Notes on Quantum Mechanics, Statistical Physics and Quantum Field Theory

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Abstract

The material reality interacts with our conscience and registering and reflecting the events of material reality we take over the random structures of this reality, building our own corresponding structures as conceptual systems and ideas, which allows us to recognize patterns of reality and make predictions of further interactions with the reality, understanding it and organizing our survival strategies.
One of the most abstract such conceptual systems consists in mathematics.
The goal of physics is to build conceptual models of the material reality, mostly based on mathematics, that can predict the way in which initial interactions with the reality determine final interactions, in a process that is always similar to the physical laws correspondence of measured values which reflect specific recognized reality events, such that any interaction with the physical reality is in fact a measuring process.
Fundamental abstractions in physics are the space-time continuum (events can have or not the same place of happening and can happen or not simultaneously, in a specific reference frame that establishes specific measurement devices for length distances and time intervals, to associate for each event a space-time equivalent in the frame) and the material particles (the smallest part that can be considered of a system) . In classical physics, particles have a well defined path in space-time (at each time moment the particle can be at a single space location).
Experience (repeated interaction with the physical reality: the famous double-slit experiment for example) shows that as we zoom in in the the space-time continuum, things get blurry and particles present uncertainities when we try to determine a precise path. Thus the Quantum mechanics formalism imposes himself, beginning with the theory of de'Broglie wave packets associated to a particle, with the explanation of path uncertainities, leading to the concepts of Hilbert space of system states and observables expressing measurable quantities asssociated with the system, as linear operators acting on states.
Special relativity and Lorentz invariance of physical laws which was initially brought up by the theory of electromagnetism plays a fundamental role in choosing the right mathematical structure for the space-time.
Possible symmetries that a quantum system can have (space-time translations, rotations), defined as Lie groups, determine observables as their generators, corresponding to the calssical concepts of energy, momentum , angular momentum and the necessary evolution of states that is taken unitary to conserve the number of quantum states and transition probabilities, according to the Hilbert space of states interpretation, leads to the time dependent Schroedinger equation.
The necessity of Lorentz invariance and the fact that a quantum particle can take between an initial state and a final state any path (acording to the wave function defined probability distribution) justify the introduction of Lagrangian field theory and path integral formalism following the canonical quantization picture of a

quantum particle field that fluctuates in vacuum creating and anihilating at any space-time location virtual particles.
The theory of electromagnetic field (and its interaction with charged particles) is a fundamental theory and provide the context for deriving the relations of relativistic dynamics.
The physical relevance of the electromagnetic field four-potential appears in the interaction of the electromagnetic field with the electron in the Aharonov-Bohm effect and the relevance of quantum electromagnetic field vacuum fluctuations appears in the Casimir effect.
The uncertainity relation for momentum and position of a real quantum particle and quantum fluctuations of the particle quantum field produce a limitation in measurement precision for position of the particle determined by the Compton wavelenght of the particle.
Thermodynamics has the main concepts necessary to understand many particles systems through the ideas of classical and quantum statistical ensembles, defining the probability density of the system which describes the distribution of microstates corresponding to a given thermodynamical macrostate. The entropy of the system measures the loss of information about the system by assigning all possible microstates of a macrostate to one averaging set of macrostate determining thermodynamical quantities.
At low temperature a quantum statistical ensemble condensates in the ground state, the lowest energy state (if the ground state is not degenerate). If the quantum statistical system system describes a many particle system at low temperature, all particles will be in the same lowest energy state forming a one state condensat and behaving in the same way.
Measurements are made by observables. Repeated measurements made on a statistical ensemble prepared in a macrostate with a defined probability density matrix results in a probability distribution over the eigenvalue spectrum of the measuring observable, the measured density matrix ‘collapsing’ through projection into the measuring observable eigenspaces. Any quantum operation, as a interaction with the environment, must be similar to a measurement, acting on a system probability density matrix.
The limits of predictability of quantum systems through collecting information about them by environmental measurements arise by decoherence: the system loses information into the environment, its evolution becomes non-unitary, quantum behaviour (additive probability amplitudes) becomes classical (additive probabilities) and it can be described poorly only by the evolution equations of the averaged expectation values of the quantum observables (as momentum and position operators) involving the system Hamiltonian expression that are similar to the classical Hamilton-Jacobi equations of the system.
Also violation of Bell inequalities by cross measurements performed on entangled states leads to the fact that local realism is forbidden by quantum mechanics, excluding the existence of hidden variables that should determine the measurement on entangled pairs outcome.

Although no bits of information can be transmitted by carefull preparing entangled systems, quantum entanglement has various applications in quantum information processing.
From the fact that any recursive problem answer can be verified through interaction with entangled provers follows that the maximum winning probability of a specific non-local game is not computable and further that the tensorial product model of enatanglement is not equivalent with the commuting operators model of entanglement (some Tsirelson bound values in the both models do not coincide) and therefore the answer to Connes embeding conjecture is negative having as cosequence that the infinite dimensional matrices (of quantum operators) cannot be approximate by finite dimensional matrices. Thus a quantum system cannot be entirely described as a computable limit : we must limit ourselves to finite dimensional subspaces for the possible eigenstates of observables.
The classical physical world emerges from the quantum world as a zero limit of distances scale (equivalent zero limit of numerical value of the Planck constant) , according to the steepest descent approximation of the path intergral, losing its significant submicroscopical information: in the classical limit the paths that are away from the classical Euler-Lagrange motion equation path of the Lagrangian field theory compensate each other through the integration, remaining only the classical path.
The spin of a particle defines the way which the particle field transforms under a rotation (or Lorentz transformation) of the coordinate system generating a spin representation of the rotations (or restricted Lorentz) group.
The Dirac Lagrangian density (leading to the Dirac equation as its Euler-Lagrange equation) describes the fermion Dirac spinor systems of quarks and leptons of the Standard model in particular of the electron.
The chiral projections of the Dirac spinor as irreducible subrepresentations of the Dirac spinor representation, having a positive helicity for the left handed spinor and a negative helicity for the right handed spinor play an important role since only left handed spinors participate in the weak interaction.
The spin statistics theorem clasifies the particles as fermions and bosons that is particles that combine as antisymmetric respective symmetric tensorial product wave functions of multiparticles systems and satisfying therefore Fermi-Dirac respective Bose-Einstein statistics of quantum statistical ensembles.
Quantum electrodynamics describes the interaction of the electromagnetic field with charged particles.
The relevant discrete symmetries of a Lagrangian field theory are charge conjugation C, parity P and time reversal T. Even though each of these symmetries can be violated, any Lorentz invariant local quantum field theory has CPT symmetry, that is an antimatter, mirrored and time reversed universe would behave exactly the same as our regular universe.
Feynman amplitudes can be calculated for various processes in direct relation with the corresponding probability amplitudes, in the perturbative approach of

Lagrangian field theory knowing the field propagator and the various coupling constants that appear in the Lagrangian field density interaction terms.
Otherwise, when for a right approximation of the amplitude all higher order fluctuation diagrams must be considered, the amplitudes for the various scattering or decay processes can be calculated using lattice gauge theory.
The Quantum harmonic oscillator provides a fundamental example for further canonical quantizations of scalar fields , Dirac fields and even the quantization of an electromagnetic field, considering creation and anihilation operators that must satisfy commutation (or anticommutation) relations.
The quantum nature of radiation reveals itself in transitions between various states of a quantum system, generating spontaneous and stimulated emission or absorption of photons, governed by Fermi's golden rule.
The energy states and levels of the electron in the Hydrogen like atom can be determined by solving directly the Dirac equation in presence of the Coulomb electromagnetic field of the nucleus or applying perturbation theory to the two-component Dirac equation considering the relativistic correction , spin-orbit interaction with Thomas precession term and Larmor term, and the Darwin term.
Quantum fluctuations of the electromagnetic field determine an anomalous magnetic moment of the electron and also the Lamb shift of energy levels in the Hydrogen like atom.
Perturbation theory can also be applied for the Hydrogen like atom in presence of a constant magnetic field (Zeeman effect, Paschen-Back effect) .
Linear combination of atomic orbitals and thight binding approximation can be used to determine the energy states and levels of electrons in covalent crystal lattices.
Phonons are quasiparticles that correspond to oscillations of crystal lattice atomic nodes.
The photonic gas inside a cavity, in thermal equilibrium with the cavity walls describes the thermal radiation of a black body and obeys to Bose-Einstein statistics of photons. The so called black body catastrophe, which happens if we would consider a classical law of energy equipartition for the photons, leaded Planck to the conclusion of quantum nature of radiation.
Phonons in a three-dimensional crystal correspond to longitudinal and transversal elastic waves in the material and also form a gas that obeys to Bose-Einstein statistics that determines the specific heat of the crystal.
Electrons in a three-dimensional crystal can absorb or emit phonons and also can interact with each other exchanging a phonon according to a phonon-electron interaction Lagrangian density. The last process determines the forming of Cooper electron pairs which behave like bosons and at low temperatures condensate in the same ground state, the material becoming a superconductor.
The emission and absorption of phonons by conduction electrons is the source of mobility effects like electric conductivity and thermal conductivity which are in direct relation with the phonon-electron interaction coupling constant.
Magnetic flux quantization is a consequence of considering theoretical magnetic monopoles and electric – magnetic duality in electrodynamics.

The Hall effect is a mobility effect of conduction electrons in presence of a magnetic field.
Perturbation theory applied to the Hamiltonian of conduction electrons from a crystal lattice explains the apparition of Landau energy levels and of the quantum Hall effect by the integer filling number of Landau levels. Fractional quantum Hall effect is caused by the interaction of electrons as fractional quasiparticles satisfying a fractional statistics (experiencing a fractional phase shift when moving around each other) tied to a flux quanta in the case of of a fractional (inverse odd integer) filling number.
Spin dependent Mott scattering of conduction electrons on the spinless impurity atoms in a crystal lattice determine a spin Hall effect of spin current normal to a charge current.
Non-abelian gauge theories, involving several tuples of fermion fields transforming under a unitary gauge symmetry group representation which can interact through gauge boson fields, are the natural generalization of the quantum electrodynamics of electrons and photons, needed to describe the interactions of particles in the Standard Model.
Adding various interaction terms to the Lagrangian density, the symmetry of the theory can be spontaneously broken when the vacuum expectation value of the field not vanishes. Every time a continuous symmetry is spontaneously broken so called Nambu-Goldstone massless bosons appear so that he theory can be reduced to a broken zero expectation value field theory, after redefining the field by extracting the vacuum expectation value.
The effective potential minimizes at the vacuum expectation value of the field.
The mass terms in the Lagrangian theory can be seen as interaction terms of the theory fields with an additional Higgs field that has non-zero expectation value and by the Anderson-Higgs mechanism, the gauge bosons also can achieve mass, at the same time ‘eating’ the Nambu Goldstone bosons that appear through the spontaneous symmetry breaking.
The necessity of CP-violation which is one of the Sakharov conditions for creation of an imbalance between matter and antimatter in the early universe, requires complex phases in the Cabibo-Kobayashi-Maskawa matrix (and/or Pontecorvo-Maki-Nakagawa-Sakata matrix) and so at least three families of leptons and quarks must exist in nature.
The necessity that baryons, as fermions, have an antisymmetrical tensorial product wave function and also the ratio between (experimental measured) crosss sections of electron-positron anihilation into hadrons and of electron-positron anihilation into a muon-antimuon pair confirm the number of three quark colors and so the $SU(3)$ symmetry of chromodynamics.
The $SU(3)$x$SU(2)$x$U(1)$ Georgi-Glashow model unifies the electromagnetic, electroweak and chromodynamics strong interactions between the Standard Model fermions mediated by gluons.
Beta decay allowed by the $SU(2)$x$U(1)$ electroweak symmetry group determines transmutation of atomic nuclei .

The strong coupling of chromodynamics determines the confinement of quarks at low energies.
The theory is renormalizable and by renormalization the electroweak and chromodynamics coupling constants become smaller and smaller as the energy or momentum transfer scale increases, determining asymptotic freedom, the quarks appearing free as isolated particles at high energies.
As the energy scale increases the renormalized three coupling constants of the Georgi-Glashow model draw closer each to other until at certain mass-energy scale the $SU(3)xSU(2)xU(1)$ symmetry is unified to a $SU(5)$ symmetry.
The $SU(5)$ symmetry group allows proton decay by emission of a quark-lepton mixing gauge boson which must have a huge mass compared to the mass scales we usually encounter for the mean life time of the proton being sufficiently long to assure the stability of universum.Thus the stability of the world implies that the unifying mass-energy scale, since quark-lepton mixing bosons are allowed only in the unified group, must be huge compared to regular mass scales that implies weakness of electromagnetism (of the fine structure constant).
It must be noticed that the $SU(5)$ unified theory breaks baryon number conservation (which is another Sakharov condition) in interactions mediated by the same quark-lepton mixing bosons.
The two $SU(5)$ representations that appear in the Georgi-Glashow model can be unified in one irreducible spin representation of $SO(10)$ which naturally allows the introduction of the (sterile) right handed neutrino. The seesaw mechanism applied to the right handed neutrino (Majorana) mass matrix generates for the (observed) left handed neutrino a small mass.

1. Special relativity
Lorentz transformations

Special relativity, Lorentz transformations

Consider the affine euclidean space of space-time events in special relativity, U
A reference frame will be identified with a bijective function $R:U\to\mathbb{R}^4$
For a space-time event $P\in U$ we have $R(P)=(\bar{x},t)$ with $\bar{x}=(x_1,x_2,x_3)$ spatial coordinates and t time coordinate.
$R^{-1}(\bar{0})=O$ with $\bar{0}=(0,0,0,0)$ and $\overline{OP}=(\bar{x},t)$
For two reference frames *R* , *R'* we have the coordinate transformations
$T:\mathbb{R}^4\to\mathbb{R}^4$, $T=R'\circ R^{-1}$, $R(O)=\bar{0}$, $R'(O')=\bar{0}$
$T(\overline{OP})=\overline{O'P'}=T(\bar{0})+M(\overline{OP})$
$T(\bar{0})=\overline{O'O}$, $M(\bar{0})=\bar{0}$
We consider now $\mathbb{R}^4=E$ as the four dimensional euclidean space of points which has at the same time the four dimensional real vector space structure.
Suppose that *R* , *R'* are inertial reference frames. The fact that if a particle is moving uniformly rectilinear as it is seen in the frame *R* then it will be seen moving uniformly rectilinear in the frame *R'* leads to the fact that *T* transforms any straight line of *E* into a straight line :
for any points $A,B\in E$ we have $T(AB)=T(A)T(B)$
If $(A_1A_2A_3)$ is a plane in E and $P\in(A_1A_2A_3)$ we can take, after eventually renumbering, a point $Q=PA_1\cap A_2A_3$. Therefore we will have
$Q'=T(Q)=T(PA_1)\cap T(A_1A_2)=P'A'_1\cap A'_2A'_3$ and so $P'=T(P)\in(A'_1A'_2A'_3)$
T transforms any plane into a plane.
Thus if $AB\|CD$, $A,B,C,D\in E$ then A,B,C,D are coplanar and so *A',B',C',D'* are also coplanar and $A'B'\cap C'D'=T(AB)\cap T(CD)=\emptyset$ which means $A'B'\|C'D'$
On $E=\mathbb{R}^4$ we have the compatible affine structure given by $\overline{AB}=B-A$ for any $A,B\in E$
For any $A,B\in E$, considering $S=\bar{0}$ and the parallelogram $[SACB]$ we will have also $[S'A'C'B']$ as a parallelogram and so

$$C=A+B$$

$T(C)=T(A)+T(B)-T(S)$ which easily leads to

$$M(A+B)=M(A)+M(B)$$

For *A, B, C, D* in *E* such that *C* is the middle of the segment *AB* and *B* is the middle of the segment *AD*, considering the parallelograms [*AGBF*] and [*AKDH*] where *B* is the middle of the segment *KH* we will have that [*A'G'B'F'*] and [*A'K'D'H'*] are also parallelograms with centres at *C'* respective *B'* and so *C'* is the middle of segment *A'B'* and *B'* is the middle of the segment *A'D'*.
Therefore it is easy to prove by induction that
any $A\in E=\mathbb{R}^4$, $m,n\in\mathbb{Z}$ satisfy $M(\frac{m}{2^n}A)=\frac{m}{2^n}M(A)$

Lemma
$\{\frac{m}{2^n}\in\mathbb{Q}\,|\,m\in\mathbb{Z},n\in\mathbb{N}\}$ is dense in $\mathbb{R}$

Proof :
For $\alpha\in\mathbb{R}$, $\epsilon\in\mathbb{R}_+$
we can take $p,m\in\mathbb{Z}$, $q,n\in\mathbb{N}^*$ such that
$\frac{1}{q}<\frac{\epsilon}{2}$, $\left|\frac{p}{q}-\alpha\right|<\frac{\epsilon}{2}$, $\frac{1}{2^n}<\frac{1}{2q}$, $\frac{m}{2^n}\in\left(\frac{p}{q},\frac{p+1}{q}\right)$

and so $\left|\frac{m}{2^n}-\alpha\right|<\frac{1}{q}+\left|\frac{p}{q}-\alpha\right|<\epsilon$
If *T* is continuous it follows now that $M(\alpha A)=\alpha M(A)$ for any $A\in\mathbb{R}^4$, $\alpha\in\mathbb{R}$

Hence, under the considered assumptions, *M* is linear continuous.

$T(u)=T(\bar{0})+M(u)$ for $u\in\mathbb{R}^4$

For $(\bar{x},t)=(x_1,x_2,x_3,x_4)$ and $(\bar{x}',t')=(x'_1,x'_2,x'_3,x'_4)$ we have

$x'_k=M_{kl}x_l$ (with Einstein summation convention) , or taking $(\bar{x},t)$ and $(\bar{x}',t')$ as column vectors *X* respective *X'*, we write *X' = MX*.

Let $G=(\gamma_{pq})$ with $\gamma_{\alpha\beta}=\delta_{\alpha\beta}$, $\gamma_{4\alpha}=\gamma_{\alpha 4}=0$, $\gamma_{44}=-c^2$ for $\alpha,\beta=1,2,3$

(where *c* is the speed of light constant)

Considering $O,P\in U$ separated by a light signal, for $\overline{OP}=X^T$ we have $X^TGX=0$ because the light signal travels from *O* to *P* with the speed *c*.

We assume, according to special relativity, that the speed of light is the same constant in any inertial reference frame and so it follows that if $X^T\in\mathbb{R}^4$ satisfies $X^TGX=0$ then $X'^TGX'=0$

Therefore if $X^T\in\mathbb{R}^4$ and $X^TGX=0$ then $X^TM^TGMX=0$ (1)

Taking $X^T=(\pm ct,0,0,t)$, $M^TGM=(a_{kl})$ it follows

$a_{11}c^2t^2+a_{44}t^2\pm 2a_{14}ct^2=0$ for any $t\in\mathbb{R}$ and so $a_{14}=a_{41}=0$, $-a_{44}=c^2a_{11}$

In the same way we have $a_{44}=c^2a_{\alpha\alpha}$, $a_{\alpha 4}=a_{4\alpha}=0$ for $\alpha=1,2,3$

(the matrix M^TGM being obviously symmetric)

Taking $X^T=(cx_1,\pm cx_2,0,\sqrt{x_1^2+x_2^2})$ it follows now

$a_{44}x_1^2+a_{44}x_2^2-a_{44}(x_1^2+x_2^2)\pm 2a_{12}x_1x_2=0$ for any $x_1,x_2\in\mathbb{R}$ and so $a_{12}=0$

In the same way we obtain $a_{\alpha\beta}=0$ for $\alpha\neq\beta$

Hence exists $l\in\mathbb{R}$ such that $lG=M^TGM$

We suppose now that the frame R moves with constant velocity $\bar{v}'$ in R' (i.e. a point at rest in R moves with velocity $\bar{v}'$ in R') and R' moves with constant velocity $\bar{v}$ in R

We take $S:\mathbb{R}^4\to\mathbb{R}^4$, $S=T-T(\bar{0})$ and we have $S\circ R'\circ R^{-1}=M$

Let $Ort=\{(a_{kl})\in M_{4\times 4}(\mathbb{R})\,|\,a_{\alpha 4}=a_{4\alpha}=0$, $(a_{\alpha\beta})=Q$, $\alpha,\beta=1,2,3$, $Q^TQ=\mathbf{I}$, $a_{44}=1\}$

Rotating adequately the frames $S\circ R'$ and R we can find $Q,P\in Ort$ such that $P\circ R=R_1$ moves with velocity $(0,0,v')$, $v'=\|\bar{v}'\|$ in $Q\circ S\circ R'=R_0$ and R_0 moves with velocity $(0,0,v)$, $v=-\|\bar{v}\|$ in R_1

Obviously we have $R_0\circ R_1^{-1}=QMP^T=\bar{M}$, $lG=\bar{M}^TG\bar{M}$ (2)

It follows that for $\bar{M}=(m_{kl})$ and $\bar{M}^{-1}=(m^*_{kl})$ we have

$(m_{k4})_k=(0,0,sv',s)$, $s\neq 0$

$(m^*_{k4})_k=(0,0,s^*v,s^*)$, $s^*\neq 0$

Let $N=(\sqrt{\gamma_{pq}})$ (with $\sqrt{-c^2}=ic$, $p,q=\overline{1,4}$) , $Z=N\bar{M}N^{-1}$ (5)

From (2) follows $l\mathbf{I}=Z^TZ$, $lZ^{-1}=Z^T$ (6)

By calculus from (5) , (3) , (4) we have

$$Z=\begin{pmatrix} . & . & . & 0 \\ . & . & . & 0 \\ . & . & . & -i\,s\,v'/c \\ . & . & . & s \end{pmatrix},\ Z^{-1}=\begin{pmatrix} . & . & . & 0 \\ . & . & . & 0 \\ . & . & . & -i\,s^{*}v/c \\ . & . & . & s^{*} \end{pmatrix}$$

Hence , considering (6) we will have

$$Z=\begin{pmatrix} . & . & . & 0 \\ . & . & . & 0 \\ . & . & . & -i\,s\,v'/c \\ . & . & -i\,s^{*}l\,v/c & s \end{pmatrix},\ s=s^{*}l\ ,\ l=-s^{*2}l^{2}v^{2}/c^{2}+s^{2}=-s^{2}v'^{2}/c^{2}+s^{2}$$

Therefore $v=-v'$ (because we have chosen $v'>0$ and $v<0$)

Since $v^{2}<c^{2}$ we have $l>0$
By calculus, it follows

$$\bar{M}=N^{-1}ZN=\begin{pmatrix} . & . & . & 0 \\ . & . & . & 0 \\ . & . & . & s\,v' \\ . & . & -s\,v/c^{2} & s \end{pmatrix},\ \bar{M}^{-1}=N^{-1}Z^{-1}N=\begin{pmatrix} . & . & . & 0 \\ . & . & . & 0 \\ . & . & . & s^{*}v \\ . & . & -s^{*}v'/c^{2} & s^{*} \end{pmatrix}$$

$$t=s'\left(t'-\frac{v'}{c^{2}}x'_{3}\right)\ ,\ t'=s\left(t-\frac{v}{c^{2}}x_{3}\right)\ ,\ x'_{3}=s(x_{3}-vt)$$

We admit the causality principle so that if an event precedes an other event at the same spatial point as it is seen in the inertial reference frame R_1 then that one event precedes the other one event also in the inertial reference frame R_0 . Therefore we have

$s>0$, $s=\sqrt{l}\,\beta$ where $\beta=\dfrac{1}{\sqrt{1-\dfrac{v^{2}}{c^{2}}}}$

Since we have $l>0$ such that $lG=M^{T}GM$ if we consider $|\det M|=1$ we will have

$l^{4}=(\det M)^{2}$, $l=1$ and so M leaves invariant the symmetric bilinear form product on the Minkowski space $V=\mathbb{R}^{4}$ defined by $X\cdot Y=X^{T}GY$ with X,Y as column vectors in $\mathbb{R}^{4}$

Consider now $M\in M_{4\times 4}(\mathbb{R})$ such that $G=M^{T}GM$. It is obbvious that also $G=M^{-T}GM^{-1}$ and |det *M*| = 1 and so if linearly independent vectors
$(E_k)k=\overline{1,4}$ are a Minkowski base in V (i.e.$E_p\cdot E_q=\gamma_{pq}$ for $p,q=\overline{1,4}$) then (E'_k)
with $E'_k=m^{*}_{lk}E_l$, $(m^{*}_{kl})=M^{-1}$ for $k,l=\overline{1,4}$ is also a Minkowski base of linearly independent vectors.
Obviously, if $x_kE_k=x'_kE'_k$ then $x'_k=m_{kl}x_l$
$m_{pk}m_{ql}\gamma_{pq}=\gamma_{kl}$ (7)

$m^*_{pk}m^*_{ql}\gamma_{pq}=\gamma_{kl}$ (8)

We have $m^*_{\alpha 4}m^*_{\alpha 4}-c^2m^{*2}_{44}=-c^2$ and so $m^{*2}_{44}\geq 1$ (9)

The assumed causality principle means

$m^*_{44}>0$. Hence we can take $v\in\mathbb{R}$, $v^2<c^2$ such that $m^*_{44}=\beta=\dfrac{1}{\sqrt{1-\dfrac{v^2}{c^2}}}$

If $v=0$, from (8) follows $m^*_{\alpha 4}=0$ and now for any $((x'_\alpha),t')\in\mathbb{R}^4$ we have

$m^*_{\alpha\gamma}m^*_{\alpha\epsilon}x'_\gamma x'_\epsilon-c^2(m^*_{4\alpha}x'_\alpha+t')^2=x'_\alpha x'_\alpha-c^2t'^2$

This leads to $m^*_{4\alpha}=0$ and $m^*_{\alpha\gamma}m^*_{\alpha\epsilon}=\delta_{\gamma\epsilon}$ and finally to M^{-1} , $M\in Ort$

We suppose now $v\neq 0$ and we can take

$A=\dfrac{1}{v\beta}m^*_{\alpha 4}E_\alpha$ with $\alpha=1,2,3$

$E''_3=\beta A+\dfrac{v\beta}{c^2}E_4$ (10)

It is easy to prove that we have $E'_4=v\beta A+\beta E_4$ (11)

and $A\cdot E_4=0$, $A\cdot A=1$, $E''_3\cdot E'_4=0$, $E''_3\cdot E''_3=1$ (12)

Consider the following system in unknown variable $X\in V$

$E'_4\cdot X=0$ (13)

$E_4\cdot X=0$ (14)

$A\cdot X=0$ (15)

$E''_3\cdot X=0$ (16)

Because of (10) , (11) the system is satisfied if and only if (14) and (15) are satisfied.

Obviously we can take $E_k=(\delta_{kl})_l$ for $l,k=\overline{1,4}$ and so it is easy to prove that we can take (E''_i) such that $E''_i\cdot E''_j=\delta_{ij}$ and for $X=E''_i$ are satisfied (13)-(14) for $i,j=1,2$

Therefore from (14) , (15) , (12) follows that (E''_1 , E''_2 , A) is an orthonormal basis of [E_1 , E_2 , E_3] and from (13) , (16) , (12) follows that (E''_1, E''_2 , E''_3) is an orthonormal basis of [E'_1 , E'_2, E'_3].

We can transform the Minkowski base (E_1 , E_2 , E_3 , E_4) to Minkowski base (E''_1, E''_2 , A , E_4) by orthonormal coordinate transformation $Q\in Ort$.

However we can choose E''_1 , E''_2 such that det$Q$ = 1 (if not we take -E''_1 instead of E''_1)

We can transform the Minkowski base (E''_1. E''_2 , A , E) to Minkowski base (E''_1 , E''_2 , E''_3 , E'_4) by the boost coordinate transformation

$$M_v=\begin{pmatrix}1 & O & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & \beta & -v\beta\\ 0 & 0 & -v\beta/c^2 & \beta\end{pmatrix}$$

We can transform the Minkowski base (E''_1 , E''_2 , E''_3 , E'_4) to Minkowski base (E'_1 , E'_2 , E'_3 ,E'_4) by orthonormal coordinate transformation $P\in Ort$

Therefore we have $M=PM_vQ$ with $P,Q\in Ort$, $\det Q=1$

If $\det M=1$ we will have $\det P=\det Q=1$

From the relation $M=PM_vQ$ follows without difficulties that we have :

$$M_{\alpha\gamma}=\bar{R}_{\alpha\gamma}+\frac{\beta-1}{v^2}\bar{R}_{\alpha\epsilon}v_\epsilon v_\gamma \text{ where } \bar{R}_{\alpha\gamma}=P_{\alpha\epsilon}Q_{\epsilon\gamma}$$
$$M_{4\gamma}=-\frac{\beta}{c^2}v_\gamma \ , \ M_{\gamma 4}=-\beta\bar{R}_{\gamma\epsilon}v_\epsilon \ , \ M_{44}=\beta \qquad (17)$$
$$\text{with } v_\alpha=Q_{3\alpha}v \ , \ v_\alpha v_\alpha=v^2 \ , \ \beta=\frac{1}{\sqrt{1-\frac{v^2}{c^2}}} \ , \ v^2<c^2$$

for $\alpha,\gamma,\epsilon=1,2,3$

and so M is described by 6 parameters (3 parameters for the rotation $\bar{R}$ and 3 parameters for $\bar{v}=(v_\alpha)$)

Thus we have proven that

$$\mathcal{L}=\{M\in M_{4\times 4}(\mathbb{R})|\exists P,Q\in Ort \ , \ v\in\mathbb{R} \text{ such that } \det P=\det Q=1 \ , \ v^2<c^2 \ , \ M=PM_vQ\}=$$
$$=\{M\in M_{4\times 4}(\mathbb{R})|m_{44}^*>0 \ , \ G=M^TGM \ , \ \det M=1\}$$

We notice that if $M\in\mathcal{L}$ then according to (17) $m_{44}=\beta=m_{44}^*>0$ and if $M\in\{M\in M_{4\times 4}(\mathbb{R})|m_{44}>0 \ , \ G=M^TGM \ , \ \det M=1\}$ then $M^{-1}\in\mathcal{L}$ and from the above we can deduce $m_{44}^*=m_{44}>0$ and so we have also

$$\mathcal{L}=\{M\in M_{4\times 4}(\mathbb{R})|m_{44}>0 \ , \ G=M^TGM \ , \ \det M=1\}$$

If $M,M'\in\mathcal{L}$ we have for $M''=M'M$ calculating according to (17)

$$M''_{44}=\beta'\beta\left(\frac{\bar{v}'\cdot\bar{R}\bar{v}}{c^2}+1\right)$$

We have $\bar{v}'\cdot\bar{R}\bar{v}>-|vv'|>-c^2$ and so $M''_{44}>0$

Also $M_v^{-1}=M_{-v}$

Therefore , from the above follows that $\mathcal{L}$ is a connected 6 – dimensional Lie group, $SO^+(3,1)$ the restricted Lorentz group. The more general set of transformations that also includes 4 – dimensional translations in space-time is known as the Poincare group.

2. Representations of the rotation group and of the restricted Lorentz group. Spin representations

Representations of the rotation group and of the restricted Lorentz group
Spin representations

For a finite dimensional vector space V, we have the general linear group
$GL(V)=\{T:V\to V|T \text{ linear homeomorphism}\}$
with the usual composition operation and topology and for a given Lie group G (as a real manifold with continuous differentiable group inversion and multiplication) we consider group representations U such that for any map of G, $h:D\to G$, U is considered to be definite on the map domain D by a function $U:D\to GL(V)$ and there exists a map
$h_0:D_0\to G$ with $\mathbf{I}_G\in h_0(D_0)$ such that for any map $h:D\to G$ of the manifold G ,
for any $R\in h(D)$ exist neighbourhoods of $\mathbf{I}_G$ and R , W_0 respective W_1 such that

$U(h^{-1}(R_0R_1))=U(h_0^{-1}(R_0))U(h^{-1}(R_1))$ for any $R_0\in W_0$, $R_1\in W_1$.
if there is no confusion we will denote $U\circ h_0^{-1}$ by U and $U\circ h^{-1}$ by U_h
Moreover we consider that U is continuous differentiable on map domain for any map of G.
In the following we will denote indexing from 1 to 3 by Latin characters and indexing from 1 to 4 by Greek characters and also use the Einstein summation convention for repeating indexes.
Let $G=\{R\in M_{3\times 3}(\mathbb{R})|R^TR=\mathbf{I}\ ,\ det\,R=1\ ,\ R=(R_{ij})\}=SO(3)$ the rotation group.
Any $R\in SO(3)$ can be written as $R=R(\varphi,n)$ a rotation around an axis of versor
$n=(n_i)$ by an angle of φ radians and we will have :
$R_{ij}=-\epsilon_{ijk}n_k\sin(\varphi)+(\delta_{ij}-n_in_j)\cos(\varphi)+n_in_j$
Obviously we have :
$R(\varphi+\delta\varphi,n)=R(\delta\varphi,n)R(\varphi,n)$
$\frac{dR}{d\varphi}(\varphi,n)=\frac{dR}{d\varphi}(0,n)R(\varphi,n)$
$R(\delta\varphi,n)=\mathbf{I}-i\,\delta\varphi n_k\bar{J}_k+O(\delta\varphi^2)$ with $(\bar{J}_k)_{ij}=-i\,\epsilon_{ijk}$ (1)
$\frac{dR}{d\varphi}(0,n)=-i\,n_k\bar{J}_k$
$R(\varphi,n)=\exp(-i\,\varphi n_k\bar{J}_k)$ (1')
Therefore SO(3) is a 3-dimensional manifold with maps given from the parametrisation in $(\varphi_1,\varphi_2,\varphi_3)=(\varphi n_1,\varphi n_2,\varphi n_3)$ as local coordinates and further we will take as h_0 the map from the (0, 0, 0) containing domain.
It is easy to verify that we have the commutation relations:
$[\bar{J}_i,\bar{J}_j]=i\,\epsilon_{ijk}\bar{J}_k$ where $[A,B]=AB-BA$ denotes the commutator of A and B.
Let U be a representation of SO(3) over a finite dimensional complex vector space V such that U takes unitary operators as values. We have :
$U_h(R(\varphi+\delta\varphi,n))=U(R(\delta\varphi,n))U_h(R(\varphi,n))$ if $\delta\varphi$ is small enough
and so , differentiating with respect to $\delta\varphi$ we obtain
$\frac{dU}{d\varphi}(R(\varphi,n))=\frac{dU}{d\varphi}(R(0,n))U(R(\varphi,n))$ for $R(\varphi,n)\in h_0(D_0)$

and if we define the operators J_k by $\frac{dU}{d\varphi}(R(0,n))=-i\,n_kJ_k$ we will have :

$U(R(\varphi,n))=\exp(-i\,\varphi n_kJ_k)$ for $R(\varphi,n)\in h_0(D_0)$ (2)
and
$U(R(\delta\varphi,n))=\mathbf{I}-i\,\delta\varphi n_kJ_k+O(\delta\varphi^2)$ (2')

The representation being unitary it follows that the operators J_k must be self-adjoint.
For any $R\in SO(3)$, because $detR=1$ we have
$R_{jp}\epsilon_{ijk}R_{kq}=R_{im}\epsilon_{mpq}$, $R^T\bar{J}_iR=R_{im}\bar{J}_m$ and thus
$R^T\exp(-i\theta\bar{J}_j)R=\exp(-i\theta R_{jk}\bar{J}_k)$ (3) and for φ,θ small enough with $R=R(\varphi,n)$
we will have :
$U(R)^{-1}U(\exp(-i\theta\bar{J}_j))U(R)=U(\exp(-i\theta R_{jk}\bar{J}_k))$ (4) and from (1') and (2) we obtain now
$U(R)^{-1}\exp(-i\theta J_l)U(R)=\exp(-i\theta R_{lj}J_j)$ (5)
Differentiating with respect to θ we obtain
$U(R)^{-1}J_lU(R)=R_{lj}J_j$ (5')
Taking $\varphi=\delta\varphi$ from (1) and (2') follows
$(\mathbf{I}+i\delta\varphi n_kJ_k)J_l(\mathbf{I}-i\delta\varphi n_kJ_k)=(\delta_{lj}-i\delta\varphi n_k(\bar{J}_k)_{lj})J_j+O(\delta\varphi^2)$
and so, because $(\bar{J}_k)_{lj}=-i\epsilon_{klj}$ we have the commutation relations :

$[J_k,J_l]=i\epsilon_{klj}J_j$ (6)

We say that the representation U is irreducible if and only if there are no proper invariant subspaces of V ,i.e. if
V_1 is a subspace of V satisfying $U(R)(V_1)\subset V_1$ for any $R\in h_0(D_0)$ then $V_1=\{0\}$ or $V_1=V$
Consider now U a finite dimensional complex unitary representation of SO(3).
Because of the commutation relations (6) we find that $J^2=J_kJ_k$ commutes with all of the generators J_l and by (2) with $U(R)$ for any $R=R(\varphi,n)\in h_0(D_0)$
U being unitary J^2 is selfadjoint positive semi-definite and so it has an eigenvalue $\lambda\in\mathbb{R}_+$
For $R\in h_0(D_0)$,if $J^2v=\lambda v$ we have $J^2U(R)v=U(R)J^2v=\lambda U(R)v$ and $U(R)$ leaves the eigenspace of λ invariant . Therefore , because the representation is irreducible, the eigenspace must be the whole space V.
Let denote $(J_k)=(J_x,J_y,J_z)$. We can take $j\geq 0$ such that $\lambda=j(j+1)$
J_z being self-adjoint and V finite dimensional, there will be a finite number of distinct eigenvalues of $J_z:\lambda_1<\lambda_2<\ldots<\lambda_p$
Let $J_+=J_x+iJ_y$. Then if $J_zv=\mu v$ with $v\neq 0$ from (6) follows $J_zJ_+v=(\mu+1)v$
Hence, because V is finite dimensional we can take $m_0=\max\{m\in\mathbb{N}|J_+^mv\neq 0\}$.
Let $v_0=J_+^{m_0}v$ and we will have $J_zv_0=(\mu+m_0)v_0$
For $J_-=J_x-iJ_y$. Then if $J_zw=\rho w$ with $w\neq 0$ follows $J_zJ_-w=(\rho-1)J_-w$ and we take
$m_1=\max\{m\in\mathbb{N}|J_-^mv_0\neq 0\}$, $v_k=J_-^kv_0$ for $k=\overline{0,m_1}$.
From (6) follows $J_+J_-=J^2-J_z^2+J_z$ and therefore for $k=\overline{1,m_1}$ we have
$J_+v_k=(j(j+1)-(\mu+m_0-k+1)^2+(\mu+m_0-k+1))v_{k-1}$ and also $J_+v_0=0$
Hence the subspace generated by $v_0,v_1\ldots,v_{m_1}$, $S=Sp[v_0,v_1\ldots,v_{m_1}]$ is invariant under J_+,J_-,J_z and so under $U(R)$ for any $R\in h_0(D_0)$ which leads to $S=V$ and
$\{\lambda_1,\lambda_2,\ldots,\lambda_p\}=\{\mu+m_0-m_1,\mu+m_0-m_1+1,\ldots,\mu+m_0\}$, $m_1+1=p$ the eigenspace for each eigenvalue $\lambda_k=\mu+m_0-m_1+k-1$ being unidimensional and so we have $\alpha_k\in\mathbb{C}$ such that
$J_+v_k=\alpha_kv_{k-1}$ for $k=\overline{1,m_1}$ and also we have $J_-v_k=v_{k+1}$ for $k=\overline{0,m_1-1}$,
$J_+v_0=0$, $J_-v_{m_1}=0$ and $J_+^+=J_-$ because J_x and J_y are self-adjoint. Therefore we have
$|\alpha_k|^2\langle v_{k-1}|v_{k-1}\rangle=\langle v_k|J_-J_+|v_k\rangle=\langle v_k|v_k\rangle(j(j+1)-(\mu+m_0-k)(\mu+m_0-k+1))$ and
$\langle v_{k+1}|v_{k+1}\rangle=\langle v_k|J_+J_-|v_k\rangle=\langle v_k|v_k\rangle(j(j+1)-(\mu+m_0-k)(\mu+m_0-k-1))$
for $k=\overline{1,m_1}$ and respective $k=\overline{0,m_1-1}$ and
$\mu+m_0=j$, $-\mu-m_0+m_1=j$
Hence we have

$m_1=2j$ and $-j\le\mu+m_0-k\le j$ for $k=\overline{0,m_1}$, $dimV=2j+1$

Unitary complex finite dimensional irreducible representations of SO(3) have 2 j + 1 dimensional

J_z having eigenvalues with one-dimensional eigenspaces : $-j,-j+1,\ldots,j-1,j$

J^2 has only eigenvalue $j(j+1)$ and j is a non-negative half-integer multiple.

If we take for V the wave functions Hilbert space of a quantum particle, because of the commutation relations for coordinates operators and momentum operators ,

$[\hat{x}_l,\hat{p}_j]=i\,\delta_{lj}\hbar$

it follows that the angular momentum operators $J_i=\frac{1}{\hbar}\hat{L}_i$ with $\hat{L}=\hat{X}\times\hat{P}$

satisfy the commutation relations (6) and therefore they can generate an unitary complex representation of SO(3). In polar coordinates (r,θ,φ) we have:

$$\frac{1}{\hbar^2}\hat{L^2}=-\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2}-\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)$$

the spherical functions operator , which has the eigenvalues $l(l+1)$ with eigenstates the spherical harmonics

$Y_l^k(\theta,\varphi)=P_l^{|k|}(\cos(\theta))\exp(ik\varphi)$ with $k,l\in\mathbb{N}|k|\le l$ and $P_l^{|k|}$ the associated Legendre polynomials. Also we will have :

$$\frac{1}{\hbar}\hat{L_+}=\exp(i\varphi)\frac{\partial}{\partial\theta}+i\cot(\theta)\exp(i\varphi)\frac{\partial}{\partial\varphi}$$

$$\frac{1}{\hbar}\hat{L_-}=-\exp(-i\varphi)\frac{\partial}{\partial\theta}+i\cot(\theta)\exp(-i\varphi)\frac{\partial}{\partial\varphi}$$

$$\frac{1}{\hbar}\hat{L_z}=-i\frac{\partial}{\partial\varphi}$$

where we have taken

$z=r\cos(\theta)$, $y=r\sin(\theta)\sin(\varphi)$, $x=r\sin(\theta)\cos(\varphi)$

The eigenstates of the $l(l+1)$ generate (for constant r) the invariant subspace of the irreducible spin l representation.

Let (σ_k) be the Pauli matrices

$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $\sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

For $M\in SU(2)=\{S\in M_{2\times2}(\mathbb{C})|S^+S=\mathbf{I}\ ,\ detS=1\}$ we have uniquely determined $(\alpha_k)\in\mathbb{C}^3$ and $\alpha_0\in\mathbb{C}$ such that $M=\alpha_0\mathbf{I}-i\,\alpha_k\sigma_k$, because $(\mathbf{I},\sigma_1,\sigma_2,\sigma_3)$ provide a basis for the complex vector space $M_{2\times2}(\mathbb{C})$

For $a=\Re(\alpha_0)$, $b=\Im(\alpha_0)$, $\vec{X}=\Re(\vec{\alpha})$, $\vec{Y}=\Im(\vec{\alpha})$ the conditions $M\in SU(2)$ lead to $a^2+b^2+\vec{X}^2+\vec{Y}^2=1$ and $a^2+\vec{X}^2-b^2-\vec{Y}^2=1$ and so we have a versor (n_k) and an angle $\frac{\theta}{2}$ uniquely determining $a=\cos(\frac{\theta}{2})$, $\vec{X}=n\sin(\frac{\theta}{2})$, $b=0$, $\vec{Y}=0$

Therefore SU(2) is a 3-dimensional Lie group with local mappings given by the parametrisation

$(\varphi n_k)\in\mathbb{R}^3$, $h((\varphi n_k))=\exp(-i\frac{1}{2}n_k\sigma_k)=\cos(\frac{\varphi}{2})\mathbf{I}-i\sin(\frac{\varphi}{2})n_k\sigma_k$

We can verify that we have a local diffeomorphism

$T:SU(2)\to SO(3)$ which in any map parametrisation (φn_k) has the expression

$$T(\exp(-i\frac{1}{2}\varphi n_k\sigma_k))=R(\varphi,n)$$

Moreover, considering the factor group

$SU(2)/\{-\mathbf{I},\mathbf{I}\}$ with the projection $p:SU(2)\to SU(2)/\{-\mathbf{I},\mathbf{I}\}$ we have that

$p\circ T^{-1}$ is well defined as diffeomorphism from $SO(3)$ to $SU(2)/\{-\mathbf{I},\mathbf{I}\}$ which has a differential manifold structure that can be considered as induced by the local diffeomorphism T.

$SU(2)$ is a double covering of $SO(3)$, for any $R(\varphi,n)$ corresponding $\pm(\cos(\frac{\varphi}{2})\mathbf{I}-i\sin(\frac{\varphi}{2})n_k\sigma_k)$ because we have $R(\varphi,n)=R(\varphi+2\pi,n)$

For $R=R(\varphi,n)\in SO(3)$, $S\in SU(2)$, $T(S)=R$ we have that $S^{-1}\sigma_k S=R_{kj}\sigma_j$ and so if $S_i\in SU(2)$ satisfies $T(S_i)=R_i\in SO(3)$ for $i=1,2$ then for $S=S_1S_2$, $R=R_1R_2$ we have that $S^{-1}\sigma_k S=R_{kj}\sigma_j$ with $k=1,2,3$

If $W\in SU(2)$ satisfies $T(W)=R$ we will have also $W^{-1}\sigma_k W=R_{kj}\sigma_j$ and therefore for $H=SW^{-1}$ we have $H\sigma_k=\sigma_k H$ with $k=1,2,3$

Thus $(\mathbf{I},\sigma_1,\sigma_2,\sigma_3)$ being a basis of $M_{2\times 2}(\mathbb{C}),H$ commutes with any 2x2 complex matrix so exists $\lambda\in\mathbb{C}$ such that $H=\lambda\mathbf{I}$ and because $det\,H=1$ follows $H=\pm\mathbf{I}$ therefore $S=\pm W$ and because $T(W)=T(-W)$ we conclude that $T(S_1)T(S_2)=T(S_1S_2)$ for any $S_1,S_2\in SU(2)$ and $p\circ T^{-1}$ is a groups isomorphism.

Let U the so called spin $\frac{1}{2}$ representation $U(R(\varphi,n))=\exp(-i\frac{1}{2}\varphi n_k\sigma_k)$

For any map h of $SO(3)$ we have obviously $T(U\circ h^{-1}(R))=R$ and so $T(U\circ h^{-1}(R_0R_1))=T(U\circ h_0^{-1}(R_0))T(U\circ h^{-1}(R_1))$ and as we have proven above it follows $U_h(R_0R_1)=\pm U(R_0)U_h(R_1)$ for R_0,R_1 in some neighbourhoods of $\mathbf{I}$ respective R (*)

Because U_h and $U\circ h_0$ are continuous in neighbourhoods of R and respective $\mathbf{I}$ and $U\circ h_0^{-1}(\mathbf{I})=\mathbf{I}$, from the relation (*) we can derive the condition for U to be indeed a representation of SO(3).

For U^i a $GL(V_i)$ valued representation of $SO(3)$ with $i=\overline{1,n}$ we can consider the $GL(\bigotimes_{i=1}^{n}V_i)$ valued representation which in any map $h:D\to SO(3)$ has the expression $U_h(R)(\varphi_1\otimes\varphi_2\ldots\otimes\varphi_n)=U_h^1(R)\varphi_1\otimes U_h^2(R)\varphi_2\otimes\ldots\otimes U_h^n(R)\varphi_n$

If we denote the generators of U^k by $J_{k,i}i=1,2,3$ then for the generators J_i of U we have $J_i=\sum_{k=1}^{n}\mathbf{I}\otimes\ldots\otimes J_{k,i}\otimes\ldots\otimes\mathbf{I}$ and so J_z carries eigenvalues $m_1+m_2+\ldots+m_n$ with $m_k\in\{-j_k,\ldots,j_k\}$ if U^k is a spin j_k representation for $k=\overline{1,n}$

Take now $n=2j$ and $U^k=U^{(1)}$,the same spin $\frac{1}{2}$ representation , valued on $GL(V^{(1)})$ having generators $J_i^{(1)}$ with eigenstates e_+,e_- for eigenvalues $\frac{1}{2}$ respective $-\frac{1}{2}$ of $J_z^{(1)}$

We can consider the subspace of symmetric tensors of the tensorial product space $V^{(n)}=\bigotimes_{k=1}^{2j}V^{(1)}$ namely

$$S=\{\sum_{i1,i2,\ldots,in=\pm}a_{i1i2\ldots in}\sum_{\tau\in S_n}e_{i\tau(1)}\otimes e_{i\tau(2)}\otimes\ldots\otimes e_{i\tau(n)}|a_{i1i2\ldots in}\in\mathbb{C}\text{ for }i1,i2,\ldots,in=\pm\}$$

The product representation is $U^{(n)}$ with generators $J_i^{(n)}$

The subspace S is invariant under $U^{(n)}$ carries the eigenstate $e_+\otimes e_+\otimes\ldots\otimes e_+$ of eigenvalue j of $J_z^{(n)}$ and has dimension $n+1=2j+1$ and therefore the restriction of $U^{(n)}$ to S must be a spin j irreducible representation of $SO(3)$.

In the same way we conclude that the representation given by

$U(R)=R$ for any $R\in SO(3)$ is a spin 1 irreducible representation
and the representation given by
$U(R)((\varepsilon_{ij})_{i,j=1,2,3})=(R_{ki}R_{lj}\varepsilon_{ij})_{k,l}$ with invariant space
$V=\{\varepsilon\in M_{3\times 3}(\mathbb{C})|\varepsilon_{ij}=\varepsilon_{ji}\ ,\ \varepsilon_{kk}=0$ with $i,j=1,2,3\}$, the symmetric traceless tensors, is a spin 2 representation.

Consider now $G=SO^{+}(3,1)$ the restrict Lorentz group (by suitable measuring units for time we can consider the speed of light constant to be c = 1) and the Minkowski space with pseudo-metric
$(\eta^{\alpha\beta})$, $\eta^{jj}=-\delta_{ij}$, $\eta^{j4}=\eta^{4i}=0$, $\eta^{44}=1$
For any $M\in G$ we have uniquely determinated $B=B(\chi,q)$, $R=R(\theta,n)$ with
$n=(n_i)$, $q=(q_i)$ versors and $\chi,\theta\in\mathbb{R}$ such that $M=BR$
$R_{ij}=-\epsilon_{ijk}n_k\sin(\theta)+(\delta_{ij}-n_in_j)\cos(\theta)+n_in_j$, $R_{i4}=R_{4i}=0$, $R_{44}=1$
$B_{ij}=\delta_{ij}+(\cosh(\chi)-1)q_iq_j$, $B_{i4}=B_{4i}=-q_i\sinh(\chi)$, $B_{44}=\cosh(\chi)$
(see Chap. Special relativity. Lorentz transformation $)v_i=q_i\tanh(\chi)$
$G=SO^{+}(3,1)$ is therefore a 6-dimensional Lie group with maps by parametrisation in
$((\chi q_i),(\theta n_i))$ and as the map h_0 we will take the map which contains $(0)\in\mathbb{R}^6$ in its domain.

We can verify that
$B(\chi+\delta\chi,q)=B(\delta\chi,q)B(\chi,q)$ (7)
$R(\theta+\delta\theta,n)=R(\delta\theta,n)R(\theta,n)$ (8)

and we can define $(\bar{J}_i)$, $(\bar{K}_i)$ such that

$n_k\bar{J}_k=\frac{dR}{d\theta}(0,n)$, $q_k\bar{K}_k=-\frac{dB}{d\chi}(0,q)$ with
$(\bar{J}_i)_{jk}=-\epsilon_{ijk}$, $(\bar{J}_i)_{4\alpha}=(\bar{J}_i)_{\alpha 4}=0$, $(\bar{K}_i)_{jk}=0$, $(\bar{K}_i)_{4j}=(\bar{K}_i)_{j4}=\delta_{ij}$, $(\bar{K}_i)_{44}=0$
and so we will have :
$B(\chi,q)=\exp(-\chi q_k\bar{K}_k)$, $R(\theta,n)=\exp(\theta n_k\bar{J}_k)$ (9)
$M(\delta\chi,q;\delta\theta,n)=B(\delta\chi,q)R(\delta\theta,n)=\mathbf{I}-\delta\chi q_k\bar{K}_k+\delta\theta n_k\bar{J}_k+O(\varepsilon^2)$ (9')
for $\delta\chi$, $\delta\theta\in O(\varepsilon)$
$[\bar{J}_i,\bar{J}_j]=\epsilon_{ijk}\bar{J}_k$, $[\bar{K}_i,\bar{K}_j]=-\epsilon_{ijk}\bar{J}_k$, $[\bar{J}_i,\bar{K}_j]=\epsilon_{ijk}\bar{K}_k$ (10)

For a representation U of $SO^{+}(3,1)$ we can define (J_i) , (K_i) such that

$n_kJ_k=\frac{dU}{d\theta}(R(0,n))$, $q_kK_k=-\frac{dU}{d\chi}(B(0,q))$ and we will have:
$U(B(\chi,q))=\exp(-\chi q_kK_k)$, $U(R(\theta,n))=\exp(\theta n_kJ_k)$ (11)
$U(M(\delta\chi,q;\delta\theta,n))=\mathbf{I}-\delta\chi q_kK_k+\delta\theta n_kJ_k+O(\varepsilon^2)$ (11')
for $\delta\chi$, $\delta\theta\in O(\varepsilon)$

Let $A_l(\theta)=R(-\theta,n)\bar{J}_lR(\theta,n)$. Then from (9) and (10) follows
$\frac{dA_l}{d\theta}=\epsilon_{lkj}A_j=(\bar{J}_k)_{lj}A_j$ and because $A_l(0)=\bar{J}_l$ we have the solution
$A_l=R_{lj}\bar{J}_j$ where $R=R(\theta,n)$ and so we have
$R^{-1}\exp(\varphi\bar{J}_l)R=\exp(\varphi R_{lj}\bar{J}_j)$
Therefore, according (9) and (11) , for θ , φ small enough we obtain
$U(R)^{-1}\exp(\varphi J_l)U(R)=\exp(\varphi R_{lj}J_j)$ and taking the second order approximation in φ:

$U(R)^{-1} J_l U(R) = R_{lj} J_j$ and so for $\theta = \delta\theta$ follows

$(\mathbf{I} - \delta\theta n_k J_k) J_l (\mathbf{I} + \delta\theta n_k J_k) = (\delta_{lj} - \delta\theta n_k \epsilon_{ljk}) J_j + O(\delta\theta^2)$

$[J_l, J_k] = \epsilon_{lkj} J_j$ (12)

In the same way, taking $A_l(\theta) = R(-\theta, n) \bar{K}_l R(\theta, n)$ we obtain

$R^{-1} \exp(-\chi \bar{K}_l) R = \exp(-\chi R_{lj} \bar{K}_j)$ with $R = R(\theta, n)$ and further, if $\theta = \delta\theta$ is small enough :

$(\mathbf{I} - \delta\theta n_k J_k) K_l (\mathbf{I} + \delta\theta n_k J_k) = (\delta_{lj} - \delta\theta n_k \epsilon_{klj}) K_j + O(\delta\theta^2)$

(n_k) being an arbitrary versor, we will have

$[J_k, K_l] = \epsilon_{klj} K_j$ (13)

We take now

$A_l(\chi) = B(-\chi, q) \bar{K}_l B(\chi, q)$, $C_l(\chi) = B(-\chi, q) \bar{J}_l B(\chi, q)$ and we have from (9) and (10)

$$\frac{dA_l}{d\chi} = -q_k \epsilon_{klj} C_j$$

$$\frac{dC_l}{d\chi} = -q_k \epsilon_{klj} A_j$$

Therefore , for $B = B(\chi, q)$ and $R = R(\chi, q)$ the solution

$B^{-1}(\bar{K}_l + \bar{J}_l) B = R_{lj}(\bar{K}_j + \bar{J}_j)$ (14)

From (10) we obtain $[\bar{K}_i + \bar{J}_i, \bar{K}_j + \bar{J}_j] = 0$, $[\bar{K}_i, \bar{J}_i] = 0$ for $i, j = 1, 2, 3$ and so we have:

$\exp(\chi'(\bar{K}_l + \bar{J}_l)) = \exp(\chi' \bar{K}_l) \exp(\chi' \bar{J}_l)$ and

$$\exp(\chi' R_{lj}(\bar{K}_j + \bar{J}_j)) = \prod_{j=1}^{3} \exp(\chi' R_{lj} \bar{K}_j) \exp(\chi' R_{lj} \bar{J}_j)$$

Multiplying (14) by χ' , exponentiating , applying U for small enough χ and χ' and after that considering (11) we obtain now:

$$U(B)^{-1} \exp(\chi' K_l) \exp(\chi' J_l) U(B) = \prod_{j=1}^{3} \exp(\chi' R_{lj} K_j) \exp(\chi' R_{lj} J_j)$$

Taking the second order approximation in χ' we obtain, for small enough χ that:

$U(B)^{-1}(K_l + J_l) U(B) = R_{lj}(K_j + J_j)$ and for $\chi = \delta\chi$

$(\mathbf{I} + \delta\chi q_k K_k)(K_l + J_l)(\mathbf{I} - \delta\chi q_k K_k) = (\delta_{lj} - \delta\chi q_k \epsilon_{klj})(K_j + J_j)$

With (13) we can now conclude that

$[K_k, K_l] = -\epsilon_{klj} J_j$ (15)

We have therefore the commutation relations (12) , (13) , (15) for the generators.

Consider now the Dirac equation for a four component wave function $\psi = (\psi_\alpha)$ (as a column vector) of a mass *m* particle :

$i \gamma^\mu \partial_\mu \psi - m \psi = 0$

with the 4x4 matrices

$$\gamma^k = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix} , \quad \gamma^4 = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & -\mathbf{I} \end{pmatrix}$$

Under a Lorentz transformation $M = (M_{\alpha\beta})$ with

$x'^\mu = M_{\mu\delta} x^\delta$, $(x^\mu) = (x, y, z, t)$, $(x'^\mu) = (x', y', z', t')$ (we consider the speed of light c = 1)

we suppose that the wave function transforms like

$\psi'_\alpha = S_{\alpha\delta}\psi_\delta$

We have $M_{\nu\mu}\partial_\nu' = \partial_\mu$, $\gamma^\mu M_{\nu\mu}\partial_\nu' S^{-1}\psi' = mS^{-1}\psi'$ and so requiring Lorentz invariance of the Dirac equation we come to

$S^{-1}\gamma^\nu S = M_{\nu\mu}\gamma^\mu$

We can verify that:

$\gamma^\alpha\gamma^\beta + \gamma^\beta\gamma^\alpha = 2\eta^{\alpha\beta}$ (16)

Considering (16), for $M = B(\chi, q)$ we can take

$S = P(\chi, q) = \cosh(\frac{\chi}{2})\mathbf{I} + \sinh(\frac{\chi}{2})q_k\gamma^k\gamma^4$

and for $M = R(\theta, n)$ we can take

$S = Q(\theta, n) = \cos(\frac{\theta}{2})\mathbf{I} + \frac{1}{2}\sin(\frac{\theta}{2})n_k\epsilon_{kij}\gamma^j\gamma^j$

Let $SL(2,\mathbb{C}) = \{S \in M_{2\times 2}(\mathbb{C}) | det\, S = 1\}$

Since $(\mathbf{I}, \sigma_1, \sigma_2, \sigma_3)$ is a basis of $M_{2\times 2}(\mathbb{C})$ we have $\alpha_0, \alpha_1, \alpha_2, \alpha_3 \in \mathbb{C}$, uniquely determined for $S \in SL(2,\mathbb{C})$ such that $S = \alpha_0\mathbf{I} + \alpha_k\sigma_k$ (17)

and $\alpha_0^2 - \vec{\alpha}^2 = 1$ which leads to

$(\Re\,\alpha_0)^2 - (\Im\,\alpha_0)^2 = (\Re\,\vec{\alpha})^2 - (\Im\,\vec{\alpha})^2 + 1$ (18)

$(\Re\,\alpha_0)(\Im\,\alpha_0) = (\Re\,\vec{\alpha})(\Im\,\vec{\alpha})$ (18')

If we suppose now that $S = (a\mathbf{I} - X_k\sigma_k)(b\mathbf{I} - iY_k\sigma_k)$ (19)

with $a, b \in \mathbb{R}$, $a \geq 1$, $(X_k), (Y_k) \in \mathbb{R}^3$

$a^2 - \vec{X}^2 = 1$ (19')

$b^2 + \vec{Y}^2 = 1$ (19'') , then (17) leads to

$ab + i\vec{X}\vec{Y} = \alpha_0$ (20) and

$b\vec{X} + ia\vec{Y} + \vec{X}\times\vec{Y} = -\vec{\alpha}$ (21) , or , by taking real and imaginary parts :

$ab = \Re\,\alpha_0$ (22)

$b\vec{X} + \vec{X}\times\vec{Y} = \Re\,\vec{\alpha}$ (23)

$\vec{X}\vec{Y} = \Im\,\alpha_0$ (24)

$a\vec{Y} = -\Im\,\vec{\alpha}$ (25)

Also from (17) we have :

$b\mathbf{I} - iY_k\sigma_k = (a\mathbf{I} + X_k\sigma_k)(\alpha_0\mathbf{I} + \alpha_k\sigma_k)$ and so

$b = a\alpha_0 + \vec{\alpha}\vec{X}$ (26)

$\vec{Y} = i\alpha_0\vec{X} + ia\vec{\alpha} - \vec{X}\times\vec{\alpha}$ (27)

1. If $(\Re\,\vec{\alpha})\times(\Im\,\vec{\alpha}) = 0$

1.1 if $\Im\,\vec{\alpha} = 0$ we obtain $\vec{Y} = 0$ from (25) and so, from (19") $b^2 = 1$

By (18) and (18') we will have in this case $\Im\,\alpha_0 = 0$ and taking the real part of (27) it follows

$\vec{X}\times\Re\,\vec{\alpha} = 0$, $\vec{X} = \lambda\Re\,\vec{\alpha}$ with $\lambda \in \mathbb{R}$

From (26) we have now $b = a\alpha_0 + \lambda(\Re\,\vec{\alpha})^2$ and multiplying by a , using (22) we have:

$\alpha_0(1 - a^2) = \lambda\vec{\alpha}^2$ and so with (19') follows $-\alpha_0\lambda^2\vec{\alpha}^2 = \lambda\vec{\alpha}^2 a$ (28)

If in this case $\alpha_0^2 = 1$ from (18) we will have $\vec{\alpha} = 0$ and so $\vec{X} = 0$ and by (19') and (22)

$a = 1$, $b = \alpha_0 a$. Hence $a, b, \vec{X}, \vec{Y}$ are uniquely determined from (19) by $\alpha_0, \vec{\alpha}$

If in this case $\alpha_0^2 \neq 1$ from (18) follows $\Re\,\vec{\alpha} \neq 0$ and from (22) and (19') follows

$a^2 \neq 1$ and $\vec{X} \neq 0$. Therefore $\lambda \neq 0$ and (28) leads to $-\lambda\alpha_0 = a$

and so, by (19') and (18) $a^2=(\Re\alpha_0)^2=1+(\Re\vec{\alpha})^2>1$ provides the correct uniquely determination of $a,b,\vec{X}$, $\vec{Y}$ from (19) by $\alpha_0,\vec{\alpha}$.

1.2. If $\Im\vec{\alpha}\neq 0$ follows

$\Re\vec{\alpha}=\lambda\Im\vec{\alpha}$ with $\lambda\in\mathbb{R}$ and because from (25) and (27) we have

$(a^2-1)\Im\vec{\alpha}=-a\Im\alpha_0\vec{X}-a\vec{X}\times\Re\vec{\alpha}$, we will also have

$a(\vec{X}\times\Re\vec{\alpha})^2=0$ and $(a^2-1)\Im\vec{\alpha}=-a\Im\alpha_0\vec{X}$ (29) which by (19') leads to

$(a^2-1)^2(\Im\vec{\alpha})^2=a^2(a^2-1)(\Im\alpha_0)^2$ (30)

1.2.1 If $(\Re\alpha_0)(\Im\alpha_0)=0$

In this subcase, from (18') follows $\Re\vec{\alpha}=0$ and with (23) and (25) we obtain

$b\vec{X}^2=0$ and $\vec{X}=\mu\vec{Y}$, $\mu\in\mathbb{R}$

From (22), (25) , (19'') and (18) we have $a^2=(\Re\alpha_0)^2+(\Im\vec{\alpha})^2=1+(\Im\alpha_0)^2+(\Re\vec{\alpha})^2\geq 1$

From (24) and (25) we have $\mu(\Im\vec{\alpha})^2=a^2\Im\alpha_0$ and so $a,b,\vec{X},\vec{Y}$ are correctly uniquely determined.

1.2.2 If $(\Re\alpha_0)(\Im\alpha_0)\neq 0$

In this subcase, (24) leads to

$\vec{X}\neq 0$ and so, by (19') $a^2\neq 1$ and from (30) follows $a^2((\Im\vec{\alpha})^2-(\Im\alpha_0)^2)=(\Im\alpha_0)^2$ (31)

In this case $(\Re\vec{\alpha})^2(\Im\vec{\alpha})^2=((\Re\vec{\alpha})(\Im\vec{\alpha}))^2$ and therefore, by (18) and (18') taking

$\mu^2=\dfrac{(\Im\alpha_0)^2}{(\Im\vec{\alpha})^2}$ we obtain $(1-\mu^2)((\Re\vec{\alpha})^2+(\Im\alpha_0)^2+1)=1$ and so $\mu^2<1$

Hence, by (31) , (29) , (22) , and (25) a,b , $\vec{X}$, $\vec{Y}$ are again correctly uniquely determined.

2. If $(\Re\vec{\alpha})\times(\Im\vec{\alpha})\neq 0$

we have $\lambda,\mu,\rho\in\mathbb{R}$ such that

$\vec{X}=\lambda\Re\vec{\alpha}+\mu\Im\vec{\alpha}+\rho(\Re\vec{\alpha})\times(\Im\vec{\alpha})$ the relations (25) , (21) and (24) leading to

$\lambda\Re\alpha_0+\rho(\Im\vec{\alpha})^2=-a$ (32)

$\mu\Re\alpha_0-\rho(\Re\vec{\alpha})(\Im\vec{\alpha})=0$ (33)

$\lambda-\rho\Re\alpha_0=0$ (34)

$\lambda(\Re\vec{\alpha})(\Im\vec{\alpha})+\mu(\Im\vec{\alpha})^2=-\Im\alpha_0$ (35)

From (22) , (25) , (19'') and (18) we have $a^2=(\Re\alpha_0)^2+(\Im\vec{\alpha})^2=1+(\Im\alpha_0)^2+(\Re\vec{\alpha})^2\geq 1$

which determines correctly

$a\geq 1$ and now (32),(34) and (35) determine λ,μ,ρ and therefore $\vec{X}$; (25) determines $\vec{Y}$

$a,b,\vec{X},\vec{Y}$ are correctly uniquely determinated from (19) by α_0 and $\vec{\alpha}$

Taking $a=\cosh(\frac{\chi}{2})$, $\vec{X}=\sinh(\frac{\chi}{2})q$, $b=\cos(\frac{\theta}{2})$, $\vec{Y}=\sin(\frac{\theta}{2})n$ with versors q,n ,

we see that $SL(2,\mathbb{C})$ can be considered as a 6-dimensional Lie group with mappings given by local parametrisation in

$((\chi q_k),(\theta n_k))\in\mathbb{R}^6$, $h((\chi q_k),(\theta n_k))=\exp(-\frac{1}{2}\chi q_k\sigma_k)\exp(-i\frac{1}{2}\theta n_k\sigma_k)$,

because we can easily verify by differentiation and same initial conditions that

$\cosh(\frac{\chi}{2})\mathbf{I}-\sinh(\frac{\chi}{2})q_k\sigma_k=\exp(-\frac{1}{2}\chi q_k\sigma_k)$ and

$\cos(\frac{\theta}{2})\mathbf{I}-i\sin(\frac{\theta}{2})n_k\sigma_k=\exp(-i\frac{1}{2}\theta n_k\sigma_k)$

We define $T:SL(2,\mathbb{C})\to SO^+(3,1)$ and $H:SL(2,\mathbb{C})\to M_{4\times 4}(\mathbb{C})$ such that if

$S=\exp(-\frac{1}{2}\chi q_k\sigma_k)\exp(-i\frac{1}{2}\theta n_k\sigma_k)$ then

$T(S)=B(\chi,q)R(\theta,n)$ and $H(S)=P(\chi,q)Q(\theta,n)$

For S_1 , $S_2\in SL(2,\mathbb{C})$ we can verify that:

$H(S_i)^{-1}\gamma^\mu H(S_i)=(T(S_i))_{\mu\nu}\gamma^\nu$ for $i=1,2$, $\mu=\overline{1,4}$ and therefore

$(H(S_1)H(S_2))^{-1}\gamma^\mu(H(S_1)H(S_2))=(T(S_1)T(S_2))_{\mu\nu}\gamma^\nu$

Let be S such that $T(S)=B(\chi,q)R(\theta,n)=T(S_1)T(S_2)$. Then we can have only

$S=\pm\exp(-\frac{1}{2}\chi q_k\sigma_k)\exp(-i\frac{1}{2}\theta n_k\sigma_k)$ and we have also:

$H(S)^{-1}\gamma^\mu H(S)=(T(S_1)T(S_2))_{\mu\nu}\gamma^{ny}$ and for $W=H(S)(H(S_1)H(S_2))^{-1}$ we will have

$\gamma^\mu W=W\gamma^\mu$ for $\mu=\overline{1,4}$ (36)

We take $W=\begin{pmatrix}A & B\\ C & D\end{pmatrix}$ with $A,B,C,D\ \in\ M_{2\times2}(\mathbb{C})$

Taking $\mu=4$ in (36) we obtain $B=-B$ and $C=-C$ and so $B=C=0$

For $\mu=i$ in (36) follows $A\sigma_i=\sigma_i D$ (37)

From (36) we obtain $W\gamma^j\gamma^j=\gamma^j\gamma^j W$ and so, because for $i\neq j$ we have

$\gamma^j\gamma^j=\begin{pmatrix}-i\epsilon_{ijk}\sigma_k & 0\\ 0 & -i\epsilon_{ijk}\sigma_k\end{pmatrix}$ it follows

$A\sigma_k=\sigma_k A$ and $D\sigma_k=\sigma_k D$ (38)

Hence, $(\mathbf{I},\sigma_1,\sigma_2,\sigma_3)$ being a basis of $M_{2\times2}(\mathbb{C})$, (37) and (38) lead to

$A=D=\lambda\mathbf{I}$ with $\lambda\in\mathbb{C}$ and so $W=\lambda\mathbf{I}$, $H(S)=\lambda H(S_1)H(S_2)$ (39)

For the subspace of $\mathbb{C}^4$ (cosidered as column vectors), namely $K=\{(X,X)\in\mathbb{C}^2\times\mathbb{C}^2|\}$ we can verify that for any $S_0\in SL(2,\mathbb{C}),Z=(X,X)\in K$ we have $H(S_0)Z=(S_0X,S_0X)$

Therefore, from (39) we obtain

$S=\lambda S_1S_2$ and because $det\,S=det\,S_1=det\,S_2=1$ it follows $\lambda=\pm1$

Obviously $T(S)=T(-S)$ for any $S\in SL(2,\mathbb{C})$ and so $T(S_1S_2)=T(S_1)T(S_2)$

Thus we have a well defined groups isomorphism

$p\circ T^{-1}:SO^+(3,1)\to SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$ where *p* is the projection operator

$p:SL(2,\mathbb{C})\to SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$

Moreover, *T* is a local diffeomorphism , is a double covering of $SO^+(3,1)$ by $SL(2,\mathbb{C})$ and determines also the differential structure of $SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$

Considering $F=(p\circ T^{-1})^{-1}$ the inverse group isomorphism defined above we have that U is a representation of $SO^+(3,1)$ if and only if $U\circ F$ is a representation of $SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$.

By composition with the projection operator at left, any representation of $SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$ determines a representation of $SL(2,\mathbb{C})$

Consider now the functions $U:D\to SL(2,\mathbb{C})$ defined for any map $h:D\to SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$ such that $U((\chi q_k),(\theta n_k))=\exp(-\frac{1}{2}\chi q_k\sigma_k)\exp(-i\frac{1}{2}\theta n_k\sigma_k)$ for $((\chi q_k),(\theta n_k))\in D$

We have that $T(U\circ h^{-1}(\hat{S}))=R$ for any $R\in SO^+(3,1)$ where $\hat{S}=p\circ T^{-1}(R)$

Therefore $T(U_h(\hat{S}_0\hat{S}_1))=T(U(\hat{S}_0))T(U_h(S_1))$ and so, as already proven above, we must have $U_h(\hat{S}_0\hat{S}_1)=\pm U(\hat{S}_0)U_h(\hat{S}_1)$ for $\hat{S}_0$, $\hat{S}_1$ in some neighbourhoods of $\mathbf{I}$ respective $\hat{S}\in h(D)$

Because $U\circ h^{-1}$ and $U\circ h_0^{-1}$ are continuous, if these neighbourhoods, W_0 respective W_1 , are connected then $U_h(\hat{S}_0\hat{S}_1)=U(\hat{S}_0)U_h(\hat{S}_1)$ for $(\hat{S}_0,\hat{S}_1)\in W_0\times W_1$

Hence if $\bar{U}$ is a representation of $SL(2,\mathbb{C})$ then $\bar{U}\circ U$ is a representation of $SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$.

Therefore any representation of $SL(2,\mathbb{C})$ determines a representation of $SL(2,\mathbb{C})/\{-\mathbf{I},\mathbf{I}\}$ and backwards.

Determining irreducible representations of $SO^+(3,1)$ reduces to determining irreducible representations of $SL(2,\mathbb{C})$.

Let U be a representation of $SL(2,\mathbb{C})$. We denote

$A(\chi,q)=\exp(-\frac{1}{2}\chi q_k\sigma_k)$; $C(\theta,n)=\exp(-i\frac{1}{2}\theta n_k\sigma_k)$ and we will have

$A(\chi+\delta\chi,q)=A(\delta\chi,q)A(\chi,q)$; $C(\theta+\delta\theta,n)=C(\delta\theta,n)C(\theta,n)$ (40)

As we mentioned , we denote by U the same function $U\circ h_0^{-1}$ where $h_0:D_0\to GL(V)$ is the map around the origin from the representation definition.

In the same way as we proven in the case of $SO^+(3,1)$, considering the relations (40), if we define $(M_k),(N_k)$ by

$\frac{dU}{d\chi}(A(0,q_k))=-q_kM_k$, $\frac{dU}{d\theta}(C(0,n))=-in_kN_k$

$U(A(\chi,q))=\exp(-\chi q_kM_k)$, $U(C(\theta,n))=\exp(-i\theta n_kN_k)$ –

We will in addition suppose that the functions defined in $\chi+i\theta\in\mathbb{C}$ by

$f_j(\chi+i\theta)=U(A(\chi,(\delta_{jk}))C(\theta,(\delta_{jk})))=U(\exp(-\frac{1}{2}(\chi+i\theta)\sigma_j))$ are complex differentiable, or that the function defined on the complex variables (α_k)

$F((\alpha_k))=U(\sqrt{1+\vec{\alpha}^2}\mathbf{I}+\alpha_k\sigma_k)$ is complex differentiable in each variable α_k in some neighbourhood of (0 , 0, 0).

We can prove that we have $f_j(\chi+i\theta)=U(\cosh(\frac{1}{2}(\chi+i\theta))\mathbf{I}-\sinh(\frac{1}{2}(\chi+i\theta))\sigma_j)$ and so any of these two suppositions will lead to $M_k=N_k$.

Let $E_l(\theta)=\frac{1}{2}C(-\theta,n)\sigma_lC(\theta,n)$ and considering the commutation relations satisfied by $(\frac{1}{2}\sigma_k)$ we obtain $\frac{dE_k}{d\theta}=-n_k\epsilon_{klj}E_j$ and so we have the solution

$E_l=R_{lj}\frac{1}{2}\sigma_j$. Therefore for $\delta\chi,\delta\theta$ small enough we will have:

$C(-\delta\theta,n)\exp(-\frac{1}{2}\delta\chi\sigma_l)C(\delta\theta,n)=\exp(-\frac{1}{2}\delta\chi R_{lj}\sigma_j)$ and

$U(C)^{-1}\exp(-\delta\chi M_l)U(C)=\exp(-\delta\chi R_{lj}M_j)$ where $C=C(\delta\theta,n)$

Taking the second order approximation in $\delta\chi$ and after that in $\delta\theta$ it follows

$(\mathbf{I}+i\delta\theta n_kM_k)M_l(\mathbf{I}-i\delta\theta n_kM_k)=(\mathbf{I}-\delta\theta n_k\epsilon_{klj})M_j+O(\delta\theta^2)$ and so we will have the commutation relations:

$[M_k,M_l]=i\epsilon_{klj}M_j$ (41)

We take $X=M_1+iM_2$, $Y=M_1-iM_2$, $H=2M_3$ and we will have:

$[X,Y]=H$, $[H,X]=2X$, $[H,Y]=-2Y$ (42)

$M_1=N_1=\frac{1}{2}(X+Y)$, $M_2=N_2=\frac{1}{2}(iY-iX)$, $M_3=N_3=\frac{1}{2}H$

Suppose that U is finite-dimensional complex and irreducible.

Then exists an eigenvalue $\lambda\in\mathbb{C}$ of H with an eigenvector $v\in V$, $Hv=\lambda v$, $v\neq0$

From $[H,X]=2X$ follows $HX^jv=(\lambda+2j)X^jv$ and the space being finite-dimensional we can take $i_0=\max\{i\in\mathbb{N}|X^iv\neq0\}$. Let $v_0=X^{i0}v$, $v_j=Y^jv_0$.

From $[H,Y]=-2Y$ follows $Hv_j=(\lambda+2(i_0-j))v_j$ and the space being finite-dimensional we can take $m=\max\{i\in\mathbb{N}|v_i\neq0\}$

We have

$Xv_0=0$, $Xv_{j+1}=XYv_j=YXv_j+Hv_j=YXv_j+(\lambda+2(i_0-j))v_j$, $Yv_j=v_{j+1}, Yv_m=0$

v_0, v_1, … v_m are linearly independent being eigenvectors of *H* for distinct eigenvalues and by induction follows from the above relations that *H, X, Y* leave invariant the subspace generated by them. The representation being irreducible, that subspace must be the whole space and *H* has therefore one-dimensional eigenspaces for each eigenvalue $\lambda+2(i_0-j)$, $j=\overline{0,m}$ with eigenvectors respective v_j . Therefore for the trace of *H* we have:

$$trH=\sum_{j=0}^{m}(\lambda+2(i_0-j))=(m+1)(\lambda+2i_0-m) \ .$$

Since $trH=tr[X,Y]=0$ it follows $\lambda=m-2i_0$

By induction we can prove $Xv_j=j(m-j+1)v_{j-1}$ for $j=\overline{1,m}$ having $Xv_0=0$.

In conclusion we will have $V=Sp[v_0,v_1,\ldots,v_m]$, $Hv_j=(m-2j)v_j$ for $j=\overline{0,m}$ and also $Yv_m=0$, $Yv_j=v_{j+1}$ for $j=\overline{0,m-1}$ for the spin m/2 irreducible representation representation.

It can be proved without difficulties that if the *V* is the subspace of complex polynomials given by

$$V_m=\left\{\sum_{j=0}^{m}a_j x^{m-j}y^j\in P[x,y]\,\middle|\,a_j\in\mathbb{C} \text{ for } j=\overline{0,m}\right\}$$

then $U:SL(2,\mathbb{C})\to GL(V_m)$ with $U(A)p(x,y)=p(A^{-1}(x,y))$ for any $A\in SL(2,\mathbb{C})$ and any $p(x,y)\in V_m$, A^{-1} acting on the column vector (x,y) , provides a m+1-dimensional irreducible representation of $SL(2,\mathbb{C})$

For $A=\exp(-i\frac{1}{2}\theta\sigma_3)$ we have $A^{-1}=\cos(\frac{\theta}{2})\mathbf{I}+i\sin(\frac{\theta}{2})\sigma_3$ and

$$\exp(-i\frac{1}{2}\theta H)(x^{m-j}y^j)=U(A)(x^{m-j}y^j)=$$

$$=(\cos(\frac{\theta}{2})+i\sin(\frac{\theta}{2}))^{m-j}(\cos(\frac{\theta}{2})-i\sin(\frac{\theta}{2}))^{j}x^{m-j}y^j=\exp(i\frac{m-2j}{2}\theta)x^{m-j}y^j$$

Differentiating with respect to θ and taking $\theta=0$ we obtain

$H(x^{m-j}y^j)=(m-2(m-j))x^{m-j}y^j$ and so we have obtained the eigenvalues and eigenvectors of *H* in the representation.

3. On the rotation groups and the restricted Lorentz group

On the rotation groups and the restricted Lorentz group

Consider the n-dimensional rotations group

$SO(n)=\{R\in M_{n\times n}(\mathbb{R})|RR^T=\mathbf{I}\ ,\ det\,R=1\}$.

On the rotations group we take the topology induced from the square real matrices space such that a fundamental system of neighbourhoods of $R_0\in SO(n)$ is $(V_\varepsilon(R_0))_{\varepsilon>0}$ with

$V_\varepsilon(R_0)=\{R\in SO(n)|\|R_{ij}-R_{0ij}|<\varepsilon \text{ for } i,j=\overline{1,n}\}$

For any $R=(Q_{ij})_{i,j}\in SO(n+1)$ if $Q_{k1}\neq 0$ we consider

$e_1^k=(Q_{i1})_{i=\overline{1,n+1}}$, $e_j^k=(\delta_{j-1i})_{i=\overline{1,n+1}}$ for $j=\overline{2,k}$, $e_j^k=(\delta_{ji})_{i=\overline{1,n+1}}$ for $j=\overline{k+1,n+1}$ and

$f_1^k=e_1^k$

$f_{p+1}^k=\text{vers}(e_{p+1}^k-\sum_{j=1}^{p}\langle f_j^k,e_{p+1}^k\rangle f_j^k)$ for $p=\overline{1,n-1}$

$f_{n+1}^k=\text{sign}\,(Q_{k1})\,\text{vers}(e_{n+1}^k-\sum_{j=1}^{n}\langle f_j^k,e_{n+1}^k\rangle f_j^k)$

Then if $Q_{k1}\neq 0$ for $Q^{(k)}=(f_{ij}^k)_{i,j=\overline{1,n+1}}$ we have $Q^{(k)}\in SO(n+1)$ and

$Q^{(k)}R=\begin{pmatrix}1 & 0_{1\times n}\\ 0_{n\times 1} & R^{(k)}\end{pmatrix}=M^{(k)}$ with

$R^{(k)}\in SO(n)$

where $\langle .,.\rangle$ denotes the euclidean scalar product and δ the Kronecker symbol

We suppose as a induction hypothesis that we have a C^∞ class mapping with

$W\ni(\psi_j)_{j=\overline{1,n(n-1)/2}}\to\overline{R}((\psi_j)_j)\in SO(n)$

W an open set of $\mathbb{R}^{n(n-1)/2}$ and $\text{rank}\left(\frac{\partial\overline{R}_{pq}}{\partial\psi_j}\right)_{pq,j}=\frac{n(n-1)}{2}$, $p,q=\overline{1,n}$, $j=\overline{1,n(n-1)/2}$

We take $(\psi_s)_{s=\overline{n(n-1)/2+1,n(n+1)/2}}\to(Q_{s1})_{s=\overline{1,n+1}}\in S_n$ where $S_n=\{x\in\mathbb{R}^{n+1}|\|x\|=1\}$ is the n+1- dimensional sphere, a mapping of S_n.

We have $Q^{(k)T}=\begin{pmatrix}Q_{11} & A\\ B & C\end{pmatrix}$ with $A\in M_{1\times n}(\mathbb{R})$, $B\in M_{n\times 1}(\mathbb{R})$, $C\in M_{n\times n}(\mathbb{R})$.

$B=\begin{pmatrix}Q_{21}\\ \cdot\\ \cdot\\ Q_{n+11}\end{pmatrix}$ and $\begin{pmatrix}A\\ C\end{pmatrix}$ has an inverse $S\in M_{(n+1)\times n}(\mathbb{R})$: $S\begin{pmatrix}A\\ C\end{pmatrix}=\mathbf{I_n}$

It follows

$Q^{(k)T}M^{(k)}=\begin{pmatrix}Q_{11} & AR^{(k)}\\ B & CR^{(k)}\end{pmatrix}$ (1) and we can consider now a mapping $\overline{R}^{(k)}$ such that

$\overline{R}^{(k)}((\psi_s)_{s=\overline{1,n(n+1)/2}})=Q^{(k)T}\begin{pmatrix}1 & 0_{1\times n}\\ 0_{n\times 1} & \overline{R}\end{pmatrix}$

$Q^{(k)}=Q^{(k)}((\psi_s)_{s=\overline{n(n-1)/2+1,n(n+1)/2}})$

$\overline{R}=\overline{R}((\psi_j)_{j=\overline{1,n(n-1)/2}})$

Since $\text{rank}\left(\frac{\partial Q_{i1}}{\partial\psi_s}\right)_{i,s}=n$ with $i=\overline{1,n+1}$, $s=\overline{n(n-1)/2+1,n(n+1)/2}$

and the mapping $\overline{R}$ has rank $n(n-1)/2$ and we have the inverse S for

$\begin{pmatrix} A \\ C \end{pmatrix}$ it follows that if $\sum_{j=1}^{n(n+1)/2} \alpha_j \frac{\partial (Q^{(k)} M^{(k)})}{\partial \psi_j} = 0$ with $\alpha_j \in \mathbb{R}$, $j = \overline{1, n(n+1)/2}$

then $\alpha_j = 0$ for $j = \overline{1, n(n+1)/2}$ and so $\operatorname{rank} \left(\frac{\partial R_{pq}^{(k)}}{\partial \psi_j} \right)_{pq, j} = \frac{n(n+1)}{2}$

where $p, q = \overline{1, n+1}$, $j = \overline{1, n(n+1)/2}$

The application $\Phi^{(k)} : S_n \times SO(n) \to SO(n+1)$

$\Phi^{(k)}((Q_{i1})_{i=\overline{1,n+1}}, R^{(k)}) = M^{(k)}$

is a local homeomorphism, defined in the neighbourhood of each

$((Q_{i1})_{i=\overline{1,n+1}}, R^{(k)})$ with $Q_{k1} \neq 0$ and so by induction we can define a smooth class C^∞ manifold structure on $SO(n+1)$ having dimension $n(n+1)/2$ that generates the same topology on $SO(n+1)$ as induced from $M_{(n+1)\times(n+1)}(\mathbb{R})$.

Suppose now the induction assumption that for any $R \in SO(m)$, $m \leq n$ exists

$W \in M_{m \times m}(\mathbb{R})$ such that $W = -W^T$ and $R = \exp(W)$

For $Q \in SO(n+1)$ if Q invariates a subspace V of $\mathbb{R}^{n+1}$ (i.e. $Q(V) = V$)

then Q invariates also $V^\perp$

If $\lambda \in \mathbb{C}$, $x \in M_{(n+1)\times 1}(\mathbb{C})$, $x \neq 0$, $Qx = \lambda x$ it follows $\lambda \overline{\lambda} = 1$, since $QQ^T = \mathbf{I}$

($\overline{\lambda}$ the complex conjugate of λ)

If further $\lambda \in \mathbb{C} \setminus \mathbb{R}$ taking $u = \Re x$, $v = \Im x$ we have

$\lambda = \cos(\theta) + i \sin(\theta)$, $\sin(\theta) \neq 0$, $v \neq 0$

$Qu = u \cos(\theta) - v \sin(\theta)$, $Qv = u \sin(\theta) + v \cos(\theta)$ and since $QQ^T = \mathbf{I}$ we will have

$\|u\|^2 = \|u\|^2 \cos^2(\theta) + \|v\|^2 \sin^2(\theta) - 2\langle u, v \rangle \sin(\theta) \cos(\theta)$

$\|v\|^2 = \|u\|^2 \sin^2(\theta) + \|v\|^2 \cos^2(\theta) + 2\langle u, v \rangle \sin(\theta) \cos(\theta)$

$\langle u, v \rangle = (\|u\|^2 - \|v\|^2) \sin(\theta) \cos(\theta) + \langle u, v \rangle (\cos^2(\theta) - \sin^2(\theta))$

$(\|u\|^2 - \|v\|^2)(\cos(2\theta) - 1) - 2\langle u, v \rangle \sin(2\theta) = 0$

$(\|u\|^2 - \|v\|^2) \sin(2\theta) + 2\langle u, v \rangle (\cos(2\theta) - 1) = 0$

Therefore, since $\sin(\theta) \neq 0$ it follows $\langle u, v \rangle = 0$, $\|u\| = \|v\| \neq 0$

Q invariates $\operatorname{Sp}(u, v)$ and $\operatorname{Sp}(u, v)^\perp$ and so we can find $R \in SO(n+1)$ such that

$RQR^T = \begin{pmatrix} B & 0_{2\times(n-1)} \\ 0_{(n-1)\times 2} & Q_0 \end{pmatrix}$

with $Q_0 = \exp(W_0) \in SO(n-1)$, $W_0 = -W_0^T \in M_{(n-1)\times(n-1)}(\mathbb{R})$

$B = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} = \exp(\theta A)$ where $A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

Taking $W = R^T \begin{pmatrix} \theta A & 0_{2\times(n-1)} \\ 0_{(n-1)\times 2} & W_0 \end{pmatrix} R$ we obtain $Q = \exp(W)$

If $\lambda \in \mathbb{R}$ we must have $\lambda \in \{-1, 1\}$

Then if $x \in M_{(n+1)\times 1}(\mathbb{R})$, $Qx = -x$, $x \neq 0$ since $\det Q = 1$ there it exists another $y \neq 0$, $y \in \{x\}^\perp$ such that $Qy = -y$ and we will have

$R \in SO(n-1)$ with $RQR^T = \begin{pmatrix} \exp(\pi A) & 0_{2\times(n-1)} \\ 0_{(n-1)\times 2} & Q_0 \end{pmatrix}$, $Q_0 = \exp(W_0)$, $W_0 = -W_0^T$

and we can take $Q = \exp(W)$ with $W = R^T \begin{pmatrix} \pi A & 0_{2\times(n-1)} \\ 0_{(n-1)\times 2} & W_0 \end{pmatrix} R = -W^T \in M_{(n+1)\times(n+1)}(\mathbb{R})$

If $x\in M_{(n+1)\times 1}(\mathbb{R})$, $x\neq 0$, $Qx=x$ we will have $R\in SO(n+1)$ such that

$RQR^T=\begin{pmatrix}1 & 0_{1\times n}\\ 0_{n\times 1} & Q_0\end{pmatrix}$ where by induction assumption $Q_0=\exp(W_0), W_0=-W_0^T$

Taking $W=R^T\begin{pmatrix}0 & 0_{1\times n}\\ 0_{n\times 1} & W_0\end{pmatrix}R=-W^T\in M_{(n+1)\times(n+1)}(\mathbb{R})$ we will have $Q=\exp(W)$

Therefore , by induction we have proved that for any

$Q\in SO(n)$ exists $W\in M_{n\times n}(\mathbb{R})$ such that $W=-W^T$ and $Q=\exp(W)$

Also it is obvious that if $W=-W^T$ then $WW^T=W^TW$ and so for $Q=\exp(W)$:

$QQ^T=\exp(W+W^T)=\mathbf{I}$, $Q\in O(n)$

Moreover we have $W=JSJ^{-1}$ where S is the Jordan normal form of W

$\det\exp(W)=\det\exp(S)=\prod_{i=1}^{n}\exp(\lambda_i)$, where

$\det(W-\lambda\mathbf{I})=\prod_{i=1}^{n}(\lambda-\lambda_i)$

For $W=-W^T\in M_{n\times n}(\mathbb{R})$, $Wx=\lambda x$, $x\in M_{n\times 1}(\mathbb{C})$, $\lambda\in\mathbb{R}$ we can take $x\in M_{n\times 1}(\mathbb{R})$

and so $x^TWx=x^TW^Tx=-x^TWx=0$, $0=x^TWx=\lambda\|x\|^2$ and

all real eigenvalues of *W* must vanish and since *W* is real we can split the eigenvalues as

$E=\{i\in\{1,..n\}|\lambda_i\in\mathbb{C}\setminus\mathbb{R}\}=E_1\cup E_2$, $E_1\cap E_2=\emptyset$, $\operatorname{card}E_1=\operatorname{card}E_2$

$E_1=\{i_1,...,i_k\}$, $E_2=\{j_1,...,j_k\}$, $\lambda_{is}=\overline{\lambda}_{js}$ for $s=\overline{1,k}$

Therefore it follows $\prod_{i=1}^{n}\exp(\lambda_i)>0$, $Q=\exp(W)\in SO(n)$.

We will prove now that the function

$\Phi:M_{n\times n}(\mathbb{R})\to M_{n\times n}(\mathbb{R})$ with $\Phi(W)=\exp(W)$ for any $W\in M_{n\times n}(\mathbb{R})$ satisfies

$\det\left(\frac{\partial\Phi_{pq}}{\partial t_{ij}}\right)_{pq,ij}\neq 0$ for any $W=(t_{ij})_{i,j}\in M_{n\times n}(\mathbb{R})$ where $i,j,p,q=\overline{1,n}$ (2)

$\Phi=(\Phi_{pq})_{p,q}=(e^W_{pq})_{p,q}$

(2) is equivalent to the fact that

for any W , $\beta\in M_{n\times n}(\mathbb{R})$ the relation $\frac{\partial}{\partial h}\exp(W+h\beta)¿\Big|_{h=0}=0$ implies $\beta=0$.

Suppose we have $W,\beta\in M_{n\times n}(\mathbb{R})$ such that $\frac{\partial}{\partial h}\exp(W+h\beta)\Big|_{h=0}=0$

Since for any $J\in M_{n\times n}(\mathbb{C})$ with $\det J\neq 0$ we have

$\frac{\partial}{\partial h}\exp(JWJ^{-1}+hJ\beta J^{-1})=J\left(\frac{\partial}{\partial h}\exp(W+h\beta)\right)J^{-1}$ it is sufficient to prove (2) only for *W*

having the upper triangular normal Jordan form

$W=\begin{pmatrix}C_1 & 0 & .. & 0\\ 0 & C_2 & .. & 0\\ . & .. & . & 0\\ 0 & .. & 0 & C_r\end{pmatrix}$ with C_i cells of the form $C_i=\lambda_i\mathbf{I}_{si}+N_{si}$, $\lambda_i\in\mathbb{C}$, $s_i\in\mathbb{N}^*$

$N_{si}=(n_{kl})_{k,l=\overline{1,si}}$, $n_{kl}=\begin{cases}1 & \text{if } l=k+1,1\leq k\leq s_i-1\\ 0 & \text{otherwise}\end{cases}$ for $k,l=\overline{1,s_i}$

We denote $W_{ii}=\mu_i$ for $i=\overline{1,n}$

Let *W* having the Jordan normal form and we have :

$\frac{\partial e^W}{\partial t_{ij}}=\sum_{m=1}^{\infty}\frac{1}{m!}\sum_{k=0}^{m-1}W^{m-1-k}E_{ij}W^k$ where $E_{ij}=(\delta_{ik}\delta_{jl})_{k,l=\overline{1,n}}$ (3)

For any $k\in\mathbb{N}$, W^k is upper triangular and has diagonal coefficients $(W^k)_{ii}=\mu_i^k$ and therefore calculating the terms $W^{m-1-k}E_{ij}W^k$ it follows that $\frac{\partial e^W_{pq}}{\partial t_{ij}}=0$ if $q<j$ or $p>i$.

We consider for pq and ij pass the ordering (1n)(2n))...((n-1)n)(nn)(1(n-1))...(n(n-1))(1(n-2))….. (11)((21)...((n-1)1)(n1) we find that the matrix

$\left(\frac{\partial e^W_{pq}}{\partial t_{ij}}\right)_{pq,ij}$ has an upper triangular form and so

$\det\left(\frac{\partial e^W_{pq}}{\partial t_{ij}}\right)_{pq,ij}=\prod_{p,q=1}^{n}\frac{\partial e^W_{pq}}{\partial t_{pq}}$

Calculation from (3), with W having the Jordan normal form leads to

$\frac{\partial e^W_{pq}}{\partial t_{pq}}=\sum_{m=1}^{\infty}\frac{1}{m!}\sum_{k=0}^{m-1}\mu_p^{m-1-k}\mu_q^k=\begin{cases}\frac{\exp(\mu_p)-\exp(\mu_q)}{\mu_p-\mu_q} & \text{if } \mu_p\neq\mu_q\\ \frac{\exp(\mu_p)-1}{\mu_p} & \text{if } \mu_p=\mu_q\end{cases}$

and so $\det\left(\frac{\partial e^W_{pq}}{\partial t_{ij}}\right)_{pq,ij}\neq 0$ for any $W\in M_{n\times n}(\mathbb{R})$ (3')

Let $(J_s)_{s=\overline{1,n(n-1)/2}}$ a system of linear independent generators for the antisymmetric real matrices so that we have

$W=-W^T\in M_{n\times n}(\mathbb{R})\ W=\psi_s J_s$, $\psi_s\in\mathbb{R}$ (with Einstein summation convention for indexes $s=\overline{1,n(n-1)/2)}$

Because we have (3'), it follows that for

$R_0\in SO(n)$ and $\psi^0=(\psi_s^0)_s$ such that $\exp(\psi_s^0 J_s)=R_0$ we have an open neighbourhood U_0 of ψ^0, an open neighbourhood G_0 of R_0 and the injective function $\Phi:U_0\to G_0$, $\Phi(\psi)=\exp(\psi_s J_s)$, $\psi=(\psi_s)_s$

As we proved, we can choose G_0 such that we have a mapping

$\overline{R}:V_0\to G_0$ of $SO(n)$ from some open neighbourhood V_0 of φ^0 such that $\varphi^0=(\varphi_s^0)_s$ and $\overline{R}(\varphi^0)=R_0$, $\operatorname{rank}\left(\frac{\partial\overline{R}_{pq}}{\partial\varphi_s}\right)_{pq,s}=\frac{n(n-1)}{2}$ (4)

Thus we have $\overline{R}(\varphi^0)=\exp(\psi_s^0 J_s)$ and for $\varphi=\overline{R}^{-1}\circ\Phi(\psi)$ we have $\overline{R}(\varphi)=\exp(\psi_s J_s)$ for any $\psi\in U_0$ and the function $\overline{R}^{-1}\circ\Phi:U_0\to V_0$ is continuous and injective .

Therefore, since U_0 is open and U_0, V_0 have the same dimension it follows that $\overline{R}^{-1}\circ\Phi(U_0)=W_0$ is an open set and $\varphi^0\in W_0$ and we have a homeomorphism $\overline{R}^{-1}\circ\Phi:U_0\to W_0$

Since (4), by the implicit function theorem we will have a C^1 class function $h:U_1\to V_1$ with U_1 open neighbourhood of ψ^0, V_1 open neighbourhood of φ^0 such that $\overline{R}(h(\psi))=\exp(\psi_s J_s)$ for any $\psi\in U_1$ and for any $(\varphi,\psi)\in V_1\times U_1:\overline{R}(\varphi)=\exp(\psi_s J_s)$ if and only if $\varphi=h(\psi)$

Since (3') we have that

$\operatorname{rank}\left(\frac{\partial \exp(\psi_s J_s)_{pq}}{\partial \psi_k}\right)_{pq,k}=\frac{n(n-1)}{2}$ and we will have also a C^1 class function

$g: V_2 \to U_2$ with U_2 open neighbourhood of ψ^0 , V_2 open neighbourhood of φ^0 such that $\overline{R}(\varphi)=\exp(g_s(\varphi) J_s)$ for any $\varphi \in V_2$

and for any $(\varphi, \psi)\in V_2\times U_2: \overline{R}(\varphi)=\exp(\psi_s J_s)$ if and only if $\psi=g(\varphi)$.

It follows $(g\circ h)(\psi)=\psi$, $(h\circ g)(\varphi)=\varphi$ for any $(\varphi,\psi)\in V_1\cap V_2\times U_1\cap U_2$

Therefore we can find *U, V* open neighbourhoods of ψ^0 respective φ^0 such that

$h(U)=V$, $g(V)=U$, $h\big|_U=g^{-1}\big|_U$, $\overline{R}(h(\psi))=\exp(\psi_s J_s)$, $\overline{R}(\varphi)=\exp(g_s(\varphi) J_s)$ for any $(\varphi, \psi)\in V\times U$.

Intermediating through the $\overline{R}$ mappings of the manifold structure $SO(n)$ we obtain that for any ψ^0 , ψ^1 with $\exp(\psi^0_s J_s)=\exp(\psi^1_s J_s)$ there exist

W_0 an open neighbourhood of ψ^0 and W_1 an open neighbourhood of ψ^1 and a C^∞ class function $f: W_0 \to W_1$ such that for any $(\psi, \psi')\in W_0\times W_1$:

$\exp(\psi_s J_s)=\exp(\psi'_s J_s)$ if and only if $\psi'=f(\psi)$ and so we have the same manifold structure on $SO(n)$ with topology induced from $M_{n\times n}(\mathbb{R})$ given by the mappings $(\psi_s)_{s=\overline{1,n(n-1)/2}} \to \exp(\psi_s J_s)$ having the continuous surjective function $\Phi: \mathbb{R}^{n(n-1)/2} \to SO(n)$ with $\Phi(\psi)=\exp(\psi_s J_s)$ and so we find $SO(n)$ as a $n(n-1)/2$- dimensional connected Lie group.

Consider now the Minkowski space

$\mathbb{R}^4$ identified with $M_{4\times 1}(\mathbb{R})$ having the pseudometric $(\eta_{\alpha\beta})_{\alpha,\beta}$ with

$\eta_{\alpha\beta}=0$ if $\alpha\neq\beta$, $\eta_{ii}=-1$ for $i=\overline{1,3}$, $\eta_{00}=1$

(we use greek characters for indexing from 0 to 3 and latin characters for indexing from 1 to 3)

We have the pseudo-scalar product $\mathbb{R}^4\times\mathbb{R}^4\ni(x,y)\to x\cdot y=y^T\eta x\in\mathbb{R}$

x , y as column vectors $x=x^\alpha E_\alpha$, $(E_\alpha)_\alpha$ Minkowski base with

$E_\alpha=(\delta_{\alpha\beta})_\beta$ (as column vector) , $E_\alpha\cdot E_\beta=\eta_{\alpha\beta}$

We remind that , as a consequence of the Cauchy-Bunyakowsky-Schwarz inequality, we have:

i) if $x, y\in\mathbb{R}^4$ and $x\neq 0$, $x^T\eta x\geq 0$, $y^T\eta x=0$ then $y^T\eta y\leq 0$

ii) if x , $y\in\mathbb{R}^4$ and $x\neq 0$, $x^T\eta x=0$, $y^T\eta x=0$ then exists $\lambda\in\mathbb{R}$ with $y=\lambda x$.

For $M\in SO^+(3,1)$ (see Chap. Representations of the rotations group and of the restricted Lorentz group , Spin representations) we have :

$M=R(\theta,n)B(\chi,q)=M(\vec{\theta},\vec{\chi})$ where $\vec{\theta}=\theta n$, $\vec{\chi}=\chi q$, $\vec{\theta}=(\theta_i)_i$, $\vec{\chi}=(\chi_i)_i$

$R(\theta,n)=(R_{\alpha\beta})_{\alpha,\beta}$, $B(\chi,q)=(B_{\alpha\beta})_{\alpha,\beta}$,

$R_{ij}=-\epsilon_{ijk}n_k\sin(\theta)+(\delta_{ij}-n_i n_j)\cos(\theta)+n_i n_j$, $R_{i0}=R_{0i}=0$, $R_{00}=1$

$B_{ij}=\delta_{ij}+(\cosh(\chi)-1)q_i q_j$, $B_{0i}=B_{i0}=-q_i\sinh(\chi)$, $B_{00}=\cosh(\chi)$

B is symmetric positive definite and so $M=RB$ must be the polar decomposition of M , $B=\sqrt{M^T M}$, $R=M(\sqrt{M^T M})^{-1}$ and we can find $k\in\{1,2,3\}$ such that :

$n=\operatorname{vers}(\epsilon_{ijk}(R_i-\delta_i)\times(R_j-\delta_j))$ with $R_i=(R_{il})_l$, $\delta_i=(\delta_{il})_l$

$\sin(\theta)=-\frac{1}{2}\epsilon_{ijl}n_l R_{ij}$, $\cos(\theta)=\frac{1}{2}(R_{ii}-1)$

$\cosh(\chi)=B_{00}$, $\sinh(\chi)=\sqrt{B_{00}^2-1}$, $q_i=-\frac{B_{i0}}{\sqrt{B_{00}^2-1}}$

Therefore we have a local homeomorphism :

$\mathbb{R}^6 \ni (\vec{\theta},\vec{\chi}) \to M(\vec{\theta},\vec{\chi}) \in SO^+(3,1)$ when $SO^+(3,1)$ is considered with the topology which is induced from $M_{4\times 4}(\mathbb{R})$ and a 6-dimensional connected Lie group structure on $SO^+(3,1)$ given by the mappings $(\vec{\theta},\vec{\chi}) \to M(\vec{\theta},\vec{\chi})$.

Suppose now we have

$(\alpha_k)_k$, $(\beta_k)_k \in \mathbb{R}^3$ such that $\alpha_k \frac{\partial M}{\partial \theta_k} + \beta_k \frac{\partial M}{\partial \chi_k} = 0$ for a value of $(\vec{\theta},\vec{\chi})$

It follows :

$0 = \beta_k \frac{\partial B_{0i}}{\partial \chi_k} = \beta_k \left(-\frac{\delta_{ik}}{\chi} + \frac{1}{\chi} q_i q_k \right) \sinh(\chi) - \beta_k q_k q_i \cosh(\chi)$

$0 = \beta_k \frac{\partial B_{00}}{\partial \chi_k} = \beta_k q_k \sinh(\chi)$ and so we obtain $\beta_i = 0$ for $i = \overline{1,3}$

$\alpha_k \frac{\partial R}{\partial \theta_k} = 0$ with $(R_{ij})_{i,j} = \exp(\theta_k J_k)$, $(J_k)_{ij} = -\epsilon_{ijk}$, for $i,j,k = \overline{1,3}$.

Since $\det\left(\frac{\partial e^W_{pq}}{\partial t_{ij}} \right)_{pq,ij} \neq 0$ for any $W = (t_{ij})_{i,j} \in M_{3\times 3}(\mathbb{R})$ as we have proven, it follows :

$\operatorname{rank}\left(\frac{\partial \exp(\theta_k J_k)_{ij}}{\partial \theta_l} \right)_{ij,l} = 3$ and so we must have also $\alpha_k = 0$ for $k = \overline{1,3}$.

Therefore taking $(\psi_l)_{l=\overline{1,6}} = (\vec{\theta},\vec{\chi})$ we have $\operatorname{rank}\left(\frac{\partial M_{\alpha\beta}}{\partial \psi_l} \right)_{\alpha\beta,l} = 6$

We remind that we rise or lower the indexes according to

$V_\alpha = \eta_{\alpha\beta} V^\beta$, $V^\alpha = \eta^{\alpha\beta} V_\beta$, $(\eta_{\alpha\beta}) = (\eta^{\alpha\beta})$

Let $\epsilon_{\alpha\beta\gamma\delta}$ be the signature of the permutation $\begin{pmatrix} \alpha & \beta & \gamma & \delta \\ 0 & 1 & 2 & 3 \end{pmatrix}$ and we define

$\overline{J}^{\alpha\beta}_{\gamma\delta} = \epsilon^{\alpha\beta\gamma\varepsilon} \eta_{\varepsilon\delta}$. We will have:

$\overline{J}^{0i} = -\overline{J}^{i0} = -J_i$, $\overline{J}^{ij} = \epsilon_{ijk} K_k$ where J_i , K_k are the Lorentz group generators

$(J_k)_{ij} = -\epsilon_{ijk}$, $(J_k)_{i0} = (J_k)_{0i} = (J_k)_{00} = 0$, $(K_k)_{ij} = 0$, $(K_k)_{i0} = (K_k)_{0i} = \delta_{i0}$, $(K_k)_{00} = 0$

$R(\theta,n) = \exp(\theta n_k J_k)$, $B(\chi,q) = \exp(-\chi q_k K_k)$.

We define also

$J^{\alpha\beta}_{\gamma\delta} = \frac{1}{2} \epsilon^{\alpha\beta}{}_{\psi\varphi} \overline{J}^{\psi\varphi}_{\gamma\delta} = -\frac{1}{2} \epsilon^{\alpha\beta\psi\varphi} \epsilon_{\psi\varphi\delta\rho} \eta^{\gamma\rho}$ obtaining

$J^{ij} = -\epsilon_{ijk} J_k$, $J^{0i} = -J^{i0} = -K_i$.

For a Lorentz coordinates transformation $x'^\mu = \Lambda^\mu{}_\nu x^\nu$, $(\Lambda^\mu{}_\nu)_{\mu,\nu} = \Lambda \in SO^+(3,1)$

we denote $(\Lambda_\mu{}^\nu)_{\nu,\mu} = \Lambda^{-1}$.

The relation $\Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \overline{J}^{\alpha\beta} = \Lambda^{-1} \overline{J}^{\mu\nu} \Lambda$ (5) is equivalent to

$\Lambda^\varepsilon{}_\gamma \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \Lambda_\rho{}^\delta \overline{J}^{\alpha\beta}_{\gamma\delta} = \overline{J}^{\mu\nu}_{\varepsilon\rho}$.

Since $\Lambda \in SO^+(3,1)$ we have $\Lambda_\rho{}^\delta = \Lambda^\varphi{}_\psi \eta_{\psi\delta} \eta_{\rho\varphi}$ and so (5) is equivalent to

$\Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \Lambda^\varepsilon{}_\gamma \Lambda^\kappa{}_\psi \epsilon^{\alpha\beta\gamma\psi} = \epsilon^{\mu\nu\varepsilon\kappa}$ which is true since $\det \Lambda = 1$

Also, since $\Lambda \in SO^+(3,1)$ we have

$\epsilon^{\gamma\varepsilon}{}_{\mu\nu} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta = \eta^{\kappa\gamma} \eta^{\rho\varepsilon} \epsilon_{\alpha\beta\psi\varphi} \Lambda_\kappa{}^\psi \Lambda_\rho{}^\varphi = \epsilon^{\kappa\rho}{}_{\alpha\beta} \Lambda^\gamma{}_\kappa \Lambda^\varepsilon{}_\rho$.

Therefore, from (5) follows :

$\Lambda^\nu{}_\alpha \Lambda^\nu{}_\beta J^{\alpha\beta} = \Lambda^{-1} J^{\mu\nu} \Lambda$ (6)

We will prove further that if $M\in SO^+(3,1)$ then exists $\Lambda\in SO^+(3,1)$ such that $M=\Lambda^{-1}\exp(\theta J_3+\chi K_3)\Lambda$ or $M=\Lambda^{-1}\exp(\alpha(J_1+K_2))\Lambda$ for some $\theta,\chi,\alpha\in\mathbb{R}$.

If exists $\mu\in\mathbb{C}\setminus\mathbb{R}$ such that we have $x\in\mathbb{C}^4$ (x as a column vector) $x\neq 0$ with $Mx=\mu x$, then if $x^T\eta x\neq 0$ it follows, since $M^T\eta M=\eta$ that $\mu^2=1$ and because $\mu\in\mathbb{C}\setminus\mathbb{R}$, we must have $x^T\eta x=0$ and so

$\Re x^T\eta\Re x=\Im x^T\eta\Im x$, $\Re x^T\eta\Im x=0$ (7)

If also $\Re x^T\eta\Re x=0$, since $\Im x\neq 0$ (because $\mu\notin\mathbb{R}$) we have $\lambda\in\mathbb{R}$ with $\Re x=\lambda\Im x$.

This leads to $(i+\lambda)M\Im x=(i+\lambda)\mu\Im x$ which again contradicts $\mu\notin\mathbb{R}$.

Therefore we have $u=\Re x$, $v=\Im x$, $x=u+iv$

$u^T\eta u=v^T\eta v\neq 0$, $u^T\eta v=0$ (8)

$\overline{x}^T\eta x=u^T\eta u+v^T\eta v\neq 0$ (9) which from $Mx=\mu x$ leads to $\mu\overline{\mu}=1$ and $\alpha\in\mathbb{R}$ with

$Mu=u\cos(\alpha)-v\sin(\alpha)$

$Mv=u\sin(\alpha)+v\cos(\alpha)$

As a consequence of Cauchy-Bunyakowsky-Schwarz inequality, from (8) we obtain

$u^T\eta u=v^T\eta v<0$ and we can therefore consider $u^T\eta u=v^T\eta v=-1$.

M invariates $V=\mathrm{Sp}(u,v)$ and for $V^\perp=\{w\in M_{4\times 1}(\mathbb{R})|w^T\eta z=0$ for any $z\in V\}$,

M invariates also $V^\perp$.

We can take $\Lambda\in SO^+(3,1)$ such that $\Lambda^{-1}E_1=u$ and $\Lambda^{-1}E_2=v$.

For $\overline{M}=\Lambda M\Lambda^{-1}$ we will have:

$\overline{M}E_1=E_1\cos(\alpha)-E_{\sin}(\alpha)$, $\overline{M}E_2=E_1\sin(\alpha)+E_2\cos(\alpha)$ and that

$\overline{M}$ invariates $\mathrm{Sp}(E_1,E_2)$ and $\mathrm{Sp}(E_3,E_0)=\mathrm{Sp}(E_1,E_2)^\perp$.

Hence exist θ , $\chi\in\mathbb{R}$ such that $\overline{M}=\exp(\theta J_3)\exp(\chi K_3)=\exp(\theta J_3+\chi K_3)$

$$M=\Lambda^{-1}\exp(\theta J_3+\chi K_3)\Lambda$$

Therefore, to prove the statement we can further suppose that

if $\mu\in\mathbb{C}$, $x\in M_{4\times 1}(\mathbb{C})$, $x\neq 0$, $Mx=\mu x$ then $\mu\in\mathbb{R}^*$ and $x\in M_{4\times 1}(\mathbb{R})$

Let $x\in M_{4\times 1}(\mathbb{R})$, $\lambda\in\mathbb{R}^*$, $x\neq 0$, $Mx=\lambda x$

If $x^T\eta x=0$ we can choose $x\in M_{4\times 1}(\mathbb{R})$ and take $\Lambda\in SO^+(3,1)$ such that $\Lambda x=E$ where $E=E_3+E_0$. Then for $\overline{M}=\Lambda M\Lambda^{-1}$, $\overline{M}$ invariates $\{E\}^\perp=\mathrm{Sp}(E_1,E_2,E)=V$ and we will have:

$\overline{M}E_1=\alpha E_1+\beta E_2+\gamma E$

$\overline{M}E_2=\alpha' E_1+\beta' E_2+\gamma' E$ (10)

$\overline{M}E=\lambda E$

Since $\overline{M}\in SO^+(3,1)$ we obtain:

$\alpha^2+\beta^2=1$, $\alpha'^2+\beta'^2=1$, $\alpha\alpha'+\beta\beta'=0$

$\alpha=\cos(\theta)$, $\beta=\sin(\theta)$, $\alpha'=\cos(\theta')$, $\beta'=\sin(\theta')$, $\theta-\theta'=\frac{2k+1}{2}\pi$, $k\in\mathbb{Z}$.

Let $S=\begin{pmatrix}\alpha & \alpha' & 0\\ \beta & \beta' & 0\\ \gamma & \gamma' & \lambda\end{pmatrix}$

After some calculus we find that solutions for the characteristic equation in μ are:

$\mu=\lambda$ and $\mu=\frac{1}{2}(1+(-1)^{k+1}\pm\sqrt{(1+(-1)^{k+1})\cos^2(\theta)+4(-1)^k})$

If $k\equiv 1(\mathrm{mod}\,2)$ and $\cos^2(\theta)\neq 1$, S and therefore also M has an eigenvalue which is not real and so we can consider that $k\equiv 0(\mathrm{mod}\,2)$ if $\cos^2(\theta)\neq 1$.

If $k\equiv 0(\mathrm{mod}\,2)$ or $\cos^2(\theta)\neq 1$, $\overline{M}$ must have an eigenvalue $\mu\in\mathbb{R}^*$, $\mu\neq\lambda$, $\mu^2=1$.
$\overline{M}y=\mu y$, $\overline{M}E=\lambda E$, $y\in V=\{E\}^{\perp}=\mathrm{Sp}(E_1,E_2,E)$.
$\overline{M}$ invariates $\mathrm{Sp}(y,E)$ and $\mathrm{Sp}(y,E)^{\perp}=W$ having $\dim W=2$.

For $z\in W$ we have $z^T\eta E=0$ and as a consequence of the Cauchy-Bunyakowsky-Schwarz inequality, for any $z\in W$ which is independent of E follows $z^T\eta z<0$.

Let $E'\in W$, $E'^T\eta E'=-1$ and we have β'' , $\alpha''\in\mathbb{R}$, $\beta''^2=1$ with

$$\overline{M}y=\mu y$$
$$\overline{M}E'=\beta''E'+\alpha''E \quad (10')$$
$$\overline{M}E=\lambda E$$

$y^T\eta E'=0$, $E'^T\eta E=0$, $E^T\eta y=0$, $y^T\eta y=-1$, $E'^T\eta E'=-1$, $E^T\eta E=0$ (10'')

$\mathrm{Sp}(y,E',E)=\mathrm{Sp}(E_1,E_2,E)$ and from (10) , (10') follows

$\det(S-\rho\mathbf{I})=\det(S'-\rho\mathbf{I})$ for any $\rho\in\mathbb{C}$ where $S'=\begin{pmatrix}\mu & 0 & 0\\ 0 & \beta'' & 0\\ 0 & \alpha'' & \lambda\end{pmatrix}$ and so we must have

$(\mu=1$ and $\beta''=-1)$ or $(\mu=-1$ and $\beta''=1)$.

Because $\det M=1$, the characteristic equation in ρ , $\det(M-\rho\mathbf{I})=0$ must have another solution $\rho=-\frac{1}{\lambda}$ and since $\lambda\in\mathbb{R}$ we have $\lambda\neq-\frac{1}{\lambda}$ and $z\in M_{4\times 1}(\mathbb{R})$, z independent of

x such that $Mz=-\frac{1}{\lambda}z$, $Mx=\lambda x$, $z^T\eta x=-z^T\eta x=0$.

Hence because $x^T\eta x=0$, *x* cannot be independent of *z* , and so, when all eigenvalues of *M* are real, as we can consider , we must suppose that we are in case a) or case b) described below:

a) for any $\lambda\in\mathbb{C}$, $x\in M_{4\times 1}(\mathbb{C})$, $x\neq 0$ with $Mx=\lambda x$ we can consider that

$$\lambda\in\mathbb{R}^*\ ,\ x\in M_{4\times 1}(\mathbb{R})\ ,\ x\neq 0\ ,\ Mx=\lambda x\ ,\ x^T\eta x\neq 0\ ,\ \lambda^2=1$$

(the last equality in case a) follows because *M* is a Lorentz transformation)

b) there exist an eigenvalue $\lambda\in\mathbb{R}^*$ such that the corresponding x , θ , k which we have for λ satisfy $x^T\eta x=0$, $\cos^2(\theta)=1$, $k\equiv 1(\mathrm{mod}\,2)$.

In case a), taking $x_0\in M_{4\times 1}(\mathbb{R})$ with $x_0\neq 0, \lambda_0\in\mathbb{R}^*$, $Mx_0=\lambda_0 x_0$ we have that M invariates $\{x_0\}$ and $\{x_0\}^{\perp}$ and we can take successively $x_i\in M_{4\times 1}(\mathbb{R})$, $x_i\neq 0$, $\lambda_i\in\mathbb{R}^*$ such that after eventually a permutation of indexes we have:

$Mx_\alpha=\lambda_\alpha x_\alpha$, $\lambda_\alpha^2=1$, $x_\alpha^T\eta x_\beta=\eta_{\alpha\beta}$ for α , $\beta=\overline{0,3}$.

Then we can find $\varepsilon_\alpha\in\{1,-1\}$, $\Lambda\in SO^+(3,1)$ with $\Lambda^{-1}E_\alpha=\varepsilon_\alpha x_\alpha$.

In the basis (E_1,E_2,E_3,E_0) the transformation $\overline{M}'=\Lambda M\Lambda^{-1}$ has the diagonal form

$\begin{pmatrix}\lambda_1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & \lambda_0\end{pmatrix}$ and since $\overline{M}'\in SO^+(3,1)$ we have $\lambda_0=1$.

If $\lambda_3=-1$ it follows $\lambda_1\lambda_2=-1$ and we can take $Q\in SO^+(3,1)$ with $Q^T=Q^{-1}$, $Q\overline{M}'Q^T=\exp(\pi J_3+0K_3)$. If $\lambda_3=1$ it follows $\lambda_1\lambda_2=1$ and also we can take $Q\in SO^+(3,1)$ with $Q^T=Q^{-1}$, $Q\overline{M}'Q^T\in\{\exp(\pi J_3+0K_3)\ ,\ \exp(0J_3+0K_3)\}$

In case b) we must have $\mu=\beta''=\cos(\theta)\in\{\pm 1\}$ and the characteristic equation has another solution $\rho=\frac{1}{\lambda}$, $\det(M-\rho\mathbf{I})=0$.

If $\beta''\neq\lambda$, taking $z=E'+\frac{\alpha''}{\beta''-\lambda}E$ we obtain:

$$\overline{M}y=\mu y\ ,\ \overline{M}z=\mu z\ ,\ \overline{M}E=\lambda E\ ,$$

$y^T\eta z=0$, $y^T\eta y=z^T\eta z=-1$, $E\in\{y,z\}^\perp$ and we find $\Lambda\in SO^+(3,1)$ with $\varepsilon\in\{\pm1\}$, $\rho\in\mathbb{R}^*$, $\Lambda^{-1}E_1=y$, $\Lambda^{-1}E_2=\varepsilon z$, $\Lambda^{-1}E=\rho E$.

For $M'=\Lambda\overline{M}\Lambda^{-1}$ we obtain $M'E_1=\mu E_1$, $M'E_2=\mu E_2$, $M'E=\lambda E$

Since $M'\in SO^+(3,1)$ it follows $\lambda>0$, M' invariates $\mathrm{Sp}(E_1,E_2)=H$ and $\mathrm{Sp}(E_3,E_0)=H^\perp$

We will have therefore :

$M'=\exp(\theta J_3+\chi K_3)$, $\theta\in\{0,\pi\}$, $\cosh(\chi)+\sinh(\chi)\in\left\{\lambda,\frac{1}{\lambda}\right\}$

If $\lambda^2\neq1$ we have obviously $\beta''\neq\lambda$ and so we have now left the case

$\lambda^2=1$, $\beta''=\lambda$ having now the situation:

$\mu=\lambda=\beta''=\cos(\theta)\in\{\pm1\}$, $k\equiv1\pmod 2$, $\sin(\theta)=\cos(\theta')=0$, $\sin(\theta')=\cos(\theta)$

$\overline{M}E_1=\mu E_1+\gamma E$, $\overline{M}E_2=\mu E_2+\gamma' E$, $\overline{M}E=\mu E$ and so in the basis (E_1,E_2,E_3,E_0):

$\overline{M}=\begin{pmatrix}\mu & 0 & \delta & -\delta\\ 0 & \mu & \varepsilon & -\varepsilon\\ \gamma & \gamma' & \rho & \mu-\rho\\ \gamma & \gamma' & \varphi & \mu-\varphi\end{pmatrix}$ and $\overline{M}\in SO^+(3,1)$ leading to:

$\gamma=-\delta$, $\gamma'=-\varepsilon$, $\mu(\rho-\varphi)=1$, $\mu(\delta^2+\varepsilon^2)=-2\varphi$, $\mu\geq\varphi+1$

If $\mu<0$ it will follow $\varphi\geq0$, $\mu\geq1$ and so we must have $\mu=1$, $\rho=\varphi+1$, $\delta^2+\varepsilon^2=-2\varphi$

Taking $\overline{Q}=\begin{pmatrix}Q & 0_{2\times2}\\ 0_{2\times2} & \mathbf{I}_2\end{pmatrix}$ with $Q=\begin{pmatrix}\cos(\zeta) & \sin(\zeta)\\ -\sin(\zeta) & \cos(\zeta)\end{pmatrix}\in SO(2)$ where

$\zeta\in\mathbb{R}$, $\delta\cos(\zeta)+\varepsilon\sin(\zeta)=0$ we have that $\overline{Q}\overline{M}\overline{Q}^T$ has the form:

$S(\alpha)=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & \alpha & -\alpha\\ 0 & -\alpha & 1-\alpha^2/2 & \alpha^2/2\\ 0 & -\alpha & -\alpha^2/2 & 1+\alpha^2/2\end{pmatrix}$ with $\alpha\in\mathbb{R}$.

After some calculus we find out that $S(\alpha+\alpha')=S(\alpha)S(\alpha')$ for any $\alpha,\alpha'\in\mathbb{R}$ and so

$\frac{dS}{d\alpha}=S\frac{dS}{d\alpha}(0)=-S(J_1+K_2)$, $S(\alpha)=\exp(-\alpha(J_1+K_2))$

Thus the statement is completely proved :

For any $M\in SO^+(3,1)$ exist $\Lambda\in SO^+(3,1)$, $\theta,\chi,\alpha\in\mathbb{R}$ such that

$M=\Lambda^{-1}\exp(\theta J_3+\chi K_3)\Lambda$ or $M=\Lambda^{-1}\exp(\alpha(J_1+K_2))\Lambda$

In conclusion, for any $M\in SO^+(3,1)$ exist $\Lambda\in SO^+(3,1)\omega=(\omega_{\alpha\beta})_{\alpha,\beta}\in M_{4\times4}(\mathbb{R})$

with $\omega=-\omega^T$, $M=\Lambda^{-1}\exp(\omega_{\alpha\beta}J^{\alpha\beta})\Lambda$

Above we have already proven that

$\Lambda^{-1}J^{\alpha\beta}\Lambda=\Lambda^\alpha_\mu\Lambda^\beta_\nu J^{\mu\nu}$ and so, taking $\overline{\omega}=\Lambda^T\omega\Lambda$ we obtain:

$\overline{\omega}^T=-\overline{\omega}$, $M=\exp(\overline{\omega}_{\mu\nu}J^{\mu\nu})$

For any $M\in SO^+(3,1)$ exists $\omega\in M_{4\times4}(\mathbb{R})$ such that $\omega=-\omega^T$ and $M=\exp(\omega_{\alpha\beta}J^{\alpha\beta})$

Let $\omega=(\omega_{\alpha\beta})_{\alpha,\beta}\in M_{4\times4}(\mathbb{R})$ with $\omega=-\omega^T$ and we suppose $\det\omega\neq0$. (11)

For $\Lambda\in SO^+(3,1)$ we have $\Lambda^{-1}\eta\omega\Lambda=\eta\Lambda^T\omega\Lambda$, $\Lambda^T\omega\Lambda=\eta\Lambda^{-1}\eta\omega\Lambda$. (12)

If $x,y\in M_{4\times1}(\mathbb{C})$ and $x,y\neq0$, $\mu,\lambda\in\mathbb{C}$ such that:

$\eta\omega x=\lambda x$, $\eta\omega y=\mu y$ then, because of (11) we have:

$\lambda,\mu\neq 0$ and $\overline{y}^T\omega x=\lambda\overline{y}^T\eta x$, $-\overline{y}^T\omega x=\overline{\mu}\overline{y}^T\eta x$. (the overline means that we are taking the complex conjugate) Therefore, if $\overline{y}^T\eta x\neq 0$ we must have $\lambda=-\overline{\mu}$.

Since we have also $\eta\omega\overline{x}=\overline{\lambda}\overline{x}$ it follows that if $\overline{x}^T\eta x\neq 0$ then $\lambda=-\overline{\lambda}$ (13)

and if $x^T\eta x\neq 0$ then $\lambda=-\lambda$.

Because we assumed $\det\omega\neq 0$ we must have $x^T\eta x=0$

for any $x\neq 0$ with $x\in M_{4\times 1}(\mathbb{C})$, $\lambda\in\mathbb{C}$, $\eta\omega x=\lambda x$

Let $x\in M_{4\times 1}(\mathbb{C})$, $x\neq 0$, $\lambda\in\mathbb{C}$ with $\eta\omega x=\lambda x$ and consider the case $\overline{x}^T\eta x=0$

Since $x^T\eta x=0$, for $u=\Re x$, $v=\Im x$ it follows $u^T\eta u=v^T\eta v=0$, $u^T\eta v=0$ and so:

$u=cv$ or $v=c'u$, $c,c'\in\mathbb{R}$ and we can consider $x\in M_{4\times 1}(\mathbb{R})$, $\lambda\in\mathbb{R}^*$

We have $\det(\omega-\lambda\eta)=\det(\omega^T-\lambda\eta)=\det(\omega+\lambda\eta)$ and therefore

we can take $y\in M_{4\times 1}(\mathbb{R})$ with $y\neq 0$, $\eta\omega y=-\lambda y$

Supposing $y^T\eta y\neq 0$ it follows $\lambda=-\lambda=0$ which cannot be since we assumed $\det(\eta\omega)\neq 0$

Hence, in the considered case we have :

$x,y\in M_{4\times 1}(\mathbb{R})$ linear independent each of other with

$\lambda\in\mathbb{R}^*$, $y^T\eta y=x^T\eta x=0$, $\eta\omega x=\lambda x$, $\eta\omega y=-\lambda y$.

Taking $u=x+y$, $v=x-y$ we obtain $u^T\eta v=0$, $u^T\eta u=-v^T\eta v$.

Since *x* and *y* are independent, *u* and *v* are independent too and so we cannot have

$u^T\eta u=-v^T\eta v=0$.

Hence we can take $u,v\in M_{4\times 1}(\mathbb{R})$ with $u^T\eta v=0$, $u^T\eta u=1$, $v^T\eta v=-1$ and

$\eta\omega u=\lambda v$, $\eta\omega v=\lambda u$.

$\eta\omega$ invariates $\mathrm{Sp}(u,v)$.

If $\eta\omega$ invariates the subspace $V\subset M_{4\times 1}(\mathbb{R})$,for any $z\in V^\perp$ we have

$z^T\eta w=0$ for any $w\in V$ and so $(\eta\omega z)^T\eta w=-z^T\omega w=-z^T\eta w'=0$ for some $w'\in V$

Since $\det(\eta\omega)\neq 0$ weobtain that $\eta\omega$ invariates also $V^\perp$.

So $\eta\omega$ invariates $\mathrm{Sp}(u,v)^\perp$.

In the case $\overline{x}^T\eta x\neq 0$ we have $\lambda=i\mu$, $\mu\in\mathbb{R}^*$ and we take $u=\Re x$, $v=\Im x$.

We obtain: $\eta\omega u=-\mu v$, $\eta\omega v=\mu u$, $u^T\eta u=v^T\eta v\neq 0$, $u^T\eta v=0$

where we can take $u^T\eta u=v^T\eta v=-1$, u , v being independent since $\mu\neq 0$.

Therefore we have two Minkowski-orthogonal subspaces , in both considered cases,

$\mathrm{Sp}(u_1,v_1)$ and $\mathrm{Sp}(u_2,v_2)$ invariated by $\eta\omega$ with $u_i^T\eta v_i=0$, $i=1,2$ one and only

one of them having a vector, say v_1 with $v_1^T\eta v_1=1$ the other u_i,v_i having the

Minkowski norm equal to -1.

So we have :

$$\eta\omega u_1=\lambda v_1\ ,\ \eta\omega v_1=\lambda u_1\ ,\ \eta\omega u_2=-\mu v_2\ ,\ \eta\omega v_2=\mu u_2\ ,\ \lambda,\mu\in\mathbb{R}^*$$

$$u_i^T\eta v_j=0 \text{ for } i,j=1,2;u_i^T\eta u_j=0\ ,\ v_i^T\eta v_j=0 \text{ for } i\neq j\ ,\ i,j=1,2$$

$u_2^T\eta u_2=v_2^T\eta v_2=u_1^T\eta u_1=-1$, $v_1^T\eta v_1=1$ and we can choose u_i,v_i such that $v_{10}>0$.

Then we can take $\Lambda\in SO^+(3,1)$ with:

$\Lambda E_1=\varepsilon u_2$, $\Lambda E_2=\varepsilon v_2$, $\Lambda E_3=\varepsilon u_1$, $\Lambda E_0=v_1$, $\varepsilon\in\{\pm 1\}$.

For $\varphi=\Lambda^{-1}\eta\omega\Lambda$ we will have:

$\varphi E_1=-\mu E_2$, $\varphi E_2=\mu E_1$, $\varphi E_3=\varepsilon\lambda E_0$, $\varphi E_0=\varepsilon\lambda E_3$ and in the basis (E_1,E_2,E_3,E_0),

we have the matrix form :

$$\Lambda^T\omega\Lambda=\eta\varphi=\begin{pmatrix}0&-\mu&0&0\\ \mu&0&0&0\\ 0&0&0&-\varepsilon\lambda\\ 0&0&\varepsilon\lambda&0\end{pmatrix}$$

$\exp(\omega_{\alpha\beta}J^{\alpha\beta})=\Lambda\exp(\omega_{\alpha\beta}\Lambda^{-1}J^{\alpha\beta}\Lambda)\Lambda^{-1}=\Lambda\exp(\omega_{\alpha\beta}\Lambda^{\alpha}{}_{\gamma}\Lambda^{\beta}{}_{\delta}J^{\gamma\delta})\Lambda^{-1}=$
$=\Lambda\exp(2\mu J_3-2\varepsilon\lambda K_3)\Lambda^{-1}$
Since J_3 commutes with K_3 we will have $\exp(\omega_{\alpha\beta}J^{\alpha\beta})\in SO^+(3,1)$,
if as we assumed $\omega=-\omega^T\in M_{4\times4}(\mathbb{R})$ with $\det\omega\neq0$.
If we have $\overline{\omega}=-\overline{\omega}^T\in M_{4\times4}(\mathbb{R})$ and $\det\overline{\omega}=0$ we observe that the set
$A=\{\omega\in M_{4\times4}(\mathbb{R})|\omega=-\omega^T,\ \det\omega\neq0\}$ is dense in $\{\omega\in M_{4\times4}(\mathbb{R})|\omega=-\omega^T\}=\overline{A}$.
The function $M_{4\times4}(\mathbb{R})\ni\omega\to\exp(\omega_{\alpha\beta}J^{\alpha\beta})\in M_{4\times4}(\mathbb{R})$ being continuous,
since $SO^+(3,1)$ is closed in $M_{4\times4}(\mathbb{R})$ it follows $\exp(\overline{\omega}_{\alpha\beta}J^{\alpha\beta})\in SO^+(3,1)$ for any $\overline{\omega}\in\overline{A}$

The above proven results lead to the following three facts:
i) We have 6 independent matrices $\{H_k\}_{k=\overline{1,6}}$ where
$H_k=-\frac{1}{2}\epsilon_{ijk}J^{ij}=J_k$, $H_{k+3}=-J^{0k}$ for $k=\overline{1,3}$
ii) We have a surjective C^∞ class function
$\Phi:\mathbb{R}^6\to SO^+(3,1)$, $\Phi((\psi_s)_s)=\exp(\psi_sH_s)$ such that $\operatorname{rank}\left(\frac{\partial\Phi_{pq}}{\partial\psi_k}\right)_{pq,k}=6$
with $p,q=\overline{0,3}$, $k=\overline{1,6}$
iii) Φ is local injective (Since $\det\left(\frac{\partial e^W_{pq}}{\partial t_{ij}}\right)_{pq,ij}\neq0$, $p,q,i,j=\overline{0,3}$
for any $W\in M_{4\times4}(\mathbb{R})$, $W=(t_{ij})_{i,j}$)

As we proved for the rotation group *SO(n)* we conclude that the manifold structure
on $SO^+(3,1)$(with the topology induced from $M_{4\times4}(\mathbb{R})$) is equivalent to a structure given by the mappings $((\psi_s)_s)\to\exp(\psi_sH_s)$.
Having the continuous surjective function Φ we find $SO^+(3,1)$ as a 6-dimensional connected Lie group (as well as by the mapping $(\vec{\theta},\vec{\chi})\to\exp(\vec{\theta}\vec{J})\exp(\vec{\chi}\vec{K})$).

For $U\in M_{n\times n}(\mathbb{C})$, $n\in\mathbb{N}^*$ we denote U^+ the conjugate transpose of U .
Let $SU(n)=\{U\in M_{4\times4}(\mathbb{C})|U^+U=\mathbf{I}$, $\det U=1\}$
Consider $M_{n\times n}(\mathbb{C})$ as its natural complex Hilbert space .
Then if $x\in M_{(n+1)\times(n+1)}(\mathbb{C})$, $\lambda\in\mathbb{C}$, $U\in SU(n+1)$ with $Ux=\lambda x$ we will have that
U invariates $\mathrm{Sp}(x)$ and also $\mathrm{Sp}(x)^\perp$ and $\lambda\overline{\lambda}=1$.
Therefore we can obviously prove by induction (in a sampler way as we did for *SO(n)*) that for any $U\in SU(n)$ exists $H\in M_{n\times n}(\mathbb{C})$ with $H^+=H$, $U=\exp(iH)$. (14)
Since $\mathrm{tr}(H)=\mathrm{tr}(JHJ^{-1})$, $\det U=$ for any $J\in M_{n\times n}(\mathbb{C})$ with $\det J\neq0$, taking *H* in the normal Jordan form, from (14) we deduce for H that $\mathrm{tr}H=0$.
From the way we proved it , it is obvious that the relation (3') works even for complex *W*.
Therefore are no difficulties in proving that we have a surjective and local injective mapping
$\Psi:\mathbb{R}^r\to SU(n)$, $\Psi(\varphi)=\exp(i\varphi_aT_a)$ where $\varphi=(\varphi_a)_{a=\overline{1,r}}$, $r=n^2-1$,

$(T_a)_a$ is a basis of the real vector space $S=\{H\in M_{4\times 4}(\mathbb{C})|H^+=H\ ,\ \mathrm{tr}H=0\}$.

For $n=2$ we can take $(T_a)_a=(\sigma_i)_{i=\overline{1,3}}$ the Pauli matrices (see Chap. Representations of the rotations group and the restricted Lorentz group. Spin representations).

Let $M=\exp(\omega_{\mu\nu}J^{\mu\nu})$ with $\omega=-\omega^T\in M_{4\times 4}(\mathbb{R})$

Then,as we proved above, if $\det\omega\neq 0$ we can find $\Lambda\in SO^+(3,1)$ such that

$$\Lambda^T\omega\Lambda=\omega'\ ,\ \omega'_{\alpha\beta}=0 \text{ for } (\alpha,\beta)\notin\{(1,2),(2,1),(0,3),(3,0)\} \text{ and} \qquad (15)$$
$$\Lambda^{-1}M\Lambda=\exp(-2\omega'_{12}J_3-2\omega'_{03}K_3)$$

We have the representation

$S:SO^+(3,1)\to M_{4\times 4}(\mathbb{C})$ such that for any $M\in SO^+(3,1)$, $S=S(M)$ satisfies

$S^{-1}\gamma^\mu S=M_{\mu\nu}\gamma^\nu$ for $\mu=\overline{0,3}$ (16) (see Chap. Representations of the rotations group and the restricted Lorentz group. Spin representations).

$$S(\exp(\theta J_3))=\cos(\frac{\theta}{2})\mathbf{I}+\sin(\frac{\theta}{2})\gamma^1\gamma^2=\exp(\frac{\theta}{4}[\gamma^1,\gamma^2])$$
$$S(\exp(\chi K_3))=\cosh(\frac{\chi}{2})\mathbf{I}+\sinh(\frac{\chi}{2})\gamma^0\gamma^3=\exp(\frac{\chi}{4}[\gamma^0,\gamma^3]) \qquad (17)$$

where $[A,B]=AB-BA$ denotes the commutator of A and B

We denote $\sigma^{\mu\nu}=\frac{i}{2}[\gamma^\mu,\gamma^\nu]$.

Since $[J_3,K_3]=0$ and $[\sigma^{12},\sigma^{03}]=0$, from (15) and (17) , after some calculus we obtain:

$$S(M)=\exp(\frac{i}{2}2\omega'_{12}S(\Lambda)\sigma^{12}S(\Lambda)^{-1}+\frac{i}{2}2\omega'_{03}S(\Lambda)\sigma^{03}S(\Lambda)^{-1}) \ . \ (18)$$

From (16) we can deduce $S(\Lambda)^{-1}\sigma^{\mu\nu}S(\Lambda)=\Lambda^\mu{}_\alpha\Lambda^\nu{}_\beta\sigma^{\alpha\beta}$ and so (15) and (18) will lead to:

$S(M)=\exp(\frac{i}{2}\omega_{\alpha\beta}\sigma^{\alpha\beta})$ if as we assumed $\det\omega\neq 0$

If $\det\omega=0$ we have $\omega=\lim_{n\to\infty}\omega_n$ with $\omega_n=-\omega_n^T\in M_{4\times 4}(\mathbb{R})$, $\det\omega_n\neq 0$ and

since the representation S is continuous, for $M_n=\exp(\omega_{n\,\alpha\beta}J^{\alpha\beta})$ we have

$\lim_{n\to\infty}S(M_n)=S(M)$ deducing $S(M)=\exp(\frac{i}{2}\omega_{\alpha\beta}\sigma^{\alpha\beta})$ for any $\omega=-\omega^T\in M_{4\times 4}(\mathbb{R})$.

The Dirac spinorial function $\psi=(\psi_\alpha)_\alpha(x)$ (as a column 4x1 matrix) ,

$x=(x^\alpha)_\alpha$ space-time coordinates, which satisfies the Dirac equation

$$i\gamma^\mu\partial_\mu\psi-m\psi=0$$

transforms under a Lorentz coordinates transformation

$x'^\mu=M_{\mu\nu}x^\nu$ according to $\psi'=S(M)\psi$ and considering

$M=\exp(\omega_{\alpha\beta}J^{\alpha\beta})$, $\overline{\psi}=\psi^+\gamma^0$ with ψ^+ the complex conjugate transpose of ψ

we have for the transformation of the conserved current , $J^\mu=\overline{\psi}\gamma^\mu\psi$, the expression:

$$J'^\mu=\psi^+S^+(M)\gamma^0\gamma^\mu S(M)\psi=\psi^+\exp(-\frac{i}{2}\omega_{\alpha\beta}\sigma^{+\alpha\beta})\gamma^0\gamma^\mu\exp(\frac{i}{2}\omega_{\alpha\beta}\sigma^{\alpha\beta})\psi$$

We have $\sigma^{+\alpha\beta}=\gamma^0\sigma^{\alpha\beta}\gamma^0$ and so we obtain:

$$J'^\mu=\psi^+\gamma^0\exp(-\frac{i}{2}\omega_{\alpha\beta}\sigma^{\alpha\beta})\gamma^\mu\exp(\frac{i}{2}\omega_{\alpha\beta}\sigma^{\alpha\beta})\psi=\psi^+\gamma^0S(M)^{-1}\gamma^\mu S(M)\psi=M_{\mu\nu}\overline{\psi}\gamma^\nu\psi \ .$$

Therefore, the conserved current transforms like a contravariant Lorentz vector.

4. Representations of the restricted Lorentz group (final)

Representations of the restricted Lorentz group

Consider the restricted Lorentz group $G=SO^{+}(3,1)$. We have the Lie group stucture on G defined by zhe mappings:
$\mathbb{R}^6\ni(\vec{\theta},\vec{\chi})\to\exp(\vec{\theta}\vec{J}+\vec{\chi}\vec{K})\in SO^{+}(3,1)$ where $\vec{J}=(\bar{J}_k)_{k=\overline{1,3}}$, $\vec{K}=(\bar{K}_k)_{k=\overline{1,3}}$ are the generators of G (see Chap. Spin representations and Chap. Rotations and restricted Lorentz groups).
We have the commutation relations:
$[\bar{J}_i,\bar{J}_j]=\epsilon_{ijk}\bar{J}_k$, $[\bar{K}_i,\bar{K}_j]=-\epsilon_{ijk}\bar{J}_k$, $[\bar{J}_i,\bar{K}_j]=\epsilon_{ijk}\bar{K}_k$ $\quad(1)$ and taking

$\bar{M}_{\pm l}=\frac{1}{2}(i\bar{J}_l\mp\bar{K}_l)$ for $l=\overline{1,3}$ we have $[\bar{M}_{+l},\bar{M}_{-k}]=0$ and $[\bar{M}_{\pm l},\bar{M}_{\pm k}]=i\epsilon_{lkj}\bar{M}_{\pm j}$ for $l,k=\overline{1,3}$. Let $\bar{X}_{\pm}=\bar{M}_{\pm 1}+i\bar{M}_{\pm 2}$, $\bar{Y}_{\pm}=\bar{M}_{\pm 1}-i\bar{M}_{\pm 2}$, $\bar{H}_{\pm}=2\bar{M}_{\pm 3}$ and we have

$$\exp(\vec{\theta}\vec{J}+\vec{\chi}\vec{K})=\exp((-i\vec{\theta}-\vec{\chi})\vec{\bar{M}}_{+}+(-i\vec{\theta}+\vec{\chi})\vec{\bar{M}}_{-})=$$
$=\exp(-i(\vec{\theta}-i\vec{\chi})\vec{\bar{M}}_{+})\exp(-i(\vec{\theta}+i\vec{\chi})\vec{\bar{M}}_{-})$ because $\bar{M}_{+l}$ and $\bar{M}_{-k}$ commute.

For W a finite dimensional vector space, as a representation U of G (see for definition Chap. Spin representations), we can consider the corresponding generators of the representation:
$H_{\pm},X_{\pm},Y_{\pm}\in GL(W)\simeq M_{n\times n}(\mathbb{C})$ with $n=\dim W$ and we have

$[S_{-},S_{+}]=0$ for any $S_{-}\in\{H_{-},X_{-},Y_{-}\}$, $S_{+}\in\{H_{+},X_{+},Y_{+}\}$,

$$U(\exp(\vec{\theta}\vec{J}+\vec{\chi}\vec{K}))=$$
$$=\exp(-\frac{1}{2}i(\theta_1-i\chi_1)(X_{+}+Y_{+})-\frac{1}{2}i(-i\theta_2-\chi_2)(X_{+}-Y_{+})-\frac{1}{2}i(\theta_3-i\chi_3)H_{+})\cdot$$
$$\cdot\exp(-\frac{1}{2}i(\theta_1+i\chi_1)(X_{-}+Y_{-})-\frac{1}{2}i(-i\theta_2+\chi_2)(X_{-}-Y_{-})-\frac{1}{2}i(\theta_3+i\chi_3)H_{-}).$$

For $(H,X,Y)\in\{(H_{\pm},X_{\pm},Y_{\pm})\}$ it follows
$[X,Y]=H$, $[H,X]=2X$, $[H,Y]=-2Y$ and that for any eigenvector $v\in W$ of H , $Hv=\lambda v$, $\lambda\in\mathbb{C}$, $v\neq 0$ we will have: $HX^{j}v=(\lambda+2j)X^{j}v$ for any $j\in\mathbb{N}$.
The space W being finite dimensional we take
$i_0=\max\{i\in\mathbb{N}|X^{i}v\neq 0\}$. Let $v_0=X^{i0}v$, $v_j=Y^{j}v_0$ and it follows
$Hv_j=(\lambda+2(i_0-j))v_j$ so that taking $m=\max\{i\in\mathbb{N}|v_i\neq 0\}$ for $j\in\mathbb{N}$ we have:

$Xv_0=0$, $Xv_{j+1}=YXv_j+Hv_j$, $Yv_j=v_{j+1}$, $Yv_m=0$.

v_0 , v_1 , … , v_m are linearly independent, being eigenvectors of H for distinct eigenvalues, and by induction follows that H , X , Y satisfy

$S(V)\subseteq V$ for $S\in\{H,X,Y\}$, $V=\mathrm{Sp}[v_0,...,v_m]$.

Since $Hv_j=(\lambda+2(i_0-j))v_j$ we have $\mathrm{tr}\,H\Big|_V=\sum_{j=0}^{m}(\lambda+2(i_0-j))=\mathrm{tr}[X,Y]\Big|_V=0$.
Therefore $\lambda=m-2i_0\in\mathbb{Z}$, $Hv_j=(m-2j)v_j$, $Yv_m=0$, $Xv_0=0$, $Yv_j=v_{j+1}$ for $j=\overline{0\ ,\ m-1}$. By induction we also prove that $Xv_j=j(m-j+1)$ for $j=\overline{1,m}$

We notice that $V = \mathrm{Sp}[v_0,\ldots, v_m]$ is an irreducible representation space, that is, if $V'\subseteq V$ such that $H(V')\subseteq V'$, $X(V')\subseteq V'$, $Y(V')\subseteq V'$ then $V'\in\{\{0\}\ ,\ V\}$.
A representation W of $g=\mathrm{Sp}[\bar{H},\bar{X},\bar{Y}]$ is given by $H,X,Y\in GL(W)$ with $[H,X]=2X$, $[H,Y]=-2Y$, $[X,Y]=H$ and any irreducible representation of g is a $V=\mathrm{Sp}[v_0,...,v_m]$ type representation as presented above.
We will prove now that if W is a finite dimensional representation of g then H is diagonalizable and following the introductory considerations we have

$W=\bigoplus_{i=1}^{n}V_i$ with V_i irreducible representations $V_i=\mathrm{Sp}[v_{i0},...v_{imi}]$ as above .
Indeed suppose we proved that H is diagonalizable and we have set
$V_i=\mathrm{Sp}[v_0^{(i)},...,v_{mi}^{(i)}]$, $W'=\bigoplus_{i=1}^{n}V_i$ with V_i irreducible representation for $i=\overline{1,n}$.
If $W'\neq W$, since H is diagonalizable we choose $v\in W\setminus W'$, $\lambda\in\mathbb{C}$, $Hv=\lambda v$.
Let $V=\mathrm{Sp}[v_0,...,v_m]$ the irreducible representation to which $v=v_k$ belongs.
Assuming that $v_l\in W'$ we have $v_l=\sum_{k,i}\alpha_{ki}Y^k v_0^{(i)}$ and applying X^l we obtain

$v_0=\sum_{p,q}\beta_{pq}Y^p v_0^{(q)}$ and further applying Y^k we obtain $v_k=\sum_{s,j}\gamma_{sj}Y^s v_0^{(j)}$

contradicting $v\in W\setminus W'$. Thus we can conclude $W=\bigoplus_{i=1}^{n}V_i$.

Let the induction over dim$W$ assumption be: “For any representation W of g with dim$W = k < n$ the corresponding H generator is diagonalizable.”
Let W with dim$W = n$ the invariant representation vector space for a representation of g. Assuming that the corresponding H generator is not diagonalizable, from its Jordan canonical form, we derive

$W=W_0\oplus W_1$, $W_1=\mathrm{Sp}[v_i]_{i=\overline{1,m}}$, $(H-\lambda_i\boldsymbol{I})v_i=0$, $v_i\neq 0$, $\lambda_i\in\mathbb{C}$ for $i=\overline{1,m}$
$(H-\lambda_i\boldsymbol{I})w_{ij}=w_{ij-1}$, $j=\overline{1,m_i}$, $w_{i0}=v_i$ and at least one $i\in\{1,...,m\}$ we have $m_i\geq 1$
$W_0=\mathrm{Sp}[w_{ij}]_{\substack{i=\overline{1,m}\\ j=\overline{1,mi}}}$

Since the commutation relations lead to

$(H-\lambda \boldsymbol{I})X=X(H-(\lambda-2)\boldsymbol{I})$, $(H-\lambda \boldsymbol{I})Y=Y(H-(\lambda+2)\boldsymbol{I})$ for any $\lambda\in\mathbb{C}$,
we can derive that for $W'=\mathrm{Sp}[\{w\in W|$ exists $\lambda\in\mathbb{C}$ such that $(H-\lambda \boldsymbol{I})^2 w=0\}]$ (2)
we have $H(W')\subseteq W'$, $X(W')\subseteq W'$, $Y(W')\subseteq W'$.

If $W'\neq W$, obviously $\dim W'<n$ and by induction hypothesis H is diagonalizable on W' which contradicts H not diagonalizable.
Therefore we can assume that $W'=W$ and so $m_i\leq 2$ for $i=\overline{1,m}$ and we have
$k,r,s\in\mathbb{N},v_0,...v_k\in W$ with $v_j=Y^j v_0$, $H v_j=(k-2j)v_j$, $Y v_k=0$, $X v_0=0$,
$\lambda_j=k-2j$, $X w_0=q_{(r-k)/2-1}$, $Y^{k+1}w_0=u_{(s+k)/2+1}$, $w_j=Y^j w_0$, $r,s\geq k$ for $j=\overline{0,k}$
and $H q_j=(r-2j)q_j$, $Y q_j=q_{j+1}$, $X q_j=j(r-j+1)q_{j-1}$ for $j=\overline{0,r}$ and
$H u_j=(s-2j)u_j$, $Y u_j=u_{j+1}$, $X u_j=j(s-j+1)u_{j-1}$ for $j=\overline{0,s}$ and
$Y q_r=0$, $X q_0=0$, $Y u_s=0$, $X u_0=0$,
$(q_l=0$ for $l<0$ or $l>r)$ and $(u_l=0$ for $l<0$ or $l>s)$.
(considering (2) , since H is not diagonalizable, for any $l\in\{0,...,k\}$ we have $w\in W$, $\lambda\in\mathbb{C}$ such that $(H-\lambda \boldsymbol{I})w=v_l$ and the rest follows from (2) and the Jordan canonical structure).
By induction hypothesis and commutation relations we can reduce W to
$W=\mathrm{Sp}[X^l Y^n H^j(\{w_0,v_0\})]_{l,n,j\in\mathbb{N}}=\mathrm{Sp}[q_0,...,q_r,u_0,...,u_s,v_0,...,v_k,w_0,...,w_k]$
where $w_j=Y^j w_0$, $w_l=0$ for $(l<0$ or $l>k)$.
We must therefore have:

$$Y w_j=w_{j+1}+\gamma_j v_{j+1}+\alpha_j q_{(r-k)/2+j+1}+\beta_j u_{(s-k)/2+j+1}$$
$$X w_j=j(k-j+1)w_{j-1}+\bar{\gamma}_j v_{j-1}+\bar{\alpha}_j q_{(r-k)/2+j-1}+\bar{\beta}_j u_{(s-k)/2+j-1} \text{ for } j=\overline{0,k}$$

with $\gamma_k=\alpha_k=\bar{\gamma}_0=\bar{\beta}_0=0$, $\bar{\alpha}_0=\beta_k=1$
$\gamma_l=\bar{\gamma}_l=\alpha_l=\bar{\alpha}_l=\beta_l=\bar{\beta}_l=0$ for $(l<0$ or $l>k)$.
Hence

$$XY w_j=(j+1)(k-j)w_j+(\bar{\gamma}_{j+1}+(j+1)(k-j)\gamma_j)v_j+$$
$$+(\bar{\alpha}_{j+1}+((r-k)/2+j+1)((r+k)/2-j)\alpha_j)q_{(r-k)/2+j}+$$
$$+(\bar{\beta}_{j+1}+((s-k)/2+j+1)((s+k)/2-j)\beta_j)u_{(s-k)/2+j}$$
$$Y X w_j=j(k-j+1)w_j+(j(k-j+1)\gamma_{j-1}+\bar{\gamma}_j)v_j+$$
$$+(j(k-j+1)\alpha_{j-1}+\bar{\alpha}_j)q_{(r-k)/2+j}+(j(k-j+1)\beta_{j-1}+\bar{\beta}_j)u_{(s-k)/2+j} \text{ for } j=\overline{0,k}$$

and it follows :

$$0=(\bar{\gamma}_{j+1}-\bar{\gamma}_j+(j+1)(k-j)\gamma_j-j(k-j+1)\gamma_{j-1}-1)v_j+$$
$$+(\bar{\alpha}_{j+1}-\bar{\alpha}_j+((r-k)/2+j+1)((r+k)/2-j)\alpha_j-j(k-j+1)\alpha_{j-1})q_{(r-k)/2+j}+ \quad (3)$$
$$+(\bar{\beta}_{j+1}-\bar{\beta}_j+((s-k)/2+j+1)((s+k)/2-j)\beta_j-j(k-j+1)\beta_{j-1}) \text{ for } j=\overline{0,k}$$

If $s = k$ and $r = k$, the $(q_j)_j$ and $(u_j)_j$ must be respective all independent of or parallel to the $(v_j)_j$. In all of this cases we have therefore a relation

$\bar{\gamma}_{j+1}-\bar{\gamma}_j+(j+1)(k-j)\gamma_j-j(k-j+1)\gamma_{j-1}-1=0$ for $j=\overline{0,k}$ (4)

If $s > k$ or $r > k$ and if we can take

$j\in\{0,...,k\}$ such that $\bar{\gamma}_{j+1}-\bar{\gamma}_j+(j+1)(k-j)\gamma_j-j(k-j+1)\gamma_{j-1}-1\neq 0$

then for this j we have

$\bar{\alpha}_{j+1}-\bar{\alpha}_j+((r-k)/2+j+1)((r+k)/2-j)\alpha-j(k-j+1)\alpha_{j-1}\neq 0$ (5) or

$\bar{\beta}_{j+1}-\bar{\beta}_j+((s-k)/2+j+1)((s+k)/2-j)\beta_j-j(k-j+1)\beta_{j-1}\neq 0$ (6).

If (5) is satisfied, applying X^{j+1} to (3) we obtain

$q_{(r-k)/2-1}\|u_{(s-k)/2-1}$ and so $\mathrm{Sp}[q_0,...,q_r]=\mathrm{Sp}[u_0,...,u_s]$, $s=r$, $q_l\|u_l$ for $l=\overline{0,r}$

and $v_j\|q_{(r-k)/2+j}$, $\mathrm{Sp}[v_0,...,v_k]=\mathrm{Sp}[q_0,...,q_r]=\mathrm{Sp}[u_0,...,u_s]$

contradicting $(s>k$ or $r>k)$.

If (6) is satisfied, applying Y^{k-j+1} to (3) we obtain in a similar way a contradiction with ($s > k$ or $r > k$).

Therefore (4) is satisfied and taking the summation over j we obtain $k+1 = 0$ which contradicts $k\geq 0$. and so we complete the proof of $H_{\pm}$ diagonalizable .

Because H_+ and H_- commute and are diagonalizable, H_+ invariate any eigenspace of H_- , we have that we can find $V_i=\mathrm{Sp}[v_k^{(i)}]_{k=\overline{0,mi}}$ such that V_i are corresponding to irreducible representations of $g_-=\mathrm{Sp}[\bar{H}_-,\bar{X}_-,\bar{Y}_-]$ for $i=\overline{1,n}$,

$W=\bigoplus_{i=1}^{n} V_i$ and $v_k^{(i)}$ is an eigenvector of H_+ for any $k=\overline{0,m_i}$, $i=\overline{1,n}$.

For any $v\in\{v_k^{(i)}\}_{\substack{k=\overline{0,mi}\\ i=\overline{1,n}}}=S$ we can take $S_j(v)\subseteq S$, $j=1,2$ such that

$X_+ v=\sum_{w\in S_1(v)}\alpha_w w$ with $\alpha_w\neq 0$ for any $w\in S_1(v)$ (7)

$Y_+ v=\sum_{w\in S_2(v)}\beta_w w$ with $\beta_w\neq 0$ for any $w\in S_2(v)$ (8)

Without difficulties, because H_+,X_+,Y_+ commute with H_-,X_-,Y_- , considering the minimal character of the chosen $S_i(v)$ (such that $\alpha_w\neq 0$ for any $w\in S_1(v)$ and $\beta_w\neq 0$ for any $w\in S_2(v)$), repeatedly applying X_+ , Y_+ , X_- , Y_- to change back and forward the levels of the H operators eigenvalues , we find for any $v\in S$ the values $r,p,k,l\in\mathbb{N}$ with $l\leq r$, $k\leq p$ such that for any $i=1,2$, $w\in S_i(v)$ we have

$a_i(w)$, $c(w)\in W$ with

$w=Y_+^k a_i(w)=Y_-^l c(w)$, $Y_+^{p+1}a_i(w)=X_+ a_i(w)=Y_-^{r+1}c(w)=X_- c(w)=0$,

$Y_+^p a_i(w)\neq 0$, $Y_-^r c(w)\neq 0$.

Also, if $S_1(v)\cup S_2(v)=\emptyset$ we have $d(v)\in W$, $h,t\in\mathbb{N}$, $h\leq t$ with

$Y_+ Y_-^j d(v)=X_+ Y_-^j d(v)=0$ for $j=\overline{0,t}$, $v=Y_-^h d(v)$, $X_- d(v)=Y_-^{t+1}d(v)=0$

$Y_-^t d(v)\neq 0$.

For $v\in S$ we can consider

$W(v)=\{u\in S|$ exist $x_1,...,x_f$ such that for any $i=\overline{1,f-1}$ exist $a,b\in\{1,2\}$ with $S_a(x_i)\cap S_b(x_{i+1})\neq\emptyset$, $x_1=v$, $x_f=u\}$

The above defined *r,p,l,k* depend on *v* and we denote $(r,p,l,k)=(r,p,l,k)(v)$ having $(r,p,l,k)(u)=(r,p,l,k)(v)$ for any $u\in W(v)$ and the space $R(v)=\mathrm{Sp}[X_+^\alpha Y_+^\beta H_+^\gamma X_-^\mu Y_-^\lambda H_-^\nu (S_j(u))]_{\substack{\alpha,\beta,\gamma,\mu,\lambda,\nu\in\mathbb{N}\\ u\in W(v)\ ,\ j=1,2}}$

is a direct sum of spaces of the form

$\mathrm{Sp}[Y_-^j Y_+^s a(u), X_-^i Y_+^s a(u)]_{j=\overline{0,r-l}\ ;\ i=\overline{0,l}\ ;\ s=\overline{0,p}}=K(u)$

with $u\in W(v)$, $(r,l,p)=(r,l,p)(v)$.

Also, if $R(v)\cap R(v')\neq\{0\}$ then $R(v)=R(v')$ and we have

$W=\mathrm{Sp}[\bigcup_{v\in S} R(v)]\oplus W_0$ where $W_0=\{u\in S|S_1(u)\cup S_2(u)=\emptyset\}$.

Thus *W* is a direct sum of irreducible representations of type *K*(*u*) and identical representations.

The *K*(*u*) representations can be indexed after (*r* /2 , *p*/2) : a spin *r*/2 representation for the (H_- , X_- , Y_-) generators and a spin *p*/2 representation for the (H_+ , X_+ , Y_+) generators.

5. Wave propagation. Wave packets . Uncertainity relations

Wave propagation. Wave packets
Uncertainity relations

Consider the general complex form of a plane wave

$\psi(t,\vec{x})=A_0\exp(i(\omega t-\vec{k}\cdot\vec{x}))$, with $(t,\vec{x})\in\mathbb{R}^4$, $A_0\in\mathbb{R}$, $\omega=2\pi\nu$, $k=\|\vec{k}\|=\frac{2\pi}{\lambda}$ (ν -frequency , λ -wavelenght) which propagates in the direction $\vec{k}$ having the amplitude A_0 and pulsation ω .

Placing a slit (we restrict ourselves to the $z = 0$ plane) which has the width l and is normal to the propagation direction x in the (x , y) plane, the wave can be detected on a screen parallel to the slit and to z -direction . The coordinate system is chosen such that the lower y coordinate of the slit is at the origin (see fig.) .

With the screen at a large distance D_0 from the origin O (0,0,0) , by the Huygens-Fresnel principle , the oscillations propagate from the slit to a point $A(D_0,y_A,0)$ on the screen (where $\widehat{xOA}$ has α rad measure) and combine to a wave function value $\psi_A(t)=\gamma\int_0^l\exp(i(\omega t-k(D+s\sin\alpha)))ds$

where $D=\|\overrightarrow{BA}\|$ (see fig. and (*) below) and γds is the amplitude corresponding to a Fresnel zone ds of the slit.

For the normal direction $(\alpha=0)$ we must have $\psi_A=A_0\exp(i(\omega t-kD_0))$ and so it follows $\gamma=\frac{A_0}{l}$.

For arbitrary α we have $\psi_A=\frac{\gamma i}{k\sin\alpha}\exp(i(\omega t-kD))(\exp(-ikl\sin\alpha)-1)$.

The intensity of the wave, for the α -angle propagation direction is

$I(\alpha)=\psi_A\psi_A^*=\frac{2|\gamma|^2}{k^2\sin^2\alpha}(1-\cos(kl\sin\alpha))=I_0\frac{\sin^2\eta}{\eta^2}$ with $I_0=|A_0|^2$, $\eta=\frac{kl\sin\alpha}{2}$.

The minima of I , near to the central maximum at $\alpha = 0$ are obtained for $\sin\alpha=\frac{n\lambda}{l}$ with $n\in\mathbb{Z}^*$ and other extremes of I are obtained from the transcedental equation $\eta=\tan\eta$. Therefore the first minimum of intensity is at $\sin\alpha=\pm\frac{\lambda}{l}$.

The slit and screen device provide a model for detection and measuring the position and momentum of a quantum particle with wave function ψ^* . The slit determines the y -coordinate of the particle with a precision $\Delta y = l/2$. Since the first minimum of intensity of the wave function is at $\sin\alpha=\frac{\lambda}{l}$, a particle entering the slit in x direction with momentum $\vec{p}=(p_x,0,0)$ can be detected at the screen with a precision in momentum determination $\Delta p_y=p_x\tan\alpha$.

Therefore $\Delta p_y = p_x \tan\alpha = \frac{h}{\lambda}\tan\alpha > \frac{h}{\lambda}\sin\alpha = \frac{h}{l}$ and so we derive a uncertainity relation about determinitation precisions of position and momentum as $\Delta p_y \Delta y \geq \frac{h}{2}$. Obviously we will have similar relations for all directions:

$\Delta p_x \Delta x \geq \frac{h}{2}$, $\Delta p_y \Delta y \geq \frac{h}{2}$, $\Delta p_z \Delta z \geq \frac{h}{2}$

and we can compare these relations with the general Heisenberg uncertainity relations we obtained in Chap. Quantum mechanics formalism.

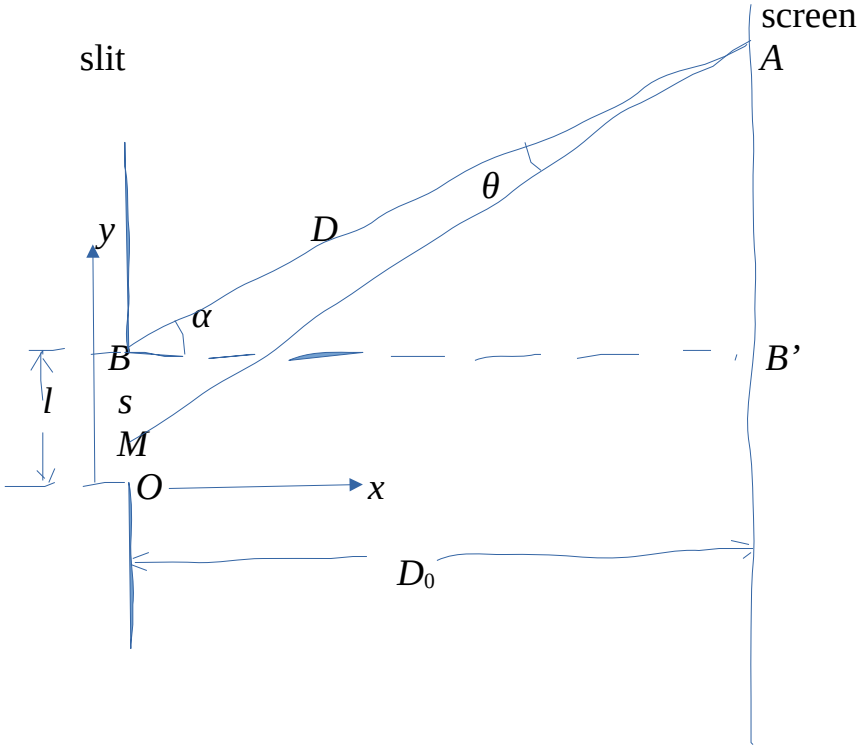


fig. (*)

The segment $|OB|$ represents the slit. $\|\overrightarrow{OB}\| = l$, $M \in |OB|$, $\|\overrightarrow{BM}\| = s$, $\overrightarrow{BB'} \| Ox$, $\widehat{ABB'} = \alpha$, $\widehat{MAB} = \theta$; A, B' are on the screen, $\overrightarrow{B'A} \| Oy$, $\|\overrightarrow{BB'}\| = D_0$, $\|\overrightarrow{BA}\| = D = \frac{D_0}{\cos\alpha}$, $l \ll D_0$, $\frac{l}{D_0} = O(\varepsilon) \ll 1$

We have $\frac{\sin\theta}{l} \leq \frac{\sin\theta}{s} = \frac{\cos\alpha}{\|\overrightarrow{AM}\|} \leq \frac{1}{D_0}$ and so $\theta = O(\varepsilon)$,

$\frac{s\sin\alpha}{D} = \frac{s\sin(\alpha+\theta)}{D} + O(\varepsilon^2)$, $\frac{\|\overrightarrow{AM}\|}{D} = \sqrt{1 + \frac{s^2}{D^2} + 2\frac{s}{D}\sin\alpha} = 1 + \frac{s}{D}\sin\alpha + O(\varepsilon^2)$.

Therefore we can approximate $\|\overrightarrow{AM}\| = D + s\sin\alpha$ even if we take $\alpha = \widehat{AOx}$.

(*)

For $k:[\omega_0-\Delta\omega,\omega_0+\Delta\omega]\to\mathbb{R}$, $\Delta\omega\ll\omega_0$ we take a wave packet propagating in direction x given by the function $\psi(t,x)=a\int_{\omega_0-\Delta\omega}^{\omega_0+\Delta\omega}\exp(-i(\omega t-k(\omega)x))d\omega$.

We have $k(\omega)\approx k_0+\left(\frac{dk}{d\omega}\right)_{\omega 0}(\omega-\omega_0)$ and so integrating we obtain

$\psi(t,x)=2a\Delta\omega\frac{\sin\alpha}{\alpha}\exp(-i(\omega_0 t-k_0 x))$ where $\alpha=\alpha(t,x)=\left(t-x\left(\frac{dk}{d\omega}\right)_{\omega 0}\right)\Delta\omega$

$A(t,x)=2a\Delta\omega\frac{\sin\alpha}{\alpha}$ is the variable amplitude .

The maximum amplitude is $A_{max}=A_0=2a\Delta\omega$ which is achieved at $\alpha=0$ and for $\alpha=\pm n\pi$, $n\in\mathbb{N}$ we have $A=0$. The secundary maxima of the amplitude for which we must have $\tan\alpha=\alpha$ have significant lower values and so the resultant wave amplitude has significant values only in the interval for $\alpha\in[-\pi,\pi]$ around the maximum which occurs at $\alpha=0$.

Also a constant value of the amplitude $A(t,x)=const.$ is held on the planes $t-x\left(\frac{dk}{d\omega}\right)_{\omega 0}=const.$ and so we can consider as the group velocity of he packet the value $v_g=\left(\frac{dx}{dt}\right)_{A=const.}=\left(\frac{d\omega}{dk}\right)_{k0}$ or vectorial for $\vec{k}=k(\omega)\vec{u}$ with $\vec{u}$ the constant versor of propagation direction we will have $\vec{v}_g=\left(\frac{d\omega}{dk}\right)_{k0}\vec{u}$.

If $v=\frac{\omega}{k}$ is the phase velocity we obtain

$$v_g=\left(\frac{d(kv)}{dk}\right)_{k0}=v+k\left(\frac{dv}{d\omega}\right)_{\omega 0}\left(\frac{d\omega}{dk}\right)_{k0}=v+kv_g\left(\frac{dv}{d\omega}\right)_{\omega 0}$$

$$v_g=\frac{v}{1-k\left(\frac{dv}{d\omega}\right)_{\omega 0}} .$$

Therefore for $\left|k\left(\frac{dv}{d\omega}\right)_{\omega 0}\right|\ll 1$ we can write $v_g\approx v+\omega\left(\frac{dv}{d\omega}\right)_{\omega 0}$.

For $\frac{dv}{d\omega}=0$ (that is $\frac{dv}{d\lambda}=0$ since $\lambda=\frac{2\pi}{k(\omega)}$) we have $v_g=v$ and a non-dispersive medium.

For $\frac{dv}{d\omega}\neq 0$ (that is $\frac{dv}{d\lambda}\neq 0$) the medium is dispersive and $v_g\neq v$.

If we take $t_1,t_2\in\mathbb{R}$ we have $\alpha_i=\alpha(t_i,x)=\left(t_i-x\left(\frac{dk}{d\omega}\right)_{\omega 0}\right)\Delta\omega$, $i=1,2$.

Since as we noticed the detection of the perturbation is significant possible only in the [- π , π] interval for α , the time interval in which the perturbation can be

detected at a position x has the length $2\,\Delta t = |\,t_1 - t_2\,|$ where Δt is the precision in determination of the time coordinate.

Hence for the considered wave packet, the precision in determination of time and the precision in determination of the pulsation satisfy the relation

$2\Delta t \geq |t_1 - t_2| = \frac{|\alpha_1 - \alpha_2|}{\Delta\omega} = \frac{2\pi}{\Delta\omega}$, $\Delta\omega\Delta t \geq \pi$.

So if the wave packet represents a pilot wave group of a quantum particle, the precision in measuring the particles energy which is $\Delta E = \hbar\,\Delta\omega$ and the precision in determining the time coordinate , Δt , satisfy the uncertainity relation

$\Delta E\,\Delta t \geq \frac{h}{2}$ (with $h = 2\pi\hbar$ -the Planck constant) .

In the same way , taking the values of α at a same time coordinate and different spatial coordinates we obtain for the width of spatial interval in which a perturbation can be detected $2\pi = |\alpha_1 - \alpha_2| = \left|(x_2 - x_1)\left(\frac{dk}{d\omega}\right)_{\omega 0}\Delta\omega\right| \approx 2\,\Delta x\,\Delta k$ and so because $\vec{p} = \hbar\vec{k}$ for the de Broglie wave vector $\vec{k}$ associated to a momentum $\vec{p}$ quantum particle, for the precision in determination of momentum and the precision in determination of the spatial coordinate in a motion on the x axis of a quantum particle we have $\Delta p_x\,\Delta x \geq \frac{h}{2}$ as we already proved.

Since similar relations are valid for all three orthogonal propagation directions this shows that if we have a bundle $\vec{k} = \vec{k}_0 + \Delta\vec{k}(\omega)$ of waves sent from the origin having central wave vector $\vec{k}_0$ say in x -direction we will have $\|\Delta\vec{x}\|\|\Delta\vec{k}\| \geq \pi$ then the width of the region in which we can significantly detect the waves being d at distance D from the origin, it follows $\frac{|k_y|}{\|\vec{k}_0\|} = \frac{d}{2D}$, $\|\Delta\vec{x}\| = \frac{d}{2}$,

$|k_y| = \|\Delta\vec{k}\|$, $\|\vec{k}_0\| = \frac{2\pi}{\lambda}$ with λ -the central wavelenght of the bundle and so $d \geq \sqrt{2\,D\,\lambda}$ concluding that the directivity of the bundle decreases when the central wavelenght of the bundle increases.

6. Lagrangian field theory. Noether theorem Symmetries in quantum mechanics

Lagrangian field theory. Noether theorem
Symmetries in quantum mechanics

Consider a set of fields $\Phi=(\Phi_a)_{a=\overline{1,n}}$, $\Phi_a=\Phi(x)\in\mathbb{R}$ defined on a manifold M which is parametrized through coordinates $x=(x^\mu)_\mu$ the manifold M can be for example the time continuum $(t\in\mathbb{R})$ or the $1+3$ time-space continuum with a metric (pseudometric) $(g^{\mu\nu})_{\mu,\nu}$ or the Minkowski space-time $((ct,x,y,z)\in\mathbb{R}^4)$ with signature (+,-,-,-) , c -speed of light in vacuum.

The dynamic of the fields system will be described by a real Lagrangian density $\mathscr{L}=\mathscr{L}(\Phi,\partial\Phi,x)$ with $\partial\Phi=(\partial_\mu\Phi_a)_{a,\mu}$ depending on the coordinates x , the fields $(\Phi_a)_a$ and the fields derivatives $(\partial_\mu\Phi_a)_{a,\mu}$ such that for any sufficiently smooth domain $D\subset M$ the action $S=\int_D \mathscr{L}(\Phi(x),\partial\Phi(x),x)d^f x$ (where f is the dimension of M) is stationary upon variations $(\delta\Phi_a)_a$ which vanish on ∂D.

The stationarity of the action for any domain is equivalent to the Euler-Lagrange equations $\frac{\partial\mathscr{L}}{\partial\Phi_a}-d_\mu\left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu\Phi_a)}\right)=0$ (where the Einstein summation convention applies to the μ index) .

We consider a family of transformations ($\Omega(\omega))_\omega$ which depend on a real infinitesimal parameter ω such that

$\Omega=\boldsymbol{I}+\omega P+O(\omega^2)$, $P=\left(\frac{d\Omega}{d\omega}\right)_{\omega=0}$.

The family $\Omega=(\Omega(\omega))_\omega$ induces coordinate transformations

$x^\mu\to\bar{x}_\mu=x^\mu+\alpha^\mu\omega+O(\omega^2)$ and field transformations

$\Phi_a\to\overline{\Phi}_a=\Phi_a+\beta_a\omega+O(\omega^2)$

(where α^μ,β_a may depend on x or Φ).

The domain also transforms becoming D_ω.

If the system is invariant under the considered family of transformations we will have

$\delta S=S_\omega-S=\int_{D_\omega}\mathscr{L}(\overline{\Phi}(\bar{x}),\partial\overline{\Phi}(\bar{x}),\bar{x})d^f\bar{x}-\int_D\mathscr{L}(\Phi(x),\partial\Phi(x),x)d^f x=0$.

We can verify that we have :

$\frac{\partial\bar{x}^\mu}{\partial x^\nu}=\delta_{\mu\nu}+\omega d_\nu\alpha^\mu+O(\omega^2)$, $\det\left(\frac{\partial\bar{x}^\mu}{\partial x^\nu}\right)_{\mu\nu}=1+\omega\partial_\lambda\alpha^\lambda+O(\omega^2)$,

$\mathscr{L}(\overline{\Phi}(\bar{x}),\partial\overline{\Phi}(\bar{x}),\bar{x})-\mathscr{L}(\Phi(\bar{x}),\partial\Phi(\bar{x}),\bar{x})=O(\omega)$,

$\delta S=A+B$ where

$A=\int_{D_\omega}(\mathscr{L}(\overline{\Phi}(\bar{x}),\partial\overline{\Phi}(\bar{x}),\bar{x})-\mathscr{L}(\Phi(\bar{x}),\partial\Phi(\bar{x}),\bar{x}))d^f\bar{x}$,

$B=\int_{D_\omega}\mathscr{L}(\Phi(\bar{x}),\partial\Phi(\bar{x}),\bar{x})d^f\bar{x}-\int_D\mathscr{L}(\Phi(x),\partial\Phi(x),x)d^f x$.

Thus by changing the variable from $\bar{x}$ to x in the integral expression of A it follows

$$A=\int_D (\mathscr{L}(\overline{\Phi}(x),\partial\overline{\Phi}(x),x)-\mathscr{L}(\Phi(x),\partial\Phi(x),x)+O(\omega^2))d^f x=$$

$$=\int_D \left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu\Phi_a)}\Delta(\partial_\mu\Phi_a)+\frac{\partial\mathscr{L}}{\partial\Phi_a}\Delta\Phi_a+O(\omega^2)\right)d^f x$$

where $\Delta\Phi_a=\overline{\Phi}_a(x)-\Phi_a(x)=\overline{\Phi_a}(\bar{x})-\Phi_a(x)-(\overline{\Phi}_a(\bar{x})-\overline{\Phi}_a(x))=$

$$=\beta_a\omega-\alpha^\mu\partial_\mu\omega+O(\omega^2)$$

$$\Delta(\partial_\mu\Phi_a)=\partial_\mu\overline{\Phi}_a-\partial_\mu\Phi_a=\partial_\mu(\Delta\Phi_a)$$

Therefore considering the Euler-Lagrange equations we obtain that on motion we have $A=\int_D (d_\mu\left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu\Phi_a)}(\beta_a-\alpha^\nu\partial_\nu\Phi_a)\right)\omega+O(\omega^2))d^f x$.

we have also $\mathscr{L}(\Phi(\bar{x}),\partial\Phi(\bar{x}),\bar{x})-\mathscr{L}(\Phi(x),\partial\Phi(x),x)=d_\mu\mathscr{L}|_x\alpha^\mu\omega+O(\omega^2)$

and so changing the $\bar{x}$ variable to x variable in the D_ω integral we obtain

$$B=\int_D \mathscr{L}(\Phi(\bar{x}),\partial\Phi(\bar{x}),\bar{x})(1+d_\mu\alpha^\mu\omega+O(\omega^2))d^f x-\int_D \mathscr{L}(\Phi(x),\partial\Phi(x),x)d^f x=$$

$$=\int_D (d_\mu(\alpha^\mu\mathscr{L})\omega+O(\omega^2))d^f x$$

Hence $0=\delta S=-\int_D (d_\mu\left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu\Phi_a)}(\alpha^\nu\partial_\nu\Phi_a-\beta_a)-\alpha^\mu\mathscr{L}\right)\omega+O(\omega^2))d^f x$

and so since D and ω are arbitrary we conclude that if the action is invariant under the Ω transformations then during any motion, the Noether current is conserved, that is $d_\mu N^\mu=0$ where $N^\mu=\frac{\partial\mathscr{L}}{\partial(\partial_\mu\Phi_a)}(\alpha^\nu\partial_\nu\Phi_a-\beta_a)-\alpha^\mu\mathscr{L}$ is the Noether current.

If $N^i(t,\vec{x})$ for $(x^\mu)_\mu=(t,\vec{x})=(t,(x^i)_{i=\overline{1,3}})\in\mathbb{R}^4$ vanishes sufficiently fast as $\|\vec{x}\|\to\infty$, for example as at least $\|\vec{x}\|^{-2-\alpha}$ with $\alpha>0$ we have that $d_\mu N^\mu=0$ implies that the total Noether amount $\int N^0(t,\vec{x})d^3\vec{x}$ is constant in time, since

$$\frac{d}{dt}\int N^0 d^3\vec{x}=-\int\partial_i N^i d^3\vec{x}=-\lim_{R\to\infty}\int_{S(\vec{0},R)} N^i(t,x)\frac{x^i}{\|\vec{x}\|}d\sigma(x)=0$$

where $S(\vec{0},R)=\{\vec{x}\in\mathbb{R}^3|\|\vec{x}\|=R\}$.

If $\Phi=q=(q_i(t))_{i=\overline{1,n}}\in\mathbb{R}^n$ are the generalized coordinates of a system with Lagrangian $L=L(q,\dot{q},t)$ and Ω is given by the s -coordinate infinitesimal translations transforms defined as $t\to\bar{t}=t$, $q_i\to\bar{q}_i=q_i+\delta_{si}\omega+O(\omega^2)$ we have with the notations from above $\mu=1$, $a=1$, $\alpha^\mu=0$, $\beta_a=(\delta_{si})_{i=\overline{1,n}}$ and the Noether statement is that the s -generalized momentum $\frac{\partial L}{\partial\dot{q}_s}=p_s$ is constant on any motion if the system is invariant under s -generalized coordinate translations: $\dot{p}_s=0$ on motion.

If $L=L(x,y,z,\dot{x},\dot{y},\dot{z},t)$ is a single particle Lagrangian and Ω is given by the z -axis infinitesimal rotations

$t\to\bar{t}=t$,

$x\to\bar{x}=x-\omega y+O(\omega^2)$

$y\to\bar{y}=y+\omega x+O(\omega^2)$

$z\to\bar{z}=z$

(ω -infinitesimal rotation angle) the conserved quantity on any motion if the system is invariant under z -axis infinitesimal rotations follows to be the z -component of the angular momentum : $L_z=p_y x-p_x y=\frac{\partial L}{\partial \dot{y}}x-\frac{\partial L}{\partial \dot{x}}y$

For a time translations invariance of a $q=q(t), L=L(q,\dot{q},t)$ system we have Ω described by $t\to\bar{t}=t+\omega$, $q\to\bar{q}=q$ and the conserved quantity on any any motion is the energy $H=\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i-L=p\dot{q}-L$: $\frac{dH}{dt}=0$.

(Obviously the notation $\dot{F}$ means $\frac{dF}{dt}$) .

Consider now for the wave functions of a quantum system

(Let $\psi(t)\in V$, V Hilbert space of quantum system (see Chap. Quantum mechanics formalism) $\psi=\psi(t,\vec{x})$, $(t,\vec{x})\in\mathbb{R}^4$) a group G of coordinates transforms $(t,\vec{x})\to(t',\vec{x}')$. Then G induces a representation group $U(G)$ of wave function transforms which are supposed to be unitary operators on V such that if $g\in G$ with $g(t,\vec{x})=(t',\vec{x}')$ then for $\Omega=U(g)$ we have $\Omega:V\to V$ so that for any $(t,\vec{x})$ we have $\Omega\,\psi(t,\vec{x})=\psi(t',\vec{x}')$, $\Omega\in L(V)$ (Ω is linear continuous) and $\Omega^+\Omega=\Omega\Omega^+=\boldsymbol{I}$ (Ω is an unitary operator).

To say that an observable $A=A(t)\in L(V), A=A^+$ is invariant under G is clearly the statement $\Omega A=A\Omega$ for any $\Omega\in U(G)$ that is $[\Omega,A]=\Omega A-A\Omega=0$ for any $\Omega\in U(G)$.

If we take G the x -coordinate translations of $(t,x,y,z)\in\mathbb{R}^4$ we have the Lie group representation of infinitesimal translations $\Omega(dx)$ with

$\Omega(dx)\,\psi(t,x,y,z)=\psi(t,x+dx,y,z)$ (1)

Obviously we have

$\Omega(dx_1+dx_2)=\Omega(dx_2)\Omega(dx_1)$, $\Omega(0)=\boldsymbol{I}$, $\Omega^{-1}(dx)=\Omega(-dx)$ and so

$\frac{d\Omega}{d\omega}(\omega)=\Omega'(0)\Omega(\omega)$, $\Omega'(0)\,\psi=\nabla_x\psi$ and so $\Omega(dx)=\exp((dx)\nabla_x)$

$\Omega(dx)=\exp(\frac{i}{\hbar}dx(-i\hbar\nabla_x))$

Because $-i\hbar\nabla_x$ is a self-adjoint operator, if we require that the system is invariant under x -coordinate translations and so the x -component of momentum must be a conserved measurable quantity on system evolution being therefore an observable which depends on the infitesimal translations group only which group is

determined by its Lie group generator, the linear self adjoint operator $-i\hbar\nabla_x$ we take as the x -momentum observable $\hat{p}_x$ the operator $-i\hbar\nabla_x$ having

$\Omega(dx)=\exp(\frac{i}{\hbar}dx\,\hat{p}_x)$, $\hat{\vec{p}}=-i\hbar\nabla$ (2) .

The $\hbar$ constant appears in the expression of momentum operator so that the operator eigenvalues have the dimension of momentum.

In a similar way considering time translations invariance we conclude that as the energy observable on system evolution we can take the operator $i\hbar\partial_t$ which on the unitary evolutions of the system is equal to a self-adjoint operator (see Quantum mechanics formalism) which must be the Hamiltonian operator of the system.

Also considering rotations invariance we derive as the z -angular momentum operator $\hat{L}_z=\hat{x}\,\hat{p}_y-\hat{y}\,\hat{p}_x=i\hbar\frac{\partial}{\partial\theta}$ (where (r,θ,z) are the cilindrical z axis coordinates $(x,y,z)=(r\cos\theta,r\sin\theta,z)$ (see Chap.Representations of the rotations group).

Thus $\hat{\vec{p}}=-i\hbar\nabla$ -momentum operator , $\hat{\vec{L}}=\hat{\vec{x}}\times\hat{\vec{p}}$ angular momentum operator, $\hat{E}=i\hbar\frac{\partial}{\partial t}$ -energy operator

$[\hat{E},\hat{\vec{p}}]=0$, $[\hat{p}_x,\hat{p}_y]=[\hat{p}_z,\hat{p}_x]=[\hat{p}_y,\hat{p}_z]=0$ and we can therefore simultaneously measure energy and momentum .

If momentum is determined to be $\vec{p}$ we have $\hat{\vec{p}}\,\psi=\vec{p}\,\psi$ and from (1) and (2) follows $\psi(t,\vec{x})=\exp(\frac{i}{\hbar}\vec{p}\cdot\vec{x})\,\psi(t,\vec{0})$.

In a similar way, if energy is determined to be E on a particle system evolution, we have $\hat{E}\,\psi=E\,\psi$ and $\psi(t,\vec{x})=\exp(-\frac{i}{\hbar}Et)\,\psi(0,\vec{x})$

Thus if energy and momentum are determined on a particle system evolution we have $\psi(t,\vec{x})=\psi(0,\vec{0})\exp(-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x}))=\exp(-i(\omega t-\vec{k}\cdot\vec{x}))$ having a plane wave function with $\nu=\frac{\omega}{2\pi}$ frequency, $\lambda=\frac{2\pi}{\|\vec{k}\|}$ wavelenght of the associated (3) de Broglie wave of the particle $\hbar\omega=E$, $\hbar\vec{k}=\vec{p}$.

The wave function formula can be obtained also in another way as follows.

An associated wave function to a relativistic particle in its rest frame with $(t',\vec{x}')$ coordinates in the rest frame , must be $\psi(t)=\psi_0\exp(-i\omega' t')$ where $\hbar\omega'=m_0c^2$ is the rest energy of the particle with rest mass m_0 (see Chap. Relativistic dynamics) .

If the particle moves with velocity v in x -direction we have the Lorentz coordinate transforms (see Chap. Special relativity) :

$x'=\frac{x-v\,t}{\sqrt{1-\frac{v^2}{c^2}}}$, $t'=\frac{t-\frac{v}{c^2}x}{\sqrt{1-\frac{v^2}{c^2}}}$ and so requiring Lorentz invariance of the wave function , the wave function will be

$\psi(t,x)=\psi_0\exp\left(-i\,\omega\left(t-\frac{x\,v}{c^2}\right)\right)=\exp(-i(\omega t-k\,x))$ with

$\omega=\frac{\omega'}{\sqrt{1-\frac{v^2}{c^2}}}$, $\hbar\,\omega=\frac{m_0c^2}{\sqrt{1-\frac{v^2}{c^2}}}=m\,c^2=E$ -relativistic energy,

$\hbar\,k=\frac{\hbar\,\omega\,v}{c^2}=\frac{m_0\,v}{\sqrt{1-\frac{v^2}{c^2}}}=p$ -relativistic momentum ,

$\psi=\psi_0\exp\left(-\frac{i}{\hbar}(E\,t-p\,x)\right)$.

Note that the phase velocity of the wave must be $v_f=\frac{\omega}{k}=\frac{c^2}{v}>c$.

Therefore we consider for the propagation of the particle an associated pilot wave group which has a group velocity $v_g=\frac{d\,\omega}{d\,k}=\frac{d\frac{c^2}{\sqrt{1-\frac{v^2}{c^2}}}}{d\frac{v}{\sqrt{1-\frac{v^2}{c^2}}}}=v$.

The group velocity appears to be in fact the supposed velocity of the particle.

7. Quantum mechanics formalism. Quantum field theory Path integral formalism. Renormalization Calculation of Feynman integrals

Quantum mechanics formalism

In quantum mechanics, a system with *f* degrees of freedom is described by a complex wave function $\psi=\psi(t,q)$ depending on time $t\in\mathbb{R}$ and f degrees of freedom generalized spatial coordinate $q=(q_i)_{i=\overline{1,f}}$.

We have $\psi=\psi(t)\in C^1(\mathbb{R},H)$ where $(H,\langle\cdot,\cdot\rangle)$ is a complex Hilbert space of functions like $L^2_{\mathbb{C}}(D)$ with $D\in\mathbb{R}^f$ a (bounded) domain in $\mathbb{R}^f$.

The function $\frac{|\psi(t)|^2}{\langle\psi(t)|\psi(t)\rangle}=w(t,q)$ can be interpreted as the probability density of the system to have the coordinates *q* at time *t*.

An obsevable which describes the system through its measurable real average values will be a time dependent function linear operator valued function

$A:\mathbb{R}\to L(H,H)$ with average values

$\langle A\rangle_t=\int\psi^*(t)(q)(A(t)\,\psi(t))(q)d^fq=\langle\psi|A|\psi\rangle(t).$

Since the average values must be real we will consider that *A* is self-adjoint : $A = A^+$.

As usual we can consider a discretization of *D* by a *f*-dimensional lattice grid

$\Gamma=\{(n_ia)_{i=\overline{1,f}}|n_i\in\mathbb{Z}\text{ for }i=\overline{1,f}\}\cap D$ with $\operatorname{card}\Gamma=N$ such that H becomes $\mathbb{R}^N$ with the scalar product $\langle(\psi'_i)_{i=\overline{1,N}},(\psi_i)_{i=\overline{1,N}}\rangle=\frac{1}{a^f}\sum_{i=1}\psi'^*_i\,\psi_i$ where $\psi_i=\psi(n^i_ja)_{j=\overline{1,f}}$ with $((n^i_ja)_{j=\overline{1,f}})_{i=\overline{1,N}}$ being an enumeration of the elements of Γ and $\psi\in H$.

Obviously, for the derivatives we have the correspondence by discretization

$$\partial_i\psi=\frac{\partial\psi}{\partial q_i}\to\left(\pm\frac{1}{a}\left(\psi(an_1,an_2,\ldots,a(n_i\pm1),an_{i+1},\ldots,an_f)-\right.\right.$$
$$\left.\left.-\psi(an_1,\ldots,an_f)\right)\right)_{(an1,\ldots,anf)\in\Gamma}$$

The $-$ sign in $\pm$ is taken eventually if $(an_1,\ldots,a(n_i+1),\ldots,n_f)\notin\Gamma$ and $(an_1,\ldots,an_i,\ldots,an_f)$ is on the boundary of the grid.

We have also the correspondence by discretization $\int F(q)d^fq\to a^f\sum_{q\in\Gamma}F(q)$,

$$\delta^f(q'-q)=\frac{1}{a^f}\delta_{q'q}$$

Considering the discretization we can suppose that the observables are compact self-adjoint linear operators on *H*.

Thus any observable has an orthonormal complete set of eigenvectors $(\psi_i)_i$ with $A\,\psi_i=\lambda_i\,\psi_i$, $\langle A\rangle_{\psi_i}=\lambda_i$, the measurable real eigenvalues of observable A .

Moreover, by the discretization, *A* can be considered a trace operator, that is it exists a number $\operatorname{tr}A$ such that for any complete orthonormal set $(\psi_i)_{i\in\mathbb{N}}$ of H we have $\operatorname{tr}A=\sum_{i\in\mathbb{N}}\langle\psi_i|A|\psi_i\rangle$.

If φ, ψ are wave functions describing states of the system, the value $\frac{|\langle\varphi|\psi\rangle|^2}{\|\varphi\|^2\|\psi\|^2}$ can be interpreted as the probability of transition from state φ to state ψ.

For simplification we will consider the measure units for length [L] such that $1\hbar m^2=[\mathrm{L}]^2$ where $2\pi\hbar=h$ and h is the value of the Planck constant in SI units.

We consider the position states $|q\rangle\in H$ for $q=(q_i)_{i=\overline{1,f}}\in D$ normalized such that

$$\langle q'|q\rangle=\delta^f(q'-q)=\int\frac{1}{(2\pi)^f}\exp(ip(q'-q))d^f p \quad (1)$$

$$\int\delta^f(q'-q)\psi(q')d^f q'=\psi(q)\ ,\int\delta^f(q)d^f q=1\ ,q(q')=\delta^f(q'-q) \quad (2)$$

$$\langle q|\psi\rangle=\psi(q)\ ,\quad \int|q\rangle\langle q|d^f q=\boldsymbol{I} \quad (3)$$

We will have the normalized states of momentum

$|p\rangle\in H$ for $p\in\mathbb{R}^f$ such that $\langle q|p\rangle=\exp(ipq)$ for any position state $\langle q|\in H$ and $\int\frac{1}{(2\pi)^f}|p\rangle\langle p|d^f p=\boldsymbol{I}$ (4).

Hence $\langle p'|p\rangle=\int\langle p'|q\rangle\langle q|p\rangle d^f q=\int\exp(iq(p-p'))d^f q=(2\pi)^f\delta^f(p'-p)$ (5)

and so $\delta^f(p'-p)=\frac{V}{(2\pi)^f}\delta_{p'p}$ where $V=\int\limits_D d^f q$ is the spatial volume taken by the system.

We define the coordinates operators $\hat{q}=(\hat{q}_i)_{i=\overline{1,f}}$, $\hat{q}_i\in L(H,H)$ as observables satisfying $\hat{q}_i|q\rangle=q_i|q\rangle$ for any $q=(q_i)_{i=\overline{1,f}}$.

The commutator of two operators A, B is defined as $[A,B]=AB-BA$ and since $(|q\rangle)_{q\in D}$ is complete it follows $[\hat{q}_i,\hat{q}_j]=0$ for $i,j=\overline{1,f}$.

With the chosen length measure units the reduced Planck constant is $\hbar=1$ and so the momentum operator is $\hat{p}=-i\nabla_q$, $\hat{p}=(\hat{p}_i)_{i=\overline{1,f}}$, $\hat{p}_i|p\rangle=p_i|p\rangle$ for any $p=(p_i)_{i=\overline{1,f}}$, $\hat{p}_k=-i\frac{\partial}{\partial q_k}$ for $k=\overline{1,f}$

For $dq\in\mathbb{R}$ infinetisimal we take the i-translation vector $(dq)_i=(dq\,\delta_{ik})_{k=\overline{1,f}}$ and the spatial translation operator $T_i(dq)$ defined by $(T_i(dq)\psi)(t,q)=\psi(t,q+(dq)_i)$ for any $\psi(t)\in H$ and we will have :

$$T_i(dq)=\boldsymbol{I}+i\hat{p}_i dq+O((dq)^2)$$

$$T_i(dq)\hat{q}_j|q'\rangle=q'_j T_i(dq)|q'\rangle+O((dq)^2)=q'_j|q'-(dq)_i\rangle+O((dq)^2)$$

$$\hat{q}_j T_i(dq)|q'\rangle=\hat{q}_j|q'-(dq)_i\rangle=(q'_j-\delta_{ij}(dq))|q'-(dq)_i\rangle$$

$$[T_i(dq),\hat{q}_j]|q'\rangle=\delta_{ij}(dq)|q'\rangle+O((dq)^2) \text{ and so}$$

$$i[\hat{p}_i,\hat{q}_j]dq=\delta_{ij}dq+O((dq)^2).$$

Dividing by dq and taking $dq\to 0$ we obtain $[\hat{p}_i,\hat{q}_j]=-i\delta_{ij}$.

Restoring the Planck constant by dimensional analysis we obtain the commutation $[\hat{p}_i,\hat{q}_j]=-i\hbar\delta_{ij}$.

For an observable $A=A(t)$ we have a complete orthonormate system $(\psi_i)_{i\in\mathbb{N}}$ of eigenvectors: $A\,\psi_i=\lambda_i\,\psi_i$ such that for any normalized $\psi\in H$ we have

$$|\psi\rangle=\sum_i\langle\psi_i|\psi\rangle|\psi_i\rangle=\sum_i c_i|\psi_i\rangle\ ,\ c_i=\langle\psi_i|\psi\rangle\ ,\ A|\psi\rangle=\sum_i\lambda_i c_i|\psi_i\rangle\ .$$

The average value of A for ψ is $\langle\psi|A|\psi\rangle=\sum_i|c_i|^2\lambda_i$ with $\sum_i|c_i|^2=1$

We define $\Delta A=A-\langle A\rangle\boldsymbol{I}$ and it follows: $\langle(\Delta A)^2\rangle=\|(\Delta A)\,\psi\|^2=\sum_i|c_i|^2|\lambda_i-\langle A\rangle|^2$.

Hence $\langle(\Delta A)^2\rangle$ is the averaged square deviation in measuring the observable A ,

$\langle(\Delta A)^2\rangle\le\|\Delta A\|^2$ where $\|\Delta A\|=\max_i|\lambda_i-\langle A\rangle|$ is the maximal error in measuring A (if we measure the obervable A , ψ collapses to an eigenvector ψ_i and the measured value is $\lambda_i=\langle\psi_i|A|\psi_i\rangle$) .

Obviously $[\Delta\hat{p}_k,\Delta\hat{q}_k]=[\hat{p}_k,\hat{q}_k]=-i$ and for any $\lambda\in\mathbb{R}$ it follows:

$$0\le\|(\lambda\Delta\hat{q}_k-i\Delta\hat{p}_k)\,\psi\|^2=\lambda^2\langle(\Delta\hat{q}_k)^2\rangle+\langle(\Delta\hat{p}_k)^2\rangle+\langle i\lambda[\Delta\hat{p}_k,\Delta\hat{q}_k]\rangle$$

$\lambda^2\langle(\Delta\hat{q}_k)^2\rangle+\langle(\Delta\hat{p}_k)^2\rangle+\lambda\ge0$ for any $\lambda\in\mathbb{R}$ and therefore $\langle(\Delta\hat{q}_k)^2\rangle\langle(\Delta\hat{p}_k)^2\rangle\ge\frac{1}{4}$,

$|\Delta q_k||\Delta p_k|\ge\frac{\hbar}{2}$ which is the Heisenberg uncertainity relation satisfied by the maximal measuring errors $|\Delta q_k|$ and $|\Delta p_k|$ of coordinates and momentum.

It is supposed that for any quantum system exists a time evolution operator $U(t,\Delta t):H\to H$ defined for $t\in\mathbb{R}$, $\Delta t\in\mathbb{R}$ with $U(t,\Delta t)\,\psi(t)=\psi(t+\Delta t)$ for any wave function $\psi=\psi(t)\in H$ such that U is an unitary operator: $UU^+=U^+U=\boldsymbol{I}$ and twice continuous differentiable in both time variables.

Thus $U(t,0)=\boldsymbol{I}$, $U(t,\Delta t)$ is linear unitary and we have a self-adjoint operator $\widehat{H}=\widehat{H}(t)=i\hbar\frac{\partial U}{\partial(\Delta t)}(t,0)\in L(H,H)$ such that $U(t,\Delta t)=\boldsymbol{I}-\frac{i}{\hbar}\widehat{H}(t)\Delta t+O((\Delta t)^2)$.

Therefore

$\psi(t+\Delta t)=\psi(t)-\frac{i}{\hbar}\widehat{H}(t)\,\psi(t)+O((\Delta t)^2)$ and according to Chap. Lagrangian field theory. Noether theorem $\widehat{H}$ is the energy observable satisfying the time dependent Schroedinger equation $i\hbar\,\partial_t\,\psi=\widehat{H}\,\psi$.

In analogy with classical mechanics, $\widehat{H}$ will be considered as a function of time and the momentum and coordinates observables :

$\widehat{H}=\widehat{(t)}(\hat{p},\hat{q})$ for example in the non-relativistic case for a spin 0, mass m particle we consider $\widehat{H}=\frac{\hat{p}^2}{2m}+V(q)$ where the potential energy is defined by $V(\hat{q})|\psi\rangle(t,q)=V(q)\,\psi(t,q)$.

Hence in this case we have

$$\hat{H}\,\psi=\frac{-\hbar^2}{2m}\nabla^2\,\psi+V\,\psi\,.$$

If $\hat{H}=\hat{H}(\hat{p},\hat{q})$ not depends explicitly on time the solution of the Schroedinger equation is $|\psi(t)\rangle=\exp(-\frac{i}{\hbar}\hat{H}\,t)|\psi(0)\rangle$ so we have to solve the time independent eigenvalue problem $\hat{H}\,\psi=E\,\psi$ with $E\in\mathbb{R}$, $\psi=\psi(q)$, $\psi\in H$
to get a complete set of energy eigenfunctions:
$(\psi_k)_{k\in\mathbb{N}}$, $\hat{H}\,\psi_k=E_k\,\psi_k$ and the wave functions of the system can be determined by

$$\psi(t,q)=\sum_k \exp(-\frac{i}{\hbar}E_k t)c_k\,\psi_k(q)\ ,\ c_k=\langle\,\psi_k|\,\psi(0,.)\rangle\ .$$

(the last equality holds if the eigenfunctions system is orthonormalized).

Quantum field theory. Path integral formalism. Feynman diagrams. Theory renormalization

For simplification we will use natural units for length and time such that the reduced Planck constant $\hbar=h/2\pi=1$ and the speed of light in vacuum constant $c=1$.
We consider the Minkowski space of time-space coordinates $(c\,t,\vec{x})=(t,\vec{x})=(x^\alpha)_{\alpha=\overline{0,3}}$ with the diagonal Minkowski metric coefficients $(\eta^{\alpha\beta})_{\alpha,\beta=\overline{0,3}}=\mathrm{diag}(1,-1,-1,-1)$ of signature $(+,-,-,-)$.
Contextual, if x , y are involved four-vectors, we denote the product $x\,y=\eta_{\alpha\beta}x^\alpha y^\beta=x^0y^0-x^1y^1-x^2y^2-x^3y^3$. We use Einstein summation covention also. We denote $\partial_\alpha=\frac{\partial}{\partial x^\alpha}$, $\partial^\alpha=\eta^{\alpha\beta}\partial_\beta$.
In quantum field theory , a system can be described by a time-space dependent coordinate field system of functions $\varphi_b=\varphi_b(t,\vec{x})=\varphi_b(x)$ with $b=\overline{1,m}$ which are considered also as operator valued functions $\hat{\varphi}_b=\hat{\varphi}_b(x)$, $b=\overline{1,m}$; $\hat{\varphi}_b(x)$ is an operator acting on a Hilbert space H of state functions
$\psi=\psi(t)\in H$, $\psi(t)=\psi(t)((\varphi_b(t,\vec{x}))_{b,\vec{x}})$; $(\varphi_b(t,\vec{x}))_{b,\vec{x}}$ is assimilated with the generalizated coordinates $q=q(t)$ evolution from quantum mechanics formalism.
The states Hilbert space has a vacuum state corresponding to $|0\rangle=|q\rangle$ with $q(t)$ assimilating as a generalizated coordinates position the field values

$$\varphi_b(t,\vec{x})=0 \text{ for any } b \text{ and } \vec{x}\ .$$

A quantum field theory is a Lagrangian field theory (see Chap. Lagrangian field theory) defined by a Lagrangian density $\mathscr{L}=\mathscr{L}((\varphi_b,d_\mu\varphi_b)_{\mu=\overline{0,3}\ ,\ b})(t,\vec{x})$.
We can consider discretizations of the field functions spatial domain so that with $\varphi_b:\mathbb{R}\times D\to\mathbb{C}$ and $a\in\mathbb{R}_+^*$ lattice constant, we take

$\Gamma=\{a(n_1,n_2,n_3)\in D|n_1,n_2,n_2\in\{1,...,N_0\}\}$ and the system is considered the continuum limit of quantum systems having wave functions $\psi=\psi(t,q)$ whose time dependent generalized coordinates and Lagrangian are given respectively by

$$q(t)=(\varphi_b(t,ja))_{b=\overline{1,m},\ j\in\{0,...,N0\}^3} \text{ and}$$

$$L(q(t),\dot{q}(t))=\sum_j a^3\mathscr{L}((\varphi_b(t,ja),d_\mu\varphi_b(t,ja))_{b,\mu,j}) \quad \text{where}$$

$$(d_0\varphi_b(t,ja))_{b,j}=\left(\frac{\partial\varphi_b}{\partial t}(t,ja)\right)_{b,j}=\dot{q}(t) \text{ for } \mu=0$$

$d_i\varphi(t,ja)=\frac{1}{a}(\varphi(t,(j+(\delta_{ik})_{k=\overline{1,3}})a)-\varphi(t,ja))$ for any $j\in\mathbb{N}^3$, $\mu=i=\overline{1,3}$

and we take $\varphi_b(t,ja)=0$ if exists $i\in\{1,2,3\}$ such that $(j_i<0$ or $j_i>N_0)$

The simplest Lorentz invariant Lagrangian densities are

$\mathscr{L}(\varphi,\partial\varphi)=\frac{1}{2}(\partial\varphi)^2-V(\varphi)$ (1) with V and φ real functions ,

$\mathscr{L}(\varphi,\partial\varphi)=\partial\varphi^+\partial\varphi-V(\varphi^+,\varphi)$ (2) with V a real function and $\varphi=\varphi_1+i\varphi_2$ a complex function.

In particular we can have :

$\mathscr{L}(\varphi,\partial\varphi)=\frac{1}{2}(\partial^\alpha\varphi\partial_\alpha\varphi-m^2\varphi^2)+J\varphi$ (1') with $J=J(t,\vec{x})$ a real source function ,

$\mathscr{L}(\varphi,\partial\varphi)=\partial^\alpha\varphi^+\partial_\alpha\varphi-m^2\varphi^+\varphi+J^+\varphi+J\varphi^+$ (2') with $J=J(t,\vec{x})$ a complex source function.

For the (1') , (2') Lagrangian densities we derive from the Euler-Lagrange equation $\frac{\partial\mathscr{L}}{\partial\varphi}-d_\mu\left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu\varphi)}\right)=0$ the motion equations

$\square\varphi+m^2\varphi=J$ (*) where $\square=\partial^\alpha\partial_\alpha$ is the d'Alembert operator.

Thus in the absence of a source J (restoring the Planck and speed of light constants) it follows that $m\frac{c^2}{\hbar}$ is the lowest pulsation that a wave solution of (*) can have , so m is the mass of the quantum particle described by the field under Lagrangian density (1') or (2').

Consider now that we have

$L(q,\dot{q})=\frac{1}{2}\bar{m}\dot{q}^2-V(q)$ (3) with $q=(q_i)_{i=\overline{1,f}}$ for the discretization Γ, $\text{card}\,\Gamma=f$, $\bar{m}$ a discretization dependent constant.

For the Hamiltonian corresponding to the (3) Lagrangian we have

$H=H(p,q)$, $p=\frac{\partial L}{\partial\dot{q}}$, $H=p\dot{q}-L=\frac{p^2}{2\bar{m}}+V(q)$

The undiscretized system with Lagrangian density

$\mathscr{L}=\mathscr{L}(\varphi,\partial\varphi)$ leads to a generalized momentum field $\pi(t,\vec{x})=\frac{\partial\mathscr{L}}{\partial(\partial_0\varphi)}(t,\vec{x})$

and so the Hamiltonian density will be

$H=\pi(t,\vec{x})\partial_0\varphi(t,\vec{x})-\mathscr{L}(t,\vec{x})=\frac{1}{2}((\partial_0\varphi)^2+(\nabla\varphi)^2+m^2\varphi^2)-J\varphi$ for the (1')

Lagrangian density and

$H=\partial_0\varphi^+\partial_0\varphi+(\nabla\varphi^+)(\nabla\varphi)+m^2\varphi^+\varphi-J^+\varphi-J\varphi^+$ for the (2') Lagrangian density.

The corresponding Hamiltonian observables are given by

$$\widehat{H}=\widehat{H}(t)=\int_D\frac{1}{2}((\partial_0\hat{\varphi})^2+(\nabla\hat{\varphi})^2+m^2\hat{\varphi}^2-J\hat{\varphi})(t,\vec{x})d^3\vec{x}$$ and

$$\widehat{H}=\widehat{H}(t)=\int_D(\partial_0\hat{\varphi}^+\partial_0\hat{\varphi}+(\nabla\hat{\varphi}^+)(\nabla\hat{\varphi})+m^2\hat{\varphi}^+\hat{\varphi}-J^+\hat{\varphi}-J\hat{\varphi}^+)(t,\vec{x})d^3\vec{x}$$

Given an initial state ψ_I and a final state ψ_F, since the Schroedinger equation solution with initial condition $\psi(0)=\psi_I$ is $\psi(t)=\exp(-i\widehat{H}t)\psi_I$ we consider the transition amplitude from state ψ_I at $t=0$ to state ψ_F at $t=T$:

$M=C\langle\psi_F|\exp(-i\widehat{H}T)|\psi_I\rangle$ where $C=1/(\|\psi_I\|\|\psi_F\|)$ is a normalization constant.

$|M|^2$ can be interpreted as the probability of the system to be in the given final state at time moment T if at time moment 0 the system is in the given initial state.

Approximating by taking the discretization Γ and initial state at position state q_I, final state at position state q_F with a discretized Hamiltonian function

$\widehat{H}(\hat{p},\hat{q})=\frac{\hat{p}^2}{2\bar{m}}+V(\hat{q})$ we take also $\delta t=\frac{T}{N+1}$, $q^j=(\varphi_b^j(j\delta t,\vec{x}))_{b=\overline{1,m},\vec{x}\in\Gamma}$, $j=\overline{0,N+1}$

and we have:

$$\frac{M}{C}=\langle q_F|\exp(-i\widehat{H}T)|q_I\rangle=\int\ldots\int\prod_{j=0}^{N}\langle q^{j+1}|\exp(-i\widehat{H}\delta t)|q^j\rangle d^fq^1d^fq^2\ldots d^fq^N$$

(because $\int|q^j\rangle\langle q^j|d^fq^j=\boldsymbol{I}$ with $f=m\,\mathrm{card}\,\Gamma$) .

Since $|q^j\rangle$ is an approximating function for $\delta^f(q-q^j)$ we can write

$\exp(-i\widehat{H}\delta t)|q^j\rangle=\exp\left(-i\frac{\hat{p}^2}{2\bar{m}}\delta t-iV(q^j)\delta t\right)|q^j\rangle$ and therefore we have

$$\langle q^{j+1}|\exp(-i\widehat{H}\delta t)|q^j\rangle=\int\langle q^{j+1}|\exp\left(-i\delta t\frac{\hat{p}^2}{2\bar{m}}-i\delta tV(q^j)\right)|p\rangle\langle p|q^j\rangle\frac{1}{(2\pi)^f}d^fp=$$

$$=\frac{1}{(2\pi)^f}\exp\left(i\delta t\frac{\bar{m}}{2}\left(\frac{q^{j+1}-q^j}{\delta t}\right)^2-i\delta tV(q^j)\right)\int\exp\left(-i\frac{\delta t}{2\bar{m}}\left(p-\frac{\bar{m}}{\delta t}(q^{j+1}-q^j)\right)^2\right)d^fp$$

Using the Fresnel integral $\int_{-\infty}^{\infty}\exp(-is^2)ds=\sqrt{-i\pi}$ we obtain :

$$\langle q^{j+1}|\exp(-i\widehat{H}\delta t)|q^j\rangle=\left(-\frac{1}{2\pi}\frac{i\bar{m}}{\delta t}\right)^{f/2}\exp\left(i\delta t\left(\frac{\bar{m}}{2}\left(\frac{q^{j+1}-q^j}{\delta t}\right)^2-V(q^j)\right)\right)$$

Hence

$$\frac{M}{C}=\left(\frac{-i\bar{m}}{2\pi\delta t}\right)^{(N+1)f/2}\int\ldots\int\exp\left(i\delta t\frac{\bar{m}}{2}\sum_{j=0}^{N}\left(\left(\frac{q^{j+1}-q^{j}}{\delta t}\right)^{2}-V(q^{j})\right)\right)d^{f}q^{1}\ldots d^{f}q^{N}\ .$$

In the limit $N\to\infty$, the integrand becomes $\exp(i\int_0^T L(q(t),\dot{q}(t))dt)$ and we are integrating over all paths $q = q(t)$ with $q(0) = q_I$ and $q(T) = q_F$, from the initial state to the final state.

We can denote the path integral

$\int\ldots Dq=\lim_{N\to\infty}\left(\frac{-i\bar{m}}{2\pi\delta t}\right)^{(N+1)f/2}\int\ldots\int\ldots d^{f}q^{1}\ldots d^{f}q^{N}$ and therefore we can write:

$$M=C\int Dq\exp(i\int_0^T L(q,\dot{q})dt)$$

For a (1) type Lagrangian density we can take the discretization lattice constant $a=\delta t$ and for given T take the continuum limit $a\to 0$ following $\bar{m}=a^{3}$ (4)

$f=\frac{V}{a^{3}}$, $V=\int_D d^{3}\vec{x}$ (5)

$N+1=\frac{T}{a}$ (6)

In the continuum limit we denote $\int Dq\ldots=\int D\varphi\ldots$ the path integral integrand becoming $\exp(i\int_{[0,T]\times D}\mathscr{L}(\varphi,\partial\varphi)d^{4}x)$ and we integrate over all $(\varphi(t,.))_t$ paths with $\left|(\varphi(0,\vec{x}))_{\vec{x}\in D}\right\rangle=|\psi_I\rangle$ and $\left|(\varphi(T,\vec{x}))_{\vec{x}\in D}\right\rangle=|\psi_F\rangle$.

Also we take $\varphi(t,\vec{x})=0$ for any $\vec{x}\in\mathbb{R}^3\setminus D$ or $t\notin[0,T]$ and we will calculate transition amplitudes when $|\psi_I\rangle=|0\rangle$, $\langle\psi_F|=\langle 0|$.

In that case, for a (1') or (2') Lagrangian density, with the discretization we made, the transition amplitude becomes

$$M=C\int D\varphi\exp(i\int\mathscr{L}(\varphi,\partial\varphi)d^{4}x)=$$

$=\bar{C}\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\exp\left(i\left(\frac{1}{2}\tilde{q}^{T}A\tilde{q}+J^{T}\tilde{q}\right)\right)dq_1^1\ldots dq_f^1dq_1^2\ldots dq_f^2\ldots dq_f^N$ where

$\tilde{q}=(q_1^1,\ldots,q_f^1,q_1^2,\ldots,q_f^N)$ as a column vector , $q^j=(q_k^j)_{k=\overline{1,f}}$ for $j=\overline{0,N+1}$ and A is a symmetric real $Nf\times Nf$ matrix and J is the discretized column source vector that couples to the discretization of $\varphi(t,\vec{x})$, $\bar{C}$ being a discretization dependent constant.

Hence, following the calculation we have done in the Appendix, we have

$\langle\psi_F|\exp(-i\hat{H}T)|\psi_I\rangle=Z(J)=\bar{C}\left(\frac{(2\pi i)^{Nf}}{\det A}\right)^{1/2}\exp(-(i/2)J^{T}A^{-1}J)$.

For the (1') Lagrangian density, because we integrate in the path integral over

φ with $\varphi(t,\vec{x})=0$ for $\vec{x}\notin D$, the domain D being bounded and $\varphi(0,\vec{x})=\varphi(T,\vec{x})=0$ for any $\vec{x}\in D$ we have, integrating by parts,

$\int \mathscr{L}(\varphi,\partial\varphi)d^4x=\int d^4x(-\frac{1}{2}\varphi(\partial^2+m^2)\varphi+J\varphi)$ and so the relation $AA^{-1}=\boldsymbol{I}$ in terms of discretized operators corresponds to

$-(\partial^2+m^2)D(x-y)=\delta^4(x-y)$ (5) so that $-\frac{1}{2}J^T A^{-1}J$ becomes in the continuum limit :

$W(J)=-\frac{1}{2}\int J(x)D(x-y)J(y)d^4x\,d^4y$ leading to $Z(J)=Z(0)\exp(iW(J))$.

The solution to the (5) partial differentials equation is the propagator

$D(x-y)=\int \frac{d^4k}{(2\pi)^4}\frac{\exp(ik(x-y))}{k^2-m^2+i\varepsilon}$ with $\varepsilon>0$, $\varepsilon\to 0$ a small value.

To evaluate $D(x)$ we integrate over k_0 by the method of contours.

Let $\omega_k=\sqrt{\vec{k}^2+m^2}$, $k=(k_0,\vec{k})$

The integrand has two poles which for $\varepsilon\to 0$, $\varepsilon>0$ are equal to $\omega_k-i\varepsilon$ and $-\omega_k+i\varepsilon$.

For $x^0>0$ the factor $\exp(ik_0x^0)$ is exponentially damped for k_0 in the upper plane. Hence w extend the contour from $-\infty$ to ∞ on the real axis to include the infinite semicircle in the upper half plane, enclosing the pole at $-\omega_k+i\varepsilon$ obtaining by the residues theorem

$\int \frac{d^4k}{(2\pi)^4}\frac{\exp(ikx)}{k^2-m^2+i\varepsilon}=-i\int \frac{d^3\vec{k}}{(2\pi)^3}\frac{1}{2\omega_k}\exp(-i(\omega_k t-\vec{k}\vec{x}))$.

For $x^0 < 0$, we close the contour in the lower half plane, enclosing the pole at $\omega_k-i\varepsilon$, obtaining $-i\int \frac{d^3\vec{k}}{(2\pi)^3}\frac{1}{2\omega_k}\exp(i(\omega_k t-\vec{k}\vec{x}))$ and so we will have

$D(x)=-i\int \frac{d^3\vec{k}}{(2\pi)^3 2\omega_k}(\theta(x^0)\exp(-i(\omega_k t-\vec{k}\vec{x}))+\theta(-x^0)\exp(i(\omega_k t-\vec{k}\vec{x})))$ (6)

where θ is the Heaviside function $\theta(x^0)=\begin{cases}1 & \text{if } x^0>0\\ 0 & \text{if } x^0<0\end{cases}$

As we observe in (6) , in the future cone ($x^0 > 0$) we integrate with a positive energy ω_k of a virtual particle, that justifies the choosing $\varepsilon>0$ in the propagator solution.

For the (2') Lagrangian density we have

$\varphi=\varphi_1+i\varphi_2$, $J=J_1+iJ_2$

$\int \mathscr{L}(\varphi,\partial\varphi)d^4x=\int d^4x\left(-\frac{1}{2}\varphi_i K_{ij}\varphi_j+2J_i\varphi_i\right)$ with

$K_{ij}=2\delta_{ij}(\partial^2+m^2)$, $i,j=1,2$

The $A A^{-1}=\boldsymbol{I}$ in the discretized formula is like $K_{ij} D_{jk}(x-y)=\delta_{ik}\delta^4(x-y)$ so that $D_{jk}(x-y)=\frac{1}{2}\delta_{jk} D(x-y)$ and after some calculus we have

$$W(J)=-2\int J_i(x) D_{jk}(x-y) J_k(y) d^4x\, d^4y=$$

$$=-\frac{1}{2}\int (J(x) D(x-y) J^+(y)+J^+(x) D(x-y) J(y)) d^4x\, d^4y$$

$Z(J)=Z(0)\exp(iW(J))$.

Obviously, $(\mathbb{R}^4\ni x\to D(x-y))$ is a temperate distribution, as an inverse Fourier transform of a temperate distribution which is $\mathbb{R}^4\ni k\to\frac{1}{k^2-m^2+i\varepsilon}$.

For the Fourier transform we use the momentum space notation of the argument:

$D(k)=\int D(x)\exp(-ikx) d^4x=\frac{1}{k^2-m^2+i\varepsilon}$.

In the distributions space, for the distribution $x\to D(x-y)$ we have

$D(x-y)=\lim_{n\to\infty}\int_{A_n}\frac{\exp(ik(x-y))}{k^2-m^2+i\varepsilon}\frac{d^4k}{(2\pi)^4}$ (7) for any sequence $(A_n)_{n\in\mathbb{N}}$ with $\bigcup_n A_n=\mathbb{R}^4$, $A_{n+1}\supset A_n$ and therefore we can separate integration variables in (7) which allows the contour method we used to derive (6).

Taking $J(k)=\int J(x)\exp(-ikx) d^4x$ in the momentum space we have :

$$W(J)=-\frac{1}{2}\int\frac{1}{(2\pi)^4} J^*(k) D(k) J(k) d^4k$$

We add to the (1') Lagrangian density an interaction term so that the Lagrangian density becomes

$$\mathcal{L}(\varphi,\partial\varphi)=\frac{1}{2}((\partial\varphi)^2-m^2\varphi^2)-\frac{1}{4!}\lambda\varphi^4+J\varphi \quad (8)$$

(to the (2') Lagrangian density we add the interaction term $-\frac{1}{2!2!}\lambda(\varphi^+\varphi)^2$

In the discretized formula we have

$$\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty}\exp(i(\frac{1}{2}\tilde{q}^T A\tilde{q}-\frac{\lambda}{4!}\tilde{q}^4+J\tilde{q}))d^{Nf}\tilde{q}=$$

$$=\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty}\exp(i(\frac{1}{2}\tilde{q}^T A\tilde{q}+J\tilde{q}))\sum_{s=0}^{\infty}\sum_{i1,\dots,1s}\frac{1}{s!}(-\frac{i\lambda}{4!})^s\tilde{q}_{i1}^4\dots\tilde{q}_{is}^4 d^{Nf}\tilde{q}=$$

$$=\exp\left(-i\frac{\lambda}{4!}\sum_j\left(\frac{\partial}{\partial(iJ_j)}\right)^4\right)\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty}\exp(i(\frac{1}{2}\tilde{q}^T A\tilde{q}+J\tilde{q}))d^{Nf}\tilde{q}$$ and so we derive:

$$Z(J,\lambda)=\int D\varphi\exp\left(i\int \mathscr{L}(\varphi,\partial\varphi)d^4x\right)=$$
$$=Z(0,0)\exp\left(-i\frac{\lambda}{4!}\int d^4w\left(\frac{\delta}{\delta(iJ(w))}\right)^4\right)\exp\left((-i/2)\int J(x)D(x-y)J(y)d^4xd^4y\right) \quad (9)$$

where $\frac{\delta}{\delta(iJ(w))}$ is the partial derivative with respect to the infinetisimal variable $iJ(w)d^4w$.

Consider now a process of a system described by the (8) Lagrangian density in which the source field J generates incoming matter $J(x_1^a)$,..., $J(x_n^a)$ at space-time locations x_1^a ,..., x_n^a, involves matter $J(w_1)$,..., $J(w_m)$ at interaction locations w_1 ,..., w_m and generates outgoing matter $J(x_1^b)$,..., $J(x_s^b)$ at space-time locations x_1^b ,... x_s^b .

$I=\{x_1^a,...,x_n^a\}$, $V=\{w_1,...,w_m\}$, $O=\{x_1^b,...,x_s^b\}$.

The process assumes field incoming propagation from x_k^a to w_{ik} for each $k=\overline{1,n}$, internal field propagation from w_{lj} to w_{mj} for $j=\overline{1,r}$ and outgoing field propagation from w_{fu} to x_u^b for each $u=\overline{1,s}$ with f_u , i_k , l_j , $m_j\in\{1,...,m\}$.

We label to each propagation : x_k^a to w_{ik} , w_{lj} to w_{mj} , w_{fu} to x_u^b respectively the four-momenta k_k^a , k_j^i , k_u^b for $k=\overline{1,n}$, $j=\overline{1,r}$, $u=\overline{1,s}$.

$((x_k^a,w_{ik})$, $k_k^a)_{k=\overline{1,n}}$ are the incoming external legs,

$((w_{fu},x_u^b)$, $k_u^b)_{u=\overline{1,s}}$ are the outgoing external legs,

$((w_{lj},w_{mj})$, $k_j^i)_{j=\overline{1,r}}$ are the internal lines and

$V=\{w_1,...,w_m\}$ are the vertices of the corresponding Feynman diagrams considered in space-time and in momentum space.

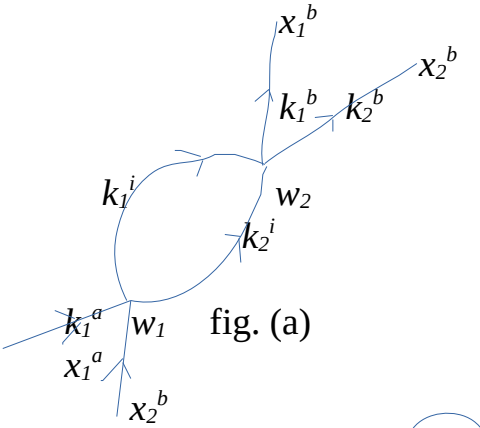


fig. (a)

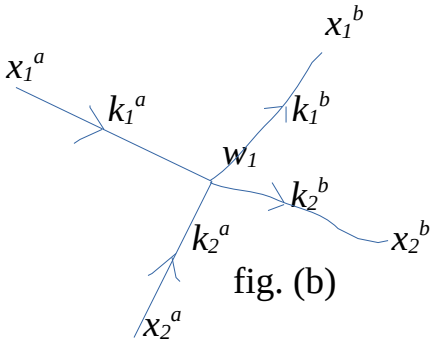


fig. (b)

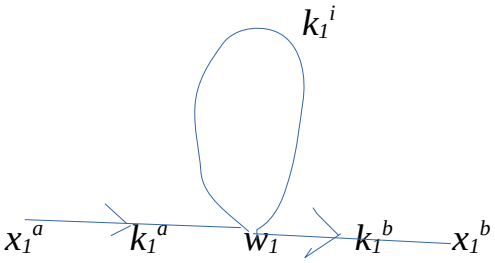


fig. (c)

To calculate the amplitude of the process we observe that the process corresponds to terms from the expansion of $\exp\left((-i/2)\int J(x)D(x-y)J(y)d^4xd^4y\right)$ in (9) that contain the following (10) expression:

$$\prod_{k=1}^{n} iJ(x_k^a)iD(x_k^a-w_{ik})iJ(w_{ik})d^4x_k^a d^4w_{ik}\prod_{j=1}^{r} iJ(w_{lj})iD(w_{lj}-w_{mj})iJ(w_{mj})d^4w_{lj}$$

$$d^4w_{mj}\prod_{u=1}^{s} iJ(w_{fu})iD(w_{fu}-x_u^b)iJ(x_u^b)d^4w_{fu}d^4x_u^b$$

These terms carry a factor $\frac{1}{2^{n+r+s}}\frac{1}{(n+r+s)!}$ and must be multiplied by a symmetry factor S_F which comes from the fact that the terms appear from the product $\left(\int J(x)D(x-y)J(y)d^4xd^4y\right)^{n+r+s}$ and $D(x-y)=D(y-x)$ and therefore each pair $(x,y)\in\{(x_k^a,w_{ik}),(w_{lj},w_{mj}),(x_u^b,w_{fu})|k=\overline{1,n}\ ,\ j=\overline{1,r}\ ,\ u=\overline{1,s}\}$ can be chosen two times if $x\neq y$ and one time if $x=y$ from any of the $n+r+s$ factors of the product $\left(\int J(x)D(x-y)J(y)d^4xd^4y\right)^{n+r+s}$ unless the factor was not already used for choosing previously a pair.

Then we get rid of the $J(w_{lj})$ and $J(w_{mj})$, $j=\overline{1,r}$ factors by applying a term from the expansion of the operatorial function $\exp\left(-i\frac{\lambda}{4!}\int d^4w\left(\frac{\delta}{\delta(iJ(w))}\right)^4\right)$ which must be

$$\left(-i\frac{\lambda}{4!}\right)^m\frac{1}{m!}\int\ldots\int d^4w_1d^4w_2\ldots d^4w_m\left(\frac{\delta}{\delta(iJ(w_1))}\right)^4\ldots\left(\frac{\delta}{\delta(iJ(w_m))}\right)^4 .$$

The integration over w_i means that the internal process can occur anywhere in space-time.

Expressing

$$J(x_l^a)=\int\frac{1}{(2\pi)^4}\exp(ik_l^ax_l^a)J(k_l^a)d^4k_l^a=\int\frac{1}{(2\pi)^4}\exp(-ik_l^ax_l^a)J^+(k_l^a)d^4k_l^a\ ,$$

$$D(x_l^a-w_{il})=\int\frac{1}{(2\pi)^4}\exp(ik_l^a(x_l^a-w_{il}))D(k_l^a)d^4k_l^a\ \text{ for } l=\overline{1,n}$$

$$J(x_l^b)=\int\frac{1}{(2\pi)^4}\exp(ik_l^bx_l^b)J(k_l^b)d^4k_l^b\ ,$$

$$D(w_{fl}-x_l^b)=\int\frac{1}{(2\pi)^4}\exp(ik_l^b(w_{fl}-x_l^b))D(k_l^b)d^4k_l^b\quad\text{for } l=\overline{1,s}$$

$$D(w_{lj}-w_{mj})=\int\frac{1}{(2\pi)^4}\exp(ik_j^i(w_{lj}-w_{mj}))D(k_j^i)d^4k_j^i\quad\text{for }\ j=\overline{1,r}$$

and integrating over all space-time variables we obtain the relevant term :

$$Z(0,0)S_F\frac{1}{2^{n+r+s}}\frac{1}{(n+r+s)!}\int\left(\prod_{j=1}^{n}\frac{i}{k_j^{a2}-m^2+i\varepsilon}iJ^+(k_j^a)\right)\left(\prod_{j=1}^{s}\frac{i}{k_j^{b2}-m^2+i\varepsilon}iJ(k_j^b)\right)\frac{1}{m!}$$
$$(-i\lambda)^m\left(\prod_{j=1}^{r}\frac{i}{k_j^{i2}-m^2+i\varepsilon}\right)\left(\prod_{i=1}^{m}\delta^4\left(\sum_{k\in Ai}k-\sum_{k\in Bi}k\right)\right)(2\pi)^{4(m-n-r-s)} \qquad (11)$$

$\prod_{j=1}^{n}d^4k_j^a\prod_{j=1}^{s}d^4k_j^b\prod_{j=1}^{r}d^4k_j^i$ where A_i , $B_i\subset\{k_k^a,k_j^b,k_l^i|k=\overline{1,n}\ ,\ j=\overline{1,s}\ ,\ l=\overline{1,r}\}$

$A_i\cap B_i=\emptyset$ for $i=\overline{1,m}$ and the momenta in A_i , B_i are occurring as labels.

Because each interaction vertex has four incoming or outgoing lines we have $n + s + 2r = 4m$ and so, as we expect, the amplitude term A defined by the (11) expression is adimensional.

For a simple propagation process we have to consider the zero-th order Feynman diagram with $I=\{x^a\}$, $O=\{x^b\}$, $V=\emptyset$ and the first order in λ diagram fig.(c)

The zero-th order amplitude for the propagation is

$$A_0=-Z(0,0)\frac{i}{(2\pi)^4}\int J^+(k)\frac{1}{k^2-m^2+i\varepsilon}J(k)d^4k \qquad (12)$$

For the fig.(c) diagram we have a symmetry factor $2^2\cdot 3!$ and so from this diagram we have an amplitude

$$A_1=Z(0,0)2^2\cdot 3!\frac{1}{2^3}\frac{1}{3!}(-i\lambda)(2\pi)^{-8}\int\frac{i}{k'^2-m^2+i\varepsilon}iJ^+(k')\frac{i}{k''^2-m^2+i\varepsilon}J(k'')$$
$$\frac{i}{k^2-m^2+i\varepsilon}\delta^4(k'-k'')d^4k'\,d^4k''\,d^4k=$$
$$=\frac{1}{2}\frac{\lambda}{(2\pi)^8}Z(0,0)\int\frac{d^4k}{k^2-m^2+i\varepsilon}\int\frac{J^+(k')J(k')}{(k'^2-m^2+i\varepsilon)^2}d^4k'$$

The integral over k (the loop from fig.(c) momentum integral) in the above expression is divergent and so we will integrate over a cutoff of momentum range we consider :

$\|k\|_4\le\Lambda$ where $\Lambda\in\mathbb{R}_+^*$ is an upper bound for the momentum range we take in consideration and $\|\cdot\|_4$ is a specified four-dimension euclidean equivalent norm.

The first order approximation amplitude for a k- four-momentum propagation process with $|k_\alpha-k_{1\alpha}|<\frac{1}{2}|dk_\alpha|$, $\alpha=\overline{0,3}$ is therefore (taking the Λ cutoff):

$$A=A_0+A_1=Z(0,0)\left(-\frac{i}{(2\pi)^4}\frac{J^+(k_1)J(k_1)}{k_1^2-m^2+i\varepsilon}d^4k_1+\right.$$
$$\left.+\frac{1}{2}\frac{\lambda}{(2\pi)^8}\left(\int^{\Lambda}\frac{1}{k^2-m^2+i\varepsilon}d^4k\right)\frac{J^+(k_1)J(k_1)}{(k_1^2-m^2+i\varepsilon)^2}d^4k_1\right) \qquad (12')$$

$|A|^2$ will be the probability for the considered *k*- momentum propagation process to occur for a given source *J*. The probability has a resonance pike for $|k_1^2-m^2|\leq\delta$ with δ small , that is $\delta\to 0$.
If we set the source to produce or remove virtual particles having an arbitrary four-momentum k_1 which is on mass shell (that is $|k_1^2-m^2|<\delta$ with $\delta\to 0$) , the probability $|A|^2$ must be bounded (for $\delta\to 0$, $\varepsilon\to 0$) and not dependent on k_1 .

Therefore we must have $J(k_1)=(k_1^2-m^2)P$ where P may depend only on the k-space discretization constant $|d\,k_{1\alpha}|$ and on k_1 .
Hence if we set the source to produce or remove virtual particles with *k*-four-momentum on mass shell, the general scattering process amplitude for $k_1^a,\ldots,k_n^a$ incoming particles four-momenta on mass shell and $k_1^b,\ldots,k_s^b$ outgoing particles four-momenta on mass shell will be proportional to the Feynman amplitude ***M*** defined by a relation as follows :

$$A=S_F(2\pi)^{4(m-r-n-s)}(-i\lambda)^m\frac{1}{m!}\frac{1}{2^{n+r+s}}\frac{1}{(n+r+s)!}(-1)^{n+s}\int\left(\prod_{j=1}^{r}\frac{i}{k_j^{i\,2}-m^2+i\,\varepsilon}\right)$$
$$\prod_{i=1}^{m}\delta^4\Big(\sum_{k\in A\,i}k-\sum_{k\in Bi}k\Big)\prod_{j=1}^{r}d^4k_j^i=(2\pi)^4(-1)^{n+s}\frac{1}{(2\pi)^{4(n+s)}}\boldsymbol{M}\,\delta^4\Big(\sum_{j=1}^{n}k_j^a-\sum_{j=1}^{s}k_j^b\Big)$$

M is obtained after progresively transforming the integral by changing variables to obtain the combination of k_i^a , k_j^b , $i=\overline{1,n}$, $j=\overline{1,s}$ reducing the delta functions. ***M*** depends on k_i^a , k_j^b and may depend on the Λ cutoff which can be a four-ball with radius Λ , $B_4(K,\Lambda)=\{k\in\mathbb{R}^4\,|\,\|K-k\|_4<\Lambda\}$ where the integration variables k_j^i , $j=\overline{1,r}$ take values if the integral is divergent and we integrate over the cutoff.

Consider now a diagram with $B_E = n + s$ external legs of incoming and outgoing particles. Let $B_I = r$ the number of internal lines and $V = m$ the number of interaction vertices. We have $4\,V = B_E + 2\,B_I$. We can see that the number of loops (elementar cycles of the unoriented graph corresponding to the Feynman diagram) is *L*, equal to the number of $\int\ldots\frac{d^4k}{(2\pi)^4}$ integrals we have to do in the expression of ***M*** (the number of B_I integrals we seem have to do is decreased to $L = B_I - (V - 1)$ (Euler theorem) by the momentum conservation delta functions associated with the vertices, one to each vertex, but one of them is associated with overall momentum conservation $\sum_{j=1}^{n}k_j^a-\sum_{j=1}^{s}k_j^b=0$).
We say that we have a superficial degree of divergence *D* for a Λ dependent expression if it diverges like Λ^D for $\Lambda\to\infty$ (a logarithmic divergence counts as *D*=0).

For each loop there is a $\int^{\Lambda} d^4k$ when cutoff integrating the $\boldsymbol{M}$ expression and each vertex brings the degree of divergence down by a power of 2 (from the propagator factor). Therefore the total degree of divergence for the $\boldsymbol{M}$ expression integrated on the Λ-cutoff of the momentum space is $D = 4\,L - 2\,B_I = 4 - B_E$.
For the fig.(b) Feynman diagram we have $m = 1$, $n = 2$, $s = 2$, $r = 0$, $S_F = 2^4.4!$ and the Feynman amplitude $\boldsymbol{M_1} = -i\,\lambda$.
For the fig.(a) Feynman diagram we have $m = n = s = r = 2$, the symmetry factor is $S_F = \binom{6}{4} 4! \cdot 2^6$ and the Feynman amplitude $\boldsymbol{M_2} = \frac{1}{(2\pi)^4} M_2(\Lambda, m, K)\,\lambda^2$ with

$$M_2 = (1/4)\int^{\Lambda} \frac{1}{k^2 - m^2 + i\varepsilon} \frac{1}{(K-k)^2 - m^2 + i\varepsilon} d^4k \quad \text{where } K = k_1 + k_2,\ k_1 = k_1^a,\ k_2 = k_2^a.$$

When we consider the whole meson-meson scattering process with k_1 , k_2 incoming particles four-momenta , k_3 , k_4 outgoing particles four-momenta in λ-second order approximation we must consider in additon to fig.(b) and fig.(a) diagrams the other two relevant Feynman diagrams fig.(d) and fig.(e) ; $k_3 = k_1^b$, $k_4 = k_2^b$, $x_3 = x_1^b$, $x_4 = x_2^b$, $x_1 = x_1^a$, $x_2 = x_2^a$

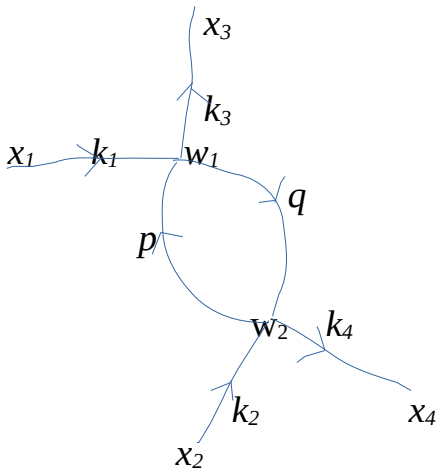


fig.(d)

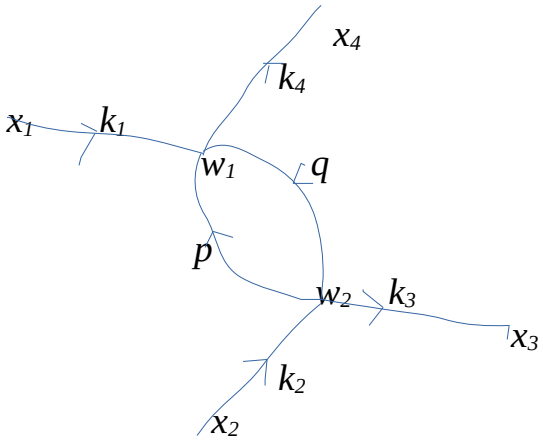


fig.(e)

with Feynman amplitudes
$\frac{1}{(2\pi)^4} M_2(\Lambda, m, k_1 - k_3)\,\lambda^2$ and respective $\frac{1}{(2\pi)^4} M_2(\Lambda, m, k_1 - k_4)\,\lambda^2$.
The final scattering process amplitude will be

$$A = \left(C\,\boldsymbol{M_1} + \frac{C}{(2\pi)^4}\lambda^2 \left(M_2(\Lambda, m, k_1 + k_2) + M_2(\Lambda, m, k_1 - k_3) + \right.\right.$$

$$\left.\left. + M_2(\Lambda, m, k_1 - k_4) \right) \right) \delta^4(k_1 + k_2 - k_3 - k_4)$$ where C is a constant independent of Λ , k_1, k_2, k_3, k_4 .

We prove in the Appendix that

$M_2(\Lambda, m, K) = E + i F \log \frac{\Lambda^2}{f(K^2, m)}$ where E, F are constants independent of Λ, K and F is real and f is a positive function of K^2, m .
Thus for $s = f((k_1+k_2)^2, m)$, $t = f((k_1-k_3)^2, m)$, $u = f((k_1-k_4)^2, m)$ we have geometrical momentum space discretization determined constants G, D, C with G, C real, such that the scattering amplitude to $O(\bar{\lambda}^3)$ approximation is given by

$$A = -i\bar{\lambda} + D\bar{\lambda}^2 + iC\bar{\lambda}^2\left(\log\frac{\Lambda^2}{s} + \log\frac{\Lambda^2}{t} + \log\frac{\Lambda^2}{u}\right) \text{with } \bar{\lambda} = G\lambda \ .$$

By real scattering experiments we can determine the probability $|A|^2$ for given values of s_0 , t_0 , u_0 and so determine positive real λ_P such that for this values we have an amplitude $A = -i\lambda_P$.

Hence $-i\lambda_P = -i\bar{\lambda} + D\bar{\lambda}^2 + iC\bar{\lambda}^2\left(\log\frac{\Lambda^2}{s_0} + \log\frac{\Lambda^2}{t_0} + \log\frac{\Lambda^2}{u_0}\right) + O(\bar{\lambda}^3)$ (13)

and for arbitrary s, t, u: $A = -i\bar{\lambda} + D\bar{\lambda}^2 + iC\left(\log\frac{\Lambda^2}{s} + \log\frac{\Lambda^2}{t} + \log\frac{\Lambda^2}{u}\right) + O(\bar{\lambda}^3)$ (14)

From (13) follows:

$$-i\bar{\lambda} = -i\lambda_P - D\lambda_P^2 - iC\lambda_P^2\left(\log\frac{\Lambda^2}{s_0} + \log\frac{\Lambda^2}{t_0} + \log\frac{\Lambda}{u_0}\right) + O(\lambda_P^3)$$

and now from (13) , (14) we obtain :

$$A = -i\lambda_P + iC\lambda_P^2\left(\log\frac{s}{s_0} + \log\frac{t}{t_0} + \log\frac{u}{u_0}\right) + O(\lambda_P^3)$$

and we have a cutoff independent description of the scattering amplitude in terms of the kinetic s , t, u and the physically measurable quantities λ_P , s_0 , t_0 , u_0 .
The scattering theory is therefore renormalizable cutoff independent when the magnitude order of the measurable λ_P coupling constant which is given by the effective amplitude $A = -i\lambda_P$ is increased requiring higher order approximation.

Consider now the k- four-momentum propagation process which corresponds to zero-th, first and second order in λ Feynman diagrams respectivefig.(g) , fig.(c) and fig.(j) (with $k_1{}^a = k_1{}^b = k$, $k_1{}^i = q$ in fig.(c))

fig.(g)

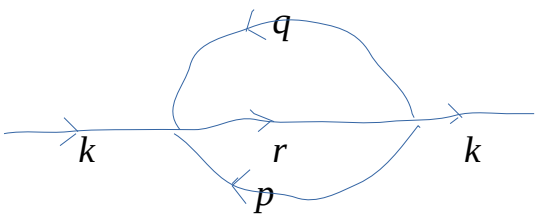


fig.(j)

For fig.(j) diagram, the cutoff dependent amplitude (with k on mass shell, $J(k)=(k^2-m^2)P$, $C=Z(0,0)$) is given by

$$A_2=-C\left(\frac{i}{2}\right)^5\frac{(-i\lambda)^2}{2!}\frac{1}{5!}\frac{1}{(2\pi)^{12}}2^5\binom{5}{2}\binom{3}{2}2!\left(\int^{\Lambda}\int^{\Lambda}\frac{1}{p^2-m^2+i\varepsilon}\frac{1}{q^2-m^2+i\varepsilon}\right.$$

$$\left.\frac{1}{(p+q+k)^2-m^2+i\varepsilon}d^4p\,d^4q\right)PP^*\,d^4k=iC\lambda^2\frac{1}{(2\pi)^4}I(k,m,\Lambda)PP^*\,d^4k \quad (15)$$

The total amplitude for fig.(g) and fig.(c) diagrams, the cutoff dependent amplitude (with k on mass shell) is (as we already determined in (12')) :

$$A_0+A_1=-\frac{i}{(2\pi)^4}C\left(k^2-m^2+\frac{i}{2}\frac{\lambda}{(2\pi)^4}\left(\int^{\Lambda}\frac{1}{q^2-m^2+i\varepsilon}d^4q\right)\right)PP^*\,d^4k$$

In order zero for λ theory of momentum on mass shell propagation the amplitude is $A_0=-\frac{i}{(2\pi)^4}C(k^2-m^2+i\varepsilon)PP^*\,d^4k$ and $k^2-m^2+i\varepsilon=\frac{1}{D(k)}$ is the inverse propagator.

In order 2 for λ theory of momentum on mass shell propagation the amplitude will be $A_0+A_1+A_2=-\frac{i}{(2\pi)^4}C(k^2-m^2+i\lambda S(\Lambda,m)-\lambda^2 I(k,m,\Lambda))PP^*\,d^4k$ and so the effective inverse propagator is $k^2-m^2+i\lambda S(\Lambda,m)-\lambda^2 I(k,m,\Lambda)=$ $=k^2-m^2+a+bk^2=(1+b)(k^2-m_P^2)$ where m_P is taken such that m_P^2 is a pole of the effective propagator in k^2 and is the physical mass , shifted from the mass m because of the quantum fluctuations corresponding to the loops in fig.(c) and fig.(j) diagrams and we defined

$$S(\Lambda,m)=\frac{1}{2}\frac{1}{(2\pi)^4}\int^{\Lambda}\frac{1}{q^2-m^2+i\varepsilon}d^4q \quad .$$

By Lorentz invariance I (k , m , Λ) is a function of k^2 which we can expand as

$$I(k,m,\Lambda)=D(m,\Lambda)+E(m,\Lambda)k^2+F(m,\Lambda)k^4+O(k^6) \qquad (16)$$

D is just I for k =0 and so it has a superficial degree of divergence 2. E is obtained by differentiating I twice with respect to k and setting k = 0. This decreases the powers of p and q in the integrand by 2 and so E has a superficial degree of divergence 0 (depends logarithmically on Λ). In the same way it follows that F has superficial degree of divergence -2 and so converges, being cutoff independent as the cutoff goes to infinity.

We evaluate S (Λ , m) in the Appendix and so we find out that a and b are quadratically respective logarithmically cutoff dependent.

Because the coefficient (1 + b) is no longer equal to 1 we must take the coefficient of $\frac{1}{2}(\partial\varphi)^2$ in an effective Lagrangian density expression considering the quantum fluctuations, not equal to 1 but to $(1+b)$. Therefore, with quantum fluctuations taken into consideration we will make a cutoff dependent renormalization of the field theory by taking a perturbed effective Lagrangian density

$$\mathscr{L}=\frac{1}{2}((\partial\varphi)^2-m_P^2\varphi^2)-\frac{\lambda_P^2}{4!}\varphi^4+A(\partial\varphi)^2+B\varphi^2+C\varphi^4 \qquad (17)$$

where A , B , C are the counterterms cutoff dependent coefficients and m_P , λ_P are respective the physical mass and physical coupling which we actually measure.
The physical mass and the physical coupling can be linked to the differential cross section of a two mesons scattering into two mesons by the relation we derive in Chap. Canonical quantization of a scalar field. Decay rate and cross section :

$$d\sigma=\frac{1}{|v_1-v_2|}\frac{1}{2\omega(k_1)2\omega(k_2)}\frac{d^3\vec{k}_3}{2\omega(k_3)}\frac{d^3\vec{k}_4}{2\omega(k_4)}\frac{1}{(2\pi)^2}|\boldsymbol{M}|^2\delta^4(k_1+k_2-k_3-k_4)$$

where $\boldsymbol{M}=-i\lambda_P$, $\omega(k_i)=\sqrt{\vec{k}_i^2+m_P^2}$, $i=\overline{1,4}$

k_1,k_2 incoming four-momenta, k_3,k_4 outgoing four-momenta,

v_1,v_2 velocities of the incoming particles.

As we derive in Chap. … Decay rate and cross section this leads to a relation satisfied in the center of mass frame of the incoming particles :

$$\frac{d\sigma}{d\Omega}=\frac{1}{|v_1-v_2|}\frac{1}{4\omega(k_1)\omega(k_2)}\frac{1}{(2\pi)^2}\frac{1}{8E_{tot}}(E_{tot}^2-4m_P^2)^{(1/2)}\left|(-i\lambda_P)^2\right| \qquad (**)$$

with $\omega(k_{1,2})=\frac{m_P}{\sqrt{1-v_{1,2}^2}}$, $E_{tot}=\omega(k_1)+\omega(k_2)$.

We can determine the physical mass at a given range of momentum or energy (expressed through the cutoff parameter Λ) considering collisions of the meson at the same energy with another particle having a known mass and applying the energy and momentum conservation during the collision process. Once determined the physical mass we can extract from (**) the physical coupling by measuring the cross section in a meson to meson scattering. (If we count N scattering events in a time interval (Δt)' in the lab frame with a n' concentration of particles in the incoming beam of mesons , considered in the lab frame, then in the center of mass frame with $\vec{w}_i=(0,0,w_i)$, $i=1,2$ velocities of incoming mesons in the lab frame

$\bar{m}_i=\frac{m_P}{\sqrt{1-w_i^2}}$, $v_i=\frac{-v_C+w_i}{1-v_C w_i}$ (relativistic velocities addition) $i=1,2$

$$v_C=\frac{\bar{m}_1 w_1+\bar{m}_2 w_2}{\bar{m}_1+\bar{m}_2} ,$$

we will have $\Delta t=\frac{(\Delta t)'}{\sqrt{1-v_C^2}}$, $n=\frac{n'}{\sqrt{1-v_C^2}}$,

$\sigma=\frac{N}{n(\Delta t)|v_1-v_2|}=\frac{N}{n'(\Delta t)'|v_1-v_2|}(1-v_C^2)$ so we have expressed σ in quantities which are determuned from the lab frame.)

Suppose now we have determined an effective Lagrangian density with m , λ as well as known :

$\mathscr{L}_N=\frac{1}{2}((\partial\varphi)^2-m^2\varphi^2)-\frac{\lambda}{4!}\varphi^4+A_N(\partial\varphi)^2+B_N\varphi^2+C_N\varphi^4$

such that taking the inverse effective propagator:

$P(k^2)=(1+2A)k^2-m^2+2B+i(\lambda-4!C)\bar{S}(\Lambda,m)-(\lambda-4!C)^2\bar{I}(k,m,\Lambda)+...=$

$=P_N(k^2,A,B,C,m,\lambda)+O((\lambda-4!C)^N)$

and the Feynman amplitude for two mesons scattering into two mesons :

$$\boldsymbol{M}=-i(\lambda-4!C)+\frac{(\lambda-4!C)^2}{(2\pi)^4}\left(\bar{M}_2(\Lambda,k_1+k_2,m)+\bar{M}_2(\Lambda,k_1-k_3,m)+\right.$$

$\left.+\bar{M}_2(\Lambda,k_1-k_4,m)\right)+...=M_N((k_i)_{i=\overline{1,4}},A,B,C,\Lambda,m,\lambda)+O((\lambda-4!C)^N)$ where

$\bar{S}(\Lambda,m)=\frac{1}{1+2A}S(\Lambda,\sqrt{\frac{1-2B}{1+2A}}m)$, $\bar{M}_2(\Lambda,K,m)=\frac{1}{(1+2A)^2}M_2(\Lambda,K,\sqrt{\frac{1-2B}{1+2A}})$,

$\bar{I}(k,m,\Lambda)=\frac{1}{(1+2A)^3}I(k,\sqrt{\frac{1-2B}{1+2A}},\Lambda)$, the physical mass m_N and the physical coupling λ_N satisfy

$P(m_N^2)=0$ (18) (we take P_N to order $O(k^3)$, $P_N=a+bk^2$ with a , b not depending on k, m_N the measured mass and that $|M_N|^2$ is linked to the event rate of the scattering process for $(k_i)_{i=\overline{1,4}}$ in a specified range of momenta and for some particular $(k_i)_{i=\overline{1,4}}$ we have $-i\lambda_N=M_N$ (19) (λ_N is the measured coupling) , for an established value $\Lambda=\Lambda_N$ and $A=A_N$, $B=B_N$, $C=C_N$.

From (18) and (19) we can determine m, λ as functions of the measured m_P, λ_P and so we can determine a squared mass shift $\delta m^2=m_P^2-m^2$ and M_N as functions depending only on the measurable quantities m_P , λ_P and the already known A_N , B_N , C_N , Λ_N . (M_N depends also on the kinematic variables $s=(k_1+k_2)^2$, $t=(k_1-k_3)^2$, $u=(k_1-k_4)^2$ and (19) leads to $O(\lambda_N^N)=O((\lambda-4!C_N)^N)$) .

If we change measuring conditions we can measure another physical mass $m_P=m_{N+1}\neq m_N$ and another physical coupling $\lambda_P=\lambda_{N+1}\neq\lambda_N$.

Then we must take higher order approximations (by considering higher order Feynman diagrams additionally) and to eliminate the cutoff dependence we will take an effective Lagrangian density

$\mathscr{L}_{N+1}=\frac{1}{2}((\partial\varphi)^2-m^2\varphi^2)-\frac{\lambda_N}{4!}\varphi^4+A_{N+1}(\partial\varphi)^2+B_{N+1}\varphi^2+C_{N+1}\varphi^4$.

For the measured m_P, λ_P to be what we say to be we require :

$P_{N+1}(k^2,A_{N+1},B_{N+1},C_{N+1},m_N,\lambda_N)=\alpha(k^2-m_P^2)$ (20) (again we take an $O(k^3)$ approximation of P_{N+1}) with α not depending on k .

$M_{N+1}((k_i)_{i=\overline{1,4}},A_{N+1},B_{N+1},C_{N+1},m_N,\lambda_N)=-i\lambda_P$ (21) for some kinematical $s=(k_1+k_2)^2$, $t=(k_1-k_3)^2$, $u=(k_1-k_4)^2$.

Considering that A_{N+1} , B_{N+1} , C_{N+1} , Λ_{N+1} are taken to be real, the relations (20) , (21) determine the counterterms coefficients A_{N+1} , B_{N+1} , C_{N+1} and the cutoff Λ_{N+1} we must take, in terms of measurable quantities

and M_{N+1} is a $O(\lambda_P^{N+1})$ approximation of $\boldsymbol{M}$ depending only on measurable determined quantities , all this in a specified range of incoming and outgoing particles on mass shell four-momenta.
Amplitudes for scattering events with more than four external legs have, according to the superficial degree of divergence relation $D = 4 - B_E$ we have proven, are determined by convergent integrals and so not cutoff dependent. We can calculate the amplitudes starting from the Lagrangian density $\mathscr{L}_{N+1}$.

Notice that the form of the Lagrangian density (8) restricts the scattering posibilities to an even number of external legs $n + s$ since if r is the number of internal lines and m is the number of interaction vertices we must have $n + s + 2\,r = 4\,m$.

We notice also that we can derive general Feynman rules for computing a Feynman amplitude as follows:
Consider a Feynman diagram determined by :
$I=\{x_1^a,...,x_n^a\}$ incoming particle endpoints, $O=\{x_1^b,...,x_s^b\}$ outging particle endpoitns,
$V=\{w_1,...,w_m\}$ interaction vertices, $k_1^a,...,k_n^a$ momenta labels to incoming endlegs,
$k_1^b,...,k_s^b$ momenta labels to outgoing endlegs,
$(w_{0j},w_{1j})_{j=\overline{1,r}}$ internal lines sequence with $w_{0j},w_{1j}\in V$ such that for $l_j=(w_{0j},w_{1j})$, l_j is incoming to w_{1j} and outgoing from w_{0j} ,
k_j moment label to line l_j , for $j=\overline{1,r}$,
$L_e=\{(x_i^a,w_i^a)|i=\overline{1,n}\}\cup\{(w_i^b,x_i^b)|i=\overline{1,s}\}$ external leg lines .
Associate with each interaction vertex w the coupling $-i\lambda$ and $(2\pi)^4\delta^4(\sum_{j\in A(w)}k_j-\sum_{j\in B(w)}k_j)$ where $A(w)=\{j\in\{1,...,r\}|l_j$ is incoming to $w\}$ and $B(w)=\{j\in\{1,...,r\}|l_j$ is outgoing from $w\}$;
Associate with each internal line the propagator $\frac{i}{k_j^2-m^2+i\varepsilon}$;
Multiply all above associated expressions obtaining an expression *E*.
Calculate the symmetry factor S_F as indicated below :
Take $a(j)=\text{card}\{q\in\{1,...,r\}|l_q=l_j\}$ for $j=\overline{1,r}$,
$\{a_1,...,a_p\}=\{a(j)|j=\overline{1,r}\}$ with $a_j\neq a_h$ for $j\neq h$, $j,h=\overline{1,p}$.
Take $l=\text{card}\{j\in\{1,...,r\}|$ exists $w\in V$ such that $l_j=(w,w)\}$.
For a real scalar field take $S_F=2^{n+r+s-l}\frac{(n+r+s)!}{a_1!...a_p!}$;
For a complex scalar field take $S_F=2^{n+r+s}\frac{(n+r+s)!}{a_1!...a_p!}$;
Multiply E with $S_F\frac{1}{2^{n+r+s}}\frac{1}{(n+r+s)!}$;

Integrate the resulting expression over each k_j , $j=\overline{1,r}$ variable with measure $\frac{d^4k_j}{(2\pi)^4}$ obtaining after elimination in the integration process of several Dirac distributions an expression $(2\pi)^4 \boldsymbol{M}\, \delta^4(\sum_{i=1}^{n} k_i^a - \sum_{i=1}^{s} k_i^b)$;

The incoming and outgoing four-momenta labels are supposed to be on mass shell and $\boldsymbol{M}$ is the resulting Feynman amplitude which is linked to the process probability amplitude as shown in Chap. Feynman amplitudes and lattice gauge theory and Chap. Canonical quantisation of a scalar field . Decay rate and cross section.

Appendix
Calculation of Feynman integrals

Let $Z(J)=\int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} \exp(i((1/2)q^T Aq+J^T q))dq_1...dq_n$

where $q=(q_j)_{j=\overline{1,n}}$, $J=(J_k)_{k=\overline{1,n}}$ are considered as column vectors in $\mathbb{R}^n$

and A is a real symmetric $n\times n$ matrix having all leading principal minors $\neq 0$:

$A=(a_{lm})_{l,m=\overline{1,n}}$, $\det(a_{lm})_{l,m=\overline{1,k}}\neq 0$, $a_{ij}=a_{ji}\in\mathbb{R}$ for $i,j,k=\overline{1,n}$

$e_i=(\delta_{ij})_{j=\overline{1,n}}$ for $i=\overline{1,n}$, $q=q_i e_i$ (Einstein summation convention), $V=\mathbb{R}^n$

$g: V\times V\to\mathbb{R}$, $g(u_i e_i\ ,\ v_j e_j)=u_i a_{ij} v_j$

Since $\Delta_k=\det(a_{lm})_{l,m=\overline{1,k}}\neq 0$ for $k=\overline{1,n}$ we can take $(f_i)_{i=\overline{1,n}}\in V^n$ with $f_i=p_i^j e_j$, $P=(p_i^j)_{i,j=\overline{1,n}}\in M_{n\times n}(\mathbb{R})$ unique determined such that $p_i^j=0$ for $j>i$ and $p_m^m=\frac{\Delta_{m-1}}{\Delta_m}$ for $m=\overline{2,n}$, $p_1^1=\frac{1}{a_{11}}$, $g(e_j,f_m)=0$ for $1\leq j<m$, $g(e_m,f_m)=1$ for $m=\overline{1,n}$. (1)

We have $g(f_k,f_m)=\sum_{j=m}^{k} p_k^j g(e_j,f_m)$ (2)

Since $g(f_k,f_m)=g(f_m,f_k)$, we can take in (2) $k\leq m$ and so we have $g(f_k,f_m)=0$ if $k\neq m$, $g(f_m,f_m)=p_m^m$.

For $P^{-1}=(\bar{p}_i^j)_{i,j=\overline{1,n}}$ we have $\bar{p}_i^j=0$ for $j>i$, $\bar{p}_m^m=\frac{1}{p_m^m}$ and it follows:

$\frac{1}{2}q^T Aq+J^T q=\frac{1}{2}\sum_{k=1}^{n} p_k^k\left(\left(\sum_{j=k}^{n}\bar{p}_j^k q_j+\frac{1}{p_k^k}\alpha_k\right)^2-\left(\frac{1}{p_k^k}\alpha_k\right)^2\right)$ where $\alpha_k=\sum_{j=1}^{k} p_k^j J_j$.

Because of translational invariance , integrating over each q_j , j = 1,2,…,n in the Z (J) integral expression, we have no dependence on the remaining q_k , $k > j$ variables and so we have :

$$Z(J)=\prod_{k=1}^{n}\exp\left(-\frac{1}{2}i\,p_k^k\left(\frac{1}{p_k^k}\alpha_k\right)^2\right)\int_{-\infty}^{\infty}\exp\left(\frac{1}{2}i\,p_k^k(\bar{p}_k^k q_k)^2\right)dq_k\ .$$

Since $\sum_{k=1}^{n}p_k^k\left(\frac{1}{p_k^k}\alpha_k\right)^2=\sum_{k=1}^{n}\frac{1}{p_k^k}\alpha_k^2=(PJ)^T(PAP^T)^{-1}(PJ)=J^TA^{-1}J$ and using the Fresnel integral formula we obtain

$\int_{-\infty}^{\infty}\exp\left(\frac{1}{2}i\frac{1}{p_k^k}q_k^2\right)dq_k=\sqrt{2\pi i\,p_k^k}$ and since $\prod_{k=1}^{n}p_k^k=(\det A)^{-1}$ it follows now :

$Z(J)=\left(\frac{(2\pi i)^n}{\det A}\right)^{1/2}\exp\left(-\frac{1}{2}iJ^TA^{-1}J\right)$ which is the formula we used above for discretized path integration.

We have further, for the above used Feynman integrals:

$$2(2\pi)^4S(\Lambda,m)=\int_{\|q\|_4<\Lambda}\frac{1}{q^2-m^2+i\varepsilon}d^4q=\int_0^{\Lambda}\int_0^{\pi}\int_0^{\pi}\int_0^{2\pi}\frac{\rho^3\sin^2(\theta)\sin(\varphi)}{\rho^2\cos(2\theta)-A}d\psi d\varphi d\theta d\rho=$$

$$=4\pi\int_0^{\Lambda}\int_0^{\pi}\frac{\rho^3\sin^2(\theta)}{\rho^2\cos(2\theta)-A}d\theta d\rho=4\pi\int_0^{\Lambda}\int_{-\infty}^{\infty}\frac{\rho^3}{\rho^2-A}\frac{1}{u^2-C^2}\frac{1}{1+u^2}du\,d\rho$$

where $A=m^2-i\varepsilon$, $C=\sqrt{\frac{\rho^2+A}{\rho^2-A}}$ with $\Im C>0$.

For $a=\frac{A}{\Lambda^2}$ it follows :

$$\frac{d}{da}\left(\frac{2(2\pi)^4S(\Lambda,m)}{\Lambda^2}\right)=\int_{\|q\|_4<\Lambda}\frac{1}{(q^2-m^2+i\varepsilon)^2}d^4q=Q(\Lambda,m)\qquad(3)$$

$$\frac{d^2}{da^2}\left(\frac{2(2\pi)^4S(\Lambda,m)}{\Lambda^2}\right)=2\Lambda^2\int_{\|q\|_4<\Lambda}\frac{1}{(q^2-m^2+i\varepsilon)^3}d^4q=2\Lambda^2R(\Lambda,m)\qquad(4)$$

Using residues theorem we derive :

$\int_{-\infty}^{\infty}\frac{1}{u^2-C^2}\frac{1}{1+u^2}du=i\pi\frac{1}{1+C^2}\left(\frac{1}{C}+i\right)$ and so after substitution $z=\sqrt{\frac{\rho^2+A}{\rho^2-A}}$

and some integration calculus we obtain for $b=\sqrt{\frac{\Lambda^2+A}{\Lambda^2-A}}$:

$$2(2\pi)^4S(\Lambda,m)=-\pi^2\Lambda^2+\pi^2Ai\left(\frac{1}{b-1}+\frac{1}{b+1}+i+\log(b^2-1)-\log(-2)\right)$$

$$\frac{2(2\pi)^4S(\Lambda,m)}{\Lambda^2}=-\pi^2-(\pi^3+\pi^2)a+\pi^2i\sqrt{1-a^2}+\pi^2a\,i\log\left(\frac{a}{1-a}\right)\qquad(5)$$

From (3) and then from (4) it follows now :

$$Q(\Lambda,m)=-(\pi^2+\pi^3)+\pi^2 i-\frac{\pi^2 i a}{\sqrt{1-a^2}}+\frac{\pi^2 i a}{1-a}+\pi^2 i\log\left(\frac{a}{1-a}\right) \quad (6)$$

$$2\Lambda^2 R(\Lambda,m)=\frac{\pi^2 i}{a}+\frac{\pi^2 i}{1-a}+\frac{\pi^2 i}{(1-a)^2}-\frac{\pi^2 i}{\sqrt{1-a^2}}-\frac{\pi^2 i a^2}{\sqrt{(1-a^2)^3}} \quad (7)$$

From (5) we obtain that for $A = a_\Lambda$,

if $\left|\frac{a_\Lambda}{\Lambda^2}\right|<d<1$ when $\Lambda\to\infty$, then $\limsup_{\Lambda\to\infty}\left|\frac{S(\Lambda,\sqrt{a_\Lambda})}{\Lambda^2}\right|<\infty$ (8)

and (considering (6) , (7)) : $R(\Lambda,\sqrt{a_\Lambda})=\frac{1}{2}\frac{H}{a_\Lambda}+O(\frac{1}{\Lambda^2})$ (9)

$$Q(\Lambda,m)=L+H\log\left(\frac{m^2}{\Lambda^2}\right)+O\left(\frac{m^2}{\Lambda^2}\right) \text{ with } H=\pi^2 i \ , \ L=\pi^2 i-\pi^3-\pi^2 \quad (10)$$

By induction we can prove that :

$\frac{1}{x_1\dots x_n}=(n-1)!\int_0^1\dots\int_0^1\delta(1-\sum_{i=1}^n\alpha_i)\frac{1}{(\alpha_1 x_1+\dots+\alpha_n x_n)^n}d\alpha_1\dots d\alpha_n$ and so we have

$$\frac{1}{xy}=\int_0^1\frac{1}{(\alpha x+(1-\alpha)y)^2}d\alpha$$

$$\frac{1}{xyz}=\int_D\frac{1}{(\alpha x+\beta y+(1-\alpha-\beta)z)^3}d\alpha d\beta \quad \text{where} \quad D=\{(\alpha,\beta)\in(0,1)^2|\alpha+\beta<1\}$$

$$M_2(\Lambda,m,K)=\frac{1}{4}\int^\Lambda\frac{1}{q^2-m^2+i\varepsilon}\frac{1}{(K-q)^2-m^2+i\varepsilon}d^4q=$$

$$=\frac{1}{4}\int_0^1\int^\Lambda\frac{1}{((q-\alpha K)^2+\alpha(1-\alpha)K^2-m^2+i\varepsilon)^2}d^4q\,d\alpha \quad .$$

In the $(0,1)\times\mathbb{R}^4$ integration domain we take the cutoff

$B_\Lambda=\{(\alpha,q)\in(0,1)\times\mathbb{R}^4|\|q-\alpha K\|_4<\Lambda\}$ and therfore we can write :

$$M_2(\Lambda,m,K)=\frac{1}{4}\int_0^1 Q(\Lambda,\sqrt{m^2-\alpha(1-\alpha)K^2-i\varepsilon})d\alpha\approx$$

$$\approx\frac{1}{4}L+\frac{1}{4}H\int_0^1\log\left(\frac{m^2+\alpha(\alpha-1)K^2-i\varepsilon}{\Lambda^2}\right)d\alpha$$

Taking $C=\sqrt{-m^2+(1/4)K^2+i\varepsilon}$ with $\Im C>0$ and $\bar{K}=\sqrt{K^2}$ we obtain

after some calculus $J=\int_0^1\log(m^2+\alpha(\alpha-1)K^2-i\varepsilon)d\alpha=$

$$=-2+\log(m^2-i\varepsilon)+2\frac{C}{\bar{K}}(\log((1/2)\bar{K}+C)-\log(C-(1/2)\bar{K})) \quad .$$

We observe that :

$\lim_{\bar{K}\to 0} J=\log(m^2)$ and we can therefore take $J=\log(f(K^2,m))$ with $\lim_{K^2\to 0} f(K^2,m)=m^2$ such that $M_2(\Lambda,m,K)=\frac{1}{4}L-\frac{1}{4}H\log\left(\frac{\Lambda^2}{f(K^2,m)}\right)$.

For the $I(K,m,\Lambda)$ integral we have:

$$4(2\pi)^8 I(K,m,\Lambda)=\int^{\Lambda}\int^{\Lambda}\frac{1}{p^2-m^2+i\varepsilon}\frac{1}{q^2-m^2+i\varepsilon}\frac{1}{(K-p-q)^2-m^2+i\varepsilon}d^4p\,d^4q= \quad (11)$$
$$=\int_D\int^{\Lambda}\int^{\Lambda}\frac{d^4p\,d^4q}{(\alpha p^2+\beta q^2+2(\alpha+\beta-1)(pq-K(p+q))+(\alpha+\beta-1)K^2-m^2+i\varepsilon)^3}$$

where $D=\{(\alpha,\beta)\in(0,1)^2|\alpha+\beta>1\}$.

For each $(\alpha,\beta)\in D$ we can take an orthogonal transformation of the $\mathbb{R}^4\times\mathbb{R}^4$ space,

$T(\alpha,\beta):\mathbb{R}^4\times\mathbb{R}^4\to\mathbb{R}^4\times\mathbb{R}^4$ with φ depending on (α,β)

$T(\alpha,\beta)(p,q)=(p\cos(\varphi)-q\sin(\varphi),p\sin(\varphi)+q\cos(\varphi))$ such that for

$2\mu=\alpha+\beta-\sqrt{(\beta-\alpha)^2+4(\alpha+\beta-1)^2}$, $2\eta=\alpha+\beta+\sqrt{(\beta-\alpha)^2+4(\alpha+\beta-1)^2}$,

$(p',q')=T(\alpha,\beta)(p,q)$ we have

$$\alpha p^2+\beta q^2+2(\alpha+\beta-1)(pq-K(p+q))+(\alpha+\beta-1)K^2-m^2+i\varepsilon=$$
$$=\mu(p'-\gamma K)^2+\eta(q'-\delta K)^2-\rho K^2-m^2+i\varepsilon\ ,\ \rho=1-\mu-\eta+\gamma^2\mu+\delta^2\eta\ , \quad (12)$$
$$\gamma=\frac{\mu+\eta-1}{\mu}(\cos(\varphi)-\sin(\varphi))\ ,\ \delta=\frac{\mu+\eta-1}{\eta}(\cos(\varphi)+\sin(\varphi))\ ,$$

$\eta>\frac{1}{2}$ and since the integral in (11) is symmetric in α,β we can integrate in (11) over $\beta\geq\alpha$ and multiply the result with 2 to get the (11) expression result.

Therefore we can consider $2\mu\geq\alpha+\beta-\beta+\alpha-2(\alpha+\beta-1)=2(1-\beta)$ (13)

We take a cutoff of the (α , β , p , q) integration space:

$$B_\Lambda=\{(\alpha,\beta,p,q)\in D\times\mathbb{R}^4\times\mathbb{R}^4\,|\,\alpha,\beta\in(\varepsilon_\Lambda,1-\varepsilon_\Lambda)\ ,\ \beta\geq\alpha\ ,$$
$$(p,q)\in(T(\alpha,\beta))^{-1}(B_4(\gamma K,\Lambda)\times B_4(\delta K,R_\Lambda))\} \text{ with} \quad (14)$$

$B_4(z,\Lambda)=\{x\in\mathbb{R}^4|\|x-z\|_4<\Lambda\}$, $\lim_{\Lambda\to\infty}\varepsilon_\Lambda=0$, $\lim_{\Lambda\to\infty}\Lambda\,\varepsilon_\Lambda=\infty$, $\lim_{\Lambda\to\infty}\frac{\Lambda}{R_\Lambda}=0$

Because of (13) , on the cutoff we have $\mu>\varepsilon_\Lambda$ and so for $\Lambda\to\infty$ we will have:

$\Lambda\mu>\Lambda\,\varepsilon_\Lambda\to\infty$, $R_\Lambda\mu\to\infty$, $\frac{\gamma K}{\Lambda}\to 0$, $\frac{\delta K}{R_\Lambda}\to 0$ and so the cutoff becomes the whole integration space as Λ goes to infinity.

Also it follows $\rho\mu\leq\gamma^2\mu^2+\delta^2\eta\mu\leq 4+16=20$,

$\lim_{\Lambda\to\infty}\frac{\mu(p'-\gamma K)^2-\rho K^2-m^2+i\varepsilon}{R_\Lambda^2}=0$ and so (9), (11) , (12) lead to :

$$I=4(2\pi)^8 I(K,m,\Lambda)=2\int_{D_\Lambda}\frac{1}{\eta^2}\int_{B_4(0,\Lambda)}\left(\frac{1}{2}\frac{H}{\mu p^2-\rho K^2-m^2+i\varepsilon}+O(\frac{1}{R_\Lambda^2})\right)d^4p\,d\alpha d\beta \ .$$

where $D_\Lambda=(\varepsilon_\Lambda,1-\varepsilon_\Lambda)^2\cap D\cap\{(\alpha,\beta)\in\mathbb{R}^2|\beta>\alpha\}$.

Hence we obtain :

$$\frac{I}{\Lambda^2}=\int_{D_\Lambda}\frac{1}{\eta^2\mu^2}H\frac{2(2\pi)^4 S(\Lambda\sqrt{\mu},\sqrt{\rho K^2+m^2+i\varepsilon})}{\Lambda^2}d\alpha d\beta+O\left(\frac{\Lambda^2}{R_\Lambda^2}\right) \ . \quad (15)$$

Since $\int_{D_\Lambda}\left|\frac{1}{\eta^2\mu}\right|d\alpha d\beta\le\frac{1}{4}\int_{\varepsilon_\Lambda}^{1/2}\int_{1-\alpha}^{1-\varepsilon_\Lambda}\frac{1}{1-\beta}d\beta d\alpha+\int_{1/2}^{1-\varepsilon_\Lambda}\int_{\alpha}^{1-\varepsilon_\Lambda}\frac{1}{1-\beta}d\beta d\alpha<\frac{1}{2}|\log(\varepsilon_\Lambda)|$.

Considering (14) , (15) and (8) it follows now that I (K , m , Λ) increases not faster than $C\Lambda^2\log\Lambda$ with C an independent positive constant as Λ goes to infinity.

This result remains valid if in (14) we take instead of the condition $\lim_{\Lambda\to\infty}\Lambda\varepsilon_\Lambda=0$ the conditions $\lim_{\Lambda\to\infty}\Lambda\varepsilon_\Lambda=c>0$ with $\frac{\sqrt{2}\|K\|_4}{c}=a<1$ and in that case we obtain $\limsup_{\Lambda\to\infty}\left|\frac{\rho K^2+m^2-i\varepsilon}{\Lambda^2\mu}\right|\le\lim_{\Lambda\to\infty}\frac{2\|K\|_4^2}{\Lambda^2\varepsilon_\Lambda^2}=a^2<1$ and

$\|\gamma K\|_4\le\frac{\sqrt{2}}{\mu}\|K\|_4\le\frac{\sqrt{2}\|K\|_4\Lambda}{\Lambda\varepsilon_\Lambda}\le\frac{1+a}{2}\Lambda<1$ for sufficiently large Λ and so

for any $z\in\mathbb{R}^4$, for sufficiently large Λ we have $\|z-\gamma K\|_4\le\|z\|_4+\frac{1+a}{2}\Lambda\le\Lambda$.

Since in the given conditions for the cutoff it is obvious that also $\lim_{\Lambda\to\infty}\frac{\|\delta K\|_4}{R_\Lambda}=0$,

we can derive that the cutoff becomes the whole integration space as $\Lambda\to\infty$.

Because $\Lambda\varepsilon_\Lambda\to c$ and $\varepsilon_\Lambda\to 0$ when $\Lambda\to\infty$ we derive in the cutoff that $\Lambda\sqrt{\mu}\to\infty$, $R_\Lambda\sqrt{\eta}\to\infty$ when $\Lambda\to\infty$ and the proof follows as above and we have

$$I(K,m,\Lambda)\sim C\Lambda^2\log\Lambda \text{ as } \Lambda\to\infty \ .$$

8. Canonical quantization of a scalar field Decay rate and cross section

Canonical quantization of a scalar field
Decay rate and cross section

We consider as in Chap. … Quantum field theory … the space-time coordinates $x=(x^{\alpha})_{\alpha=\overline{0,3}}=(t,\vec{x})$ Minkowski space with metric coefficients $(\eta_{\alpha\beta})_{\alpha,\beta=\overline{0,3}}=$ $=\mathrm{diag}(1,-1,-1,-1)$ corresponding to a choosing of time and lenght measuring units such that $\hbar=1$ (reduced Planck constant) and $c=1$ (speed of light in vacuum constant).

Consider a quantum field system described by a real scalar field $\varphi=\varphi(t,\vec{x})$ with Lagrangian density $\mathscr{L}=\frac{1}{2}((\partial\varphi)^2-m^2\varphi^2)-\frac{\lambda}{4!}\varphi^4+J\varphi$ (where $\partial=\left(\frac{\partial}{\partial x^{\alpha}}\right)_{\alpha}$ and $J=J(t,\vec{x})$ is a sources field of the theory).

The free scalar field theory with $\mathscr{L}=\frac{1}{2}((\partial\varphi)^2-m^2\varphi^2)$ leads to a motion equation (Euler-Lagrange equations) which is the Klein-Gordon equation for φ : $(\partial^2+m^2)\varphi=0$ (where $\partial^2=\partial_{\alpha}\partial^{\alpha}=\Box$ is the D'Alembert operator) and has solutions in Fourier expansion given by

$$\varphi(t,\vec{x})=\int\frac{d^3\vec{k}}{(2\pi)^{3/2}(2\omega_k)^{1/2}}(a(\vec{k})\exp(-i(\omega_k t-\vec{k}\cdot\vec{x}))+a^{+}(\vec{k})\exp(i(\omega_k t-\vec{k}\cdot\vec{x}))) \quad (1)$$

where $\omega_k=\sqrt{\vec{k}^2+m^2}$ and as usual we will use greek letters for indexing from 0 to 3 and latin letters for indexing from 1 to 3 .

As in Chap. ... Quantum field theory we will have the corresponding field operator function $\hat{\varphi}=\hat{\varphi}(t,\vec{x})$ defined according to (1) by an operator function $\hat{a}=\hat{a}(\vec{k})$

For a discretization of the field we have quantum system with generalized coordinates $q=(q^k(t))_{k=\overline{1,N}}$ a discretized Lagrangian $L=L(q,\dot{q})$, generalized momenta $p=(p^k(t))_{k=\overline{1,N}}=\frac{\partial L}{\partial\dot{q}}$ (see Chap. Feynman diagrams and lattice gauge theory).

The canonical commutation relation $[\hat{p}^k(t),\hat{q}^j(t)]=-i\delta_{kj}$ becomes in the continuous field formulation $[\hat{\pi}(t,\vec{x}),\hat{\varphi}(t,\vec{x}')]=-i\delta^3(\vec{x}-\vec{x}')$ (2) where

$$\hat{\pi}(t,\vec{x})=\frac{\partial\widehat{\mathscr{L}}}{\partial(\partial_0\varphi)}(t,\vec{x})=\partial_0\hat{\varphi}(t,\vec{x})$$

With the (1) relation, the (2) relation can be satisfied if we have the commutation relation $[a(\vec{k}),a^{+}(\vec{k}')]=\delta^3(\vec{k}-\vec{k}')$ for any $\vec{k},\vec{k}'\in\mathbb{R}^3$. (3)

We consider our system enclosed in a box, say a cube *D* with sides of length *L* disposed along the spatial axes. (*L* is considered to be much larger than the characteristic size of our system)

For periodic boundary conditions we have $\varphi(t,\vec{x}+(\delta_{ij})_{j=\overline{1,3}}L)=\varphi(t,\vec{x})$ for $i=\overline{1,3}$

We will have a Fourier expansion:

$\varphi(t,\vec{x})=\sum_{\vec{k}} \exp(i\vec{k}\cdot\vec{x})\int \varphi(t,\vec{x})\frac{1}{V}\exp(-i\vec{k}\cdot\vec{x})d^3\vec{x}$ where $\vec{k}=\frac{2\pi}{L}(n_1,n_2,n_3)$ with $(n_1,n_2,n_3)\in\mathbb{Z}^3$, $V=L^3$ and so considering (1) we obtain

$$\varphi(t,\vec{x})=\sum_{\vec{k}} \frac{1}{V^{1/2}}\frac{1}{\sqrt{2\omega_k}}(\tilde{a}(\vec{k})\exp(-ikx)+\tilde{a}^+(\vec{k})\exp(ikx))$$ where

$kx=\omega_k t-\vec{k}\cdot\vec{x}$, $\omega_k=\sqrt{\vec{k}^2+m^2}$, $\tilde{a}(\vec{k})=\left(\frac{(2\pi)^3}{V}\right)^{1/2} a(\vec{k})$.

We have obviously by discretization $\frac{V}{(2\pi)^3}\delta_{\vec{k}\vec{k}'}=\delta^3(\vec{k}-\vec{k}')$ and therefore the normalized creation and anihilation operators $\tilde{a}^+,\tilde{a}$ satisfy the commutation relation $[\tilde{a}(\vec{k}),\tilde{a}^+(\vec{k}')]=\delta_{\vec{k}\vec{k}'}$ for any $\vec{k},\vec{k}'=\frac{2\pi}{L}(n_1,n_2,n_3)$, $n_j\in\mathbb{Z}$.

We will have a ground state $|0\rangle$ with $a(\vec{k})|0\rangle=0$ for any $\vec{k}\in\mathbb{R}^3$ and the single particle of momentum $\vec{k}$ state $|k\rangle=\tilde{a}^+(\vec{k})|0\rangle$ which according to the above relations is properly normalized , having $\langle k|k'\rangle=\delta_{\vec{k}\vec{k}'}$ with $k=(k^\alpha)_\alpha=(\omega_k,\vec{k})$.

As we have seen , for periodic boundary conditions for φ with the system enclosed in the box D , the allowed momentum plane wave states are with momenta $\vec{p}=\frac{2\pi}{L}(n_1,n_2,n_3)$ with $n_j\in\mathbb{Z}$. The allowed values of momentum form a lattice of points in momentum space with spacing $\frac{2\pi}{L}$ between points. We measure momentum with finite resolution, small, but much larger than $\frac{2\pi}{L}$. Thus an infinitesimal volume $d^3\vec{p}$ in momentum space contains $d^3\vec{p}/(2\pi/L)^3=\frac{V}{(2\pi)^3}d^3\vec{p}$ states. Because $V=\int d^3\vec{x}$, requiring one single state $\frac{V\,d^3\vec{p}}{(2\pi)^3}=1$ we notice that the minimum accesible volume in phase-space $(\vec{x},\vec{p})$ of a particle can be considered to be $(2\pi)^3$ (or restoring the Planck constant in the relations by dimensional analysis it will be $(2\pi\hbar)^3$ i.e. a factor of $2\pi\hbar$ for each degree of freedom).

It follows also $\langle 0|\hat{\varphi}(t,\vec{x})|k\rangle=\frac{1}{V^{1/2}}\frac{1}{\sqrt{2\omega_k}}\exp(-i(\omega_k t-\vec{x}\cdot\vec{k}))$ which we could think of as the relativistic wave function of a single particle with momentum k .

If we define the time-ordered product

$T(\hat{\varphi}(x)\hat{\varphi}(y))=\theta(x^0-y^0)\hat{\varphi}(x)\hat{\varphi}(y)+\theta(y^0-x^0)\hat{\varphi}(y)\hat{\varphi}(x)$ with θ , the Heaviside function , we find out (see Chap. ... Quantum field theory ...) that

$\langle 0|T(\hat{\varphi}(t,\vec{x})\hat{\varphi}(0,\vec{0}))|0\rangle = i\,D(x)$ where $D(x)$ is the propagator for a particle to go from 0 to x we obtained using the path integral formalism. This further justifies by the way of contour method integration (see Chap. ...Quantum field theory ...) the $i\varepsilon$ with $\varepsilon>0$ prescription in the propagator formula

$$D(x)=\frac{1}{(2\pi)^4}\int \frac{\exp(-ikx)}{k^2-m^2+i\varepsilon}d^4k$$

with the physical meaning that we always create (operator function a^+) before we anihilate (operator function a) , a form of causality as formulated in quantum field theory.

For any function $f=f(k^0,\vec{k})$ we have

$$\int \theta(k^0)\delta(k^2-m^2)f(k^0,\vec{k})d^4k=\int\limits_{\{z>0\}\times\,\mathbb{R}^3}\delta(z-\vec{k}^2-m^2)\frac{1}{2\sqrt{z}}f(\sqrt{z},\vec{k})\,dz\,d^3\vec{k}=$$

$$=\int \frac{1}{2\,\omega_k}f(\omega_k,\vec{k})d^3\vec{k}\ .$$

For $k^2=m^2$ we have $k^2>0$ and so exists a Lorentz transformation $k\overset{T_0}{\to}k'$ such

that $k'=(k'^0,0,0,0)$.

Lorentz transformations $k'\to k''$ do not change the sign of k'^0 : $\operatorname{sign}k'^0=\operatorname{sign}k''^0$ and therefore $\operatorname{sign}k'^0=\operatorname{sign}k^0$ and considering for a Lorentz transformation $k\overset{T}{\to}p$ the Lorentz transformation $k'\overset{T\circ T_0^{-1}}{\to}p$ we obtain $\operatorname{sign}k'^0=\operatorname{sign}p^0$.

Hence Lorentz transformations do not change the sign of k^0 if $k^2=m^2$ and so $\theta(k^0)\,\delta(k^2-m^2)f(k^0,\vec{k})d^4k$ is Lorentz invariant if f is Lorentz invariant following now that $\frac{d^3\vec{k}}{2\,\omega_k}$ is a Lorentz invariant measure .

For the system considered above we look at a scattering process of two mesons having four-momenta k_1 , k_2 on mass shell into two mesons having four-momenta k_3 , k_4 on mass shell . The theory Hamiltonian is

$$H=\int d^3\vec{x}\left(\frac{\partial\mathscr{L}}{\partial(\partial_0\varphi)}\partial_0\varphi-\mathscr{L}\right)=\int\left(\frac{1}{2}((\partial_0\varphi)(\partial_0\varphi)+(\nabla\varphi)\cdot(\nabla\varphi)+m^2\varphi^2)+\frac{\lambda}{4!}\varphi^4\right)d^3\vec{x}$$

and we calculate the transition amplitude

$$A=\langle k_3,k_4|\exp(-i\hat{H}T)|k_1,k_2\rangle=\langle 0|\tilde{a}(\vec{k}_4)\tilde{a}(\vec{k}_3)\exp(-i\hat{H}T)\tilde{a}(\vec{k}_2)\tilde{a}(\vec{k}_1)|0\rangle$$

Turning the large transition time T into $\int dx^0$ and expanding in λ we get the only relevant for the scattering term

$$A=-i\frac{\lambda}{4!}\int\langle k_3,k_4|\hat{\varphi}^4(x)|k_1,k_2\rangle d^4x \qquad (4)$$

To avoid unnecessary complications we consider k_1 , k_2 , k_3 , k_4 to be distinct. Then the only non-vanishing terms in developing the right member of (4) with (1) expresion for φ are those containing the factor

$$-i\frac{\lambda}{4!}\langle 0|\tilde{a}(\vec{k}_3)\tilde{a}(\vec{k}_4)a^+(\vec{k}_4)a^+(\vec{k}_3)a(\vec{k}_2)a(\vec{k}_1)\tilde{a}^+(\vec{k}_2)\tilde{a}^+(\vec{k}_1)|0\rangle$$

$\exp\left(i(k_3+k_4-k_1-k_2)x\right)$ where we integrate over $x\in(0,T)\times D$

(Obviously we also consider the commutation $[a(\vec{k}),a(\vec{k}')]=0$ for any $\vec{k},\vec{k}'\in\mathbb{R}^3$)

$a^+(\vec{k}_4)$ can come from any of the 4 factors $\hat{\varphi}$ in $\hat{\varphi}^4$, $a^+(\vec{k}_3)$ from the remaining 3, $a(\vec{k}_2)$ from the remaining 2 and $a(\vec{k}_1)$ from the remaining 1 factor occuring in $\hat{\varphi}^4$. Therfore we have a coefficient 4! which cancels the 4! denominator from $-i\frac{\lambda}{4!}$ and we have considering the commutation relations that

$A=\frac{1}{V^2}\left(\prod_{i=1}^{4}\frac{1}{\sqrt{2\omega_{ki}}}\right)A_F$ where $A_F=(2\pi)^4\boldsymbol{M}\,\delta^4(k_4+k_3-k_1-k_2)$ with $\boldsymbol{M}=-i\lambda$ is the Feynman amplitude for the scattering process.

For the field system we considered we have an “energy of the vacuum” given by $\langle 0|\hat{H}|0\rangle=\int\frac{1}{2}\langle 0|(\partial_0\hat{\varphi})^2+(\nabla\varphi)^2+m^2\varphi^2|0\rangle d^3\vec{x}$ and after some calculus we obtain

$$\langle 0|\hat{H}|0\rangle=V\int\frac{d^3\vec{k}}{(2\pi)^3 2\omega_k}\frac{1}{2}(\omega_k^2+\vec{k}^2+m^2)=\int\frac{V}{(2\pi)^3}\frac{1}{2}\hbar\omega_k d^3\vec{k}$$

(after restoring the Planck constant) .

Since as we proved above $\frac{V}{(2\pi)^3}d^3\vec{k}$ is the number of individual states contained in the infinitesimal volume $d^3\vec{k}$ of the momentum space we recognize the vacuum energy as the zero point energy of the harmonic oscillator integrated over all momentum modes and over all space. The integral over the momentum space clearly diverges but the energy of any physical configuration is to be measured relative to this “energy of the vacuum” and we could define the correct Hamiltonian as $\hat{H}-\langle 0|\hat{H}|0\rangle$.

For a complex scalar field system with Lagrangian density

$\mathscr{L}=(\partial\varphi)^+(\partial\varphi)-m^2\varphi^+\varphi-\frac{\lambda}{2!2!}(\varphi^+\varphi)^2+J^+\varphi+J\varphi^+$ with $\varphi=\varphi_1+i\varphi_2$,

the free field theory leads also to the Klein-Gordon equation for the complex field as a motion equation and the canonical commutation relations in the continuous field theory are

$$[\frac{\partial\mathscr{L}}{\partial(\partial_0\varphi_a)}(t,\vec{x}),\varphi_b(t,\vec{x}')]=-i\delta_{ab}\delta^3(\vec{x}-\vec{x}') \ , \ a,b=1,2 \ , \ t\in\mathbb{R} \ , \ \vec{x},\vec{x}'\in\mathbb{R}^3$$

Therefore we will have for the field operator function an expression as

$$\hat{\varphi}(t,\vec{x})=\int \frac{d^3\vec{k}}{(2\pi)^{3/2}(2\omega_k)^{1/2}}(a(\vec{k})\exp(-ikx)+b^+(\vec{k})\exp(ikx)) \quad \text{with}$$

$kx=\omega_k t-\vec{k}\cdot\vec{x}$, $\omega_k=\sqrt{\vec{k}^2+m^2}$

$a(\vec{k}),a^+(\vec{k})$ anihilation , creation operators for a system particle of momentum $\vec{k}$

$b(\vec{k}),b^+(\vec{k})$ anihilation , creation operators for a system anti-particle of momentum $\vec{k}$ satisfying commutation relations :

$$[a(\vec{k}),a^+(\vec{k}')]=[b(\vec{k}),b^+(\vec{k}')]=\delta^3(\vec{k}-\vec{k}')$$

$$[a(\vec{k}),a(\vec{k}')]=[b(\vec{k}),b(\vec{k}')]=[a(\vec{k}),b(\vec{k}')]=[a(\vec{k}),b^+(\vec{k}')]=0$$

Considering as above the system enclosed in the cube *D* with sides of length *L* along the axes , volume $V = L^3$ and periodic boundary conditions we will have in a similar way as above that :

$$\hat{\varphi}(t,\vec{x})=\sum_{\vec{k}} \frac{1}{V^{1/2}}\frac{1}{\sqrt{2\omega_k}}(\tilde{a}(\vec{k})\exp(-ikx)+\tilde{b}^+(\vec{k})\exp(ikx)) \quad \text{with}$$

$$\tilde{a}(\vec{k})=\left(\frac{(2\pi)^3}{V}\right)^{1/2}a(\vec{k}) \ , \ \tilde{b}(\vec{k})=\left(\frac{(2\pi)^3}{V}\right)^{1/2}b(\vec{k})$$

$$\vec{k}=\frac{2\pi}{L}(n_1,n_2,n_3) \ , \ n_j\in\mathbb{Z} \ , \ k=(\omega_k,\vec{k})$$

Obviously the normalized anihilation and creation operators satisfy

$$[\tilde{a}(\vec{k}),\tilde{a}^+(\vec{k}')]=[\tilde{b}(\vec{k}),\tilde{b}^+(\vec{k}')]=\delta_{\vec{k}\vec{k}'}$$

$\tilde{a}^+(\vec{k})$ creates a normalized particle with four-momentum k on mass shell state and $\tilde{b}^+(\vec{k})$ creates a normalized anti-particle with four-momentum k on mass shell state and we have a ground state such that $a(\vec{k})|0\rangle=0$ and $b(\vec{k})|0\rangle=0$ for any $\vec{k}\in\mathbb{R}^3$.

The free theory Lagrangian density is invariant under the field transformations $\varphi\to\exp(i\theta)\varphi$, $\theta\in\mathbb{R}$ that is $\varphi_1\to\varphi_1-\theta\varphi_2+O(\theta^2)$, $\varphi_2\to\varphi_2+\theta\varphi_1+O(\theta^2)$ and the Noether conserved current corresponding to this transformation is

$$(J^\mu)_\mu=(-2((\partial^\mu\varphi_1)\varphi_2-(\partial^\mu\varphi_2)\varphi_1))_\mu=(i(\varphi^+\partial^\mu\varphi-\partial^\mu\varphi^+\varphi))_\mu$$

We can verify through the Klein-Gordon equation that the current is conserved: $\partial_\mu J^\mu=0$ which leads to a time independent charge $Q=\int J_0(t,\vec{x})d^3\vec{x}$

After some calculus we derive, disposing of a time independent constant vacuum charge $\int\delta^3(\vec{0})d^3\vec{k}$ a time independent charge operator with expression :

$\hat{Q}=\int\hat{J}_0(t,\vec{x})d^3\vec{x}=\int(a^+(\vec{k})a(\vec{k})-b^+(\vec{k})b(\vec{k}))d^3\vec{k}$ and we will have

$$\hat{Q}\tilde{a}^+(\vec{k})|0\rangle=\tilde{a}^+(\vec{k})|0\rangle \ , \ \hat{Q}\tilde{b}(\vec{k})|0\rangle=-\tilde{b}^+(\vec{k})|0\rangle$$

We conclude that the field operator $\hat{\varphi}^{+}$ creates particles with one unit of positive charge and anihilates anti-particles with one unit of negative charge . The field operator $\hat{\varphi}$ does the opposite.
Hence for a complex scalar field we have one particle in the box *D* since the particles come in units of charge.

We can consider the more general case of a system of *h* interacting complex scalar fields with a Lagrangian density

$\mathscr{L}=\sum_{j=1}^{h}\left((\partial\,\xi_j)^{+}(\partial\,\xi_j)-m_j^2\,\xi_j^{+}\,\xi_j\right)+P\left((\xi_j^{+},\xi_j)_{j=\overline{1,h}}\right)+\sum_{j=1}^{h}\left(J_j^{+}\,\xi_j+J_j\,\xi_j^{+}\right)$ where

P is a polynomial in $(\xi_j^{+},\xi_j)_{j=\overline{1,h}}=(\varphi_j)_{j=\overline{1,2h}}$, $P=\sum_{\bar{m}}\sum_{\substack{f\in S_{\bar{m}f,2h}\\ mf=\bar{m}}} g_f\prod_{i=1}^{mf}\varphi_{f(i)}$

with $S_{\bar{m},2h}=\{1,2,\ldots,2h\}^{\{1,2,\ldots,\bar{m}\}}$, P expresses the field to field interactions.
For a process with incoming paricles j_1 , j_2 , … , j_n having four-momenta on mass shell q_1 , q_2 , … , q_n and outgoing particles l_1 , l_2 , … , l_s having four-momenta on mass shell p_1 , p_2 , … , p_s , just as in Chap. Feynman amplitudes and lattice gauge theory we derive that the relation between the total transition probability amplitude *A* for a given couplings orders and the total Feynman amplitude A_F corresponding for all Feynman diagrams in the same couplings orders, computed using Feynman rules (see Chap. … Quantum field theory … Feynman amplitudes and Chap. Feynman amplitudes and lattice gauge theory) is given by

$$A=V^{-(s+n)/2}\left(\prod_{k=1}^{n}\frac{1}{\sqrt{2\,\omega_{qk\,jk}}}\right)\left(\prod_{k=1}^{s}\frac{1}{\sqrt{2\,\omega_{pk\,lk}}}\right)A_F \quad , \; A_F \text{ having as we know the form} \tag{5}$$

$$A_F=(2\pi)^4\,\boldsymbol{M}\,\delta^4\left(\sum_{k=1}^{s}p_k-\sum_{k=1}^{n}q_k\right) \quad \text{with } \omega_{qj}=\sqrt{\vec{q}^{\,2}+m_j^2}$$

Consider the particular case of the decay of a ξ_1 field meson having four-momentum on mass shell *k* into a ξ_2 field meson and a field ξ_3 meson having four-momenta on mass shell *p* respective *q* and the interaction term is $P=g\left(\xi_2^{+}\,\xi_3^{+}\,\xi_1+\xi_2\,\xi_3\,\xi_1^{+}\right)$.
The Feynman amplitude at first order in *g* of the process is
$A_F=(2\pi)^4\,i\,g\,\delta^4(p+q-k)$, $\boldsymbol{M}=i\,g$ and so the transition probability is

$$|A|^2=\frac{1}{V^3}\frac{1}{8\,\omega_k\,\omega_p\,\omega_q}|\boldsymbol{M}|^2\left((2\pi)^4\,\delta^4(p+q-k)\right)^2$$

Taking *T* as the transition time we have :

$\left((2\pi)^4\,\delta^4(p+q-k)\right)^2=(2\pi)^4\,\delta^4(p+q-k)\int d^4x\exp(i(p+q-k)x)=$

$=(2\pi)^4\,\delta^4(p+q-k)\,V\,T$ and so the transition decay rate is therefore

$$\frac{|A|^2}{T}=\frac{1}{V^2}\frac{1}{2\,\omega_k\,2\,\omega_p\,2\,\omega_q}(2\pi)^4|\boldsymbol{M}|^2\,\delta^4(p+q-k)$$

Recall that there are $\frac{V}{(2\pi)^3} d^3\vec{p}$ states in the volume $d^3\vec{p}$ in momentum space.

Therefore the differential decay rate of a meson with momentum $\vec{k}$ into two mesons carrying momenta in some specified ranges $d^3\vec{p}$, $d^3\vec{q}$ around the values $\vec{p}$ respective $\vec{q}$ is given by

$$d\Gamma = \frac{1}{2\omega_k} \frac{d^3\vec{p}}{(2\pi)^3 2\omega_p} \frac{d^3\vec{q}}{(2\pi)^3 2\omega_q} (2\pi)^4 |\boldsymbol{M}|^2 \delta^4(p+q-k)$$

We notice that the factors of V cancel. The decay rate for a moving particle is smaller than that of a resting particle by a factor of m/ω_k from which we can derive time dilation. To obtain the total decay rate we integrate over the $\vec{p}, \vec{q}$ variables considering that the p , q four-momenta are on mass shell.

Consider now the particular case of a scattering process of two incoming complex scalar field particles with four-momenta on mass shell k_1 , k_2 into outgoing complex scalar field particles with four-momenta on mass shell p_1 , p_2 , … , p_s . We compute the total Feynman amplitude to a specific couplings order for corresponding Feynman diagrams, using the Feynman rules, and obtain

$$A_F = (2\pi)^4 \boldsymbol{M}\, \delta^4\left(k_1 + k_2 - \sum_{j=1}^{s} p_j\right) .$$

Then the transition probability for the considered process at the desired order in coupling constants will be according to (5) :

$$|A|^2 = \frac{1}{V^{2+s}} \frac{1}{2\omega_{k1} 2\omega_{k2}} \left(\prod_{j=1}^{s} \frac{1}{2\omega_{pj}} \right) \left((2\pi)^4 \delta^4\left(k_1 + k_2 - \sum_{j=1}^{s} p_j\right) \right)^2 |\boldsymbol{M}|^2 . \qquad (6)$$

The process can be viewed as a beam of k_1 particles crashing with velocity v_1 into a k_2 particle having velocity v_2 . The density of the k_1 particles in the beam is n . The flux of the beam F is the number of k_1 particles crossing an unit area surface normal to the relative velocity $\vec{v}_1 - \vec{v}_2$ (we consider $|\vec{v}_2| \ll c = 1$) and solidar to the k_2 particle. We assume that $\vec{v}_1$ and $\vec{v}_2$ point in opposite directions and take a collinear frame (the mass center frame or the k_2 particle at rest frame) in which $k_1 = E_1(1,0,0,v_1)$, $k_2 = E_2(1,0,0,v_2)$ and we have that $F = n|v_1 - v_2|$.

The cross section σ of the scattering process is defined as the measured event rate divided by the flux of the beam . Obviously σ has the dimension of an area.

With N event particles crossing normal in time interval Δt the area ΔS we have $\Gamma = \frac{N}{\Delta t}$ the event rate, $nv = F = \frac{N}{\Delta t \Delta S}$ where $v = |v_1 - v_2|$, $\sigma = \frac{N}{nv\Delta t}$, $\Gamma = n\sigma v$ and so $\sigma = \Delta S$. Thus a k_2 particle sweeps in time Δt through a volume $\Delta S |v_1 - v_2| \Delta t = \sigma |v_1 - v_2| \Delta t$ which contains $n\sigma |v_1 - v_2| \Delta t$ particles.

For $T = \Delta t$, having $\frac{V}{(2\pi)^3} d^3\vec{p}_j$ p_j particle states in the $d^3\vec{p}_j$ volume in momentum space it follows from (6) that the differential event rate of k_1 , k_2 mesons scattering into p_1 , p_2 , …, p_s mesons in some specified ranges

$d^3\vec{p}_1, d^3\vec{p}_2, ..., d^3\vec{p}_s$ around the values $\vec{p}_1, \vec{p}_2, ..., \vec{p}_s$ respective is given by

$$d\Gamma = \frac{1}{V}\frac{1}{2\omega_{k1}2\omega_{k2}}\left(\prod_{j=1}^{s}\frac{d^3\vec{p}_j}{(2\pi)^3 2\omega_{pj}}\right)\delta^4(k_1+k_2-\sum_{j=1}^{s}p_j)|\boldsymbol{M}|^2$$

and since $n=\frac{1}{V}$, having one particle in the box, the differential cross section is

$$d\sigma = \frac{d\Gamma}{n|v_1-v_2|} = \frac{1}{|v_1-v_2|}\frac{1}{2\omega_{k1}2\omega_{k2}}\left(\prod_{j=1}^{s}\frac{d^3\vec{p}_j}{(2\pi)^3 2\omega_{pj}}\right)\delta^4(k_1+k_2-\sum_{j=1}^{s}p_j)|\boldsymbol{M}|^2$$

Because $\omega_{ki}=E_i$, $\vec{k}_i=E_i(0,0,v_i)$, $\omega_{ki}=\sqrt{\vec{k}_i^2+m_i^2}$ for $i=1,2$ we have $(k_1k_2)^2-m_1^2m_2^2=(E_1E_2(v_1-v_2))^2$ we have a more Lorentz invariant looking form of the $\omega_{k1}\omega_{k2}|v_1-v_2|$ factor showing that the differential cross section is invariant under Lorentz boosts in the direction of the beam.

(Recalling that $\frac{d^3\vec{p}}{2\omega_p}$ is a Lorentz invariant measure).

In particular we can consider the scattering of two particles into two particles in the center of mass frame of the incoming k_1 , k_2 particles.

We consider the p_1 particle detector spanning a solid angle $d\Omega = \sin\theta\, d\theta\, d\varphi$ in the p_1 directions space and count the number of events per unit time detected within the considered solid angle.

We have $d^3\vec{p}_1 = p_1^2 dp_1 d\Omega$ if we take $p_1=\|\vec{p}_1\|$

and in the mass center frame $\vec{k}_1+\vec{k}_2=0$ and so if $\boldsymbol{M}$ not depends on p_1, p_2

integrating the differential cross section over $\vec{p}_2$ and taking

$\omega=\sqrt{\vec{p}_1^2+m_1^2}+\sqrt{\vec{p}_1^2+m_2^2}$ we will have $p_1=p_1(\omega)$, $\omega_1=\sqrt{\vec{p}_1^2+m_1^2}$, $\omega_2=\sqrt{\vec{p}_1^2+m_2^2}$

$d\omega = p_1\frac{\omega_1+\omega_2}{\omega_1\omega_2}dp_1$, $E_{tot}=E_1+E_2$

$$\frac{d^3\vec{p}_1}{2\omega_{p1}}\frac{d^3\vec{p}_2}{2\omega_{p2}}\delta^4(k_1+k_2-p_1-p_2) = \frac{p_1(\omega)}{4\omega}\delta(\omega-E_{tot})d\omega d\Omega = \frac{p_1(E_{tot})}{4E_{tot}}d\Omega$$

Solving for $p_1(\omega)$ we obtain finally

$$\frac{d\sigma}{d\Omega} = \frac{1}{|v_1-v_2|}\frac{1}{4\omega_{k1}\omega_{k2}}\frac{1}{(2\pi)^2}\frac{1}{8E_{tot}^2}((E_{tot}^2-(m_1+m_2)^2)(E_{tot}^2-(m_2-m_1)^2))^{1/2}|\boldsymbol{M}|^2$$

with $\omega_{k1}=\frac{m_1}{\sqrt{1-v_1^2}}$, $\omega_{k2}=\frac{m_2}{\sqrt{1-v_2^2}}$, $E_{tot}=\omega_{k1}+\omega_{k2}$

v_1 and v_2 are velocities in the center of mass frame.

If $\vec{w}_1=(0,0,w_1)$, $\vec{w}_2=(0,0,w_2)$ are the incoming velocities in the lab frame, we can take

$$\bar{m}_i=\frac{m_i}{\sqrt{1-w_i^2}} \text{ for } i=1,2 \text{ , } v_c=\frac{\bar{m}_1 w_1+\bar{m}_2 w_2}{\bar{m}_1+\bar{m}_2} \text{ ,}$$

$v_i=\frac{w_i-v_c}{1-v_c w_i}$ for $i=1,2$, v_c mass center velocity in the lab frame.

At the end we must notice that in computing the effective transition probability amplitude according to (5) the initial and final state ψ_I respective ψ_F must be normalized.

We have $\psi_F=\langle 0|\tilde{a}_{l1}(\vec{p}_1)...\tilde{a}_{ls}(\vec{p}_s)$ and $\psi_i=\tilde{a}^+_{j1}(\vec{q}_1)...\tilde{a}^+_{jn}(\vec{q}_n)|0\rangle$ and we require $\langle\psi_I|\psi_I\rangle=\langle\psi_F|\psi_F\rangle=1$. Using the commutation relations we derive $\langle 0|\tilde{a}^l_j(\vec{q})\tilde{a}^{l+}_j(\vec{q})|0\rangle=l!$. Therefore we must normalize ψ_F and ψ_I with a factor of $\frac{1}{\sqrt{l!}}$ for each occurence of l identical particles with the same momentum and of the same sort in the outgoing or incoming particles sets and the corresponding transition probability $|A|^2$ must be adjusted by a statistical factor (eliminating double counting of events) given by :

$S=\prod_j \frac{1}{l_j!}$ where l_j is an occurence number of identical particles having the same sort and momentum.

9. Energy momentum tensor

Energy-momentum tensor

Consider the space-time continuum of special relativity as the Minkowski space with signature (+,-,-,-) of relativistic space-time coordinates ($c\,t$, x , y , z) , (c speed of light in vacuum). A collection of relativistic particles is determined by the number flux four vector field (N^t , N^x , N^y , N^z) and the four momentum vector field (P^t , P^x , P^y , P^z) where N^t is the particles density times c and (N^x , N^y , N^z) is the particles flux vector :

$$N^t=\frac{\text{' number of particles in volume } V=\Delta x\Delta y\Delta z\text{ '}}{\Delta x\Delta y\Delta z}\times c$$

$$N^x=\frac{\text{' number of particles passing the area } A_x=\Delta y\Delta z \text{ in time } \Delta t\text{ '}}{\Delta c\,t\,\Delta y\Delta z}\times c$$

similar definitions are considered for N^y , N^z.

We have $N=N(ct,x,y,z)$, $P=P(ct,x,y,z)$ for a particle at (ct,x,y,z) coordinates.

Taking $U=\left(\frac{c}{\sqrt{1-\frac{v^2}{c^2}}},\frac{v^x}{\sqrt{1-\frac{v^2}{c^2}}},\frac{v^y}{\sqrt{1-\frac{v^2}{c^2}}},\frac{v^z}{\sqrt{1-\frac{v^2}{c^2}}}\right)$ the four-velocity field (see Chap. Relativistic dynamics) we will have $N=nU$, $P=mU$

where n is the rest number of particles density and m is the rest mass of a particle. So it follows $m\,n=\rho$, the rest mass density of the particle collection.

The energy-momentum tensor component $T^{\alpha\beta}$ will be defined as the amount of α -momentum, $P^\alpha\,c$ going through a 3D -unit volume of constant β coordinate.

For dust, a collection of particles not exerting pressure on each other the energy-momentum tensor will be $T=P\otimes N=\rho U\otimes U$.

Choosing Δt , Δx , Δy , Δz such that the number of particles in volume V is 1 and the number of particles passing the area A_x in time Δt is 1 (and a similar condition for directions y , z) we will have $\Delta x=v^x\Delta t$, $\Delta y=v^y\Delta t$, $\Delta z=v^z\Delta t$ and :

$$T^{tt}=\frac{P^t c}{\Delta x\Delta y\Delta z}\text{ -energy density}$$

$$T^{tx}=\frac{P^t c}{\Delta c\,t\,\Delta y\Delta z}\text{ -energy flux}\times\frac{1}{c}$$

$$T^{xt}=\frac{P^x c}{\Delta x\Delta y\Delta z}\text{ -momentum density}\times c$$

$$T^{xy}=\frac{P^x c}{\Delta c\,t\,\Delta x\Delta z}\text{ -shear stress}$$

$$T^{xx}=\frac{P^x c}{\Delta c\,t\,\Delta y\Delta z}\text{ -strech-compression stress}$$

It follows that the energy-momentum tensor is symmetric : $T^{\beta\alpha} = T^{\alpha\beta}$ and the conservation in time of total energy and momentum of particles in any space region is equivalent with the fact that the energy-momentum tensor is a conserved tensor field, that is $\frac{\partial T^{\alpha\beta}}{\partial x^{\beta}}=0$ for $\alpha=\overline{0,3}$ with Einstein summation convention for $(x^{\beta})_{\beta=\overline{0,3}}=(ct,x,y,z)$ noticing that according to definition $(T^{\alpha\beta})_{\alpha,\beta}$ is a contravariant Lorentz tensor.

10. Electromagnetic four-potential. Electromagnetic tensor Lagrangian of electromagnetism Energy momentum tensor of electromagnetic field

Electromagnetic four-potential. Electromagnetic tensor
Lagrangian of electromagnetism
Energy-momentum tensor of elecromagnetic field

By a suitable choice of time measuring units we can consider for the speed of ligh in vacuum $c = 1$ and by a suitable choice of electric charge measuring units we can consider the electric permittivity in vacuum $\varepsilon = 1$. Therefore, because $\frac{1}{c}=\sqrt{\varepsilon\,\mu}$ for the magnetic permeability of vacuum we have also $\mu=1$.

The Maxwell equations for a electromagnetic field in vacuum will then become :

$\nabla\times E=-\frac{\partial B}{\partial t}$ (1)

$\nabla\cdot B=0$ (2)

$\nabla\cdot E=\rho$ (3)

$\nabla\times B=\vec{j}+\frac{\partial E}{\partial t}$ (4)

with $(t,x)\in\mathbb{R}^4$, $t\in\mathbb{R}$, $(t,x)=(x^\alpha)_{\alpha=\overline{0,3}}$ -time space coordinates

$E=(E_i)_i$, $E=E(t,x)\in\mathbb{R}^3$ -electric intensity field

$B=(B_i)_i$, $B=B(t,x)\in\mathbb{R}^3$ -magnetic induction field

$\rho=\rho(t,x)\in\mathbb{R}$ -charge density

$\vec{j}=\vec{j}(t,x)\in\mathbb{R}^3$ -current density (charge flux vector)

We have also the charge conservation law $\frac{\partial\rho}{\partial t}+\nabla\cdot\vec{j}=0$ (5) expressing the fact that in any space domain the total charge is conserved in time.

We consider the Minkowski space-time with signature (+,-,-,-) denoting the metric as $(\eta^{\alpha\beta})_{\alpha,\beta}$; we denote indices from 1 to 3 by latin letters and indices from 0 to 3 by greek letters.

Considering (1) and (2) it follows that we can take a four-potential $(A^\alpha)_\alpha$ auch that $B_i=\epsilon_{ijk}A^k_{,j}$, $E_i+A^i_{,0}=-A^0_{,i}$ (where as usual $F_{,\alpha}$ denotes $\frac{\partial F}{\partial x^\alpha}$) for $i=\overline{1,3}$.

$(A^\alpha)_\alpha$ is considered Lorentz contravariant so that the Maxwell system is Lorentz invariant.

From (3) and (4) we obtain now

$-A^i_{,0i}-A^0_{,ii}=\rho$ (5)

$A^k_{,pk}-A^p_{,qq}+A^p_{,00}+A^0_{,p0}=j_p$ (6)

and so if $A^\alpha_\alpha=0$ we have $\Box A=(\rho,\vec{j})=J$ with $\Box=\partial^\alpha\partial_\alpha=\partial^2$.

Taking the covariant antisymmetric electromagnetic tensor field

$$(F_{\alpha\beta})_{\alpha,\beta}=\begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{pmatrix} \ , \ F_{\alpha\beta}=\partial_\alpha A_\beta-\partial_\beta A_\alpha \ ,$$

The Maxwell equations can be written as

$\partial_\alpha F^{\alpha\beta}=J^\beta$ (7)

$\partial_\alpha \epsilon^{\alpha\beta\gamma\delta} F_{\gamma\delta}=0$ (8) where $(J^\beta)_\beta=(\rho,\vec{j})$

with $\epsilon_{\alpha\beta\gamma\delta}$ the Levi-Civita symbol (signature of permutation)

$\epsilon^{\alpha\beta\gamma\delta}=\eta^{\alpha\nu}\eta^{\beta\mu}\eta^{\gamma\rho}\eta^{\delta\varepsilon}\epsilon_{\nu\mu\rho\varepsilon}$.

It is obvious that if we take a gauge transformation of *A* given by

$A_\alpha \to A'_\alpha=A_\alpha+\partial_\alpha\Psi$ the electromagnetic tensor field not changes.

Therefore we can take the Lorentz gauge in which $\partial_\alpha A^\alpha=\partial^\alpha A_\alpha=0$ and so in the Lorentz gauge we have $\Box A^\alpha=J^\alpha$ (9) .

Solutions of the equations (9) , if exists $M>0$ such that $\|(\rho,\vec{j})(t,x')\|<\frac{M}{\|x'\|^3}$

for $\|x'\|$ sufficiently large, are given by

$$A^0=\varphi(t,x)=\frac{1}{4\pi}\int \frac{\rho(t-\|x-x'\|,x')}{\|x-x'\|}d^3x'$$

$$(A^i)_i=(A^i(t,x))_i=\frac{1}{4\pi}\int \frac{\vec{j}(t-\|x-x'\|,x')}{\|x-x'\|}d^3x'$$

For a concentrated at $x'=x'_O$ stationary charge Q we see that φ is the

Coulomb potential $\varphi(x)=\frac{Q}{4\pi\|x-x'_O\|}$.

Consider the Lagrangian density (see Chap. Lagrangian field theory)

$\mathscr{L}(A,\partial A)=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}-J^\alpha A_\alpha$ we notice that the corresponding

Euler-Lagrange equations $\frac{\partial\mathscr{L}}{\partial A_\nu}-d_\mu\left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu A_\nu)}\right)=0$ are equivalent to $J^\nu=\partial_\mu F^{\mu\nu}$.

With $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ the (8) equations are automatically satisfied.

Hence we choose for the Lagrangian density of the electromagnetic field the

expression $\mathscr{L}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}-J^\alpha A_\alpha$.

Taking a gauge such that $A_0=0$ we notice that for the field

$\vec{A}=(A_i(t,x))_i=\vec{\tilde{A}}\cos(\omega t-\vec{k}\cdot x)$ we have for

$J=0$, $\omega^2=\vec{k}^2$ (electromagnetic wave) that

$$\mathscr{L}=\frac{1}{4}\sin^2(\omega t-\vec{k}\cdot x)(\vec{\tilde{A}}^2\omega^2-(\vec{k}\times\vec{\tilde{A}})^2)=\frac{1}{4}\sin^2(\omega t-\vec{k}\cdot x)(\vec{\tilde{A}}^2(\omega^2-\vec{k}^2)+(\vec{k}\cdot\vec{\tilde{A}}))$$

and so the action $\int \mathscr{L}\,dt\,d^3x$ has a minimum at $\vec{k}\cdot\vec{\tilde{A}}=0$.

Hence we have chosen the right sign for the Lagrangian density.

Considering a charge density $\rho=\rho(t,x)$, charged particles system having a motion described by the velocity field $\vec{v}=\vec{v}(t,x)$ we will have $J=(\rho,\rho\vec{v})$ and the Lorentz forces density vector field $f=\rho(E+\vec{v}\times B)$.

The power transmitted from the electromagnetic field to the charged particles contained in the volume element dV is given by

$dP=\rho(E+\vec{v}\times B)\cdot\vec{v}\,dV=J^i E_i\,dV$ and so if W represents the energy of the particles in a domain $D_t\subset\mathbb{R}^3$ we have $\frac{dW}{dt}=\int_{D_t} J^i E_i dV=$

$$=\int_{D_t}\left(-E\cdot\frac{\partial E}{\partial t}+E\cdot(\nabla\times B)-B\cdot(\nabla\times E+\frac{\partial B}{\partial t})\right)dV=$$

$$=-\frac{\partial}{\partial t}\frac{1}{2}\int_{D_t}(E^2+B^2)dV-\int_{\partial D_t}(E\times B)\cdot\boldsymbol{n}\,d\sigma$$

with $\boldsymbol{n}$ the outwards normal on ∂D_t .

Therefore we take $w=\frac{1}{2}(E^2+B^2)$ the energy density of the electromagnetic field, $S=E\times B$ the energy flux of the electromagnetic field which is also the momentum density of the electromagnetic field.
(see Chap. Energy-momentum tensor) S is called the Poynting vector of the electromagnetic field.

Also after some calculus we obtain :

$f=(\nabla\cdot E)E+\left(\nabla\times B-\frac{\partial E}{\partial t}\right)\times B=\nabla\cdot(-\boldsymbol{I}w+B\otimes B+E\otimes E)-\frac{\partial S}{\partial t}$ with $\boldsymbol{I}=(\delta_{ij})_{i,j}$.

We define therefore the energy-momentum tensor of the electromagnetic field in vacuum :

$(T^{\alpha\beta})_{\alpha,\beta}=\begin{pmatrix} w & S \\ S & \boldsymbol{I}w-B\otimes B-E\otimes E\end{pmatrix}$ having the relation

$T^{\alpha\beta}{}_{,\beta}+G^\alpha=0$ with $(G^\alpha)_\alpha=(\vec{j}\cdot E,f)$

For a non-relativistic spinless charged particle in an electromagnetic field we consider the Lagrangian

$L(x,\dot{x})=\frac{1}{2}\dot{x}_i\dot{x}_i+q\,\dot{x}_i A^i-qA^0$ where $(A^\alpha)_\alpha$ is the four-potential of the electromagnetic field, q is the charge of the particle, m is the mass of the particle, and $x=(x_i)_i$ are the Carthesian coordinates of the particle .

The motion equations are given by the Euler-Lagrange equations

$0=\frac{\partial L}{\partial x_i}-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{x}_i}\right)=q\,v_k A^k_{,i}-q\,A^0_{,i}-m\,\ddot{x}_i-q\,A^i_{,0}-q\,v_k A^i_{,k}$ and so by the four-potential definition we recover the Lorentz force in the motion equations:

$m\ddot{x}=qE+q\vec{v}\times B$ with $\vec{v}=\frac{dx}{dt}=\dot{x}$.

The canonical momenta are $p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + qA^i$ and the Hamiltonian is

$H = \dot{x}_i p_i - L = \frac{1}{2m}(p_i - qA^i)(p_i - qA^i) + qA^0$.

Therefore we must consider in an electromagnetic field a coupling which replaces the canonical momentum with the gauge invariant kinetical momentum $p_i + qA_i$ and adds to the Hamiltonian the potential term qA_0.

In other words, considering the momentum and energy operators acting on wave functions $\psi = \psi(t,x)$ with the Schroedinger equation

$i\partial_0 \psi = \hat{H}\psi = \frac{1}{2m}(\hat{\vec{p}} + q(A_i)_i)^2 + qA_0$ with $\hat{\vec{p}} = -i(\partial_k)_k$, we introduce gauge invariant kinetical momentum $-iD_j = -i\partial_j + qA_j$ and energy $iD_0 = i\partial_0 - qA_0$ that is we replace the ∂ operator in the definition of momentum and energy operators by $\partial \to D = \partial + iq(A_\alpha)_\alpha$.

Under a gauge transformation we must take:

$\psi(t,x) \to \exp(i\Lambda(t,x))\psi(t,x)$, $A_\mu \to A_\mu - \frac{1}{q}\partial_\mu \Lambda$.

11. Electric dipole. Magnetic dipole. Dipole radiation Macroscopic Maxwell equations

Electric dipole. Magnetic dipole
Dipole radiation. Macroscopic Maxwell equations

An electric dipole consists of two equal and opposite point charges $+q$ and $-q$ placed at the ends of a rigidised segment A_+ and A_-.
With $\boldsymbol{d}=\overrightarrow{A_- A_+}$ the electric dipole moment is $\boldsymbol{p}=q\boldsymbol{d}$. For a neutral distribution of charge $\rho=\rho(\boldsymbol{r})$ ($\boldsymbol{r}$ position vector) the associated electric dipole moment will be $\boldsymbol{p}=\int \rho \boldsymbol{r}\, d^3\boldsymbol{r}$. One should always consider the 'dipole limit' where the distance between the generating charges should converge to 0 while the charge strenght should diverge to ∞ such way that the product $q\boldsymbol{d}$ remains constant.
Such dipole moments appear on molecules due the non-uniform distributions of positive and negative charges on the various atoms.
Therefore in an electromagnetic material, an electric field can induce a electric dipole density as a polarization density field $P=P(\boldsymbol{r})=\frac{d\boldsymbol{p}}{dV}$, the amount of electric dipole moment which appears at position $\boldsymbol{r}$ in the volume element $dV(\boldsymbol{r}) = d^3\boldsymbol{r}$.
The polarization density field $P=P(t,\boldsymbol{r})$ (t time coordinate) must depend on the history of electric intensity field $E^t=(E(\tau))_{\tau<t}(E(\tau)=E(\tau,\boldsymbol{r})$ electric intensity vector) having $P=f(E^t)$ and we will have an electric induction vector field $D=\varepsilon_0 E+P$ where ε_0 is the electric permittivity of vacuum with $\nabla\cdot D=\rho_f$, $\nabla\cdot P=-\rho_b$, $\rho_f=\rho_f(t,\boldsymbol{r})$ - the free charges distribution , $\rho_b=\rho_b(t,\boldsymbol{r})$ -the bound in dipoles charges distribution
$\rho=\rho_f+\rho_b$ -the total charges distribution.
There can be also permanent dipoles when two atoms in a molecule have substantially different electronegativity, causing also a polarization density field *P*.

A magnetic dipole is the closed circulation of an electric current system.
In the Amperian loop model, the magnetic dipole moment is given by $\boldsymbol{m}=\frac{1}{2}\int \boldsymbol{r}\times\vec{j}\, d^3\boldsymbol{r}$ where $\vec{j}=\vec{j}(\boldsymbol{r})$ is the electric current density vector field.
For a uniformly as ρ distributed charge we have $\vec{j}=\rho\vec{v}(t,\boldsymbol{r})$ with $\vec{v}=\vec{v}(t,\boldsymbol{r})$ -the velocities field and so the magnetic moment is proportional to the angular momentum $\vec{L}=\int \boldsymbol{r}\times\mu\vec{v}\, d^3\boldsymbol{r}$ when μ is a uniform mass distribution in fact we have $\boldsymbol{m}=\frac{Q}{2M}\vec{L}$ with Q charge and M mass.
The current density is supposed to be localized on a circular loop wire so that if the

circle is $\{(r\cos\alpha, r\sin\alpha, 0)|\alpha\in(0,2\pi)\}$ we can approximate

$$2\boldsymbol{m}=\int_0^{2\pi}\boldsymbol{r}(\alpha)\times\vec{j}(\alpha)\,A\,r\,d\alpha$$

where $\boldsymbol{r}(\alpha)=(r\cos\alpha, r\sin\alpha, 0)$, $\vec{j}(\alpha)=(-j\sin\alpha, j\cos\alpha, 0)$ and A is the area of the wire transversal section, $I=jA$ is the electric current intensity through the wire. Thus we will have, in the Amperian loop model of magnetic moment that:

$\boldsymbol{m}=\pi r^2\, jA\, e_3=IS\, e_3$ with $S=\pi r^2$ the area of the loop circle and $e_k=(\delta_{ki})_{i=\overline{1,3}}$.

The magnetic dipole limit will be obtained for *S* convergent to 0 while the current intensity diverges to infinity such that ***m*** remains constant.

The magnetic properties of a material are mainly due to the magnetic moments of their atoms orbiting magnetic moments (both orbital angular momentum and intrinsic spin magnetic moments).

Therefore in an electromagnetic material we will have a magnetic dipole moment density as a magnetization density field $M=M(\boldsymbol{r})=\frac{d\boldsymbol{m}}{dV}$ (the amount of magnetic moment at position $\boldsymbol{r}$ in the volume element $dV(\boldsymbol{r})=d^3\boldsymbol{r}$) .

Sometimes, either spontaneously, or owing to an applied external magnetic field of intensity *H* each electron magnetic moments will be on average lined up. The magnetization density field $M=M(t,\boldsymbol{r})$ must depend on the history of magnetic intensity field $H^t=(H(\tau))_{\tau<t}$ ($H(\tau)=H(\tau,\boldsymbol{r})$ magnetic intensity vector field) having $M=f(H^t)$ and we will have $B=\mu_0 H+\mu_0 M$ where μ_0 is the magnetic permeability of vacuum, $\nabla\times M=\vec{j}_b-\frac{\partial P}{\partial t}$, $\nabla\times H=\vec{j}_f+\frac{\partial D}{\partial t}$,

$\vec{j}_b$ -the bound charge current density , $\vec{j}_f$ -the free charge current density ,

$\vec{j}=\vec{j}_f+\vec{j}_b$ -the total charge current density .

Thus we have a macroscopic formulation of Maxwell's equations for materials with polarization and magnetization :

$\nabla\cdot D=\rho_f$ Gauss law

$\nabla\cdot B=0$ Gauss law for magnetism

$\nabla\times E=-\frac{\partial B}{\partial t}$ Faraday law of induction

$\nabla\times H=\vec{j}_f+\frac{\partial D}{\partial t}$ Ampere circuital law

$D=\varepsilon_0 E+P$, $H=\frac{1}{\mu_0}B-M$ electromagnetic constitutive laws for the material

$\vec{j}_b=\nabla\times M+\frac{\partial P}{\partial t}$, $\rho_b=-\nabla\cdot P$, $\rho=\rho_b+\rho_f$, $\vec{j}=\vec{j}_b+\vec{j}_f$

and we can derive the charge conservation laws :

$$\frac{\partial \rho_b}{\partial t}+\nabla\cdot\vec{j}_b=0\ ,\ \frac{\partial \rho_f}{\partial t}+\nabla\cdot\vec{j}_f=0\ ,\ \frac{\partial \rho}{\partial t}+\nabla\cdot\vec{j}=0\ .$$

Consider an electric dipole generated by the dipole charge distribution

$$\rho(\boldsymbol{r})=q\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_+)-q\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_-)\ \text{with}\ q>0\ ,\ \boldsymbol{d}_p=\boldsymbol{r}_+-\boldsymbol{r}_-\ .$$

A stationary electric field E produces forces $F_+=qE$, $F_-=-qE$ acting on the ends of the rigid segment A_+A_- which rotate the dipole in the $(E,\boldsymbol{d}_p)$ plane to a stable equilibrium at which the angle between E and $\boldsymbol{d}_p$ is 0.
Taking the coordinate system such that $\boldsymbol{r}_++\boldsymbol{r}_-=0$, $E=(-\widetilde{E},0,0)$, $\widetilde{E}>0$, $\boldsymbol{r}_+=(\frac{d_p}{2}\cos\alpha,\frac{d_p}{2}\sin\alpha,0)$ we have that during a rotation of angle $d\alpha$ of the segment A_-A_+ around the mass center $(0,0,0)$ in the $(e,\boldsymbol{d}_p)$ plane, the system does the work $L=q\,d_p\,E\sin\alpha\,d\alpha=-dU$ where U is the potential energy of the dipole in the electric stationary field.
Therefore for the potential energy of the electric dipole in a electric field we have

$$U=\int -d_p\widetilde{E}\sin\alpha\,d\alpha=d_p\widetilde{E}\cos\alpha=-\boldsymbol{p}\cdot E\ ,\ U=-\boldsymbol{p}\cdot E \qquad (1)$$

$\boldsymbol{p}$ electric dipole moment , E electric intensity field .

Consider now a magnetic dipole in the Amperian loop model given by
$I=j\,A_m$ the electric current intensity through the wire loop
$\boldsymbol{r}(\alpha,\theta)=(-r_m\sin\alpha,r_m\cos\alpha\sin\theta,-r_m\cos\alpha\cos\theta)$
$\vec{j}(\alpha,\theta)=(-j\cos\alpha,-j\sin\alpha\sin\theta,j\sin\alpha\cos\theta)$.
A stationary magnetic field $B=(0,0,\widetilde{B})$ produces by the Lorentz forces a total moment acting on the dipole $\vec{M}_O=\int_0^{2\pi}\boldsymbol{r}\times(\vec{j}\times B)A_m r_m\,d\alpha=\int_0^{2\pi}\vec{j}(\boldsymbol{r}\cdot B)A_m r_m\,d\alpha=$

$=\widetilde{B}\,\pi A_m r_m^2\,j\cos\theta e_1=M_O e_1$.
The dipole rotates therefore around the Ox_1 axis with θ as a motion parameter to an equilibrium position at $\theta=-\frac{\pi}{2}$ if $\widetilde{B}>0$ and at $\theta=\frac{\pi}{2}$ if $\widetilde{B}<0$.
Hence if $\widetilde{B}>0$ during a rotation of $-d\theta$ the system does the work $L=-M_O\,d\theta=-dU$ where U is the potential energy of the dipole in the stationary magnetic field.
For the potential energy we will have $U=\int M_O\,d\theta=\pi\widetilde{B}\,A_m r_m^2\,j\sin\theta=-\boldsymbol{m}\cdot B$
If $\widetilde{B}<0$ we have $L=M_O\,d\theta$ during a rotation of $d\theta$ and we have again $U=-\pi\widetilde{B}\,A_m r_m^2\,j\sin\theta=-\boldsymbol{m}\cdot B$
Thus $U=-\boldsymbol{m}\cdot B$ (2) with $\boldsymbol{m}$ magnetic moment , B magnetic induction field .

For a dielectric material in a slow changing electric field $E = E(t, \boldsymbol{r})$ we will have a induced variable polarization density $P = f(E^t)$ which according to (1) produces a variation of the potential energy of each dipole in the material system with

$\boldsymbol{p}=\boldsymbol{p}(t,\boldsymbol{r})$ electric dipole moment at position $\boldsymbol{r}$ by an amount of $-\frac{\partial \boldsymbol{p}}{\partial t}\cdot E(t,\boldsymbol{r})dt$.

Having $\boldsymbol{p}(t,\boldsymbol{r})=P(t,\boldsymbol{r})dV(\boldsymbol{r})$ the heat dissipated energy from polarization processes in the material during a polarization cycle $\Gamma:(E(\tau,\boldsymbol{r}),P(\tau,\boldsymbol{r}))_{\tau\in(0,T)}$, $E(0,\boldsymbol{r})=E(T,\boldsymbol{r})$ in the (E,P) plane will have a density

$$\int_0^T E\cdot\frac{\partial P}{\partial \tau}d\tau=\oint_\Gamma E\cdot dP=\oint_\Gamma E\cdot d(-\varepsilon_0 E+D)=\oint_\Gamma E\cdot dD\ .$$

The dissipated energy density is therefore $\int_0^T E\cdot\frac{\partial D}{\partial \tau}d\tau$.

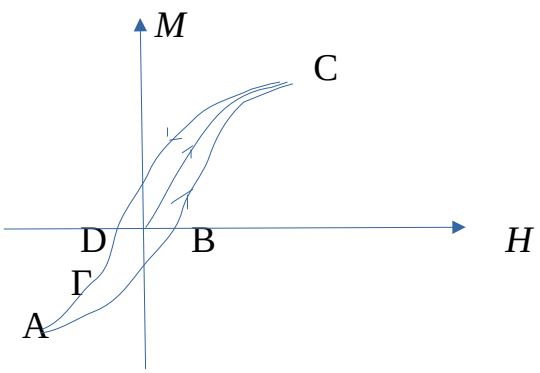
If $E=E_0\exp(-i\omega t)+E_0^*\exp(i\omega t)$ with $E_0=E_0(\boldsymbol{r})\in\mathbb{C}$ is a real harmonic oscillating electric field , the time averaged dissipated power density for $T=\frac{2\pi}{\omega}$: $\frac{1}{T}\int_0^T E\cdot\frac{\partial D}{\partial \tau}d\tau$ will be non-zero only if $\frac{\partial D}{\partial \tau}$ has a component which has the same phase as E . Therefore we consider a constitutive relation for polarisation such that $D=\varepsilon E_0\exp(-i\omega t)+\varepsilon^* E_0^*\exp(i\omega t)$ with $\varepsilon=\varepsilon_{real}+i\varepsilon_{imag}$ a complex dielectric constant.

In that case the time averaged dissipated power density is

$$\frac{1}{T}\int_0^T(E_0\exp(-i\omega t)+E_0^*\exp(i\omega t))i\omega(\varepsilon^* E_0^*\exp(i\omega t)-\varepsilon E_0\exp(-i\omega t))dt=$$
$$=2\omega\varepsilon_{imag}|E_0|^2.$$

For a material with magnetic ordering (like ferromagnetic materials) in a slow changing magnetic field $H = H(t, \boldsymbol{r})$ we will have the induced variable magnetization $M = f(H^t)$ which according to (2) , in the same way as for dielectric materials above, leads to a dissipated energy density

$\oint_\Gamma B\cdot dM=\oint_\Gamma \mu_0 H\cdot dM$ during a magnetization cycle $\Gamma:(H(\tau,\boldsymbol{r}),M(\tau,\boldsymbol{r}))_{\tau\in(0,T)}$, $H(0,\boldsymbol{r})=H(T,\boldsymbol{r})$ in the (H,M) plane.



We note that $\oint_{\Gamma} H\cdot dM$ is the 'area' of the region surrounded by the hysteresis cycle in the (H,M) plane: $\Gamma(ABCDA)$.

Consider now a harmonic oscillating electric dipole $\boldsymbol{p}(t)=\boldsymbol{p_0}\exp(-i\,\omega t)$ with constant $\boldsymbol{p_0}$ and mass center at the origin of the coordinate system.
The dipole can be considered given by a $\rho = \rho(t, \boldsymbol{r})$ neutral variable charge distribution and as two in opposite directions oscillating charges q , $-q$ having position coordinates variable $\boldsymbol{r}_+(t)$, $\boldsymbol{r}_-(t)$. Therefore we have a charge density $\rho(t,\boldsymbol{r})=q\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_+(t))-q\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_-(t))$ and a current density $\vec{j}(t,\boldsymbol{r})=q\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_+(t))\dot{\boldsymbol{r}}_+(t)-q\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_-(t))\dot{\boldsymbol{r}}_-(t)$.
It follows $\dot{\boldsymbol{p}}(\tau)=\int\frac{\partial\rho}{\partial t}(\tau,\boldsymbol{r})\boldsymbol{r}\,d^3\boldsymbol{r}=q(\dot{\boldsymbol{r}}_+(\tau)-\dot{\boldsymbol{r}}_-(\tau))=\int\vec{j}(\tau,\boldsymbol{r})d^3\boldsymbol{r}$.
The oscillating dipole generates a variable electromagnetic field which in the Lorentz gauge (see Chap. Electromagnetic four-potential) has a four-potential $(A^\alpha)_{\alpha=\overline{0,3}}=(\frac{\varphi}{c},A)$ (denoting $A=(A^i)_{i=\overline{1,3}}$) given by

$$\varphi(t,\boldsymbol{R})=\frac{1}{4\pi\varepsilon_0}\int\frac{\rho(t-\frac{\|\boldsymbol{R}-\boldsymbol{r}\|}{c},\boldsymbol{r})}{\|\boldsymbol{R}-\boldsymbol{r}\|}d^3\boldsymbol{r}$$

$$A(t,\boldsymbol{R})=\frac{\mu_0}{4\pi}\int\frac{\vec{j}(t-\frac{\|\boldsymbol{R}-\boldsymbol{r}\|}{c},\boldsymbol{r})}{\|\boldsymbol{R}-\boldsymbol{r}\|}d^3\boldsymbol{r}\ ,$$

where $\boldsymbol{R},\boldsymbol{r}\in\mathbb{R}^3$ denoting $r=\|\boldsymbol{r}\|$, $R=\|\boldsymbol{R}\|$
For large R , $\frac{r}{R}\ll 1$ we will have:

$$\varphi=\frac{1}{4\pi\varepsilon_0}\int\left(\rho(t-\frac{R}{c},\boldsymbol{r})+\frac{\partial\rho}{\partial t}(t-\frac{R}{c},\boldsymbol{r})\frac{\boldsymbol{R}\cdot\boldsymbol{r}}{c\,R}\right)\left(\frac{1}{R}+\frac{1}{R^3}\boldsymbol{R}\cdot\boldsymbol{r}\right)d^3\boldsymbol{r}+O\left(\left(\frac{r}{R}\right)^2\right)=$$

$$=\frac{1}{4\pi\varepsilon_0}\left(\frac{\boldsymbol{p}(\tau)\cdot\boldsymbol{R}}{R^3}+\frac{\dot{\boldsymbol{p}}(\tau)\cdot\boldsymbol{R}}{c\,R^2}\right)+O\left(\left(\frac{r}{R}\right)^2\right)$$

$$A=\frac{\mu_0}{4\pi}\int\left(\vec{j}(t-\frac{R}{c},\boldsymbol{r})+\frac{\partial\vec{j}}{\partial t}(t-\frac{R}{c},\boldsymbol{r})\frac{\boldsymbol{R}\cdot\boldsymbol{r}}{c\,r}\right)\left(\frac{1}{R}+\frac{1}{R^3}\boldsymbol{R}\cdot\boldsymbol{r}\right)d^3\boldsymbol{r}+O\left(\left(\frac{r}{R}\right)^2\right)=$$

$$=\frac{\mu_0}{4\pi}\frac{\dot{\boldsymbol{p}}(\tau)}{R}+O\left(\frac{r}{R}\right)$$

where $\tau=t-\frac{R}{c}$ and after some calculus, for the generated electromagnetic field, for large R:

$$E(t,\boldsymbol{R})=-\nabla\varphi-\frac{\partial A}{\partial t}=$$

$$=\left(\frac{3(\hat{\boldsymbol{R}}\cdot\boldsymbol{p_0})\hat{\boldsymbol{R}}-\boldsymbol{p_0}}{R}\left(\frac{c^2}{\omega^2R^2}-\frac{ic}{\omega R}\right)+\frac{(\hat{\boldsymbol{R}}\times\boldsymbol{p_0})\times\hat{\boldsymbol{R}}}{R}\right)\frac{\omega^2}{c^2}\frac{\exp(-i\omega\tau)}{4\pi\varepsilon_0} \qquad (3)$$

$$B(t,\boldsymbol{R})=\nabla\times A=\frac{\hat{\boldsymbol{R}}\times\boldsymbol{p_0}}{R}\left(1+\frac{ic}{\omega R}\right)\frac{\omega^2}{c^3}\frac{\exp(-i\omega\tau)}{4\pi\varepsilon_0} \qquad (3')$$

where $\hat{\boldsymbol{R}}=\frac{\boldsymbol{R}}{R}$.

For $\frac{R\omega}{c}\gg 1$ the far field has the form of a radiating 'spherical wave' with angular dependence embedded in the cross product:

$B=\frac{\hat{\boldsymbol{R}}\times\boldsymbol{p_0}}{R}\frac{\omega^2}{c^3}\frac{\exp(-i\omega\tau)}{4\pi\varepsilon_0}$, $E=cB\times\hat{\boldsymbol{R}}$, $\hat{\boldsymbol{R}}\times E=cB$, $E\times B=\frac{1}{c}E^2\hat{\boldsymbol{R}}$,

$\hat{\boldsymbol{R}}=\mathrm{vers}(E\times B)$, $E\cdot B=\hat{\boldsymbol{R}}\cdot E=\hat{\boldsymbol{R}}\cdot B=0$, $E^2=c^2B^2$ (taking for E,B the real parts of the (3) respective (3') expression approximations).

The time averaged energy flux Poynting vector is

$\langle S_P\rangle=\frac{1}{\mu_0}\langle E\times B\rangle=\frac{1}{\mu_0}c\langle B^2\rangle\hat{\boldsymbol{R}}=\frac{\mu_0}{c}p_0^2\frac{\omega^4}{R^2}\frac{\sin^2\theta}{32\pi^2}\hat{\boldsymbol{R}}$ where $\boldsymbol{p_0}=p_0e_3$,

$\hat{\boldsymbol{R}}=(\sin\theta\cos\psi,\sin\theta\sin\psi,\cos\theta)$ in spherical polar coordinates (R,θ,ψ).

Hence the total time averaged power radiated by the field is

$$P=\int_0^{2\pi}\int_0^{\pi}\langle S_P\rangle R^2\sin\theta\,d\theta\,d\psi=\frac{\mu_0\omega^4p_0^2}{c}\frac{1}{32\pi^2}4\pi\int_0^1(1-x^2)\,dx=\frac{\mu_0\omega^4p_0^2}{12\pi c} \qquad (4)\ .$$

When coming from the Sun in the Earth's atmosphere, the lightwaves oscillating electric field acts on the charges within each polarizable air molecule, causing them to move at the same frequency. The particle therefore becomes a small radiating dipole whose radiation we see as scattered light having the same frequency as the incoming lightwaves. Light of higher frequency is therefore scattered by the radiating dipoles in all directions with more radiating power and thus the light received from the sky not directly from the Sun appears more in the higher frequency domain and so it appears in the blue zone of the visible spectrum (the sky is blue). This scattering of sunlight (Rayleigh scattering) removes a significant proportion of the shorter wavelenght (blue and green) from the direct path from the Sun to the observer and the reddening of the Sun is intensified when the Sun is near the horizon because the light received directly from it must pass through more of the atmosphere. So the Sun appears yellow on day time and red on morning and evening time.

The above relations (3) , (3') lead in the case of a stationary electric dipole moment (ω = 0) for large R to expressions of potential and electric field as :

$$\varphi=\frac{1}{4\pi\varepsilon_0}\frac{\boldsymbol{p}\cdot\hat{\boldsymbol{R}}}{R^2}\ ,\ E=\frac{3(\hat{\boldsymbol{R}}\cdot\boldsymbol{p})\hat{\boldsymbol{R}}-\boldsymbol{p}}{4\pi\varepsilon_0 R^3}\qquad(5)$$

For a stationary magnetic dipole given in the Amperian loop model by :
$\boldsymbol{r}(\alpha)=(-r_m\sin\alpha, r_m\cos\alpha, 0)$, $\vec{j}(\alpha)=(-j\cos\alpha, -j\sin\alpha, 0)$, $I=jA_m$ we have the vector potential at large R expressed as

$$A(\boldsymbol{R})=\frac{\mu_0}{4\pi}\int\frac{\vec{j}(\boldsymbol{r})}{\|\boldsymbol{R}-\boldsymbol{r}\|}d^3\boldsymbol{r}\approx\frac{\mu_0}{4\pi}\int\vec{j}(\boldsymbol{r})\left(\frac{1}{R}+\frac{\hat{\boldsymbol{R}}\cdot\boldsymbol{r}}{R^2}\right)d^3\boldsymbol{r}=$$

$$=\frac{\mu_0}{4\pi}\left(\int-\frac{\hat{\boldsymbol{R}}\times(\boldsymbol{r}\times\vec{j}(\boldsymbol{r}))}{R^2}d^3\boldsymbol{r}+\int\frac{\hat{\boldsymbol{R}}\cdot\vec{j}(\boldsymbol{r})}{R^2}\boldsymbol{r}\,d^3\boldsymbol{r}\right)=$$

$$=\frac{\mu_0}{2\pi}\frac{\boldsymbol{m}\times\hat{\boldsymbol{R}}}{R^2}+\frac{\mu_0 r_m^2 A_m j}{4R^2}(\hat{R}_2,\hat{R}_1,0)$$ where

$\boldsymbol{m}=\pi r_m^2 A_m j(0,0,1)$ and $\boldsymbol{m}\times\hat{\boldsymbol{R}}=\pi r_m^2 A_m j(-\hat{R}_2,\hat{R}_1,0)$ and so for large R:

$$A=\frac{\mu_0}{4\pi}\frac{\boldsymbol{m}\times\hat{\boldsymbol{R}}}{R^2}\ ,\ B=\nabla\times A=\frac{\mu_0}{4\pi}\frac{3(\hat{\boldsymbol{R}}\cdot\boldsymbol{m})\hat{\boldsymbol{R}}-\boldsymbol{m}}{R^3}\qquad(5')\ .$$

Considering the Amperian loop model for a magnetic dipole , the torque acting on a magnetic dipole with magnetic moment $\boldsymbol{m}$ in a magnetic field $B=(0,0,\tilde{B})$ will be as we already computed above $\vec{T}=\int_C\boldsymbol{r}\times(\vec{j}\times B)\,ds=\pi r_m^2 A_m j\tilde{B}\sin\theta e_1=\boldsymbol{m}\times B$

where θ is the angle between $\boldsymbol{m}$ and B and C with arc element ds is the loop defining cycle .

Since the potential energy of a magnetic dipole in a magnetic field B is $U = -\boldsymbol{m}.B$, the force acting from a magnetic dipole $\boldsymbol{m}$ located at point P, on a magnetic dipole $\boldsymbol{m_1}$ located at point P_1 will be given by

$\vec{F}=-\nabla_{\boldsymbol{R}}U=\nabla_{\boldsymbol{R}}(\boldsymbol{m_1}\cdot B(\boldsymbol{R}))$ with $\boldsymbol{R}=\overrightarrow{PP_1}$ at large R and $B(\boldsymbol{R})=B$ given by (5').

Also the torque acting on the $\boldsymbol{m_1}$ magnetic dipole from the $\boldsymbol{m}$ magnetic dipole will be $\vec{T}=\boldsymbol{m_1}\times B(\boldsymbol{R})$ in the same conditions as above.

In a similar way, we derive for the force and torque acting from a electric dipole $\boldsymbol{p}$ located at a point P on a electric dipole $\boldsymbol{p_1}$ located at P_1 that

$\vec{F}=\nabla_{\boldsymbol{R}}(\boldsymbol{m}\cdot E(\boldsymbol{R}))$, $\vec{T}=\boldsymbol{p_1}\times E(\boldsymbol{R})$ with $E(\boldsymbol{R})=E$ given by (5).

We consider now a material domain $D\subset\mathbb{R}^3$ with no free charges and polarization density $P=P(\boldsymbol{r})$, $\boldsymbol{r}\in D$. The polarization generates an electrostatic field with potential $\varphi=\varphi(\boldsymbol{R})=\frac{1}{4\pi\varepsilon_0}\int_D\frac{P(\boldsymbol{r})\cdot(\boldsymbol{R}-\boldsymbol{r})}{\|\boldsymbol{R}-\boldsymbol{r}\|^3}d^3\boldsymbol{r}$ (according to (5))

Thus we will have :

$$\varphi(\boldsymbol{R})=\frac{1}{4\pi\varepsilon_0}\int_D P(\boldsymbol{r})\cdot\nabla_r\left(\frac{1}{\|\boldsymbol{r}-\boldsymbol{R}\|}\right)d^3\boldsymbol{r}=\frac{1}{4\pi\varepsilon_0}\left(\int_D\nabla_r\cdot\left(\frac{P(\boldsymbol{r})}{\|\boldsymbol{r}-\boldsymbol{R}\|}\right)d^3\boldsymbol{r}-\int_D\frac{\nabla_r\cdot P(\boldsymbol{r})}{\|\boldsymbol{r}-\boldsymbol{R}\|}d^3\boldsymbol{r}\right)$$

If the polarization density is constant on D , P ($\boldsymbol{r}$) = P it follows:

$\varphi(\boldsymbol{R})=\frac{1}{4\pi\varepsilon_0}\int_{\partial D}\frac{P\cdot\boldsymbol{n}}{\|\boldsymbol{r}-\boldsymbol{R}\|}d\sigma(\boldsymbol{r})$ (with $\boldsymbol{n}$ the outward normal versor on the surface ∂D , $d\sigma$ the surface area element on ∂D , which is the field created by a surface charge distribution $P\cdot\boldsymbol{n}\,d\sigma$ on the boundary ∂D of the domain.

The electric intensity field due the surface charge distribution is

$E(\boldsymbol{R})=-\frac{1}{4\pi\varepsilon_0}\nabla_{\boldsymbol{R}}\int_{\partial D}\frac{P\cdot\boldsymbol{n}}{\|\boldsymbol{R}-\boldsymbol{r}\|}d\sigma(\boldsymbol{r})$ so if D is a ball, at its center the field intensity is $E=-\frac{P}{3\varepsilon_0}$.

We take the example of a dielectric ball in an uniform electric field.

Therefore $D=\{\boldsymbol{r}\in\mathbb{R}^3\,|\,\|\boldsymbol{r}\|\le R\}$. The external electric field is $(0,0,E_\infty)$ which is created by the potential $\varphi_\infty=-E_\infty z$. We consider spherical coordinates (r,θ,ψ) $z=r\cos\theta$, $y=r\sin\theta\sin\psi$, $x=r\sin\theta\cos\psi$.

We assume for the dielectric the linear constitutive equation for the electric induction field $D=\kappa\varepsilon_0 E$, κ -dielectric constant. (There must be no confusion between the dielectric ball *D* which is notation for a set and the electric induction *D* which is notation for a vector field.)

Outside the sphere we have $D=\varepsilon_0 E$ and we assume also that the electric field in z direction E_∞ induces a constant polarization density field on the domain D and in the samedirection $P=3\varepsilon_0\frac{C}{R^3}E_\infty e_3$. Hence the potential outside the sphere is $\varphi_e(\boldsymbol{r})\approx-r\,E_\infty\cos\theta+\frac{1}{4\pi\varepsilon_0}\int_{\partial D}\left(\frac{1}{r}+\frac{\boldsymbol{r}'\cdot\boldsymbol{r}}{r^3}\right)(P\cdot\boldsymbol{n})\,d\sigma(\boldsymbol{r}')=-r\,E_\infty\cos\theta+R^3\frac{(P\cdot\boldsymbol{r})}{r^3}\frac{1}{3\varepsilon_0}$

$\varphi_e(\boldsymbol{r})\approx-r\,E_\infty\cos\theta+\frac{C}{r^2}\cos\theta$ (with C a constant) .

In the interior of the sphere, having no free charge we have $\nabla\cdot D=0$ and so $\nabla\cdot\kappa\varepsilon_0 E=0$, $-\nabla^2\varphi_i=0$ for φ_i the potential inside the sphere.

Therefore we can take $\varphi_i(\boldsymbol{r})=A\,z=A\,r\cos\theta$ (A constant) considering a z dependence of the field.

We must have the continuity of potential and radial component of the electric induction field *D* at the boundary of the sphere (see Appendix : electromagnetic boundary conditions).

Therefore we have

$$-R\,E_\infty+\frac{C}{R^2}=A\,R\ ,\quad \kappa\varepsilon_0 A=-\varepsilon_0 E_\infty-2\frac{\varepsilon_0}{R^3}C$$

leading to $A=-\frac{3}{\kappa+2}E_\infty$, $C=\frac{\kappa-1}{\kappa+2}R^3E_\infty$

Taking $P=\frac{\boldsymbol{p}}{V}$ with $V=\frac{4}{3}\pi R^3$ the domain volume and $\boldsymbol{p}$ the induced polarization we have $\boldsymbol{p}=4\pi\varepsilon_0\frac{\kappa-1}{\kappa+2}R^3E_\infty$ and we see that the induced polarization flips sign if $\kappa<1$ which happens in the case of two different dielectrics separated by a spherical surface and κ replaced by the ratio of the inner to outer region dielectric constants , ε_0 replaced by the outer electric permittivity .

We have $\varphi_i=-\frac{3}{\kappa+2}E_\infty r\cos\theta$ and the electric field intensity inside the sphere is

$$-\nabla\varphi_i=\frac{3}{\kappa+2}(0,0,E_\infty)=\left(1-\frac{\kappa-1}{\kappa+2}\right)(0,0,E_\infty)\ ,$$

$$\varphi_e=\left(-r+\frac{\kappa-1}{\kappa+2}\frac{R^3}{r^2}\right)E_\infty\cos\theta\ .$$

The surface charge density is the difference between the radial field components at the boundary :

$$(\varepsilon_0\varphi_{i,r}-\varepsilon_0\varphi_{e,r})\Big|_{r=R}=\left(-1+\frac{\kappa-1}{\kappa+2}+1+2\frac{\kappa-1}{\kappa+2}\right)\varepsilon_0E_\infty\cos\theta=3\,\varepsilon_0\frac{\kappa-1}{\kappa+2}E_\infty\cos\theta=P\cdot\boldsymbol{n}$$

Thus the dielectric constant treatment is equivalent to the uniform electric dipole moment and leads to zero charge everywhere except for the surface charge at the boundary of the sphere.

Consider now a metalic conductor material domain $D\subset\mathbb{R}^3$ in an electrostatic field $E=E(\boldsymbol{R})$, $\boldsymbol{R}\in\mathbb{R}^3$, $E=-\nabla\varphi$, $\varphi=\varphi(\boldsymbol{R})\in\mathbb{R}$.

If the electric field would not vanish inside the domain we would have a electric charges transport inside the domain. But in the electrostatic case, an equilibrium is achieved so that no electric charges transport exists inside the metal domain. The time interval needed for the redistribution of conduction electrons inside the metal so that no charge currents exist inside the metal is called relaxation time.

Due the redistribution of electric charges , since according to Ohm's law we have $J=\sigma_cE$ (σ_c -conductivity of the metal , J -electric charge current density or charge flux vector field) and since the charge current density vanishes on D after equilibrium is achieved it follows that at equilibrium we have $E(\boldsymbol{R})=0$ for any $\boldsymbol{R}\in D$.

Thus inside the domain D , the potential φ is constant and since the potential must be a continuous function it follows that the potential is equal on the boundary of D with

the same constant as in the interior of D. Hence the tangential component of the electric field $E_t = E - (E\cdot \boldsymbol{n})\boldsymbol{n}$ ($\boldsymbol{n}$ -outwards normal versor on ∂D) which as we prove in the Appendix is continuous when passing the boundary of D, must vanish on the boundary of the domain.

Let $E^{\text{ext}}(\boldsymbol{R}) = \lim\limits_{\substack{\boldsymbol{r}\to\boldsymbol{R}\\ \boldsymbol{r}\in\mathbb{R}^3\setminus D}} E(\boldsymbol{r})$, $E^{\text{int}}(\boldsymbol{R}) = \lim\limits_{\substack{\boldsymbol{r}\to\boldsymbol{R}\\ \boldsymbol{r}\in D}} E(\boldsymbol{r})$ for $\boldsymbol{R}\in\partial D$.

Then $E^{\text{ext}} = (E^{\text{ext}}\cdot\boldsymbol{n})\boldsymbol{n} = E_n$ on ∂D.

Considering the electric induction field $D = D(\boldsymbol{R})$ we must have $D^{\text{int}} = 0$ (since $E^{\text{int}} = 0$) and $D^{\text{ext}} = \varepsilon E^{\text{ext}}$ with ε -electric permittivity of vacuum exterior of the domain and as we prove in the Appendix $D^{\text{ext}}\cdot\boldsymbol{n} - D^{\text{int}}\cdot\boldsymbol{n} = \sigma_f$ on ∂D, where σ_f is the free charge density on ∂D, so $E_n = \frac{\sigma_f}{\varepsilon}\boldsymbol{n}$.

Thus when we have the conductor charged with uncompensated electric charges we have a zero density of charges $\rho = \nabla\cdot D$ in the interior of the conductor domain and the electric charges concentrate on the external surface of the conductor as a free charge surface density σ_f on ∂D so that $E^{\text{ext}}\Big|_{\partial D} = E_n = \frac{\sigma_f}{\varepsilon}\boldsymbol{n}$.

Let *E'* the electric field created in exterior of the domain by the electric charges that are located on the infinitesimal surface element $d\sigma$ of the domain boundary and *E"* the electric field created by the rest of electric charges. Then on $d\sigma$ we will have $E^{\text{ext}} = E_n = E' + E''$, $E^{\text{int}} = 0 = E'' - E'$ and so $E'' = \frac{1}{2}E_n = \frac{\sigma_f}{2\varepsilon}\boldsymbol{n}$.

The force acting on the electric charged surface element $d\sigma$ since the total charge of the element is $\sigma_f d\sigma$ will be therefore $d\vec{F} = \sigma_f d\sigma E'' = \frac{\sigma_f^2 d\sigma}{2\varepsilon}\boldsymbol{n}$.

Hence on ∂D we will have a normal electrostatic pressure acting towards the exterior of D having the value $p = \frac{\sigma_f^2}{2\varepsilon}$. If we have a metal conductor with uncompensated electric charge the electrostatic pressure pushes the electric charges towards the external surface of the metal. Thus if electric charges are communicated to a metal through interior cavities, the charges will pass immediately on the external surface of the metal and the external surfaces of the metal can be charged at high potentials.

The potential φ is as we proved constant on $D\cup\partial D$ (we assume obviously that D is connected) and we define $C = \frac{Q}{\varphi}$ where Q is the total uncompensated electric charge of the metalic domain , the electric capacity of the domain which depends only on the geometry of the conductor (when we define the potential with the condition that it vanishes at infinit large distances).

If $D = \{\boldsymbol{r}\in\mathbb{R}^3 \mid \|\boldsymbol{r}\| < R\}$ is a ball of radius R considering σ_f the constant free electric charge density on ∂D we have $Q = 4\pi R^2\sigma_f$ and computing the external

electric field generated by the constant electric charge density taking the integral on ∂D summation of infinitesimal contributions of the Coulomb fields $dE(\boldsymbol{r})=\frac{\sigma_f}{4\pi\varepsilon\|\boldsymbol{r}-R\boldsymbol{n}\|^3}(\boldsymbol{r}-R\boldsymbol{n})\,d\sigma(R\boldsymbol{n})$ we obtain $E^{\text{ext}}(\boldsymbol{r})=\frac{Q}{4\pi\varepsilon\|\boldsymbol{r}\|^3}\boldsymbol{r}$ and so $\varphi(\boldsymbol{r})=\frac{Q}{4\pi\varepsilon\|\boldsymbol{r}\|}$ for $\boldsymbol{r}\in\mathbb{R}^3\setminus D$ leading since the potential is continuous to a capacity of the sphere $C=4\pi\varepsilon R$.

The value of free charge density on the surface of a conductor can have different values from surface point to surface point.

Let σ_j the free electric charge surface density at point P_j , j=1,2 on the metal external surface such that in P_j the surface has mean curvature $1/R_j$. The infinitesimal surface region around P_j can be considered as a spherical surface with radius R_j .

Therefore the potential around P_j is $\varphi_j=\frac{4\pi R_j^2\sigma_j}{4\pi\varepsilon R_j}$. Because the potential is constant on the whole surface we have $\varphi_1=\varphi_2$ and so $R_1\sigma_1=R_2\sigma_2$.

The free electric charge surface density is proportional to the mean curvature of the surface and the electric charges tend to concentrate at the spikes of the external surface of the metal.

Appendix : boundary conditions for E , D , B , H at a separation surface between domains with different electromagnetic properties

Suppose we have two electromagnetic mediums 1 and 2 with constitutive equations $D^i=\varepsilon_i E^i$, $B^i=\mu_i H^i$, ε_i electric permittivities, μ_i magnetic permeabilities D^i electric induction fields , E^i electric intensity fields, B^i magnetic induction fields, H^i magnetic intensity fields, $i=1,2$.

We consider the separation surface as a layer of thickness δh in the direction of the normal at the actual median separation surface, on which layer E , D , B , H change continuosly and then take $\delta h\to 0$.

We take a region S of the separation surface, and the layer volume element $W_{\delta h}$ of height δh upon S . Let δS the area of S , $\delta S\,\delta h$ the volume of $W_{\delta h}$.

The Gauss laws for electric and magnetic induction lead to

$$\int_{\partial W_{\delta h}} D\cdot\boldsymbol{n}\,d\sigma=\int_{W_{\delta h}}\nabla\cdot D\,d^3\boldsymbol{r}=\int_{W_{\delta h}}\rho_f\,d^3\boldsymbol{r}\ ,$$

$$\int_{\partial W_{\delta h}} B\cdot\boldsymbol{n}\,d\sigma=\int_{W_{\delta h}}\nabla\cdot B\,d^3\boldsymbol{r}=0$$

and we have $\lim_{\delta h\to 0}\int_{\partial W_{\delta h}} D\cdot \boldsymbol{n}\, d\sigma = \boldsymbol{n}\cdot\left(D^1-D^2\right)\delta S$,

$\lim_{\delta h\to 0}\int_{\partial W_{\delta h}} B\cdot \boldsymbol{n}\, d\sigma = \boldsymbol{n}\cdot\left(B^1-B^2\right)\delta S$,

$\lim_{\delta h\to 0}\int_{W_{\delta h}} \rho_f\, d^3\boldsymbol{r} = \sigma_f\,\delta S$ where $\sigma_f = \lim_{\delta h\to 0}\rho_f\,\delta h$ is the surface free charge density on the separation surface, $d\sigma$ is the surface element on S and $\boldsymbol{n}$ is the normal on S pointing from medium 2 to medium 1.

Therefore on the separation surface we have

$B^1\cdot\boldsymbol{n} = B^2\cdot\boldsymbol{n}$, $D^1\cdot\boldsymbol{n} - D^2\cdot\boldsymbol{n} = \sigma_f$.

We take now on the separation surface a path *s* with $\boldsymbol{\tau}_s$ tangent versor and consider the surface *S* made by rising from the points of *s* segments of length *δh*/2 normal to the separation surface in both medium domains 1 and 2 . Let *Γ* the rectangular contour ∂S having tangent versor $\boldsymbol{\tau}$ and lenght element $d\,s$ and let δs be the lenght of s. We choose the orientation of *Γ* such that in the medium domain 1 the orientation of $\boldsymbol{\tau}$ on the parallel to *s* edge of *Γ* is opposite to $\boldsymbol{\tau}_s$.

Let $\boldsymbol{n}_s$ the normal on *S* inducing directly the chosen orientation of *Γ* and also let *dσ* the surface element on *S*.

Then if $\boldsymbol{n}$ is the normal on the separation surface with orientation from medium 2 to medium 1 , we have $\boldsymbol{n}_s = \boldsymbol{\tau}_s\times\boldsymbol{n}$.

We have also $\boldsymbol{\tau}_s\cdot\left(H^2-H^1\right)\delta s = \lim_{\delta h\to 0}\int_\Gamma H\cdot\boldsymbol{\tau}\, d\,s = \lim_{\delta h\to 0}\int_S (\nabla\times H)\cdot\boldsymbol{n}_s\, d\sigma =$

$= \lim_{\delta h\to 0}(\nabla\times H)\cdot(\boldsymbol{\tau}_s\times\boldsymbol{n})\,\delta s\,\delta h$.

By Ampere circuital law follows :

$\left(H^2-H^1\right)\cdot\boldsymbol{\tau}_s = \lim_{\delta h\to 0}\left(\vec{j}_f + \frac{\partial D}{\partial t}\right)\cdot(\boldsymbol{\tau}_s\times\boldsymbol{n})\,\delta h = \lim_{\delta h\to 0}\delta h\left(\boldsymbol{n}\times\vec{j}_j\right)\cdot\boldsymbol{\tau}_s$ where we used the fact that $\frac{\partial D}{\partial t}$ is obviously bounded.

Since $\boldsymbol{\tau}_s$ can be taken any versor with $\boldsymbol{n}\,.\boldsymbol{\tau}_s = 0$ we derive

$\boldsymbol{n}\times\left(H^1-H^2\right) = \vec{j}_s$ where $\vec{j}_s = \lim_{\delta h\to 0}\left(\boldsymbol{n}\times\left(\vec{j}_f\times\boldsymbol{n}\right)\right)\delta h = \lim_{\delta h\to 0}\left(\vec{j}_f - \left(\vec{j}_f\cdot\boldsymbol{n}\right)\boldsymbol{n}\right)$ is the surface free charge current density on the separation surface. The tangential to the surface component of H , namely H – (H . $\boldsymbol{n}$) $\boldsymbol{n}$ has a jump at the separation surface given by $\vec{j}_s\times\boldsymbol{n}$.

In the same way, using the Faraday law of induction we prove that the tangential component of E , namely E – (E . $\boldsymbol{n}$) $\boldsymbol{n}$ is continuous when passing the separation surface.

12. Quantum harmonic oscillator
Quantum rotator

Quantum harmonic oscillator

For a harmonic oscillator we have the classic law of thespatial coordinate evolution in time: $x(t)=A\sin(\omega t+\varphi)$ for a particle of mass m_0 under a elastic force $F_e=-k_e x$ having $\omega=\sqrt{\frac{k_e}{m_0}}$ and the potential energy of the oscillator $V(x)=\frac{m_0\omega^2 x^2}{2}$. Thus we have for the quantum harminic oscillator a Hamiltonian operator $\hat{H}=\frac{\hat{p}_x^2}{2m}+\frac{m_0\omega^2 x^2}{2}$ with $\hat{p}_x=-i\hbar\frac{\partial}{\partial x}$ which leads to the time independent Schroedinger equation $\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-\frac{m_0\omega^2 x^2}{2})\psi=0$ (1) and $\tilde{\psi}=\tilde{\psi}(t,x)=\exp(-iEt)\psi(x)$ the E -eneregy level wave function of the oscillator.

Let $\alpha=\frac{2m_0E}{\hbar^2}$, $\beta=\frac{m_0\omega}{\hbar}=\frac{1}{x_0^2}$, $\lambda=\frac{\alpha}{\beta}=\frac{2E}{\hbar\omega}$, $\xi=\frac{x}{x_0}$ and (1) becomes

$\frac{d^2\psi}{d\xi^2}+(\lambda-\xi^2)\psi=0$ (2) .

Taking $\psi(\xi)=\overline{\psi_0}\exp(-\frac{\xi^2}{2})u(\xi)$ we obtain the equivalent to (2) equation

$\frac{d^2u}{d\xi^2}-2\xi\frac{du}{d\xi}+(\lambda-1)u=0$ (3) .

If $u=u(\xi)$ is a solution of (3) , then $v=u(-\xi)$ is also a solution of (3) and so, the solutions of (3) are linear combinations of even an odd solutions of (3).

Searching for solutions $u(\xi)=\sum_{j=0}^{\infty}b_j\xi^j$ and plugging in (3) we obtain the recurence relation $b_{j+2}=\frac{2j+1-\lambda}{(j+1)(j+2)}b_j$ for $j\in\mathbb{N}$ and so with $\varepsilon=0$ for even solutions and $\varepsilon=1$ for odd solutions we have

$$u(\xi)=b_\varepsilon\xi^\varepsilon+\sum_{k=0}^{\infty}\frac{\prod_{l=0}^{k}(4l+2\varepsilon+1-\lambda)}{(2k+\varepsilon+2)!}b_\varepsilon\xi^{2k+\varepsilon+2}=$$

$$=b_\varepsilon\xi^\varepsilon+\sum_{k=0}^{p-1}b_\varepsilon\frac{\prod_{l=0}^{k}(4l+2\varepsilon+1-\lambda)}{(2k+\varepsilon+2)!}\xi^{2k+\varepsilon+2}+$$

$$+\sum_{k=0}^{\infty}b_\varepsilon\frac{(\prod_{l=0}^{p-1}(4l+2\varepsilon+1-\lambda))(\prod_{l=0}^{k}(4l+2\varepsilon+4p+1-\lambda))}{(2k+\varepsilon+2p+2)!}\xi^{2k+\varepsilon+2p+2}$$

where $p=\max\{\lfloor \lambda/4 \rfloor,1\}$.
Suppose $b_\varepsilon \neq 0$ and $4l+2\varepsilon+1-\lambda\neq 0$ for any $l\in\mathbb{N}$ and we will have a polynomial $P_{\lambda,\varepsilon}=P_{\lambda,\varepsilon}(\xi)$ of degree $2p+\varepsilon$ and a non-zero positive constant $C_{\lambda,\varepsilon}$ such that

$$|u(\xi)|\geq -|b_\varepsilon|P_{\lambda,\varepsilon}(|\xi|)+\sum_{k=0}^{\infty}|b_\varepsilon|C_{\lambda,\varepsilon}\frac{k!|\xi|^{\varepsilon-2}}{4^{p+2}((k+p+2)!)^2}|\xi|^{2(k+p+2)}\geq$$

$$\geq |b_\varepsilon|Q_{\lambda,\varepsilon}(|\xi|)+\sum_{k=0}^{\infty}|b_\varepsilon|C_{\lambda,\varepsilon}\frac{|\xi|^{\varepsilon-2}}{4^{p+2}}\frac{1}{(p+2)!}\left(\frac{2}{3}\right)^{k+2p+4}\frac{1}{(k+3p+6)!}|\xi|^{2(k+3p+6)}=$$

$$=|b_\varepsilon|\widetilde{Q}_{\lambda,\varepsilon}(|\xi|)+|b_\varepsilon|B_{\lambda,\varepsilon}\exp\left(\frac{2}{3}\xi^2\right)$$

where $Q_{\lambda,\varepsilon},\widetilde{Q}_{\lambda,\varepsilon}$ are polynomials of degree $3p+8+\varepsilon$ and
$B_{\lambda,\varepsilon}$ is a non-zero positive constant.
Thus under the supposition we made, the $\psi = \psi(\xi)$ function would be a non-normalizable function because of the behaviour at infinity . Hence we must have $n\in\mathbb{N}$ such that $\lambda-1=2n$ and for $k+1=\lfloor n/2 \rfloor$, $2(k+1)+\varepsilon=n$ it follows $u(\xi)=b_\varepsilon\sum_{l=0}^{k+1}\frac{(k+1)!}{l!(n-2l)!}(-1)^l 2^{-\varepsilon}(2\xi)^{n-2l}$ and we can take the solutions of (3) given by the Hermite polynomials: $u(\xi)=H_n(\xi)=(-1)^n\exp(\xi^2)\frac{d^n}{d\xi^n}\exp(-\xi^2)$

$$H_n(\xi)=\sum_{m=0}^{\lfloor n/2\rfloor}n!\frac{(-1)^m}{m!(n-2m)!}(2\xi)^{n-2m}.$$

The Hermite polynomials $(H_n)_{n\in\mathbb{N}}$ are a complete orthogonal system in $L^2_{\exp(-\xi^2)}(\mathbb{R})$, having $\int_{-\infty}^{\infty}H_n(\xi)H_m(\xi)\exp(-\xi^2)d\xi=\sqrt{\pi}\,2^n n!\,\delta_{nm}$
Therefore the energy levels of the quantum harmonic oscillator are quantized as $E_n=\frac{\hbar\omega\lambda}{2}=\left(n+\frac{1}{2}\right)\hbar\omega$ with the normalized n -th level wave function defined by

$$\psi_n(x)=\frac{\exp\left(-\frac{1}{2}\left(\frac{x}{x_0}\right)^2\right)}{\sqrt{x_0\sqrt{\pi}\,2^n n!}}H_n\left(\frac{x}{x_0}\right).$$

We observe that we have a zero level energy $E_0=\frac{\hbar\omega}{2}$ which can also be justified by the correlation and uncertainity relations

$$[\hat{p}_x,\hat{x}]=-i\hbar\ ,\ \langle(\Delta\hat{p}_x)^2\rangle\langle(\Delta\hat{x})^2\rangle\geq\frac{\hbar^2}{4}\qquad(4)$$

(see Chap. Quantum mechanics formalism) as follows.
Thus , if the oscillator fluctuates in a ground state ψ_0 , for the average spatial coordinate and the average momentum we have
$\langle\hat{x}\rangle=\langle\psi_0|\hat{x}|\psi_0\rangle=0$, $\langle\hat{p}_x\rangle=\langle\psi_0|\hat{p}_x|\psi_0\rangle=0$ and so

$\langle(\Delta\hat{x})^2\rangle=\langle\hat{x}^2\rangle$, $\langle(\Delta\hat{p}_x)^2\rangle=\langle\hat{p}_x^2\rangle$ and from (4) follows $\langle\hat{p}_x^2\rangle\geq\frac{\hbar^2}{4\langle\hat{x}^2\rangle}$,

$E=\langle\widehat{H}\rangle=\frac{\langle\hat{p}_x^2\rangle}{2m_0}+\frac{1}{2}m_0\omega^2\langle\hat{x}^2\rangle\geq\frac{\hbar^2}{8\langle\hat{x}^2\rangle m_0}+\frac{1}{2}m_0\omega^2\langle\hat{x}^2\rangle$ and so for abitrary dispersion of the spatial coordinates fluctuations $\langle\hat{x}^2\rangle^{1/2}$ we have a minimum value of the zero point energy which is $E_0=\frac{\hbar\omega}{2}$ interpretable as the vacuum energy of the oscillator, the average energy of the ground state.

We take $\bar{\alpha},\bar{\beta}\in\mathbb{R}$ such that for

$\hat{a}=\bar{\alpha}\hat{x}-\bar{\beta}\frac{i}{\hbar}\hat{p}_x$, $\hat{a}^+=\bar{\alpha}\hat{x}+\bar{\beta}\frac{i}{\hbar}\hat{p}_x$, $\hat{x}=\frac{1}{2\bar{\alpha}}(\hat{a}+\hat{a}^+)$, $\hat{p}_x=\frac{1}{2\bar{\beta}}i\hbar(\hat{a}-\hat{a}^+)$

we have $[\hat{a},\hat{a}^+]=1$ and the $\hat{a}^2$ and $\hat{a}^{+2}$ terms in $\widehat{H}=\frac{\hat{p}_x^2}{2m_0}+\frac{1}{2}m_0\omega^2\hat{x}^2$ vanish.

It follows $\bar{\alpha}=\frac{1}{2}\left(\frac{m_0\omega}{\hbar}\right)^{1/2}$, $\bar{\beta}=\frac{1}{2}\left(\frac{\hbar}{m_0\omega}\right)$, $\widehat{H}=(\hat{a}^+\hat{a}+\frac{1}{2})\hbar\omega$.

Consider a complete set of eigenfunctions for $\widehat{H}$, $(|\nu\rangle)_\nu$, $\widehat{H}|\nu\rangle=E_\nu|\nu\rangle$.

We have $\widehat{H}\hat{a}|\nu\rangle=\hbar\omega\left(\hat{a}\hat{a}^+-\frac{1}{2}\right)\hat{a}|\nu\rangle=\hat{a}\widehat{H}|\nu\rangle-\hbar\omega\hat{a}|\nu\rangle=(E_\nu-\hbar\omega)|\nu\rangle$

and in a similar way $\widehat{H}\hat{a}^+|\nu\rangle=(E_\nu+\hbar\omega)|\nu\rangle$.

Taking $\widehat{N}=\hat{a}^+\hat{a}$ we have $[\widehat{N},\widehat{H}]=0$ and so $(|\nu\rangle)_\nu$ is a complete set of eigenfunctions for $\widehat{N}$ and since as we proven the energy levels are quantized as $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$ we take must take $E_\nu=\left(\nu+\frac{1}{2}\right)\hbar\omega$, $\widehat{N}|\nu\rangle=\nu|\nu\rangle$,

$\hat{a}\hat{a}^+|\nu\rangle=(\nu+1)|\nu\rangle$, $\hat{a}|\nu\rangle=c_\nu|\nu-1\rangle$, $\hat{a}^+|\nu\rangle=c'_\nu|\nu+1\rangle$,

$\nu=\langle\nu|\hat{a}^+\hat{a}|\nu\rangle=|c_\nu|^2=c'_{\nu-1}c_\nu$, $\nu+1=\langle\nu|\hat{a}\hat{a}^+|\nu\rangle=|c'_\nu|^2$

Since the $|\nu\rangle$ is determined to multiplication with a complex number of unitar absolute value we can take $\hat{a}|\nu\rangle=\sqrt{\nu}|\nu-1\rangle$, $\hat{a}^+|\nu\rangle=\sqrt{\nu+1}|\nu+1\rangle$.

Acting on a quantum state $|\nu\rangle$ the operator $\hat{a}^+$ increases its energy level with a quantum $\hbar\omega$ and the operator $\hat{a}$ decreases its energy level with a quantum $\hbar\omega$.

Therefore the energy states of a quantum oscillator are made of one quantum particle states with energy $\hbar\omega$.

The operator $\widehat{N}=\hat{a}^+\hat{a}$ can be interpreted as the particle number operator (population number) , the operator $\hat{a}^+$ as the creation operator and the operator $\hat{a}$ as the anihilation operator.

Quantum rotator

Consider first a rotation with fixed rotation axis.
Let the rotation axis be *Oz* in a cartesian *Oxyz* frame.
The Hamiltonian is
$\hat{H}=\frac{\hat{L}_z^2}{2I}$ where I is the moment of inertia and $\hat{L}_z$ is the Oz axis angular
angular momentum operator: $\hat{L}_z=-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)=-i\hbar\frac{\partial}{\partial\varphi}$
with $x=r\cos\varphi$, $y=r\sin\varphi$, $z=z$.
The time independent Schroedinger equation is
$\frac{d^2\psi}{d\varphi^2}+k^2\psi=0$ where $\psi=\psi(\varphi)$, $k^2=\frac{2I}{\hbar^2}E$
We must have $\psi(\varphi)=\psi(\varphi+2\pi)$ and therefore the solution is $\psi=\bar{\psi}_0\exp(ik\varphi)$
with $2k\pi=2\pi n$, $n\in\mathbb{Z}$. The energy being quantized as
$E_n=\frac{\hbar^2}{2I}n^2$, $\psi_n=\bar{\psi}_0\exp(in\varphi)$ and we have also a quantized angular momentum
$\hat{L}_z\psi_n=\hbar n\psi_n$.

Consider now a free axis quantum rotator.
In a spherical coordinate system (r , θ , φ)
$x=r\sin\theta\cos\varphi$, $y=r\sin\theta\sin\varphi$, $z=r\cos\theta$ the rotator is localized at
a position vector $\vec{r}(x,y,z)$ and rotates with instataneous rotation axis around
the position vector.
The Hamiltonian operator is $\hat{H}=\frac{\hat{\vec{L}}^2}{2I}$ with $\hat{\vec{L}}=\vec{r}\times\hat{\vec{p}}$ angular momentum operator,
$\hat{\vec{p}}=-i\hbar\nabla$, I-momentum of inertia with respect to the instantaneous rotation axis.
We have $\hat{\vec{L}}^2=-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$ and the eigenfunctions of $\hat{\vec{L}}^2$
the spherical functions $Y_l^m(\theta,\varphi)=P_l^m(\cos\theta)\exp(im\varphi)$
with $m\in\mathbb{Z}$, $l\in\mathbb{N}$, $|m|\le l$, P_l^m -the associated Legendre polynomials ,
$\int_0^{2\pi}\int_0^{\pi}Y_l^m(\theta,\varphi)Y_k^n(\theta,\varphi)\sin\theta\,d\theta\,d\varphi=\frac{4\pi(l+m)!}{(2l+1)(l-m)!}\delta_{mn}\delta_{kl}$,
$\hat{\vec{L}}^2Y_l^m=\hbar^2l(l+1)Y_l^m$ and the energy levels are quantized as $E_l=\frac{\hbar^2}{2I}l(l+1)$ and
energy level is degenerated $g_l=2l+1$ times.
(see Chap. Representations of the rotations group)

For $l,m\in\mathbb{N}$, P_l^m is defined as

$$P_l^m(x)=\frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l=$$

$$=(-1)^m 2^l(1-x^2)^{m/2}\sum_{k=m}^{l}\frac{k!}{(k-m)!}x^{k-m}\binom{l}{k}\binom{\frac{l+k-1}{2}}{l}$$

where $x\in[-1,1]$ and $\binom{\alpha}{k}=\frac{\alpha(\alpha-1)...(\alpha-k+1)}{k!}$ for $\alpha\in\mathbb{R}$, $k\in\mathbb{N}^*$; $\binom{\alpha}{0}=1$

$$P_l^{-m}=(-1)^m\frac{(l-m)!}{(l+m)!}P_l^m \ .$$

13. Electromagnetic waves
Quantization of an electromagnetic field

Electromagnetic waves
Quantization of an electromagnetic field

In the absence of charges and current in vacuum we will have the Maxwell equations

$\nabla\cdot D=0$ (1)

$\nabla\cdot B=0$ (2)

$\nabla\times E=-\frac{\partial B}{\partial t}$ (3)

$\nabla\times H=\frac{\partial D}{\partial t}$ (4)

with constitutive vacuum relations $D=\varepsilon_0 E$ (5) and $\mu_0 H=B$ (6)

E -electric field intensity field, D -electric induction field

H -magnetic field intensity field, B -magnetic induction field

ε_0 -electric permittivity of vacuum

μ_0 -magnetic permeability of vacuum

$(E,B,D,H)=(E,B,D,H)(t,x)\in\mathbb{R}^{12}$, $x=(x^1,x^2,x^3)\in\mathbb{R}^3$, $t\in\mathbb{R}$,

$(E,B,D,H)=(E_i,B_i,D_i,H_i)_{i=\overline{1,3}}$

Applying $\nabla\times$ in (3) from (1)-(6) follows

$-\varepsilon_0\mu_0\frac{\partial^2 E}{\partial t^2}=-\frac{\partial}{\partial t}(\nabla\times\mu_0 H)=\nabla\times(\nabla\times E)=\nabla(\nabla\cdot E)-\nabla^2 E=-\nabla^2 E$ and so

$\frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}-\Delta E=\Box E=0$ (7) where $c=\frac{1}{\varepsilon_0\mu_0}$

In a similar way, applying $\nabla\times$ in (4) we obtain $\frac{1}{c^2}\frac{\partial^2 B}{\partial t^2}-\Delta B=\Box B=0$ (8)

We have the potentials φ , $A=(A_i)_{i=\overline{1,3}}$ such that

$E=-\nabla\varphi-\frac{\partial A}{\partial t}$, $B=\nabla\times A$, $(\varphi,A)=(\varphi,A)(t,x)\in\mathbb{R}^4$

(see Chap. Electromagnetic four-potential)

E,B remain the same under a gauge transformation

$\varphi'=\varphi-\frac{\partial\psi}{\partial t}$, $A'=A+\nabla\psi$ with $\psi=\psi(t,x)\in\mathbb{R}$.

Therefore we can have a Lorentz gauge such that

$\frac{1}{c^2}\frac{\partial\varphi'}{\partial t}+\nabla\cdot A'=0$ (9)

$\Box A'=0$, $\Box\varphi'=0$ (10)

The (10) equations have plane wave solutions

$\varphi'=\varphi'_0\exp(-i(\omega t-\vec{k}\cdot x))+\varphi'^{*}_0\exp(i(\omega t-\vec{k}\cdot x))$

$A'=A'_0\exp(-i(\omega t-\vec{k}\cdot x))+A'^{*}_0\exp(i(\omega t-\vec{k}\cdot x))$

with $\vec{k}=(k_i)_{i=\overline{1,3}}\in\mathbb{R}^3$, $k=\|\vec{k}\|$, $\omega=kc$, $\varphi',A'_{0i}\in\mathbb{C}$, $A'_0=(A'_{0i})_{i=\overline{1,3}}$
(z^* the complex conjugate of z)
Taking a gauge transformation defined by
$\psi=\frac{\varphi'_0}{\omega}i\exp(-i(\omega t-\vec{k}\cdot x))-\frac{\varphi'^*_0}{\omega}i\exp(i(\omega t-\vec{k}\cdot x))$
$\varphi=\varphi'-\frac{\partial\psi}{\partial t}$, $A=A'+\nabla\psi$ we obtain
$\varphi=0$, $\Box A=0$, $\Box\psi=0$, $\nabla\cdot A=0$
Therefore we have plane wave solutions of the Maxwell system given by

$$E=-\frac{\partial A}{\partial t}\ ,\ B=\nabla\times A \qquad \text{with}$$

$A=A_0\exp(-i(\omega t-\vec{k}\cdot x))+A_0^*\exp(i(\omega t-\vec{k}\cdot x))$, $A_0=(A_{0i})_{i=\overline{1,3}}\in\mathbb{C}^3$, (11)
$\vec{k}=(k_i)_{i=\overline{1,3}}\in\mathbb{R}^3$, $k=\|\vec{k}\|$, $\omega=kc$, $\vec{k}\cdot A_0=0$ and it follows
$B\cdot E=0$, $\vec{k}\cdot E=0$, $\vec{k}\cdot B=0$, $\omega B=\vec{k}\times E$, $-k^2E=\omega(\vec{k}\times B)$,
$c(E\times B)=E^2\operatorname{vers}\vec{k}$, $c^2B^2=E^2$
For any propagtion direction $\vec{k}$ we can take two independendent orthogonal polarization directions of E : $e^p_{\vec{k}}\in\mathbb{R}^3$, $p=1,2$ with $e^i_{\vec{k}}\cdot e^j_{\vec{k}}=\delta_{ij}$, $\vec{k}\cdot e^i_{\vec{k}}=0$
$\operatorname{vers}\vec{k}=e^1_{\vec{k}}\times e^2_{\vec{k}}$ for $i,j=1,2$ such that

$$A_0=A_0^1e^1_{\vec{k}}+A_0^2e^2_{\vec{k}}\ ,\ A_0^p\in\mathbb{C}\ ,\ p=1,2$$

$E=E^1e^1_{\vec{k}}+E^2e^2_{\vec{k}}$, $E^p=E^p_0\sin(\omega t-\vec{k}\cdot x+\alpha_p)$, $E^p_0,\alpha_p\in\mathbb{R}$, $p=1,2$.
From (11) follows that the energy density of the wave field is (see Chap. Electromagnetic four-potential Electromagnetic tensor) :
$w=\frac{1}{2}(\varepsilon_0E^2+\frac{1}{\mu_0}B^2)=\varepsilon_0E^2$ and the energy flux Poynting vector is
$S_P=E\times H=\frac{1}{\mu_0}E\times B=\frac{E^2}{c\mu_0}\operatorname{vers}\vec{k}=\varepsilon_0cE^2\operatorname{vers}\vec{k}.$
The energy intensity vector of the wave is $I=\langle S_P\rangle=\frac{1}{T}\int_0^T S_P\,dt=\varepsilon_0c\langle E^2\rangle\operatorname{vers}\vec{k}$
has the propagation direction and the energy intensity of the wave | I | which defines the optical behaviour of the wave (visual perception, photochemic and photoelectric effects, etc.) depends only on the time-averaged electric intensity
$\langle E^2\rangle=\frac{1}{T}\int_0^T E^2\,dt=\frac{1}{2}(E_0^{12}+E_0^{22})$ with $T=\frac{2\pi}{\omega}$.
We have $\frac{\partial w}{\partial t}+\nabla\cdot S_P=0$ (see Chap. Electromagnetic energy-momentum tensor)
$S_P=wc\operatorname{vers}\vec{k}$ is the amount of energy transported by the wave in an unit of time through an unit of surface element which is normal to propagation direction.

Consider now two dielectric mediums 1 and 2 , separated by a plane non-absorbant surface in the plane $x_1 O x_2$. The mediums have electric permittivities ε_1 respective ε_2 and magnetic permeabilities μ_1 respective μ_2 and so the electromagnetic waves speed in the mediums will be $c_1=\frac{1}{\sqrt{\varepsilon_1\mu_1}}$ and respective $c_2=\frac{1}{\sqrt{\varepsilon_2\mu_2}}$.

Let be from 1 medium to the separating surface an incident electromagnetic plane polarized plane wave which has electric intensity field given by

$E=E_0\cos(\omega t-\vec{k}\cdot x)$ and magnetic field intensity $H=\frac{1}{\mu_1\omega}\vec{k}\times E=$

$=\sqrt{\frac{\varepsilon_1}{\mu_1}}\vec{e}\times E$ where $\vec{e}=\operatorname{vers} k$ and so $H=\sqrt{\frac{\varepsilon_1}{\mu_1}}\vec{e}\times E_0\cos(\omega t-\vec{k}\cdot x)$ (12)

Then according to wave propagation laws we will have a reflected electromagnetic wave $E'=E'_0\cos(\omega' t-\vec{k}'\cdot x-\varphi_i)$

$$H'=\sqrt{\frac{\varepsilon_1}{\mu_1}}\vec{e}'\times E'=\sqrt{\frac{\varepsilon_1}{\mu_1}}\vec{e}'\,E'_0\cos(\omega' t-\vec{k}'\cdot x-\varphi_i) \quad (13)$$

and a refracted electromagnetic vave

$$E''=E''_0\cos(\omega'' t-\vec{k}'' x-\varphi_r)$$

$$H''=\sqrt{\frac{\varepsilon_2}{\mu_2}}\vec{e}''\times E''=\sqrt{\frac{\varepsilon_2}{\mu_2}}\vec{e}''\times E''_0\cos(\omega'' t-\vec{k}''\cdot x) \quad (14)$$

where $\vec{e}'=\operatorname{vers}\vec{k}'$, $k' c_1=\omega'$, $\vec{e}''=\operatorname{vers}\vec{k}''$, $k'' c_2=\omega''$.

We can consider that $\vec{k}$ is in the $x_1 O x_3$ plane $e_i=(\delta_{ij})_{j=\overline{1,3}}$ for $i=\overline{1,3}$, e_3 is normal to the separation surface and

$\vec{e}=e_1\sin\theta+e_3\cos\theta$, $\vec{e}'=e_1\sin\theta'-e_3\cos\theta'$, $\vec{e}''=e_1\sin\theta''+e_3\cos\theta''$.

According to the Appendix to Chap. Macroscopic Maxwell equations, since the separation surface $x_3 = 0$ not contains free charges , on $x_3 = 0$ we have:

$E_t+E'_t=E''_t$, $H_t+H'_t=H''_t$

where $E_t^{(i)}=E^{(i)}-(E^{(i)}\cdot e_3)e_3$, $H_t^{(i)}=H^{(i)}-(H^{(i)}\cdot e_3)e_3$ for $i=\overline{0,2}$ are the tangential to separation surface components of electric and magnetic field intensities.

We have $\vec{k}\cdot x=k x_1\sin\theta+k x_3\cos\theta$,

$$\vec{k}'\cdot x=k' x_1\sin\theta'-k' x_3\cos\theta'$$

$$\vec{k}''\cdot x=k'' x_1\sin\theta''+k'' x_3\cos\theta''$$

Therefore for any $t, x_1\in\mathbb{R}$ we must have

$E_{0t}\cos(\omega t-k x_1\sin\theta)+E'_{0t}\cos(\omega' t-k' x_1\sin\theta'-\varphi_i)=$

$=E''_{0t}\cos(\omega'' t-k'' x_1\sin\theta''-\varphi_r)$ (15)

Taking $\psi=k x_1\sin\theta$, $\psi_i=k' x_1\sin\theta'+\varphi_i$, $\psi_r=k'' x_1\sin\theta''+\varphi_r$, differentiating twice with respect to t in (15) for $t = 0$ we obtain

$$E_{0t}\cos\psi+E'_{0t}\cos\psi_i=E''_{0t}\cos\psi_r$$

$$\omega^2 E_{0t}\cos\psi+\omega'^2 E'_{0t}\cos\psi_i=\omega''^2 E''_{0t}\cos\psi_r \quad (15')$$

$$\omega^4 E_{0t}\cos\psi+\omega'^4 E'_{0t}\cos\psi_i=\omega''^4 E''_{0t}\cos\psi_r$$

This system for unknowns $(E_{0t}\cos\psi, E'_{0t}\cos\psi_i, E''_{0t}\cos\psi_r)$ must have a non-zero solution and so

$$\begin{vmatrix} 1 & 1 & 1 \\ \omega^2 & \omega'^2 & \omega''^2 \\ \omega^4 & \omega'^4 & \omega''^4 \end{vmatrix} = 0 \quad , (\ \omega=\omega' \text{ or } \omega=\omega'' \text{ or } \omega'=\omega''\ ) .$$

Supposing $\omega = \omega'$ from the first two equations in (15') will follow $\omega = \omega' = \omega''$. The cases $\omega = \omega''$ and $\omega' = \omega''$ lead in a similar way to $\omega = \omega' = \omega''$.

Differentiating twice with respect to x_1 in (15) in the same way as above we obtain $k\sin\theta = k'\sin\theta' = k''\sin\theta''$ and since $k=\frac{\omega}{c_1}=\frac{\omega'}{c_1}=k'$, $k''=\frac{\omega}{c_2}=\frac{\omega''}{c_2}$ it follows

$\theta=\theta'$, $\frac{\sin\theta}{\sin\theta''}=\frac{\sin\theta'}{\sin\theta''}=\frac{c_1}{c_2}=\frac{n_2}{n_1}$ where $n_i=\frac{c}{c_i}$ is the refraction index of i medium.

Hence as we expected from waves reflection and refraction laws we have :

$\omega=\omega'=\omega''$, $\theta=\theta'$, $\frac{\sin\theta}{\sin\theta''}=\frac{c_1}{c_2}$, $n_1\sin\theta=n_2\sin\theta''$.

We must have also $\varphi_i = \varphi_r = 0$ so that the conditions at the separation surface lead to $E_{0t}+E'_{0t}=E''_{0t}$, $H_{0t}+H'_{0t}=H''_{0t}$ relations for the tangential components of amplitudes for electric and magnetic field intensities.

We consider the transversal magnetic case (TM) : $E_0\cdot(\vec{e}\times e_3)=0$, E_0 in the $(\vec{e}, e_3)$ plane and so H_0 normal to the $(\vec{e}, e_3)$ plane and the transversal electric case (TE): $H_0\cdot(\vec{e}\times e_3)$, H_0 in the $(\vec{e}, e_3)$ plane and so E_0 normal to the $(\vec{e}, e_3)$ plane.

We have $H_0=\sqrt{\frac{\varepsilon_1}{\mu_1}}\vec{e}\times E_0$, $\sqrt{\frac{\varepsilon_1}{\mu_1}}E_0=-\vec{e}\times H_0$.

In the (TM) case we obtain

$H_{0t}=H_0=H_{0s}e_2$, $H'_{0t}=H'_0=H'_{0s}e_2$, $H''_{0t}=H''_0=H''_{0s}e_2$ with $H_{0s}^{(i)}\in\mathbb{R}$,

$H_{0s}+H'_{0s}=H''_{0s}$,

$E_0=-\sqrt{\frac{\mu_1}{\varepsilon_1}}H_{0s}\sin(\theta)e_3+\sqrt{\frac{\mu_1}{\varepsilon_1}}H_{0s}\cos(\theta)e_1=E_{0p}e_2\times\vec{e}$

$E'_0=-\sqrt{\frac{\mu_1}{\varepsilon_1}}H'_{0s}\sin(\theta')e_3-\sqrt{\frac{\mu_1}{\varepsilon_1}}H'_{0s}\cos(\theta')e_1=E'_{0p}e_2\times\vec{e}'$

$E''_0=-\sqrt{\frac{\mu_2}{\varepsilon_2}}H''_{0s}\sin(\theta'')e_3+\sqrt{\frac{\mu_2}{\varepsilon_2}}H''_{0s}\cos(\theta'')e_1=E''_{0p}e_2\times\vec{e}''$

$E_{0t}=\sqrt{\frac{\mu_1}{\varepsilon_1}}H_{0s}\cos(\theta)e_1=E_{0p}\cos(\theta)e_1$

$E'_{0t}=-\sqrt{\frac{\mu_1}{\varepsilon_1}}H'_{0s}\cos(\theta')e_1=-E'_{0p}\cos(\theta')e_1$

$E''_{0t}=\sqrt{\frac{\mu_2}{\varepsilon_2}}H''_{0s}\cos(\theta'')e_1=E''_{0p}\cos(\theta'')e_1$

Therefore in the (TM) case we have

$$\begin{aligned}&(E_{0p}-E'_{0p})\cos\theta=E''_{0p}\cos\theta''\\&\sqrt{\frac{\varepsilon_1}{\mu_1}}(E_{0p}+E'_{0p})=\sqrt{\frac{\varepsilon_2}{\mu_2}}E''_{0p}\end{aligned}\qquad(16)$$

Taking $\mu_1=\mu_2=\mu$ the last equation becomes

$(E_{0p}+E'_{0p})\sin\theta''=E''_{0p}\sin\theta$ (17) .

From (16) and (17) follows now

$$E'_{0p}=\frac{\tan(\theta-\theta'')}{\tan(\theta+\theta'')}E_{0p}\qquad(17')$$

$$E''_{0p}=\frac{2\cos(\theta)\sin(\theta'')}{\sin(\theta+\theta'')\cos(\theta-\theta'')}\qquad(17'')$$

At the limit $\theta\to 0$ with $\frac{\sin\theta}{\sin\theta''}=\frac{n_2}{n_1}=n$ we derive now

$$E'_{0p}=\frac{n-1}{n+1}E_{0p}\quad,\quad E''_{0p}=\frac{2}{n+1}E_{0p}\ .$$

In this case the energy intensities of the waves will be:

$$|I|=\frac{1}{2}\varepsilon_1 c_1 E_{0p}^2\ ,\ |I'|=\frac{1}{2}\varepsilon_1 c_1\left(\frac{n-1}{n+1}\right)^2 E_{0p}^2\ ,\ |I''|=\frac{1}{2}\varepsilon_2 c_2\frac{4}{(n+1)^2}E_{0p}^2$$

Since $\varepsilon_2 c_2=\sqrt{\frac{\varepsilon_2}{\mu}}=\frac{1}{c_2\mu}=\frac{n}{c_1\mu}=n\varepsilon_1 c_1$ we can verify that

$|I'|+|I''|=|I|$ which is the expression of energy conservation of the incident wave for a non-absorbing separation surface (that is there are no free charges on the surface).

In the (TE) case we obtain

$E_0=E_{0t}=E_{0s}e_2$, $E'_0=E'_{0t}=E'_{0s}e_2$, $E''_0=E''_{0t}=E''_{0s}e_2$ with $E_{0s}^{(i)}\in\mathbb{R}$

$$H_0=\sqrt{\frac{\varepsilon_1}{\mu_1}}E_{0s}\sin(\theta)e_3-\sqrt{\frac{\varepsilon_1}{\mu_1}}E_{0s}\cos(\theta)e_1$$

$$H'_0=\sqrt{\frac{\varepsilon_1}{\mu_1}}E'_{0s}\sin(\theta')e_3+\sqrt{\frac{\varepsilon_1}{\mu_1}}E'_{0s}\cos(\theta')e_1$$

$$H''_0=\sqrt{\frac{\varepsilon_2}{\mu_2}}E''_{0s}\sin(\theta'')e_3-\sqrt{\frac{\varepsilon_2}{\mu_2}}E''_{0s}\cos(\theta'')e_1$$

$$H_{0t}=-\sqrt{\frac{\varepsilon_1}{\mu_1}}E_{0s}\cos(\theta)e_1$$

$$H'_{0t}=\sqrt{\frac{\varepsilon_1}{\mu_1}}E'_{0s}\cos(\theta')e_1$$

$$H''_{0t}=-\sqrt{\frac{\varepsilon_2}{\mu_2}}E''_{0s}\cos(\theta'')e_1\ .$$

Therefore in the (TE) case e have:

$$\begin{aligned}&E_{0s}+E'_{0s}=E''_{0s}\\&\sqrt{\frac{\varepsilon_1}{\mu_1}}(E_{0s}-E'_{0s})\cos(\theta)=\sqrt{\frac{\varepsilon_2}{\mu_2}}E''_{0s}\cos(\theta'')\end{aligned}\qquad(18)$$

Taking $\mu_1=\mu_2=\mu$ the last relation becomes

$\sin(\theta'')\cos(\theta)(E_{0s}-E'_{0s})=E''_{0s}\sin(\theta)\cos(\theta'')$ (19) .

From (18) and (19) follows

$$E'_{0s}=-\frac{\sin(\theta-\theta'')}{\sin(\theta+\theta'')}E_{0s}$$

$$E''_{0s}=\frac{2\sin(\theta'')\cos(\theta)}{\sin(\theta+\theta'')}E_{0s}\ .$$

At the limit $\theta\to 0$ with $\frac{\sin\theta}{\sin\theta''}=\frac{n_2}{n_1}=n$ we have

$E'_{0s}=-\frac{n-1}{n+1}$, $E''_{0s}=\frac{2}{n+1}E_{0s}$ and the energy intensities of the waves are

$|I|=\frac{1}{2}\varepsilon_1 c_1 E_{0s}^2$, $|I'|=\frac{1}{2}\varepsilon_1 c_1\left(\frac{n-1}{n+1}\right)^2 E_{0s}^2$, $|I''|=\frac{1}{2}\varepsilon_2 c_2\frac{4}{(n+1)^2}E_{0s}^2$.

Again we can verify the energy conservation of the incident wave for a non-absorbing separation surface, as above in the (TM) case:

$|I'|+|I''|=|I|$.

In the general case we will have the sum of transversal and parallel to the incidence plane components:

$E_0=E_{0s}e_2+E_{0p}e_2\times\vec{e}$

$E'_0=E'_{0s}e_2+E'_{0p}e_2\times\vec{e}'$

$E''_0=E''_{0s}e_2+E''_{0p}e_2\times\vec{e}''$.

We can see from (17') that if $\theta=\theta_B$ such that $\theta_B+\theta_B''=\frac{\pi}{2}$ we have $E'_{0p}=0$ and the reflected wave will contain only the transversal electric component and will be therefore plane polarized in one direction, transversal to the incidence plane.

θ_B is the Brewster angle, having $n=\frac{\sin\theta_B}{\sin\theta_B''}=\tan\theta_B$. The Brewster angle is given by $\tan\theta_B=n$.

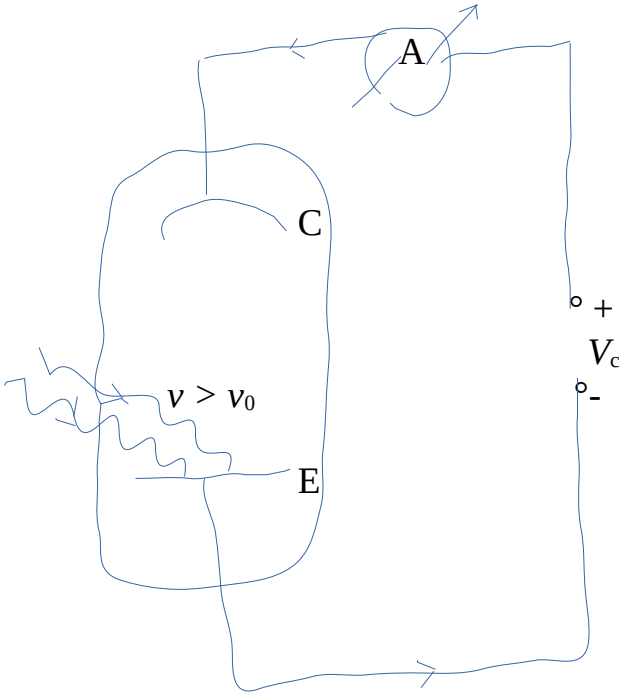
We explained some phenomenons like refraction , reflection, interference, diffraction pf light supposing that light is an electromagnetic wave. Phenomenons like photoelectric effect, Compton effect, pressure of light can be explained only supposing that electromagnetic radiation transfers energy as a quantized flux of particles called photons. With a monochromatic radiation of frequency ν and wave propagation vector $\vec{k}$ in vacuum we will therefore associate photons having wave functions of the form $\psi=\psi_0\exp(-\frac{i}{\hbar}(Et-\vec{p}\cdot x))=\psi_0\exp(-i(\omega t-\vec{k}\cdot x))$ with $E=\hbar\omega$ -energy of the photon , $\omega=2\pi\nu$, $\vec{p}=\hbar\vec{k}$ -momentum of the photon, $k=\frac{2\pi}{\lambda}$, λ -wavelenght of the photon .

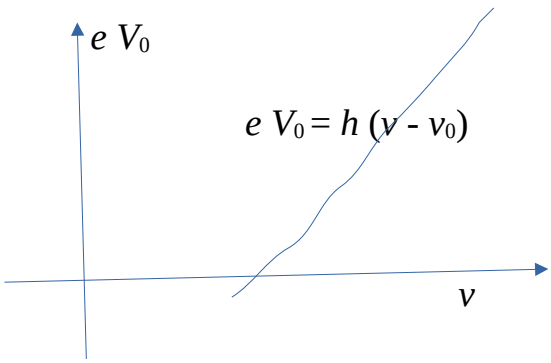
The energy of the electromagnetic wave is therefore quantized in portions of $E = h\nu$ ($h=2\pi\hbar$ -the Planck constant) $h\nu$ -energy of a single photon of a ν frequency radiation. We have $\omega=kc$, c speed of light in vacuum.

Because the photon travels with the speed of light, its rest mass m_0 must be zero so that the momentum relation $\vec{p}=\frac{m_0\vec{v}}{\sqrt{1-\frac{v^2}{c^2}}}=\hbar\vec{k}$ with $\left(\frac{m_0 c}{\sqrt{1-\frac{v^2}{c^2}}},\vec{p}\right)$ the relativistic four-momentum, can have sense for $v = c$.

Photoelectric effect

Consider a vacuum tube transparent to ultraviolet light. Monochromatized light is incident on a emitting electrode E in the vacuum tube which contains also opposite to the electrode E a collector catode C whose voltage V_c can be externally controlled. An electron within the electrode material can absorbe the $h\,v$ energy of a photon from the incident radiation, and if this energy is higher than the electron's binding energy W, $h\,v > W$, the electron aquires a maximum kinetic energy $K_{max} = h\,v - W$ and is likely to be ejected from the electrode. A positive external voltage between C and E is used to direct the ejected photo-emitted electrons onto the collector. An increasing negative voltage prevents all but the highest energy electrons from reaching the collector. When no current is observed through the tube, the value of the retarding voltage, called the stopping potential V_0 is reached. Since the work done by the retarding potential is stopping the electron of charge e is $e\,V_0$ we must have $e\,V_0 = K_{max}$ and the experiment proves the relation $e\,V_0 = K_{max} = h\,v - h\,v_0$ where $h\,v_0 = W$ and v_0 is the minimum frequency for which a current can be observed through the tube.





Compton effect

A photon γ with wavelenght λ collides with an electron e in an atom which is treated to be at rest. The collision causes the electron to recoil and a new photon γ' emerges at an angle θ from the photon's incoming path. Let e' denote the electron after the collision.
We have conservation of energy :

$E_\gamma + E_e = E_{\gamma'} + E_{e'}$ (20)

and momentum conservation:

$\vec{p}_\gamma = \vec{p}_{\gamma'} + \vec{p}_{e'}$ (21) .

With m the rest mass of the electron we have :

$E_\gamma = h\nu$, $E_{\gamma'} = h\nu'$, $E_e = mc^2$, $E_{e'} = \sqrt{(p_{e'}c)^2 + (mc^2)^2}$

(see Chap. Relativistic dynymics)
Thus from (20) we obtain

$(p_{e'}c)^2 = (h\nu - h\nu' + mc^2)^2 - (mc^2)^2$ and from (21) follows

$(p_{e'}c)^2 = p_\gamma^2 c^2 + p_{\gamma'}^2 c^2 - 2c^2 p_\gamma p_{\gamma'} \cos\theta$.

Hence after some calculus we derive $\frac{c}{\nu'} - \frac{c}{\nu} = \frac{h}{mc}(1 - \cos\theta)$.

We can observe therefore a wavelenght shift $\lambda' - \lambda = 2\frac{h}{mc}\sin^2(\frac{\theta}{2})$ at an angle θ photon deviation.

Pressure of light

Consider a surface of unit area on which a beam of monochromatic light is normal incident.
Let n_0 the number of photons hitting the surface in an unit time interval. A fraction R of them is reflected : $n_R = R\, n_0$. n_R the number of reflected photons from the unit surface in unit time interval , $n_A = (1 - R)\, n_0$ the number of photons absorbed from the unit surface in unit time interval.
Each reflected photon experiences during the reflection a momentum variation of $\frac{2\hbar\omega}{c}$ and for each absorbed photon there is a momentum variation of $\frac{\hbar\omega}{c}$ in the surface.
The total momentum variation in unit time on unit surface, gives the exerted pressure of light and will be $p = \frac{2\hbar\omega}{c} n_R + \frac{\hbar\omega}{c} n_A = \frac{n_0 \hbar\omega}{c}(1 + R)$.
$n_0 \hbar\omega = |I|$ is the energy intensity of the incident beam and so for the pressure of light we have derived the formula $p = \frac{|I|}{c}(1 + R)$.

R -reflexion coefficient of the surface ;
$|I|$ -intensity of normal incident light on the surface.
If the beam is incident at θ angle from the normal to the surface we must take $|I|\cos^2\theta$ instead of energy intensity $|I|$.
Indeed, if S_0 is the unit surface transversal to the beam and the beam is incident at angle θ with intensity $|I|=n_0\hbar\omega$ then n_0 photons hit an area of $S=\frac{1}{\cos\theta}$ in an unit time interval.
The normal to S exerted pressure by the reflected photons is
$p_R=\left(\left(\frac{2\hbar\omega}{c}\cos\theta\right)/S\right)n_0R$.
The normal to S exerted pressure by the absorbed photons is
$p_A=\left(\left(\frac{\hbar\omega}{c}\cos\theta\right)/S\right)n_0(1-R)$.
Therefore the pressure exerted by the light beam of monochromatic light with intensity $|I|=n_0\hbar\omega$ incident at θ angle will be $p=\frac{|I|}{c}(1+R)\cos^2\theta$.

Quantization of an electromagnetic field

Consider an electromagnetic field in a cubic box D of edge length L , volume $V=L^3$ determined by the potentials $(\varphi',A')=(\varphi',A')(t,x)$ in the Lorentz gauge with $A'=(A'^i)_{i=\overline{1,3}}$, $x=(x^i)_{i=\overline{1,3}}$ (see Chap. Electromagnetic four-potential) satisfying the boundary conditions $(\varphi',A')(t,x)=(\varphi,A')(t,(x^i+L\,\delta_{ij})_i)$ for any $j=\overline{1,3}$
We consider the electromagnetic field I absence of free chatges and currents ($\rho=0$, $\vec{j}=0$) in vacuum and as we have seen in Chap. Electromagnetic four-potential we have $\Box\varphi'=0$, $\Box A'=0$ with $\Box=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{\partial}{\partial x^i}\frac{\partial}{\partial x^i}$.
Therefore expanding in Fourier series we have

$$\varphi'=\sum_{\vec{k}}\varphi'_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))+\varphi'^{*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x))$$

$$A'=\sum_{\vec{k}}A'_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))+A'^{*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x))$$

with $A'_{\vec{k}}=(A'^i_{\vec{k}})_i\in\mathbb{C}^3$, $\varphi'_{\vec{k}}\in\mathbb{C}$,
$\vec{k}=\frac{2\pi}{L}(n_1e_1+n_2e_2+n_3e_3)$, $n_i\in\mathbb{Z}$, $e_i=(\delta_{ij})_j$ for $i=\overline{1,3}$, $\omega_{\vec{k}}=kc$, $k=\|\vec{k}\|$.
We have the Lorentz gauge relation $\frac{1}{c^2}\frac{\partial\varphi'}{\partial t}+\nabla\cdot A'=0$.
We can consider a gauge transformation given by
$\varphi=\varphi'-\frac{\partial\psi}{\partial t}$, $A=A'+\nabla\psi$,

where $\psi=-(A'_{\vec{0}}+A'^{*}_{\vec{0}})\cdot x+(\varphi'_{\vec{0}}+\varphi'^{*}_{\vec{0}})t+$

$+\sum_{\vec{k}}\frac{i}{\omega_{\vec{k}}}(\varphi'_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))-\varphi'^{*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x)))$

and we will have $\varphi=0$, $\frac{\partial\psi}{\partial t}=\varphi'$, $\Box\psi=0$, $\Box A=0$, $\nabla\cdot A=0$.

Also we have $\int_D \exp(-i(\vec{k}-\vec{k}')\cdot x)d^3x=\delta_{\vec{k}\vec{k}'}V$ (22)

$A=\sum_{\vec{k}\neq\vec{0}}A_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x)+A^{*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x)))$ and since $\nabla\cdot A=0$

$\sum_{\vec{k}\neq\vec{0}}\vec{k}\cdot A_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))-\vec{k}\cdot A^{*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x))=0$ (23) .

Multiplying (23) with $\exp(-i\vec{k}'\cdot x)$ and integrating over x on D we obtain:

$\vec{k}\cdot A_{\vec{k}}\exp(-i\,\omega_{\vec{k}}t)+\vec{k}\cdot A^{*}_{-\vec{k}}\exp(i\,\omega_{\vec{k}}t)=0$ for any $t\in\mathbb{R}$ and any $\vec{k}\neq\vec{0}$ (24)

Differentiating (24) with respect to t and taking $t = 0$ we obtain:

$\vec{k}\cdot A_{\vec{k}}+\vec{k}\cdot A^{*}_{-\vec{k}}=0$, $\omega_{\vec{k}}\vec{k}\cdot A_{\vec{k}}-\omega_{\vec{k}}\vec{k}\cdot A^{*}_{-\vec{k}}=0$ and so it follows

$\vec{k}\cdot A_{\vec{k}}=0$ for any $\vec{k}\neq\vec{0}$, $(\vec{k}=\frac{2\pi}{L}(n_1e_1+n_2e_2+n_3e_3)$, $n_i\in\mathbb{Z}$) .

For any $\vec{k}\neq\vec{0}$ we can choose two polarization versors $e^{p}_{\vec{k}}$, $p=1,2$ such that

$A_{\vec{k}}=A^{1}_{\vec{k}}e^{1}_{\vec{k}}+A^{2}_{\vec{k}}e^{2}_{\vec{k}}$, $\vec{k}\cdot e^{p}_{\vec{k}}=0$, $e^{p}_{\vec{k}}\cdot e^{q}_{\vec{k}}=\delta_{pq}$ for $p,q=1,2$,

$e^{1}_{\vec{k}}\times e^{2}_{\vec{k}}=\mathrm{vers}\,\vec{k}$, $\mathrm{vers}\,\vec{k}\times e^{1}_{\vec{k}}=e^{2}_{\vec{k}}$, $\mathrm{vers}\,\vec{k}\times e^{2}_{\vec{k}}=-e^{1}_{\vec{k}}$

$A=\sum_{\vec{k}\neq\vec{0}}\sum_{p=1}^{2}e^{p}_{\vec{k}}(A^{p}_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))+A^{p*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x)))$.

Taking $\vec{A}^{p}_{\vec{k}}=A^{p}_{\vec{k}}e^{p}_{\vec{k}}$ the electric intensity field and the magnetic intensity field are

$E=-\frac{\partial A}{\partial t}=\sum_{\vec{k},p-i}\omega_{\vec{k}}(\vec{A}^{p}_{\vec{k}}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))-\vec{A}^{p*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x)))$

$H=\frac{1}{\mu_0}\nabla\times A=\frac{i}{\mu_0}\sum_{\vec{k},p}(\vec{k}\times\vec{A}^{p}_{\vec{k}})\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))-(\vec{k}\times\vec{A}^{p*}_{\vec{k}})\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x))$

Integrating the energy density of the electromagnetic field $w=\frac{1}{2}(\varepsilon_0E^2+\mu_0H^2)$

over x on D , considering (22) and $\omega_{\vec{k}}=\frac{1}{\sqrt{\varepsilon_0\mu_0}}k$ we obtain after some calculus

that the energy of the electromagnetic field is is

$W=\int_D w\,d^3x=2\,\varepsilon_0V\sum_{\vec{k},p}\omega^2_{\vec{k}}A^{p}_{\vec{k}}A^{p*}_{\vec{k}}$ (25) .

Considering the transformation to $x^p_{\vec{k}}, p^p_{x\vec{k}} \in \mathbb{R}$ variables defined by

$A^p_{\vec{k}} = \frac{1}{2}\left(\frac{m}{\varepsilon_0 V}\right)^{1/2}\left(x^p_{\vec{k}} + i\frac{p^p_{x\vec{k}}}{\omega_{\vec{k}} m}\right)$ the relation (25) for energy becomes

$W = \sum_{\vec{k},p}\left(\frac{m\,\omega^2_{\vec{k}}\,x^{p\,2}_{\vec{k}}}{2} + \frac{1}{2m}\,p^{p\,2}_{x\vec{k}}\right)$ which is the form for the energy of a system of linear harmonic oscillators (see Chap. Quantum harmonic oscillator).

Therefore we can consider a system of quantum oscillators with creation and anihilation operators given by

$$\hat{a}^p_{\vec{k}} = \left(\frac{m\,\omega_{\vec{k}}}{2\hbar}\right)^{1/2}\left(\hat{x}^p_{\vec{k}} + \frac{i}{m\,\omega_{\vec{k}}}\,\hat{p}^p_{x\vec{k}}\right) = \left(\frac{2\,\varepsilon_0\,\omega_{\vec{k}}\,V}{\hbar}\right)^{1/2}\hat{A}^p_{\vec{k}}$$

$$\hat{a}^{p+}_{\vec{k}} = \left(\frac{m\,\omega_{\vec{k}}}{2\hbar}\right)^{1/2}\left(\hat{x}^p_{\vec{k}} - \frac{i}{m\,\omega_{\vec{k}}}\,\hat{p}^p_{x\vec{k}}\right) = \left(\frac{2\,\varepsilon_0\,\omega_{\vec{k}}\,V}{\hbar}\right)^{1/2}\hat{A}^{p+}_{\vec{k}}$$

where $\hat{A}^p_{\vec{k}}$ is a quantum operator associated to $A^p_{\vec{k}}$ variable.

We must assume the commutation relations $[\hat{a}^p_{\vec{k}}, \hat{a}^{p'+}_{\vec{k}'}] = \delta_{\vec{k}\vec{k}'}\,\delta_{pp'}$ suitable for creation and anihilation operators and the electromagnetic field in the *D* box is described as a quantum system with Hamiltonian operator

$\hat{H} = \sum_{\vec{k},p}\hbar\,\omega_{\vec{k}}\left(\hat{a}^{p+}_{\vec{k}}\,\hat{a}^p_{\vec{k}} + \frac{1}{2}\right)$. (like the system of quantum oscillators)

The field has a ground state (the vacuum state) $|0\rangle$ in which no field is detected and $\hat{a}^{p+}_{\vec{k}}|0\rangle$ is the single particle state that corresponds to one photon of energy $\hbar\,\omega_{\vec{k}}$ and polarization p. Also we must have $\hat{a}^p_{\vec{k}}|0\rangle = 0$ for any $\vec{k}, p$.

$\hat{N}^p_{\vec{k}} = \hat{a}^{p+}_{\vec{k}}\,\hat{a}^p_{\vec{k}}$ is the photon particles of energy $\hbar\,\omega_{\vec{k}}$ and polarization p number operator and its eigenvalues represent the number of photons of the respective energy and polarization from the field. (see Chap. Quantum harmonic oscillator)

The vacuum fluctuations give a vacuum energy $\sum_{\vec{k},p}\frac{1}{2}\hbar\,\omega_{\vec{k}} = \boldsymbol{E_0}$ and the energy levels of the field are measured relative to this level , which level generally not affects the energy transfer between field and substance, despite the fact that this energy level associated to the electromagnetic field must be infinite.

The field operator function of the electromagnetic field is

$\hat{A} = \hat{A}(t,x) = \sum_{\vec{k},p} e^p_{\vec{k}}\left(\hat{A}^p_{\vec{k}}\exp(-i(\omega_{\vec{k}}t - \vec{k}\cdot x)) + \hat{A}^{p*}_{\vec{k}}\exp(i(\omega_{\vec{k}}t - \vec{k}\cdot x))\right)$

and it acts on a Hilbert space $\boldsymbol{H}$ which contains the vacuum state $|0\rangle$ and the single photon wave functions $\hat{a}^{p+}_{\vec{k}}|0\rangle$.

We can verify that for the state $|\psi_N\rangle=\prod_{i=1}^{N}\hat{a}_{\vec{k}i}^{p\,i+}|0\rangle$ we have

$\widehat{H}|\psi_N\rangle=\sum_{i=1}^{N}\hbar\,\omega_{\vec{k}i}|\psi_N\rangle$ and

$\widehat{N}_{\vec{k}}^{p}|\psi_N\rangle=n_{\vec{k}}^{p}|\psi_N\rangle$ where $n_{\vec{k}}^{p}=\text{card}\{j\in\{1,2,\ldots,N\}|\vec{k}_j=\vec{k}$ and $p_j=p\}$.

The electromagnetic field in the box *D* can be indeed considered as a system of photons with different wave numbers $\vec{k}_i$ and polarizations p_i .

14. Doppler effect for electromagnetic waves
Relativistic dynamics
Compton wavelenght

Doppler effect for electromagnetic waves
Relativistic dynamics. Compton wavelenght

Consider an electromagnetic field in vacuum, the Minkowski space considered with signature (+,-,-,-) and space-time coordinates $(x^{\alpha})_{\alpha=\overline{0,3}}=(c\,t,x,y,z)$, c speed of light in vacuum.

We have the electromagnetic tensor (see Chap. Electromagnetic tensor) :

$$(F^{\alpha\beta})_{\alpha,\beta}=\begin{pmatrix} 0 & -\frac{E_1}{c} & -\frac{E_2}{c} & -\frac{E_3}{c} \\ \frac{E_1}{c} & 0 & -B_3 & B_2 \\ \frac{E_2}{c} & B_3 & 0 & -B_1 \\ \frac{E_3}{c} & -B_2 & B_1 & 0 \end{pmatrix} , \; F^{0i}=-F^{i0}=-\frac{E_i}{c} , \; F^{ij}=-\epsilon_{ijk}B_k , \; F^{00}=0$$

$\alpha,\beta=\overline{0,3}$, $i,j,k=\overline{1,3}$

$E=(E_i)_i$ electric field intensity , $B=(B_i)_i$ magnetic induction field.

Considering the inertial frames *R* and *R'* such that a point at rest in *R* moves with velocity $(v_i)_{i=\overline{1,3}}=\vec{v}$ in the frame R' , the coordinates transformation from R to R' is given by $x'^{\alpha}=M_{\alpha\gamma}x^{\gamma}$ (we use Einstein summation convention and Greek letters for indexing from 0 to 3 ,Latin letters for indexing from 1 to 3)

$M_{ij}=\delta_{ij}+\frac{\beta-1}{v^2}v_i v_j$, $M_{i0}=\frac{\beta v_i}{c}$, $M_{0i}=\frac{\beta v_i}{c}$, $M_{00}=\beta$ with $\beta=\frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$.

(see Chap. Special relativity. Lorentz transformations)

The electromagnetic tensor transforms like $F'^{\alpha\gamma}=M_{\alpha\delta}M_{\gamma\varepsilon}F^{\delta\varepsilon}$ and after some calculus we find out that E and B transform like $E'=\beta(E-\vec{v}\times B)+\frac{1-\beta}{v^2}(\vec{v}\cdot E)\vec{v}$ (1) , $B'=\beta(B+\frac{1}{c^2}(\vec{v}\times E))+\frac{1-\beta}{v^2}(\vec{v}\cdot B)\vec{v}$ (2)

Consider now a particle M with rest mass m_0 and charge q which moves in the frame R on trajectory $(x^{\alpha}_{\mathrm{M}})_{\alpha}=(c\,t,x^1_{\mathrm{M}}(t),x^2_{\mathrm{M}}(t),x^3_{\mathrm{M}}(t))_t$ under the action of an electromagnetic field with $E=E(t,x)$, $B=B(t,x)$ electric field intensity respective magnetic induction field in the frame R , $x=(x^i)_i$.

At time moment t_0 we have an instantaneous rest frame R'_0 of the particle which

moves with the velocity $(v_i)_i=(v_i(t_0))_i=\left(\frac{dx^i_{\mathrm{M}}}{dt}(t_0)\right)_i$ relative to frame R and therefore the coordinates trandform from R to R'_0 will be $x'^{\alpha}=M_{\alpha\gamma}x^{\gamma}$ with (*)

$M_{ij}=\delta_{ij}+\frac{\beta-1}{v^2}v_iv_j$, $M_{i0}=M_{0i}=-\frac{\beta v_i}{c}$, $M_{00}=\beta=\frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$.

Since $c^2(dt)^2-dx^idx^i$ is a Lorentz invariant we can take the proper time of the particle $d\tau=\sqrt{1-\frac{v^2}{c^2}}dt$ as a Lorentz invariant and the four-momentum

$$(p^{\alpha})_{\alpha}=\left(m_0\frac{dx^{\alpha}}{dt}\right)_{\alpha}=(m_0c\beta,m_0\beta v_1,m_0\beta v_2,m_0\beta v_3)\ ,$$

$\vec{p}=(p^i)_{i=\overline{1,3}}$ the relativistic momentum.

We have $x^{\alpha}=M^*_{\alpha\gamma}x'^{\gamma}$ where $M^*_{ij}=\delta_{ij}+\frac{\beta-1}{v^2}v_iv_j$, $M^*_{0i}=M^*_{i0}=\frac{\beta v_i}{c}$, $M^*_{00}=\beta$.

For $(v_i)_i=(v_i(t_0))_i$ as instantaneous R'_0 rest frame velocity we have for the frame R coordinates of the particle M evolution:

$$\frac{dt}{dt'}=M^*_{00}+\frac{M^*_{0i}}{c}\frac{dx'^i}{dt'}$$

$$\frac{dx^i}{dt}=\left(M^*_{ij}\frac{dx'^j}{dt'}+M^*_{i0}c\right)\frac{1}{M^*_{00}+\frac{1}{c}M^*_{0i}\frac{dx'^i}{dt'}}$$

$$\frac{d^2x^i}{dt^2}=\frac{M^*_{ij}\frac{d^2x'^j}{dt'^2}\left(M^*_{00}+\frac{1}{c}M^*_{0k}\frac{dx'^k}{dt'}\right)-\frac{1}{c}M^*_{0j}\frac{d^2x'^j}{dt'^2}\left(M^*_{ij}\frac{dx'^j}{dt'}+M^*_{i0}c\right)}{\left(M^*_{00}+\frac{1}{c}M^*_{0i}\frac{dx'^i}{dt'}\right)^3}\ .$$

In the rest frame we have $\frac{dx'^i}{dt'}(t_0)=0$ and therefore for the acceleration in the frame R at t_0 , if $a'=\left(\frac{d^2x'^i}{dt'^2}(t_0)\right)_i$ is the acceleration in the instantaneous rest frame R', we have:

$$a=\frac{d^2x^i}{dt^2}=\frac{M^*_{ij}M^*_{00}a'_j-M^*_{0j}a'_jM^*_{i0}}{M^{*3}_{00}}$$

$$a=\beta^{-3}\left(\beta a'+\frac{1-\beta}{v^2}(\vec{v}\cdot a')\vec{v}\right)\qquad(3)$$

At time moment t_0 in the rest frame we must have :
$m_0 a' = q E'(t'_0, 0)$ (4) where $E' = E'(t', x')$, $B' = B'(t', x')$ are the electric intensity field and the magnetic induction field in the instantaneous rest frame R'_0 . Thus with
$E' = E'(t'_0, 0)$, $B' = B'(t'_0, 0)$, $E = E(t_0, x_M)$, $B = B(t_0, x_M)$ since
according to (1), (2) $E = \beta(E' - \vec{v} \times B') + \frac{1-\beta}{v^2}(\vec{v} \cdot E')\vec{v}$ and

$B' = \beta(B - \frac{1}{c^2}(\vec{v} \times E)) + \frac{1-\beta}{v^2}(\vec{v} \cdot B)\vec{v}$ from (3) , (4) follows

$$\beta^3 m_0 a = q E + q\beta^2(\vec{v} \times B) - q\frac{\beta^2}{c^2}\vec{v} \times (\vec{v} \times E) \ .$$

In the frame R we have the Lorentz force
$f = qE + q\vec{v} \times B$.
Let $a_s = \frac{1}{v^2}(a \cdot \vec{v})\vec{v}$, $a_p = a - a_s$, $f_s = \frac{1}{v^2}(f \cdot \vec{v})\vec{v}$, $f_p = f - f_s$ and after some calculus we obtain $\beta^3 m_0 a_s = f_s$ (5) and $\beta m_0 a_p = f_p$ (6) .
At time moment t_0 we have also:

$$\frac{d\vec{p}}{dt} = \frac{d}{dt}\frac{\vec{v}}{\sqrt{1-\frac{v^2}{c^2}}} = \beta m_0 \frac{d\vec{v}}{dt} + \frac{\beta^3 m_0}{c^2}\left(\vec{v} \cdot \frac{d\vec{v}}{dt}\right)\vec{v} = \beta m_0 a_p + \beta m_0 \left(\vec{v} \cdot \frac{d\vec{v}}{dt}\right)\left(\frac{1}{v^2} + \frac{\beta^2}{c^2}\right)\vec{v} =$$

$= \beta m_0 a_p + \beta^3 m_0 a_s$ and so from (5) and (6) we obtain $\frac{d\vec{p}}{dt} = f$ (7)

Taking $\boldsymbol{E} = \frac{m_0 c^2}{\sqrt{1-\frac{v^2}{c^2}}}$ we have $\frac{d\vec{p}}{dt} \cdot \vec{v} = \beta m_0 \left(\vec{v} \cdot \frac{d\vec{v}}{dt}\right)\left(1 + \frac{\beta^2}{c^2}v^2\right) = \beta^3 m_0 \left(\vec{v} \cdot \frac{d\vec{v}}{dt}\right) = \frac{d\boldsymbol{E}}{dt}$

and so $\frac{d\boldsymbol{E}}{dt} = f \cdot \vec{v}$. $\boldsymbol{E} = \frac{m_0 c^2}{\sqrt{1-\frac{v^2}{c^2}}}$ (8) is the energy of the particle in the frame R , since $f \cdot \vec{v}$ is the work done by the Lorentz force in unit time in the frame R.

If we have an electromagnetic plane wave in the frame R given by
$E = E_0 \cos(\omega t - \vec{k} \cdot x)$, $B = B_0 \cos(\omega t - \vec{k} \cdot x)$ with
$E_0, B_0 \in \mathbb{R}^3$, $\vec{k} = (k_1, k_2, k_3) \in \mathbb{R}^3$, $\omega = \|\vec{k}\| c$ taking $(K^\alpha)_\alpha = (\frac{\omega}{c}, k_1, k_2, k_3)$, $(x_\alpha)_\alpha = (ct, -x_1, -x_2, -x_3)$ we will have for the electromagnetic tensor the Lorentz invariant relation of the wave: $F = F_0 \cos(K^\alpha x_\alpha)$

where $F_0=\begin{pmatrix} 0 & -E_{01}/c & -E_{02}/c & -E_{03}/c \\ E_{01}/c & 0 & -B_{03} & B_{02} \\ E_{02}/c & B_{03} & 0 & -B_{01} \\ E_{03}/c & -B_{02} & B_{01} & 0 \end{pmatrix}$.

If *R'* moves with velocity $\vec{v}=(v_i)_i$ in the frame R then in the frame R' the same electromagnetic wave will be given by :

$E'=E'_0\cos(\omega' t'-\vec{k}'\cdot x')$, $B'=B'_0\cos(\omega' t'-\vec{k}'\cdot x')$ where

$E'_0=\beta(E_0+\vec{v}\times B_0)+\frac{1-\beta}{v^2}(\vec{v}\cdot E_0)\vec{v}$

$B'_0=\beta(B_0-\frac{1}{c^2}(\vec{v}\times E_0))+\frac{1-\beta}{v^2}(\vec{v}\cdot B_0)\vec{v}$

$\omega'=c\,M_{0i}k_i+M_{00}\omega$

$k'_i=M_{ij}k_j+M_{i0}\frac{\omega}{c}$ with M , β defined by (*).

Thus in the relativistic electromagnetic wave propagation we have the Doppler effect relation $\omega'=\beta\omega\left(1-\frac{v}{c}\cos\theta\right)$ where θ is the angle between $\vec{v}$ and $\vec{k}$:

the observer in R' moves in the frame R in which the source is at rest with velocity $\vec{v}$ and the wave vector in R is $\vec{k}$.

For $\theta\in\{0,\pi\}$ we have the longitudinal Doppler effect relation $\omega'=\omega\sqrt{\frac{1\mp\frac{v}{c}}{1\pm\frac{v}{c}}}$:

if the observer moves away from the source we have $\omega'<\omega$ and so a red shift of the wave in R' relative to R.

For $\theta=\frac{\pi}{2}$ we have the transversal Doppler effect relation $\omega'=\frac{\omega}{\sqrt{1-\frac{v^2}{c^2}}}=\omega+O(\frac{v^2}{c^2})$

The transversal Doppler effect is a second order in $\frac{v}{c}$ effect and we have $\omega'>\omega$.

Suppose now the particle M moves with constant velocity $\vec{v}=(v_i)_i$ in the frame R and and emits electromagnetic waves. Then the particle remains at rest in a frame R'_0 with spatial origin at M which moves with velocity $\vec{v}$ relative to the frame R and by symmetry reasons, the emitted electromagnetic waves must be, in the R'_0 frame, identical packets of waves emitted in opposite directions. The packets consist of photons with energy $\hbar\omega'$ emitted in directions at angles $\theta',\pi+\theta'$ to the velocity $\vec{v}'=-\vec{v}$. The energy of these photons in the frame R will be

$$\hbar\,\omega_{\theta'}=\beta\hbar\,\omega'\left(1-\frac{v}{c}\cos\theta'\right) \text{ and } \hbar\,\omega_{\pi+\theta'}=\beta\hbar\,\omega'\left(1+\frac{v}{c}\cos\theta'\right).$$

Therefore if W' is the total emitted energy in the rest frame R'_0 then the energy emitted in the frame R is

$$W=\sum_{\omega'}\left(\beta\hbar\,\omega'\left(1-\frac{v}{c}\cos\theta'\right)+\beta\hbar\,\omega'\left(1+\frac{v}{c}\cos\theta'\right)\right)=\beta\sum_{\omega'}2\hbar\,\omega'=\beta W'$$

and so $W=\beta W'$.

According to (8), since *v* is constant, the energy variation of the particle must be $W=\beta\Delta m_0c^2$ where Δm_0 is the variation of the rest mass of the particle. Hence $W'=\Delta m_0c^2$. W' is the variation in rest energy of the particle which is at rest in the frame R' and so for the rest energy of the particle we take m_0c^2, proving the equivalence between rest mass and rest energy.

In conclusion, for a force f in the frame R we have

$\frac{d\vec{p}}{dt}=f$, $\frac{d\boldsymbol{E}}{dt}=f\cdot\vec{v}$ with $\vec{p}=\frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}\vec{v}$ momentum, $\boldsymbol{E}=\frac{m_0c^2}{\sqrt{1-\frac{v^2}{c^2}}}$ energy,

the four-momentum Lorentz vector $\left(P^\alpha\right)_\alpha=\left(\frac{\boldsymbol{E}}{c},\vec{p}\right)$,

the Lorentz invariant proper time $d\tau=\sqrt{1-\frac{v^2}{c^2}}dt$, velocity $\vec{v}=\left(\frac{dx^i}{dt}\right)_i$,

the four-velocity Lorentz vector $\left(V^\alpha\right)_\alpha=\left(\frac{dx^\alpha}{d\tau}\right)_\alpha=\left(\frac{c}{\sqrt{1-\frac{v^2}{c^2}}},\frac{\vec{v}}{\sqrt{1-\frac{v^2}{c^2}}}\right)$,

the four-acceleration $\left(W^\alpha\right)_\alpha=\left(\frac{d^2x^\alpha}{d\tau^2}\right)_\alpha$ so that we have

$P^\alpha=m_0\frac{dx^\alpha}{d\tau}$, $\left(m_0W^\alpha\right)_\alpha=\beta\left(\frac{dP^\alpha}{dt}\right)_\alpha=\left(\beta\frac{f\cdot\vec{v}}{c},\beta f\right)$ with $\beta=\frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$,

$m_0W=F$, $F=\left(\beta\frac{f\cdot\vec{v}}{c},\beta f\right)$ is the Lorentz vector four-force,

$$\boldsymbol{E}^2=\vec{p}^2c^2+m_0^2c^4 \qquad (9).$$

Replacing in (9) the energy and momentum with the corresponding quantum operators for a quantum particle with rest mass *m*, taking therefore

$\boldsymbol{E}\to i\hbar\frac{\partial}{\partial t}$, $\vec{p}\to-i\hbar\nabla_x$ we find out that the

wave function $\psi=\psi(t,x)$ of a mass m particle quantum system should

satisfy the following Klein-Gordon equation

$$\left(\Box+\frac{m^2c^2}{\hbar^2}\right)\psi(t,x)=0$$

where $\Box=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{\partial}{\partial x^i}\frac{\partial}{\partial x^i}=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\nabla_x^2$.

With $c=1$, $\hbar=1$ as we can have by suitable choosing of time and lenght measure units, the Klein-Gordon equation becomes: $(\partial^2+m^2)\,\psi=0$.

A mode with energy $E=m+\varepsilon$ would oscillate in time as $\psi\propto\exp(-iEt)$.

In the non-relativistic limit the kinetic energy ε is much smaller than the rest mass m. It makes sense to write

$\psi(t,x)=\exp(-imt)\,\varphi(t,x)$ with the field φ oscillating in time much more slowly than $\exp(-imt)$. Thus the Klein-Gordon equation becomes :

$$\left(-im+\frac{\partial}{\partial t}\right)^2\varphi-\nabla_x^2\varphi+m^2\varphi=0.$$

Dropping the term $\left(\frac{\partial^2}{\partial t^2}\right)\varphi$ as much smaller than $-2im\left(\frac{\partial}{\partial t}\right)\varphi$ we find

the Schroedinger equation $i\frac{\partial}{\partial t}\varphi=-\frac{\nabla_x^2}{2m}\varphi.$

Having absorbed this we can easily take the non-relativistic limit of a quantum field theory plugging $\psi(t,x)=\frac{1}{\sqrt{2m}}\exp(-imt)\,\varphi(t,x)$ in the Lorentz invariant scalar field theory with Lagrangian density

$\mathscr{L}=(\partial\psi)^+(\partial\psi)-m^2\psi^+\psi-\lambda(\psi^+\psi)^2$ (see Chap. Quantum field theory , Path integral formalism) which reduces to

$\mathscr{L}\approx\frac{1}{2}i\left(\varphi^+\frac{\partial\varphi}{\partial t}-\frac{\partial\varphi^+}{\partial t}\varphi\right)-\frac{1}{2m}\partial_i\varphi^+\partial_i\varphi-g^2(\varphi^+\varphi)^2$ where $g^2=\frac{\lambda}{4m^2}$

After integration by parts in the action $S=\int\mathscr{L}(\varphi,\partial\varphi)dtd^3x$ we can define the theory by the Lagrangian density

$\mathscr{L}=i\varphi^+\partial_0\varphi-\frac{1}{2m}\partial_i\varphi^+\partial_i\varphi-g^2(\varphi^+\varphi)^2$. (**)

The theory defines a conserved Noether current (for invariance under the transformation $(\bar{t},\bar{x})=(t,x)$, $\bar{\psi}=\exp(i\omega)\psi=\psi+i\omega\psi+O(\omega^2)$, $\omega\in\mathbb{R}$ (see Chap.Lagrangian field theory. Noether theorem)): $J_\mu=i(\psi^+\partial_\mu\psi-\partial_\mu\psi^+\psi)$ which for the (**) Lagrangian density becomes $J_0=\varphi^+\varphi$ (as expected the probability density) and $J_k=\frac{i}{2m}(\varphi^+\partial_k\varphi-\partial_k\varphi^+\varphi)$, $k=\overline{1,3}$ the charge current.

We can measure the position of a particle by bouncing light of it, but measuring the position accurately requires light of short wavelenght. Light with a short wavelenght consists of photons of high energy. If the energy of these photons exceeds mc^2 (m the mass of the particle) when one hits the particle whose position is being measured, the collision may yield enough energy to create a new particle of the same type. This renders out the question of the original particle's location.
Suppose we wish to measure the position of a particle with an accuracy Δx . Then the uncertainity relation for position and momentum says that $\Delta x \Delta p \geq \frac{\hbar}{2}$ so the uncertainity in the particle's momentum satisfies $\Delta p \geq \frac{\hbar}{2\Delta x}$.
Having the relativistic relation between energy and momentum $E^2 = (pc)^2 + (mc^2)^2$, when Δp exceeds mc , the uncertainity in energy is greater than mc^2 which is enough energy to create another particle of the same type.
This greater energy uncertainity must be excluded by the creation of one or more additional particles to keep the uncertainity of each particle's momentum at or below mc .
It follows that there is a fundamental minimum for Δx when $\Delta p \leq mc$: $\Delta x \geq \frac{\hbar}{2\Delta p} \geq \frac{\hbar}{2mc}$. The wavelenght of a photon with the same energy as the rest mass of the particle is $\frac{h}{mc}$ and $\frac{\hbar}{mc}$ is the so called reduced Compton wavelenght of the particle.
Thus the uncertainity in position must be greater than half of the reduced Compton wavelenght.

15. Free quantum particle. Potential gap. Potential barrier.Tunnel effect

Free quantum particle. Potential gap for a quantum particle Potential barrier. Tunnel effect

The Hamiltonian operator for a free one-dimensional particle is

$\hat{H}=\frac{\hat{p}^2}{2m_0}$ with $\hat{p}=-i\hbar\frac{d}{dx}$, m_0 mass of the particle .

For the wave function $\psi=\psi(t,x)\in\mathbb{C}$, $t\in\mathbb{R}$, $x\in\mathbb{R}$ the Schroedinger equation is:

$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m_0}\frac{\partial^2\psi}{\partial x^2}$ which leads to a time independent Schroedinger equation:

$\frac{d^2\psi}{dx^2}+k_x^2\psi=0$ where $k_x^2=\frac{2m_0}{\hbar^2}E$ and the solution for the energy level E will be

$\psi(t,x)=A\exp(-\frac{i}{\hbar}(Et-\hbar k_x x))+B\exp(\frac{i}{\hbar}(Et-\hbar k_x x))$.

The regresive wave (with coefficient *B*) has no physical meaning and so the energy level E solution is $\psi(t,x)=A\exp(-\frac{i}{\hbar}(Et-\hbar k_x x))$ the free quantum particle having a continuous energetic spectrum $E=\frac{\hbar^2k^2}{2m_0}$, $k\in\mathbb{R}$.

The model can be applied to study conduction electrons in metals. For the wave functions ψ of conduction electrons in a one-dimensional crystal grid of latticial constant *a* and length *L* we must have $\psi(x+L)=\psi(x)$ so $k_xL=2\pi n_x$, $n_x\in\mathbb{N}$, the energy levels being quantized as $E_n=\frac{\hbar^2 2\pi^2}{m_0L^2}n^2$, $n\in\mathbb{N}$.

The electrons can absorb or release energy quantums ε in transition from one level to another $\varepsilon=E_{n+1}-E_n=\frac{2\pi^2\hbar^2}{m_0L^2}(2n+1)$, $n\in\mathbb{N}$.

For macroscopic large *L* we can see that the spectrum will be quasicontinuous.

A potential gap is determined by a Hamiltonian operator

$\hat{H}=\frac{\hat{p}^2}{2m_0}+V(x)$ where $V(x)=\begin{cases}V_0 & \text{for } x<0\\ 0 & \text{for } x\in[0,a]\\ V_0 & \text{for } x>a\end{cases}$ with $V_0\in\mathbb{R}$ a constant.

Such potential gap appears for example in ionic crystals in an anionic vacancy (when a negative ion is missing from the lattice, leaving an empty space where the electrons coming from the neighbouring positive ionised atoms are trapped).

The corresponding time independent Schroedinger equation is

$\frac{d^2\psi}{dx^2}-\frac{2m_0}{\hbar^2}(V(x)-E)\psi=0$ and with $k_1^2=\frac{2m_0}{\hbar^2}E$, $k_2^2=\frac{2m_0}{\hbar^2}(V_0-E)$

the solutions are

$\psi=\exp(-\frac{i}{\hbar}Et)\,\psi_1(x)$, $\psi_1(x)=A_1\exp(-k_2x)+B_1\exp(k_2x)$ for $x<0$

$\psi=\exp(-\frac{i}{\hbar}Et)\,\psi_2(x)$, $\psi_2(x)=A_2\exp(ik_1x)+B_2\exp(-ik_1x)$ for $x\in[0,a]$

$\psi=\exp(-\frac{i}{\hbar}Et)\,\psi_3(x)$, $\psi_3(x)=A_3\exp(k_2(x-a))+B_3\exp(-k_2(x-a))$ for $x>a$

The function ψ must be bounded for $x\to\pm\infty$ and so $A_3=A_1=0$.

The function ψ must be also continuous differntiable in $x=0$ and $x=a$ and so

$B_1-A_2-B_2=0$

$A_2\exp(ik_1a)+B_2\exp(-ik_1a)-B_3=0$

$k_2B_1-ik_1A_2+ik_1B_2=0$

$ik_1A_2\exp(ik_1a)-ik_1B_2\exp(-ik_1a)+k_2B_3=0$.

This system in B_1 , A_2 , B_2 , B_3 has a non-zero solution if and only if

$\tan(k_1a)=\tan(2\alpha)$ where $\tan\alpha=\frac{k_2}{k_1}$ and therefore $k_1a=2\alpha+n\pi$ with $n\in\mathbb{Z}$.

The energy levels $E=\frac{\hbar^2}{2m_0}k_1^2$ are therefore quantized and we see that if $V_0=\infty$,

we have $k_1a=n\pi$, $n\in\mathbb{Z}$ leadind to quantized energy levels as $E_n=\frac{\hbar^2}{2m_0}\frac{\pi^2}{a^2}n^2$.

The absorption or releasing energy quantums only in amounts of $\varepsilon = E_{n+1} - E_n$ gives the crystal its color since a is a small quantity, determining a discrete spectrum.

For $V_0=\infty$ follows also $k_2=\infty$, $B_1=0$, $\psi_1=\psi_3=0$, $\psi_2(x)=A\sin(\frac{n\pi}{a}x)$.

The potential gap can be generalized to a three-dimensional gap for wave functions

$\psi=\psi(t,x,y,z)$ and a hamiltonian operator $\hat{H}=\frac{\hat{p}^2}{2m_0}+V(x,y,z)$, $\hat{p}=-i\hbar\nabla$

$$V(x,y,z)=\begin{cases}0 & \text{for } x,y,z\in[0,L]\\ \infty & \text{for } (x,y,z)\in\mathbb{R}^3\setminus[0,L]^3\end{cases}$$

The time independent Schroedinger equation is

$\nabla^2\psi+\frac{\hbar^2}{2m_0}(E-V)\,\psi=0$ which for $k^2=\frac{2m_0}{\hbar^2}E$, E -energy level ,

leads to solutions $\psi=A\exp(-\frac{i}{\hbar}E_nt)\,\psi_{\boldsymbol{n}}(x,y,z)$ with $\boldsymbol{n}=(n_x,n_y,n_z)\in\mathbb{N}^3$,

$\vec{k}=(k_x,k_y,k_z)=\frac{\pi}{L}\boldsymbol{n}$, $E_n=\frac{\hbar^2}{2m_0}(n_x^2+n_y^2+n_z^2)$,

$$\psi_{\boldsymbol{n}}=\left(\frac{2}{L}\right)^{3/2}\sin(\frac{\pi n_x x}{L})\sin(\frac{\pi n_y y}{L})\sin(\frac{\pi n_z z}{L}) \qquad (*)$$

The solutions (*) form a complete orthonormal system of eigenfunctons of the

operator $\hat{H}=-\frac{\hbar^2}{2m_0}\nabla^2$ on the Hilbert space $L^2([0,L]^3)$.

There are more than one normalized wave functions corresponding to an energy level E_n giving a degeneration of the energy level g_n .

$g_n=\text{card}\{(n_x,n_y,n_z)\in\mathbb{N}^3 | n_x^2+n_y^2+n_z^2=\boldsymbol{n}^2\}$.

The spectrum is quasicontionuous for macroscopic large L and we have an energetic density of states $\rho(E)=\frac{dn_x dn_y dn_z}{dE}=\left(\frac{L}{\pi}\right)^3 4\pi k^2\frac{dk}{dE}=\frac{4}{\pi^2}\frac{V}{\hbar^3}\sqrt{2m_0^3E}$ with $V=L^3$.

In the case of a one-dimensional potential barrier the free quantum particle encounters at $x = 0$ a repulsive force field having a potential $V_0 > E$ (E -energy level of the particle) on the interval [0 , a] . The solution for the whole spatial x -axis not vanishes for $x > a$ and so with a non-zero probability, the particle can pass through the potential barrier even if $V_0 > E$, which gives the tunnel effect.

For the wave function ψ we will have

$\psi=\exp(-\frac{i}{\hbar}Et)\,\psi_1(x)$ for $x\in(-\infty,0)$, $\psi=\exp(-\frac{i}{\hbar}Et)\,\psi_2(x)$ for $x\in[0,a]$,

$\psi=\exp(-\frac{i}{\hbar}Et)\,\psi_3(x)$ for $x\in[a,\infty)$

The time independent Schroedinger equations are

$\frac{d^2\psi_{1,3}}{dx^2}+\frac{2m_0}{\hbar^2}E\,\psi_{1,3}=0$ on $\mathbb{R}\setminus[0,a]$

$\frac{d\psi_2}{dx^2}-\frac{2m_0}{\hbar^2}(V_0-E)\,\psi_2=0$ on $[0,a]$

For $k_1^2=\frac{2m_0}{\hbar^2}$, $k_2^2=\frac{2m_0}{\hbar^2}(V_0-E)$ the solutions are

$\psi_1(x)=A_1\exp(ik_1x)+B_1\exp(-ik_1x)$ with $x<0$

$\psi_2(x)=A_2\exp(-k_2x)+B_2\exp(k_2x)$ with $x\in[0,a]$

$\psi_3(x)=A_3\exp(ik_1(x-a))+B_3\exp(-ik_1(x-a))$ with $x>a$

We can obviously drop the regresive wave on $[a,\infty)$ and take $B_3=0$.

The function ψ must be continuous differentiable in $x = 0$ and $x = a$ and so :

$A_1+B_1=A_2+B_2$

$ik_1(A_1-B_1)=k_2(-A_2+B_2)$

$A_2\exp(-k_2a)+B_2\exp(k_2a)=A_3$

$-k_2(A_2\exp(-k_2a)-B_2\exp(k_2a))=ik_1A_3$

Let $n=\frac{k_1}{k_2}$, $k_2a\gg1$ and we derive

$B_2=\frac{1+in}{2}A_3\exp(-ik_2a)\approx0$, $A_2=\frac{1-in}{2}A_3\exp(k_2a)$,

$A_1=\frac{i+n}{2n}A_2$, $B_1=\frac{n-i}{2n}A_2$

Tunnel effect processes (like α -decay or cold electron emission) depend on the transparency coefficient of the barrier which can be computed as

$T=\frac{|\psi_3(a)|^2}{|\psi_1(0)|^2}$ and we obtain $T=\frac{A_3 A_3^*}{(A_1+B_1)(A_1^*+B_1^*)}=\frac{4}{1+n^2}\exp(-2k_2 a)$.

16. Thermodynamics

Thermodynamics

In thermodynamics we describe systems as a union of macroscopic parts which are in local thermodynamical equilibrium, that is the state of a part P_i of the system S will be described by a set of extensive parameters X^i_0 , X^i_1 , … , X^i_n . An extensive parameter depends on the size o the part which it describes and is additive with respect to parts. So if X^1_m , X^2_m are the m-th extensive parameter for a part P_1 respective a disjoint part P_2 then the considered value X_m of the m-th extensive parameter for the system $P_1 \cup P_2$ is $X_m = X^1_m + X^2_m$.
Extensive parameters are the internal energy U , the entropy S of the system, the volume occupied by the system V , or the particles number N of the system.
The macroscopic state of the system will be described by its total internal energy U, its total entropy S and the values of the extensive parameters of its parts. The fact that such state parameters exist can be resumed as
P1. There exist so called equilibrium states of a system in which , if the system interacts only with itself (that is the system is isolated) then the extensive parameters of each part of the system do not evolve in time.

A system in thermodynamical equilibrium will be described macroscopically by its total internal energy U, its total entropy S and its other extensive parameters X_1 , X_2 , … , X_n (we take $X_0 = U$). It follows that a system is in thermodynamical equilibrium if and only if any subsystem of it is in thermodynamical equilibrium.
A quasistatic thermodynamic process is a continuous differentiable evolution in time of the extensive parameters $(X^j_k)_{k,j}$ of the parts and we will have:
P2. If the system is at thermodynamical equilibrium or it experiences a quasistatic thermodynamic process then for the whole system (and for each part of the system), the entropy is a continuous differentiable homogeneous of degree 1 function of the internal energy and the other extensive parameters.
Therefore we can write :

$$S = S(U, X_1, \dots, X_n) \qquad (1)$$

$$\lambda S = S(\lambda U, \lambda X_1, \dots, \lambda X_n) \quad \text{for any} \quad \lambda \in \mathbb{R} \qquad (2)$$

Moreover we have an intensive parameter T , the thermodynamical temperature, such that $T > 0$ and $\frac{1}{T} = \frac{\partial S}{\partial U}(U, X_1, \dots, X_n)$.
Hence from (1) and (2) we obtain

$$U = U(S, X_1, \dots, X_n) \qquad (3)$$

$$\lambda U = U(\lambda S, \lambda X_1, \dots, \lambda X_n) \qquad (4)$$

$$T = \frac{\partial U}{\partial S}(S, X_1, \dots, X_n) \qquad (5)$$

$$T(\lambda S, \lambda X_1, \dots, \lambda X_n) = T(S, X_1, \dots, X_n) \quad \text{for any} \quad \lambda \in \mathbb{R}^* \qquad (6) .$$

We can consider also the other intensive parameters :

$$P_i=\frac{\partial U}{\partial X_i}(S,X_1,...,X_n)$$

$$F_i=\frac{\partial S}{\partial X_i}(U,X_1,...,X_n)\ .$$

For $X_i=V$ we have $P=-P_i$ where P is the thermodynamical pressure.

For $X_i=N_k$ we have $\mu_k=P_i$ where μ_k is the chemical potential of particles denoted by k having N_k the number of such particles.

We will have obviously :

$P_i(\lambda S,\lambda X_1,...,\lambda X_n)=P_i(S,X_1,...,X_n)$,

$F_i(\lambda U,\lambda X_1,...,\lambda X_n)=F_i(U,X_1,...,X_n)$ for any $\lambda\in\mathbb{R}^*$.

Differentiating (2) and (4) with respect to λ and taking λ = 1 we obtain

$$dU=T\,dS+P_i\,dX_i \qquad (7)$$

$$dS=\frac{1}{T}dU+F_i\,dX_i=\frac{1}{T}dU-\frac{P_i}{T}dX_i \qquad (8)$$

$$F_i=-\frac{P_i}{T} \qquad (9)$$

Also since from the above results the vanishing of the total differential of $H=U-TS-P_iX_i$ as a function in $(S,X_1,...,X_n)$ and taking $\lambda=0$ in (4) we obtain $H(0,0,...,0)=0$ we can derive

$$U=TS+P_iX_i \qquad (10)$$

$$S=\frac{1}{T}U+F_iX_i \qquad (11)$$ (in all above relations we take summation over i index) .

We will assume also that :

P3. If the system is at thermodynamical equilibrium with constant internal energy then the entropy has a maximum when unrestrained varying the other extensive parameters.

Therefore at equilibrium we have

$$\left(\frac{\partial S}{\partial X}\right)_{U=const}=0 \text{ and } \left(\frac{\partial^2 S}{\partial X^2}\right)_{U=const}<0 \text{ (negative definite)} .$$

P4. (The third principle of thermodynamics) If $T\to 0$ then $S\to 0$.

The second princple of thermodynamics:

If a system interacts only with itself (the system is isolated) then the entropy can only increase during any natural process. (The entropy remains constant for reversible natural processes).

The first principle of thermodynamics:
A system can exchange energy with the environment only by the variation of entropy in which case the energy infinitesimal variation is given by the heat exchange $dU=\delta Q=T\,dS$ or by the variation of the other extensive parameters in which case the internal energy infinitesimal variation is given by the work exchange $dU=\delta L=P_i\,dX_i$ (for $X_i=V$ the work will be $\delta L=-P\,dV$) .
The total infinitesimal internal energy variation is given by
$dU=\delta Q+\delta L=T\,dS+P_i\,dX_i$.
An isolated system has therefore constant internal energy and by the second principle of thermodynamics evolves naturally to an equilibrium state in which the entropy is maximal.
If an isolated system consists for example of two parts we may consider the case in which the separation between the two parts is permeable only to the extensive parameters X^k_i, k = 1,2 , that is the system evolves such that for the i indexed parameters we have $X^1_i+X^2_i=X_i=constant\ \ in\ \ time$ and the other extensive parameters X^1_j , X^2_j are constant in time, then we must consider for the equilibrium state to which the system naturally evolves a restrained maximum condition for the entropy function
$S=S^1(X^1_i,X^1_j)+S^2(X^2_i,X^2_j)$ with the restraints $X^1_i+X^2_i=X_i=constant$ (12) .
Therefore for the function $\psi=S-\lambda_i(X^1_i+X^2_i)$ depending on the variables X^k_i, X^k_j and on the λ_i Lagrange coefficients additional parameters we must have:
$\frac{\partial\psi}{\partial X^1_i}=\frac{\partial\psi}{\partial X^2_i}=0$ and so $\frac{\partial S^1}{\partial X^1_i}=\frac{\partial S^2}{\partial X^2_i}=\lambda_i$, $F^1_i=F^2_i$ (13) .
The restraints (12) and the (13) relation determine the parameters X^1_i , X^2_i at equilibrium.
For $X^k_i=U^k$ the internal energy of part k , $k=1,2$ that is the separation is diathermal and the two parts exchange energy by heat it follows $T^1 = T^2$ at equilibrium: Two systems exchanging energy by heat have at equilibrium the same temperature and if the separation is also mobile (that is $V^1+V^2=V=constant$) then at equilibrium the pressures must also be equal (since we must have $\frac{P^1}{T^1}=\frac{P^2}{T^2}$ and so $P^1=P^2$) .
If the separation is X_i permeable the whole system evolves according to second principle of thermodynamics and the total entropy is increasing. We have $\Delta X^1_i+\Delta X^2_i=0$, where ΔX^k_i is the variation of X^k_i parameter in the system's evolution process,(since $X_i=X^1_i+X^2_i=const.$) and so at first order approximation

$$0<\Delta S=\Delta S^1+\Delta S^2=\frac{\partial S^1}{\partial X^1_i}\Delta X^1_i+\frac{\partial S^2}{\partial X^2_i}\Delta X^2_i=(F^1_i-F^2_i)\Delta X^1_i\ .$$

Therefore the natural evolution of the system is such that the extensive parameter X^k_i is increasing in that part of the system which has the higher conjugate intensive

parameter F^k_i . In particular for $X_i = U$ the internal energy increases or decreases in that part of the system which has the lower respective higher temperature.
We observe also that, for the infinitesimal heat exchange differential form we have $\delta Q = T\,dS$, $\frac{1}{T}\delta Q = dS = \frac{\partial S}{\partial U}dU + \frac{\partial S}{\partial X_i}dX_i$ and so $\frac{1}{T}$ is an integration factor for the heat differential form.

Consider now a monothermal engine, that is an isolated system which consists of a thermostat reservoir system R_T with temperature T , a mechanical system M and a engine system E such that E exchanges energy only in form of heat Q with R_T and only in form of work - L with M in a cyclic process. (The engine E receives heat Q and delivers work L) .
The process being cyclic the internal energy variation of E is zero:
$0 = \Delta U = Q - L$ and so $Q = L$.
From the second principle of thermodynamics we have :
$\Delta S^r + \Delta S + \Delta S^m \geq 0$.
Because E exchanges only work with M , the heat exchange amount with M will be zero : $0 = -Q^m = T\,\Delta S^m$.
We have also $-Q = T\,\Delta S^r$, the heat exchange amount with the reservoir R .
The process experienced by E is cyclic and so the entropy variation of E , which we denoted ΔS vanishes: $\Delta S = 0$.
Therefore we have $0 \leq \Delta S^r = -\frac{Q}{T}$, $Q \leq 0$, $L \leq 0$ and we derived the Kelvin principle:
“ There is no cyclic monothermal process experienced by a monothermal engine which transforms received heat in effectuated work.”
Consider now a bithermal engine E which receives heat Q_1 from the thermostat R_1 at temperature T_1 , delivers heat Q_2 to the thermostat R_2 at temperature T_2 and effectuates work L on mechanical system M in a cyclical process.
We have $\Delta U = Q_1 - Q_2 - L$ by the first principle of thermodynamics and $\Delta S^1 + \Delta S^2 + \Delta S + \Delta S^m \geq 0$ by the second principle of thermodynamics.
With the mechanical system we have zero exchanged heat: $Q^m = 0$ and so $\Delta S^m = -\frac{Q^m}{T} = 0$ for the variation in entropy of the mechanical system.
The process being cyclic we have $\Delta U = 0$, $\Delta S = 0$.
Obviously $\Delta S^1 = -\frac{Q_1}{T_1}$, $\Delta S^2 = \frac{Q_2}{T_2}$ for the entropy variations of the thermostate systems and so $Q_1 - Q_2 = L$, $\frac{Q_2}{T_2} - \frac{Q_1}{T_1} \geq 0$.
If $L = 0$, the engine delivers naturally heat from thermostate R_1 to thermostate R_2 with $Q = Q_1 = Q_2 > 0$ and therefore follows $T_1 \geq T_2$ and we have the Clausius principle formulation:

"There is no cyclic process which delivers naturally heat from a source with lower temperature to source with higher temperature."

If $L>0$ the engine transforms received heat Q_1 partially in delivered work L and for the efficiency η of the engine we will have $\eta=\frac{L}{Q_1}=1-\frac{Q_2}{Q_1}\leq 1-\frac{T_2}{T_1}$. If the cyclic process is reversible we will have $\Delta S^1+\Delta S^2=0$ and so the efficiency will be maximal $\eta=1-\frac{T_2}{T_1}$. Obviously , to deliver work by the engine we must have $Q_1>Q_2$ and so $T_2<T_1$. To deliver heat from a lower temperature T_2 source to a higher temperature T_1 source, the mechanical system of the engine must deliver work on the engine system so that $L=Q_1-Q_2<0$.

If we assume now that a system is in diathermal contact with a thermostat reservoir *R* having temperature T^r and δQ is the amount of heat which the system receives from the thermostat, then the infinitesimal variation of entropy of the reservoir will be $dS^r=-\frac{\delta Q}{T^r}$. The system and the thermostat forming a whole isolated system, the second principle of thermodynamics leads to $dS+dS^r\geq 0$ where dS is the infinitesimal variation of the entropy of the system.

Therefore $dS\geq\frac{\delta Q}{T^r}$ (14) . If the system is supposed to be at equilibrium with the reservoir then we have $T^r=T$ the temperature of the system and $dS\geq\frac{\delta Q}{T}$ (14').

We can assume that the system is in contact with many sources R_i having respective temperatures T_i , receiving heat amounts δQ_i from the source R_i (if the source R_i is instead receiving the heat we take $\delta Q_i < 0$) through its separation surface ∂D .

Then the relation (14') takes the form $dS\geq\sum_i\frac{\delta Q_i}{T_i}$ (15) or

$dS\geq\int_{\partial D}\frac{\delta Q}{T}d\sigma$ (16) which is known as the Clausius inequality.

We can have also radiative heat terms in (15) in which the heat exchange is volumic distributed in the domain *D* of the system and so we will have a heat flux vector $\vec{q}$ on the separation surface ∂D and a radiation volumic density ρr on the domain D such that if $\vec{n}$ is the outwards normal on the surface ∂D , relation (16) becomes the Clausius-Duhem inequality

$$\frac{dS}{dt}\geq\int_{\partial D}-\frac{\vec{q}\cdot\vec{n}}{T}d\sigma+\int_D\frac{\rho r}{T}dV \qquad (17)$$

where $\vec{q}$ is the amount of heat delivered from the domain D of the system to its exterior through an unit surface element normal to $\mathrm{vers}\,\vec{q}$ in an unit of time interval,

ρ is the mass density of the system,

r is the amount of heat generated in an unit mass element in an unit of time interval inside the system,

T is the temperature field defined on the domain D of the system in local equilibrium with the thermostat reservoir,
t is the time variable.
(17) is equivalent to

$$\frac{dS}{dt} \geq \int_D \left(-\nabla \cdot \left(\frac{\vec{q}}{T} \right) + \frac{\rho r}{T} \right) dV \qquad (18) .$$

Consider that we have a system E in diathermal contact with a temperature reservoir R, the separation between system and reservoit being also X_i permeable.
We suppose that we deliver to the whole system $E \cup R$ energy in form of work L.
With r index reffering to the reservoir, we will have:
$L = \Delta(U + U^r)$, $\Delta U^r = T^r \Delta S^r + P_i^r \Delta X_i^r$.
Then we let the system evolve to equilibrium with the reservoir.
The X_i permeability condition $X_i + X_i^r = const.$ leads to $\Delta X_i = -\Delta X_i^r$ and because the environment not exchanges heat with the entire system $E \cup R$ the entire entropy variation is $\Delta S + \Delta S^r \geq 0$ and so $\Delta S^r \geq -\Delta S$ by the second principle.
We also suppose that during the work delivering process, the environment, the system and the reservoir reach to an equilibrium at which we will have $T = T^r$, $P_i = P^r{}_i$.
Therefore, under this conditions we will have $L \geq \Delta(U - TS - P_i X_i)$ and the minimal possible to be delivered work to the system is $L_{min} = \Delta \bar{U}$ where $\bar{U}$ is the potential $\bar{U} = U - TS - P_i X_i$.
We have $L = L_{min}$ if the work delivering proces is reversible.
In the same way we can conclude that the maximal possible to be effectuated work by the system is $L_{max} = -\Delta \bar{U}$.
If the connection with the reservoir is only diathermal we have $\bar{U} = U - TS$, the free energy potential and if the connection is diathermal and the separation between system and reservoir is mobile (that is volume V permeable) then $\bar{U} = U - TS + PV$, the Gibbs potential.

Suppose a system can be described by $s + 1$ extensive parameters denoted as: $(X_i)_{i=\overline{0,s}}$ with $X_0 = S$. Then from the relations $P_i = \frac{\partial U}{\partial X_i}(S, X_1, \ldots, X_s)$ we can express $X_i = X_i(P_0, P_1, \ldots, P_n, X_{n+1}, \ldots, X_s)$ with $P_0 = T$, for $i = \overline{0,n}$
Let $\bar{U} = U - \sum_{i=0}^{n} P_i X_i$.
Considering (10) we obtain $d\bar{U} = -\sum_{i=0}^{n} X_i dP_i + \sum_{i=n+1}^{s} P_i dX_i$,
$\bar{U} = \bar{U}(P_0, P_1, \ldots, P_n, X_{n+1}, \ldots, X_s)$ and by the mixed derivatives symmetry we have the Maxwell relations:

$$\frac{\partial X_i}{\partial P_j}=\frac{\partial X_j}{\partial P_i} \quad \text{for} \quad i,j=\overline{0,n}$$
$$\frac{\partial P_i}{\partial X_j}=\frac{\partial P_j}{\partial X_i} \quad \text{for} \quad i,j=\overline{n+1,s}$$
$$\frac{\partial X_i}{\partial X_j}=-\frac{\partial P_j}{\partial P_i} \quad \text{for} \quad i=\overline{0,n} \ , \ j=\overline{n+1,s} \ .$$

Consider a system with $S=S(U,X)$ where X denotes the other reduced unrestrained extensive variables. If the system is at equilibrium with equilibrium internal energy U^e and X^e equilibrium other reduced unrestrained extensive variables, according to P3 we have $\left(\frac{\partial S}{\partial X}\right)_U(U^e,X^e)=0$ and $\left(\frac{\partial^2 S}{\partial X^2}\right)_U(U^e,X^e)<0$.

From $S=S(U(S,X),X)$ we obtain
$$\left(\frac{\partial U}{\partial S}\right)_X=\frac{1}{\left(\frac{\partial S}{\partial U}\right)_X}=T \ , \ \left(\frac{\partial U}{\partial X}\right)_S=-T\left(\frac{\partial S}{\partial X}\right)_U \quad \text{and so} \quad \left(\frac{\partial U}{\partial X}\right)_S(S^e,X^e)=0 \ ,$$
$$\left(\frac{\partial^2 U}{\partial X^2}\right)_S=-\left(\frac{\partial^2 U}{\partial S\partial X}\right)\left(\frac{\partial S}{\partial X}\right)_U-T\left(\left(\frac{\partial^2 S}{\partial X\partial U}\right)\left(\frac{\partial U}{\partial X}\right)_S+\left(\frac{\partial^2 S}{\partial X^2}\right)_U\right) \ ,$$
$$\left(\frac{\partial^2 U}{\partial X^2}\right)_S(S^e,X^e)=-T\left(\frac{\partial^2 S}{\partial X^2}\right)_U(U^e,X^e)<0 \ .$$
Therefore the internal energy has a minimum at equilibrium, when unrestrained varying the other than entropy extensive parameters . (Minimum energy principle).

Suppose a system is in contact with a temperature T and intensive parameters P_i reservoir. The other than internal energy unrestrained reduced extensive parameters are denoted by x . At equilibrium we have the system's entropy $S = S^e$, the extensive parameters $X_i = X^e{}_i$ and the reduced unrestrained parameters $x = x^e$ and
$$\frac{\partial U}{\partial S}(S^e,X_i^e,x^e)=T \ , \ \frac{\partial U}{\partial X_i}(S^e,X_i^e,x^e)=P_i \ .$$
Therefore , considering also stability criterions, the expression $\bar{U}=U-TS-P_iX_i$ will have a minimum when we vary S and X_i at equilibrium:

$$\bar{U}(S^e,X_i^e,x^e)=\min_{S,X_i}\left(U(S,X_i,x^e)-TS-P_iX_i\right)$$
By the above derived minimumenergy principle we have at equilibrium:

$$U(S^e,X_i^e,x^e)=\min_x U(S^e,X_i^e,x) \ .$$

Hence at equilibrium we will have:

$\bar{U}(S^e, X_i^e, x^e) = \min_{S, X_i, x} (U - TS - P_i X_i) = \min_x \tilde{U}(x)$ where $\tilde{U}$ is the potential

$\tilde{U} = \min_{S, X_i} (U - TS - P_i X_i)$

For the free energy potential we have generally with $U = U(S, V, N)$:

$$F = U - TS \ , \ F = F(T, V, N)$$
$$dF = -S\,dT - P\,dV + \mu\,dN$$
$$\frac{\partial F}{\partial T} = -S \ , \ \frac{\partial F}{\partial V} = -P$$ - the thermodynamical pressure ,

$\frac{\partial F}{\partial N} = \mu$ - the chemical potential of the particles from the system .

For the macrocanonical potential we have with $U = U(S, V, N)$

$$\Omega = U - TS - \mu N \ , \ \Omega = \Omega(T, V, \mu)$$
$$d\Omega = -S\,dT - N\,d\mu - P\,dV$$
$$\frac{\partial \Omega}{\partial T} = -S \ , \ \frac{\partial \Omega}{\partial V} = -P \ , \ \frac{\partial \Omega}{\partial \mu} = -N \ .$$

For the Gibbs potential we will have:

$$G = U - TS + PV \ , \ G = G(T, P, N)$$
$$dG = -S\,dT + V\,dP + \mu N$$
$$\frac{\partial G}{\partial T} = -S \ , \ \frac{\partial G}{\partial P} = V \ , \ \frac{\partial G}{\partial N} = \mu \ .$$

For the enthalpy potential we have:

$$H = U + PV \ , \ H = H(S, P, N)$$
$$dH = T\,dS + V\,dP + \mu\,dN$$
$$\frac{\partial H}{\partial S} = T \ , \ \frac{\partial H}{\partial P} = V \ , \ \frac{\partial H}{\partial N} = \mu \ .$$

17. Classsical statistical ensemble. Probability density Liouville theorem. Macrocanonical distribution Gibbs theorem

Classical statistical ensemble. Probability density. Liouville theorem. Macrocanonical distribution. Gibbs theorem

We consider physical systems described by a phase space of q_i – generalized coordinates and p_i – generalized momenta : $((q_i, p_i)_{i=\overline{1,s}}), q_i, p_i \in \mathbb{R}$ (for a N particles system we will have $s = 3N$), a Hamiltonian $H = H(q, p)$ and a statistical ensemble of M microstates $((q_i^a, p_i^a)_{i=\overline{1,s}})_{a=\overline{1,M}}$ (with large M) of such physical systems, all prepared in the same given macrostate described by thermodynamical parameters (U, S, X), with $X = (X_i)_{i=\overline{1,n}}$ the other extensive parameters than internal energy U and entropy S (see Chap. Thermodynamics).

For a domain $D_t \subset \mathbb{R}^{2s}$ in phase space we take

$$\bar{M}(D_t) = \text{card}\{a \in \{1, 2, ..., M\} | (q_i^a, p_i^a)_{i=\overline{1,s}} \in D_t\} \text{ and}$$

$$\Omega(D_t) = \int_{D_t} \prod_{i=1}^{s} dq_i dp_i \quad \text{- the measure in phase space}$$

with $(q_i^a, p_i^a) = (q_i^a(t), p_i^a(t))$ for time variable $t \in \mathbb{R}$, $i = \overline{1,s}$, $a = \overline{1,M}$,

so we can have $P(D_t, t) = \lim_{M \to \infty} \frac{\bar{M}(D_t)}{M}$ as the probability that a microstate $(q_i(t), p_i(t))_{i=\overline{1,s}}$ at time moment t , prepared in the given macrostate $(U(t), S(t), X(t))$ belongs to D_t .

The probability density for the given macrostate will be defined as

$$\rho(x, t) = \lim_{\Omega(D_t) \to 0, x \in D_t} \frac{P(D_t, t)}{\Omega(D_t)} \quad \text{with} \quad x = (x_i)_{i=\overline{1,2s}} = (q_i, p_i)_{i=\overline{1,s}} \text{ and we have}$$

$$\rho(x, t) \geq 0 \quad , \quad \int \rho(x, t) d^{2s}x = 1 \ .$$

The microstates evolution in time $x = x(t) = (q_i(t), p_i(t))_{i=\overline{1,s}}$ satisfies the Hamilton-Jacobi system

$$(*) \begin{cases} \dot{p}_i = -\frac{\partial H}{\partial q_i} \\ \dot{q}_i = \frac{\partial H}{\partial p_i} \ , \ i = \overline{1,s} \end{cases}$$

Therefore we can define for any $t \in \mathbb{R}$ the evolution operator on the phase space $\tilde{H} = \tilde{H}(t)$ such that $x(t) = \tilde{H}(t)x$ with $x(t) = (q_i(t), p_i(t))_{i=\overline{1,s}}$, as a function of time variable t , is the unique solution of the Cauchy problem defined by the system (*) and initial conditions $(q_i(0), p_i(0))_{i=\overline{1,s}} = x$ for given $x \in \mathbb{R}^{2s}$.

Let $D_t = \tilde{H}(t)(D)$ for $D \subset \mathbb{R}^{2s}$ and it follows :

$\Omega(D_t)=\int\limits_{D_t} d^{2s}x(t)=\int\limits_{D} J(t,0)d^{2s}x$ where $J(t,t')=\det\left(\frac{\partial x_i(t)}{\partial x_j(t')}\right)_{i,j=\overline{1,2s}}$ for $t,t'\in\mathbb{R}$.

We have $J(t,0)=J(t,t')J(t,0)$, $J(t,t)=1$ (1)

$$\frac{d}{dt}J(t,0)\Big|_{t=t'}=\frac{\partial J(t,t')}{\partial t}\Big|_{t=t'}J(t',0) \qquad (2)$$

and further , because of (1) , follows :

$$\frac{\partial J(t,t')}{\partial J_{ij}(t,t')}\Big|_{t=t'}=\delta_{ij} ,$$

$$\frac{\partial J(t,t')}{\partial t}\Big|_{t=t'}=\sum_{i,j}\frac{\partial J(t,t')}{\partial J_{ij}(t,t')}\frac{\partial J_{ij}(t,t')}{\partial t}\Big|_{t=t'}=\sum_{i=1}^{2s}\frac{\partial J_{ii}(t,t')}{\partial t}\Big|_{t=t'}=$$

$$=\sum_{i=1}^{s}\left(\frac{\partial \dot q_i(t')}{\partial q_i(t')}+\frac{\partial \dot p_i(t')}{\partial p_i(t')}\right)=\sum_{i=1}^{s}\left(\frac{\partial^2 H}{\partial q_i\partial p_i}-\frac{\partial^2 H}{\partial p_i\partial q_i}\right)(q(t'),p(t'))=0 .$$

Therefore from (1) and (2) we can derive now $J(t,0)=1$ for any $t\in\mathbb{R}$ and so $\Omega(D_t)=\Omega(D)$ for any $t\in\mathbb{R}$, $D\subset\mathbb{R}^{2s}$.

Because of the unicity of solutions for the Cauchy problem (*) for any given *x* in the phase space we have that the evolution operator is bijective at any time moment, having $(\widetilde{H}(t))^{-1}=\widetilde{H}(-t)$. Also, for suitable smooth H , $\widetilde{H}(t)$ must be continuous from $\mathbb{R}^{2s}$ to $\mathbb{R}^{2s}$ and so by a known theorem, $\widetilde{H}(t)$ is a homeomorphism from $\mathbb{R}^{2s}$ to $\mathbb{R}^{2s}$. Therefore for any $M\in\mathbb{N}^*$, $t\in\mathbb{R}$, $D\subset\mathbb{R}^{2s}$ we will have $P(D_t,t)=P(D,0)$ and since $\Omega(D_t)=\Omega(D)$ we obtain

$\rho(x(t),t)=\rho(x,0)$ for any $x\in\mathbb{R}^{2s}$, $t\in\mathbb{R}$ (3) .

Differentiating (3) with respect to time variable and using Hamilton-Jacobi relations we obtain also :

$\frac{\partial\rho}{\partial t}+[\rho,H]=0$ (4) where $[\rho,H]=\frac{\partial\rho}{\partial q}\cdot\frac{\partial H}{\partial p}-\frac{\partial\rho}{\partial p}\cdot\frac{\partial H}{\partial q}$ is the Poisson bracket.

The (3) , (4) relations represent the Liouville theorem for the probability density.

We notice that from the Hamilton-Jacobi system follows $\frac{d}{dt}H(x(t))=0$. (**)

For a dynamical function $F=F(x(t),t)$ we define the average $\langle F\rangle_t=\int\rho(x(t),t)F(x(t),t)d^{2s}x(t)=\int\rho(x,0)F(x(t),t)d^{2s}x$ and so differentiating with respect to t we obtain

$\frac{d\langle F\rangle_t}{dt}=\left\langle\frac{\partial F}{\partial t}\right\rangle_t+\langle[F,H]\rangle_t$ (5) .

The thermodynamical parameters are described as average values of some dynamical functions of the statistical ensemble.

If all systems of the statistical ensemble are prepared in the same equilibrium state (*U* , *S*, *X*) , then the virtual statistical ensemble is stationary, that is we have for the probability density a dependence in the form:

$\rho(x(t),t)=\rho(x(t))$ and according to (3) $\rho=\rho(x(t))$ is a not dependent on time integral of the system (*) . Therefore the probabibility density depends only of 2*s* independent integrals of the system (*). However, we suppose that the microstates probabilities , at equilibrium are well determined by the macroscopic state and backwards, the macroscopic state is well determined by the microstates probabilities. According to (**) , the Hamiltonian is also an integral not dependent on time of the system (*) and is in a well determination relation with the macrostate equilibrium state. Hence we will assume that for equilibrium states, the probability density dependends on the microstate *x* (*t*) only through *H*(*x*(*t*)) having $\rho = f(H)$. Measuring a macroscopic thermodynamical variable at equilibrium involves the determination of the temporal averaged value of a dynamical function $F = F(x(t))$,

namely the value $F_0(x)=\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau}F(x(t))dt=\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau}F(\widetilde{H}(t)x)dt$.

In determination of the macroscopic state, the insolvable problem (due to the large number of equations) for solutions of the Hamilton-Jacobi system is replaced to the problem of determination for probability densities by assuming the ergodic statement :

for any x we have the measurable time average $F_0(x)$ equal to the domain averaged F namely $\langle F\rangle_t=\int\rho(x)F(\widetilde{H}(t)x)d^{2s}x$ at equilibrium.

For systems which exchange particles with the environment we can consider a statistical ensemble with variable particles number of systems described by phase spaces $(\Gamma_N)_N$ ($\Gamma_N\subseteq\mathbb{R}^{2s}$, $s=3N$) , $x^{(N)}\in\Gamma_N$, Hamiltonians $H_N=H_N(x^{(N)},V)$, for each possible particles number N with V volume as an extensive parameter of the system and we will have partial probability densities $\rho_N=\rho_N(x^{(N)},t)$ with $\int_{\Gamma_N}\rho_N(x^{(N)},0)d^{2s}x^{(N)}=p_N$ - the probability that a system of the statistical ensemble has N particles.

All systems of the statistical ensemble are considered to be prepared in the same macrostate having volume *V*.

In the same way as above we will define

for $D_t^{(N)}\subset\Gamma_N$: $P_N(D_t^{(N)},t)$ the probability that a microstate $x^{(N)}\in\Gamma_N$ of the system of the ensemble when it has N particles belongs to $D_t^{(N)}\subset\Gamma_N$ at time t ,

$$\Omega(D_t^{(N)})=\int_{D_t^{(N)}}d^{2s}x^{(N)}\ ,\ \rho_N(x^{(N)},t)=p_N\lim_{\Omega(D_t^{(N)})\to 0,\,x^{(N)}\in D_t^{(N)}}\frac{P_N(D_t^{(N)},t)}{\Omega(D_t^{(N)})}\ .$$

$$P_N(D_t^{(N)},t)=\lim_{M\to\infty}\frac{\bar{M}_N(D_t^{(N)})}{M}$$

$$\bar{M}_N(D_t^{(N)})=\mathrm{card}\{a\in\{1,\dots,M\}\,|\,(q_i^a,p_i^a)_i\in D_t^{(N)}\}$$

with $(q_i^a,p_i^a)_i=x^{a(N)}$-microstates of the partial statistical ensemble $((q_i^a,p_i^a)_i)_{a=\overline{1,M}}$ corresponding to N particles systems of the total ensemble.

Consider now a system S_1 with N_1 particles , volume V_1 and Hamiltonian $H_1=H_{N1}(x_1,V_1)$, $x_1=x_1^{(N1)}$ phase space coordinates for S_1 . We assume that S_1 is in contact with a reservoir S_2 with N_2 particles, volume V_2 and Hamiltonian $H_2=H_{N2}(x_2,V_2)$, $x_2=x_2^{(N2)}$ phase space coordinates for S_2.

The total system $S=S_1\cup S_2$ has $N=N_1+N_2$ particles, volume $V=V_1+V_2$, $x=(x_1,x_2)$ phase space coordinates and a Hamiltonian $H_{tot}=H_{tot}(x,V)=H_1(x_1,V_1)+H_2(x_2,V_2)+H_{12}(x_1,x_2,V_1,V_2)$, where $H_{12}=H_{12}(x_1,x_2,V_1,V_2)$ is the interaction Hamiltonian between S_1 and S_2 particles. H_1 , H_2 are proportional sized to particle numbers from S_1 respective S_2 and H_{12} is proportional sized to the particle number from the surface surrounding the volume V_1 domain of S_1 and so H_{12} can be neglected in relation to H_1 + H_2 and so we can consider $H_{tot}(x,V)\approx H_1(x_1,V_1)+H_2(x_2,V_2)$.

According to above considerations we suppose that the systems S_1 and S_2 are prepared in macrostates with partial probability densities $\rho_{N1}=\rho_1(H_1(x_1,V_1),N_1)$ and respective $\rho_{N2}=\rho(H_2(x_2,V_2),N_2)$ and the total system is in thermodynamical equilibrium and also $N_1\ll N_2$.

Since S_1 , S_2 form together a system S which is in thermodynamical equilibrium, they must be statistical independent systems, the microstates of S_1 belong to a phase space domain D_1 independently of how microstates of S_2 belong to a phase space domain D_2 .

Therefore if $\rho=\rho_N(H_{tot}(x,V),N)$ is the partial probability density which determines the macrostate of the combined system S, as formed from S_1 and S_2 we will have $\rho(H_{tot}(x,V),N)=\rho_1(H_1(x_1,V_1),N_1)\rho_2(H_2(x_2,V_2),N_2)$ (6)

$$\rho(H_1+H_2,N_1+N_2)=\rho_1(H_1,N_1)\rho_2(H_2,N_2) \qquad (6')$$

Because the total system S is in thermodynamical equilibrium we have that H_{tot} and N are constant and so if S_1 and S_2 change energy and particles by infinitesimal amounts respective dH_1 , dH_2 , dN_1 , dN_2 we must have

$dH_1+dH_2=0$ (7)

$dN_1+dN_2=0$ (8)

H_1+H_2 and N_1+N_2 are constant and so from (6) follows :

$d\log\rho_1(H_1,N_1)+d\log\rho_2(H_2,N_2)=0$ (9) and with (7) and (8) we obtain :

$$\left(\frac{\partial\log\rho_1}{\partial H_1}(H_1,N_1)-\frac{\partial\log\rho_2}{\partial H_2}(H_2,N_2)\right)dH_1+$$

$$+\left(\frac{\partial\log\rho_1}{\partial N_1}(H_1,N_1)-\frac{\partial\log\rho_2}{\partial N_2}(H_2,N_2)\right)dN_1=0 \qquad (10)\ .$$

Since dH_1 and dN_1 are arbitrary infinitesimal values we derive now:

$$\frac{\partial \log \rho_1}{\partial H_1}(H_1(x_1,V_1),N_1)=\frac{\partial \log \rho_2}{\partial H_2}(H_2(x_2,V_2),N_2) \qquad (11)$$

$$\frac{\partial \log \rho_1}{\partial N_1}(H_1(x_1,V_1),N_1)=\frac{\partial \log \rho_2}{\partial N_2}(H_2(x_2,V_2),N_2) \qquad (12)$$

The right members of (11) and (12) depend on x_2 , N_2 , V_2 and we can consider since $N_1 \ll N_2$ and the reservoir volume is considered much larger than the S_1 system volume, that $V_2 \approx V$, $N_2 \approx N$.

The left members of (11) and (12) depend on x_1 , N_1 , V_1 which are independent of x_2 , N , V reservoir variables.

Therefore $\frac{\partial \log \rho_1}{\partial H_1}=\alpha$, $\frac{\partial \log \rho_1}{\partial N_1}=\beta$ with α,β constants depending only on the macrostate of the reservoir .

We take $\alpha=-\frac{1}{\Theta}$, $\beta=\frac{\mu}{\Theta}$ and we must have $\rho_1=\exp\left(\frac{\Omega-H_1+\mu N}{\Theta}\right)$ where Ω not depends on x_1, N_1 .

Hence a system in equilibrium with a reservoir will have partial probability densities $\rho_N=\rho_N(x^{(N)},\Theta,\mu,V)=\exp\left(\frac{\Omega-H_N(x^{(N)},V)+\mu N}{\Theta}\right)$ with $x^{(N)}\in\Gamma_N$ phase space variables for a system of the statistical ensemble with N particles , Hamiltonian $H_N=H_N(x^{(N)},V)$ and V macroscopic volume of the system such that $\int_{\Gamma_N}\rho_N d^{2s}x^{(N)}=p_N$ -probability that the system in the ensemble has N particles .

We must have $\sum_N p_N=1$ and so $\Omega=-\Theta\log Z$ with

$$Z=\sum_N \int_{\Gamma_N} \exp\left(\frac{-H_N(x^{(N)},V)+\mu N}{\Theta}\right) d^{2s}x^{(N)}$$

μ,Θ are constants depending only on the reservoir macrostate thermodynamic parameters.

Let $\langle H\rangle=\sum_N \int_{\Gamma_N} H_N\rho_N d^{2s}x^{(N)}=U$ -the internal energy parameter,

$$\left\langle\frac{\partial H}{\partial V}\right\rangle=\sum_N \int_{\Gamma_N}\frac{\partial H_N}{\partial V}\rho_N d^{2s}x^{(N)}=-P$$ -the pressure parameter,

$\langle N\rangle=\sum_N \int_{\Gamma_N} N\rho_N d^{2s}x^{(N)}=N_t$ -the particles number thermodynamic parameter.

Considering the above definitions, we will have :

$$0=\frac{\partial}{\partial V}\sum_N \int_{\Gamma_N} \rho_N d^{2s}x^{(N)}=\sum_N \frac{1}{\Theta}\frac{\partial \Omega}{\partial V}\int_{\Gamma_N}\rho_N d^{2s}x^{(N)}-\sum_N \frac{1}{\Theta}\int_{\Gamma_N}\frac{\partial H_N}{\partial V}\rho_N d^{2s}x^{(N)}=$$

$$=\frac{1}{\Theta}\frac{\partial \Omega}{\partial V}+\frac{P}{\Theta} \quad \text{and so} \quad \frac{\partial \Omega}{\partial V}=-P \qquad (13)$$

$$0=\frac{\partial}{\partial \Theta}\sum_N \int_{\Gamma_N} \rho_N d^{2s}x^{(N)}=\sum_N \frac{1}{\Theta}\frac{\partial \Omega}{\partial \Theta}\int_{\Gamma_N}\rho_N d^{2s}x^{(N)}-\sum_N \frac{1}{\Theta^2}\int_{\Gamma_N}(\Omega-H_N+\mu N)\rho_N d^{2s}x^{(N)}=$$

$$=\frac{1}{\Theta}\frac{\partial \Omega}{\partial \Theta}-\frac{1}{\Theta^2}(\Omega-U+\mu N_t) \text{ and so } U=\Omega-\Theta\frac{\partial \Omega}{\partial \Theta}+\mu N_t \qquad (14)$$

$$0=\frac{\partial}{\partial \mu}\sum_N \int_{\Gamma_N} \rho_N d^{2s}x^{(N)}=\frac{1}{\Theta}\sum_N \frac{\partial \Omega}{\partial \mu}\int_{\Gamma_N}\rho_N d^{2s}x^{(N)}+\frac{1}{\Theta}\sum_N \int_{\Gamma_N} N\rho_N d^{2s}x^{(N)}=$$

$$=\frac{1}{\Theta}\frac{\partial \Omega}{\partial \mu}+\frac{1}{\Theta}N_t \quad \text{and so} \quad \frac{\partial \Omega}{\partial \mu}=-N_t \qquad (15)$$

From (14) we obtain :

$$\frac{\partial \Omega}{\partial \Theta}=\sum_N \int_{\Gamma_N}\rho_N \log \rho_N d^{2s}x^{(N)} \qquad (16)$$

From (14) and (13) we obtain after differentiating (14) that:

$$dU=-\Theta d\frac{\partial \Omega}{\partial \Theta}-P dV+\mu d N_t \qquad (17)$$

Consider now two systems S_1 and S_2 which do not exchange particles and evolve with constant particles numbers reaching an each to other equilibrium state in the combined system $S=S_1\cup S_2$. Since the particles numbers of the systems do not change , we can consider that $\mu_1 = \mu_2 = 0$ and the system will have probability densities at equilibrium given respective as:

$$\rho_i=\exp\left(\frac{F_i-H_i(x_i,V_i)}{\Theta_i}\right) \text{ with } F_i=-\Theta_i \log\int \exp\left(-\frac{H_i(x_i,V_i)}{\Theta_i}\right)d^{2s_i}x_i \quad \text{for } i=1,2 \ ,$$

with Θ_1,Θ_2 equilibrium parameters and V_1, V_2 respective volumes at equilibrium. Because as noticed before the interaction energy H_{12} between system is small compared to H_1 , H_2 at equilibrium we suppose that, allowing an infinitesimal energy exchange between systems we have that

$$dH_1+dH_2=0 \qquad (18)$$, near to the equilibrium state.

At equilibrium the two systems are statistical independent and so the probability density of the combined system S will be at equilibrium :

$$\rho=\rho_1(x_1)\rho_2(x_2)=\exp\left(\frac{F_1}{\Theta_1}+\frac{F_2}{\Theta_2}-\frac{H_1(x_1,V_1)}{\Theta_1}-\frac{H_2(x_2,V_2)}{\Theta_2}\right).$$

The combined system is also in equilibrium and so we will have an equilibrium parameter Θ such that $\rho=\exp\left(\frac{F}{\Theta}-\frac{H}{\Theta}\right)$ with $F=-\Theta\log\int\exp\left(-\frac{H}{\Theta}\right)d^{2s_1}x_1 d^{2s_2}x_2$,

$H=H_1(x_1,V_1)+H_2(x_2,V_2)$.

Therefore , considering the (x_1 , x_2) dependence , we must have at equilibrium

$H_1\left(\frac{1}{\Theta}-\frac{1}{\Theta_1}\right)=C-H_2\left(\frac{1}{\Theta}-\frac{1}{\Theta_2}\right)$ with C not depending on x_1, x_2 .

The left member of the above relation depends only on x_1 , while the right member depends only on x_2 . Since x_1 and x_2 are independent variables it follows $C=0$, $\Theta=\Theta_1=\Theta_2$.

Hence systems which are each to other in a thermodynamic equilibrium relation have the same Θ parameter.

Considering (17) which gives Θ^{-1} as an integration factor for the heat exchange differential form $\delta Q=dU+PdV-\mu dN$ and relations (13), (14) , (15) we can therefore interpretate Θ as an absolute equilibrium temperature and we can take $\Theta=k_B T$ with T -thermodynamical absolute temperature at equilibrium ,

k_B -the Boltzmann constant,

Ω -the macrocanonical thermodynamical potential,

μ -the chemical potential parameter.

Thus the partial probability densities of a system in equilibrium will be

$$\rho_N=\exp\left(\frac{\Omega-H_N(x^{(N)},V)+\mu N}{k_B T}\right) \text{ with } \Omega=-k_B T\log Z \ ,$$

$$Z=\sum_N \int_{\Gamma_N} \exp\left(\frac{-H_N(x^{(N)},V)+\mu N}{k_B T}\right) d^{2s}x^{(N)} \ .$$

According to (16) , the entropy of the system is

$$S=-\frac{\partial\Omega}{\partial T}=-k_B\frac{\partial\Omega}{\partial\Theta}=-k_B\sum_N\int_{\Gamma_N}\rho_N\log\rho_N d^{2s}x^{(N)}.$$

If the system not exchanges particles with the environmental reservoir then we have no dependence on particles number and the probability density becomes

$$\rho=\exp\left(\frac{F-H(x,V)}{k_B T}\right) \text{ with } F=-k_B T\log Z \ , \ Z=\int\exp\left(-\frac{H(x,V)}{k_B T}\right)d^{2s}x \ ,$$

$F=U-TS$ is the free energy potential and the entropy is $S=-k_B\int\rho\log\rho d^{2s}x$.

(Notice that in all relations log is the natural logarithm.)

For a discrete probability density of W microstates with p_i the probability for the realisation of state i , i = 1,2,…,W we have $S=-k_B\langle\log\rho\rangle=-k_B\sum_{i=1}^{W}p_i\log p_i$.

We recognize the Shannon entropy of the system.

If $p_i=\frac{1}{W}$ for $i=\overline{1,W}$ we obtain $S=-k_B\sum_{i=1}^{W}\frac{1}{W}\log\left(\frac{1}{W}\right)=k_B\log W$,

$S=k_B\log W$ with W -the number of microstates corresponding to the same macrostate.

As we know, the Shannon entropy is maximal for an uniform probability distribution.

An ensemble of a system with N particles which can have states 1,2,…,s such that k_j particles can have state j for j = 1,2,…,s in the same macrostate with

$\sum_{j=1}^{s} k_j = N$ has a number of $W = \frac{N!}{k_1! \ldots k_s!}$ microstates.

The fact that for the *N* particles system the entropy must be a maximum at thermodynamical equilibrium (see Chap. Thermodynamics) can be derived as $\frac{N!}{k_1! \ldots k_s!} \leq N!$ the entropy $k_B \log W$ being maximal at $k_1 = k_2 = \ldots = k_s = 1$, $s = N$.

Hence a system who is interacting only with itself tends to evolve to thermodynamical equilibrium to a state of the highest probability among all possible *N*! states, according to:

$\frac{1}{k_1! \ldots k_s!} = \frac{W(k_1, k_2, \ldots, k_s)}{N!} \leq \frac{W(1,1,\ldots,1)}{N!}$ for $k_j \in \{1,2,\ldots,N\}$, $j = \overline{1,s}$,

$s \in \{1,\ldots,N\}$, $\sum_{j=1}^{s} k_j = N$.

Consider now a system (for example a gas of molecular particles) with the Hamiltonian having the form

$$H(q,p) = H_{kin}(p) + H_{pot}(q) ,$$

where H_{kin} -kinetic energy and H_{pot} -potential energy are quadratic forms of

$p = (p_i)_{i=\overline{1,h}}$ and respective $q = (q_i)_{i=\overline{1,h}}$, $H_{kin} = \sum_{i=1}^{h} \frac{p_i^2}{2m}$ with

m -the mass of a molecular particle (if for a degree of freedom i the p_i is an angular momentum of rotation around onre of three molecular axes then m in the $\frac{p_i^2}{2m}$ term will be replaced by the corresponding moment of inertia of the molecule).

For a gas system with *N* particles we have *h* = *s N* where

s = 3 degrees of freedom for each particle if we have a monoatomic gas,

s = 5 degrees of freedom for each particle if we have a biatomic gas (two additional degrees of freedom corresponding to rotations around two transversal to the molecule, orthogonal axes of rotation, the angular momentum of rotation around the axis along the molecule being neglected),

s = 6 degrees of freedom for each particle for more complicated molecules.

We assume that in the expression of H_{pot} (*q*) each particle is involved with with *f* degrees of freedom and therefore H_{pot}(*q*) involves *f N* degrees of freedom.

We have $2H_{kin} = \sum_{i=1}^{sN} p_i \frac{\partial H}{\partial p_i}$ (19)

$2H_{pot} = \sum_{j=1}^{fN} q_{i(j)} \frac{\partial H}{\partial q_{i(j)}}$ (20)

where $(i(j))_{j=\overline{1,fN}}$ are the degrees of freedom involved in H_{pot} which is a quadratic form if we consider elastic molecular interactions; for cristals formed by particles with 3 degrees of freedom we take *f* = 3 and for biatomic gases we consider only vibrations of atoms in the direction of molecular axis and so *f* = 1 .

Obviously, as quadratic forms, H_{kin} and H_{pot} must be considered positive strict definite in $(p_i)_{i=\overline{1,sN}}$ respective $(q_{i(j)})_{j=\overline{1,fN}}$.

For the system prepared in a thermodynamical equilibrium macrostate with a thermostat at temperature T, without exchanging particles with the thermostat we will have a probability density given by

$$\rho=\rho(q,p)=\frac{1}{Z}\exp\left(-\frac{H(q,p)}{k_BT}\right) \text{ with } Z=\int \exp\left(-\frac{H(q,p)}{k_BT}\right)d^hq\,d^hp \ .$$

Since H_{kin} is a strict positive definite quadratic form we have for $i=\overline{1,sN}$:

$$p_i\exp\left(-\frac{H}{k_BT}\right)\Bigg|_{p_i=-\infty}^{p_i=\infty}=0 \quad ,$$

$$\frac{\partial}{\partial p_i}\left(p_i\exp\left(-\frac{H}{k_BT}\right)\right)=\exp\left(-\frac{H}{k_BT}\right)-\frac{1}{k_BT}p_i\frac{\partial H}{\partial p_i}\exp\left(-\frac{H}{k_BT}\right)$$

and so with (19) we derive $\langle H_{kin}\rangle=\int H_{kin}\rho d^hq\,d^hp=\frac{1}{2}sNk_BT$.

Since H_{pot} is strict positive definite we have for $i\in\{i(j)|j=\overline{1,fN}\}$:

$$q_i\exp\left(-\frac{H}{k_BT}\right)\Bigg|_{q_i=-\infty}^{q_i=\infty}=0 \quad ,$$

$$\frac{\partial}{\partial q_i}\left(q_i\exp\left(-\frac{H}{k_BT}\right)\right)=\exp\left(-\frac{H}{k_BT}\right)-\frac{1}{k_BT}q_i\frac{\partial H}{\partial q_i}\exp\left(-\frac{H}{k_BT}\right)$$

and so with (20) we derive $\langle H_{pot}\rangle=\int H_{pot}\rho d^hq\,d^hp=\frac{1}{2}fNk_BT$.

Therefore we obtain $U=\frac{s+f}{2}k_BNT$ and we have an amount of $\frac{1}{2}k_BT$ energy for each degree of freedom in H_{kin} and for each degree of freedom involved in H_{pot}.

For example if we neglect the interactions within the molecules we will have $H_{kin}=H(p)$, $H_{pot}=0$ and $U=\frac{3}{2}Nk_BT$ for monoatomic gases,

$U=\frac{5}{2}Nk_BT$ for biatomic gases, $U=3Nk_BT$ for more general molecular gases.

A classical system can be also considered as a thermodynamical system of N subsystems which are independent and are in states $s\in S$, the state s having an energy ε_s with a g_s degeneracy (there are g_s possibilities for a subsystem to be in state s with energy ε_s).

Let N_s the number of subsystems in state s . Then the virtual statistical ensemble will have $W=\frac{N!}{\prod_s N_s!}\prod_s g_s^{N_s}$ microstates which correspond to the same macrostate

having particle number $N=\sum_s N_s$ and energy $U=\sum_s \varepsilon_s N_s$.

The entropy for this state is therefore
$S=k_B \log W$ and at thermodynamical equilibrium we must have
$S=\max\{S((N_s)_s)\,|\sum_s \varepsilon_s N_s=U\ ,\ \sum_s N_s=N\}$.

Taking α,β additional variables as Lagrange coefficients we must have:
$d(\log(N!)-\sum_s(\log(N_s!)-g_s N_s))+\beta((\sum_s N_s)-N)+\alpha((\sum_s \varepsilon_s N_s)-U)$ and so

$\log((N_s-1)!)-\log(N_s!)+\log g_s+\beta+\alpha\varepsilon_s=0$

$N_s=g_s\exp(\beta+\alpha\varepsilon_s)=\frac{g_s\exp(\alpha\varepsilon_s)}{\sum_{s'} g_{s'}\exp(\beta+\alpha\varepsilon_{s'})}N$

$\beta=\log N-\log(\sum_s g_s\exp(\alpha\varepsilon_s))$.

At equilibrium we will have also
$dS=k_B\sum_s(-\log N_s+\log g_s)dN_s=-k_B\sum_s(\beta+\alpha\varepsilon_s)dN_s=-k_B\beta dN-k_B\alpha dU$.

Considering the relation $dS=\frac{1}{T}dU-\frac{\mu}{T}dN$ (see Chap. Thermodynamics)

we must take $\alpha=-\frac{1}{k_B T}$, $\beta=\frac{\mu}{k_B T}$ with T -equilibrium temperature,

μ -chemical potential and at equilibrium we have the energy levels occupation

numbers $N_s=g_s\exp\left(\frac{\mu-\varepsilon_s}{k_B T}\right)=g_s\frac{\exp\left(-\frac{\varepsilon_s}{k_B T}\right)}{Z}N$ with $Z=\sum_s g_s\exp\left(-\frac{\varepsilon_s}{k_B T}\right)$.

18. Dirac spinors. Quantization of a Dirac field Quantum electrodynamics. Fadeev-Popov method Fermi weak theory

Dirac spinors, Quantization of a Dirac field, Quantum electrodynamics

As before we consider, by suitable choosing of length, time, electric charge units that $\hbar=1$ (reduced Planck constant) , $c=1$ (speed of light in vacuum constant) , $\varepsilon=1$ (electrical permittivity of vacuum constant), $\mu=1$ (magnetic permeability of vacuum constant) and the Minkowski space-time with metric signature(+, - , - , -)the metric coefficients $(\eta^{\alpha\beta})_{\alpha,\beta=\overline{0,3}}=\mathrm{diag}(1,-1,-1,-1)$, space-time coordinates denoted usual by $x=(x^{\alpha})_{\alpha=\overline{0,3}}=(t,\vec{x})$.

The relativistic relation $E^2=\vec{p}^2+m^2$ (1) which holds for a free particle with rest mass m , momentum $\vec{p}$ and energy E leads for the energy and momentum operators $i\frac{\partial}{\partial t}$ respective $\left(-i\frac{\partial}{\partial x^j}\right)_{j=\overline{1,3}}$ to the Klein-Gordon equation

$(\partial_{\alpha}\partial^{\alpha}+m^2)\,\psi=0$ (2) with $\psi=\psi(t,\vec{x})$.

In order to obtain a linear equation for some possible wave function from (2) we take the $\hat{H}=\pm\sqrt{\hat{\vec{p}}^2+m^2}$ expression equivalent to (2) as $\hat{H}=\alpha^j\hat{p}_j+\alpha^0 m$ where $(\alpha^{\mu})_{\mu=\overline{0,3}}$ is a set of coefficients satisfying $\alpha^{\mu}\alpha^{\lambda}+\alpha^{\lambda}\alpha^{\mu}=2\,\delta_{\mu\lambda}$ for $\mu,\lambda=\overline{0,3}$ (3).

The (3) relations are satisfied if we take

$\alpha^0=\gamma^0$, $\alpha^j=\gamma^0\gamma^j$ where γ^{μ} , $\mu=\overline{0,3}$ are the 4×4 gamma matrices:

$\gamma^0=\begin{pmatrix}\boldsymbol{I} & 0\\ 0 & -\boldsymbol{I}\end{pmatrix}$, $\gamma^j=\begin{pmatrix}0 & \sigma_j\\ -\sigma_j & 0\end{pmatrix}$ with σ_j , $j=\overline{1,3}$ the Pauli matrices

$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$, $\sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$.

Therefore we can consider for the relativistic mass *m* particle the following Dirac equation in place of a Schroedinger equation :

$(i\gamma^{\mu}\partial_{\mu}-m)\,\psi=0$,since we have $\hat{H}=i\partial_0$, $\hat{p}_j=-i\partial_j$, $j=\overline{1,3}$ where $\psi=\psi(t,\vec{x})$ as we noticed in Chap. Representations of the rotation group and of the restricted Lorentz group and Chap. On the rotations group and the restricted Lorentz group, must be a Dirac spinor field $\psi=(\psi_{\alpha})_{\alpha=\overline{0,3}}$ describing a spin 1/2 , mass m particle, so that if $\Lambda=\exp(\omega_{\alpha\beta}J^{\alpha\beta})$ with $\omega_{\alpha\beta}=-\omega_{\beta\alpha}\in\mathbb{R}$ and $J^{\alpha\beta}=-J^{\beta\alpha}$ the $SO^{+}(3,1)$ generators , is a restricted Lorentz transformation of coordinates

$x^{\alpha}\to x'^{\alpha}=\Lambda_{\alpha\beta}x^{\beta}$ then the Dirac spinor ψ transforms as $\psi'=S(\Lambda)\psi$ with

$S(\Lambda)=\exp\left((i/2)\,\omega_{\alpha\beta}\sigma^{\alpha\beta}\right)$, $\sigma^{\alpha\beta}=\frac{i}{2}[\gamma^{\alpha},\gamma^{\beta}]$, $J^{\alpha\beta}_{\gamma\delta}=-\frac{1}{2}\epsilon^{\alpha\beta\varepsilon\varphi}\epsilon_{\varepsilon\varphi\delta\rho}\eta^{\gamma\delta}$

$J^{ij}=-\epsilon_{ijk}J_k$, $J^{0i}=-J^{i0}=-K_i$.

$\epsilon_{\alpha\beta\gamma\delta}$ the signature of the permutation $\begin{pmatrix}\alpha & \beta & \gamma & \delta\\ 0 & 1 & 2 & 3\end{pmatrix}$

Hence we can have a mass *m* fermion moving in a central forces potential $V = V(r)$, $r = \|\vec{x}\|$ field Hamiltonian $\hat{H} = \alpha^0 m + \alpha^j \hat{p}_j + V(r)$ (4).

As we know from Chap. Quantum statistical ensemble , for an observable that not depends explicitely on time, $\hat{A}$, we have $\frac{d\langle \hat{A} \rangle_t}{dt} = -i\langle [\hat{A}, \hat{H}] \rangle_t$ and so the measurements of $\hat{A}$ are conserved in time if and only if $\hat{A}$ commutes with $\hat{H}$ considering $\hat{H}$ given by (4) and taking the orbital angular momentum operator $\hat{\vec{L}}_l = \hat{\vec{x}} \times \hat{\vec{p}}$, with $\vec{x} = (x, y, z)$ considering $[\hat{p}_j, \hat{x}^k] = -i\,\delta_{jk}$, we will have:

$[\hat{H}, \hat{L}_{lz}] = -i(\alpha^1 \hat{p}_y - \alpha^2 \hat{p}_x) = -\frac{1}{2}[\hat{H}, i\,\gamma^1\gamma^2]$,

$[\hat{H}, \hat{L}_{ly}] = -i(\alpha^3 \hat{p}_x - \alpha^1 \hat{p}_z) = -\frac{1}{2}[\hat{H}, i\,\gamma^3\gamma^1]$,

$[\hat{H}, \hat{L}_{lx}] = -i(\alpha^2 \hat{p}_z - \alpha^3 \hat{p}_y) = -\frac{1}{2}[\hat{H}, i\,\gamma^2\gamma^3]$

and taking $\hat{s}_k = \frac{1}{4}\epsilon_{ljk}\sigma^{lj} = \frac{1}{2}\begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}$ we can consider a spin angular momentum operator $\hat{\vec{L}}_s = \hbar \vec{S}$ (we restored the Planck constant by dimensional analysis), where $\vec{S} = \frac{1}{2}(\sigma^{23}, \sigma^{31}, \sigma^{12})$ is the spin operator, such that the total angular momentum

$\vec{L}_j = \vec{L}_l + \vec{L}_s$ is a conserved in time quantity: $[\hat{\vec{L}}_j, \hat{H}] = 0$

The spin angular momentum $\hat{L}_{sz}$ has eigenvalues $\pm\frac{1}{2}\hbar$.

Under a z-axis rotation $\Lambda = \exp(i\,\theta J^{12})$ a S_z eigenfunction ψ with $\frac{1}{2}\sigma^{12}\psi = \frac{1}{2}\psi$ transforms like $\psi \to \psi' = S(\Lambda)\psi = \exp(i\frac{\theta}{2}\sigma^{12})\psi = \exp(i\frac{\theta}{2})\psi$, so that a full 2π rotation flips the sign of the spin eigenfunction.

Given a versor $\vec{n}$ the spin along $\vec{n}$ is $\vec{S}\cdot\vec{n}$.

Further we have :

$\hat{\vec{L}}_s^2 = \hat{L}_{sx}^2 + \hat{L}_{sy}^2 + \hat{L}_{sz}^2 = \frac{3}{4}\hbar^2 \boldsymbol{I} = s(s+1)\hbar^2 \boldsymbol{I}$, $s = \frac{1}{2}$ is the spin quantum number.

Taking spherical coordinates $(x, y, z) = (r\cos(\theta), r\sin(\theta)\cos(\varphi), r\sin(\theta)\sin(\varphi))$ with $\theta \in (0, \pi)$, $\varphi \in (0, 2\pi)$ we have

$\frac{1}{\hbar^2}\hat{\vec{L}}_l^2 = -\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2} - \frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)$ the spherical functions operator having eigenvalues $l(l+1)$, $l \in \mathbb{N}$

and $\frac{1}{\hbar}\hat{L}_{lz} = -i\frac{\partial}{\partial\varphi}$ having eigenvalues $m = 0, \pm 1, ..., \pm l$ for eigenfunctions the spherical functions

$Y_l^m(\theta,\varphi)=P_l^{|m|}(\cos(\theta))\exp(im\varphi)$ where $P_l^{|m|}$ are the associated Legendre polynomials $P_l^m(x)=(-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_l^0(x)$, P_l^0 the Legendre polynomial of degree $l: P_l^0(x)=\frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l=\frac{1}{2^l}\sum_{k=0}^{\left\lfloor\frac{l}{2}\right\rfloor}(-1)^k\binom{l}{k}\binom{2l-2k}{l}x^{l-2k}$.
l is the orbital quantum number and *m* is the magnetic quantum number.
(Obviously we will not confuse the magnetic quantum number *m* which is an integer with the mass *m* of the particle which is a real positive number.)

For the free particle of mass *m* we have therefore the Dirac equation satisfied by the Dirac spinor field $\psi=\psi(t,\vec{x})$ which describes the particle system:
$(i\gamma^\mu\partial_\mu-m)\psi=0$, $\psi=(\psi_\alpha)_{\alpha=\overline{0,3}}$ as a column vector (5)

Taking the Lagrangian density
$\mathscr{L}(\psi,\partial\psi)=\overline{\psi}(i\partial\!\!\!/-m)\psi$ (6) where $\partial\!\!\!/=\gamma^\mu\partial_\mu$, $\overline{\psi}=\psi^+\gamma^0$ since ψ_α are complex functions we can vary independently $\overline{\psi}$ and ψ in (6) to obtain the Euler-Lagrange equation of motion from $d_\mu\left(\frac{\partial\mathscr{L}}{\partial(d_\mu\psi)}\right)-\frac{\partial\mathscr{L}}{\partial\psi}=0$, $\partial_\mu(i\overline{\psi}\gamma^\mu)+m\overline{\psi}=0$ which upon hermitean conjugation and multiplication with γ^0 gives the Dirac equation (5).
From the other variational equation $d_\mu\left(\frac{\delta\mathscr{L}}{\delta(\partial_\mu\overline{\psi})}\right)-\frac{\delta\mathscr{L}}{\delta\overline{\psi}}=0$ we obtain the Dirac equation (5) more directly.
Although the Lagrangian density (6) treats asymmetrically ψ and $\overline{\psi}$, integrating by parts the action $S=\int\mathscr{L}(\psi,\partial\psi)d^4x$, having ∂_μ act on $\overline{\psi}$ and then average the two forms of the Lagrangian, we can see that S treats ψ and $\overline{\psi}$ symmetrically.
Obviously, the relations (3) hold even if instead of the canonical gamma matrices we take any set $(M\gamma^\mu M^{-1})_{\mu=\overline{0,3}}$ with $M\in M_{4\times4}(\mathbb{C})$, $\det M\neq0$. We notice also that for any versor $\vec{n}$ we have $(2\vec{S}\cdot\vec{n})^2=\boldsymbol{I}$ and so the spin along $\vec{n}$ can have only eigenvalues $\pm\frac{1}{2}$.

Considering the Lagrangian density (6) the free particle system is described by the Dirac spinor field operator function $\hat{\psi}=\hat{\psi}(t,\vec{x})$ and the momentum density field operator function conjugate to $\hat{\psi}_\alpha$ is $\hat{\pi}_\alpha=\hat{\pi}_\alpha(t,\vec{x})=\frac{\delta\hat{\mathscr{L}}}{\delta(\partial_0\psi_\alpha)}(t,\vec{x})=i\hat{\psi}_\alpha^+(t,\vec{x})$.
The canonical commutation between generalized coordinates observables and generalized momentum observables, considered for the discretization of the Dirac spinor field at two locations *x* respective *x'* at the same moment in time *t* supposes a

exchange of locations between virtual particles located at *x* and *x'* and so the canonical commutation relation which would be $[\hat{\psi}_\alpha(t,\vec{x}),\hat{\pi}_\beta(t,\vec{x}')]=i\delta^3(\vec{x}-\vec{x}')\delta_{\alpha\beta}$,in consideration of spin statistics for fermions which reqiures anticommutation will lead to the anticommutation relation $\{\hat{\psi}_\alpha(t,\vec{x}),\hat{\psi}_\beta(t,\vec{x}')\}=\delta^3(\vec{x}-\vec{x}')\delta_{\alpha\beta}$ (7), where $\{A,B\}=AB+BA$ is the anticommutator of operators A and B .

Plugging in equation (5) plane wave solutions $\psi(x)=u(p,s)\exp(-ipx)$ and $\psi(x)=v(p,s)\exp(ipx)$ we obtain $p_0=\sqrt{\vec{p}^2+m^2}$ and $(\not{p}-m)u(p,s)=0$, $(\not{p}+m)v(p,s)=0$ where $\not{p}=\gamma^\mu p_\mu$

u and *v* are 4-component Dirac spinors.

Taking $u=\begin{pmatrix}u_1\\u_2\end{pmatrix}$, $v=\begin{pmatrix}v_1\\v_2\end{pmatrix}$ with u_j , v_j two component parts of u respective v

we obtain $p_0u_1-(\sigma_1p_1+\sigma_2p_2+\sigma_3p_3)u_2=mu_1$

$(\sigma_1p_1+\sigma_2p_2+\sigma_3p_3)u_1-p_0u_2=mu_2$ and since $p_0^2=\vec{p}^2+m^2$,

the system $(\not{p}-m)u(p,s)=0$ (8) has for a given $\vec{p}$ two linear independent

solutions $u(p,\pm1)$. In the same way we find two linear independent solutions $v(p,\pm1)$ for the system $(\not{p}+m)v(p,s)=0$ (9)

Under a restricted Lorentz transformation Λ , we have

$x'=\Lambda x$, $p=\Lambda^T p'$, $u'(p',s)=S(\Lambda)u(p,s)$

$\bar{u}'u'=u^+S^+\gamma^0Su=u^+\exp(-(i/2)\omega_{\alpha\beta}\sigma^{+\alpha\beta})\gamma^0\exp((i/2)\omega_{\alpha\beta}\sigma^{\alpha\beta})u=$

$=u^+\gamma^0S^{-1}\gamma^0\gamma^0Su=\bar{u}u$ and similar $\bar{v}'v'=\bar{v}v$.

In the rest frame $p=(m,0,0,0)$ (8) and (9) having the form $(\gamma^0-\boldsymbol{I})u=0$;

$(\gamma^0+\boldsymbol{I})v=0$ and so imposing normalization conditions $\bar{u}u=1$, $\bar{v}v=-1$

we obtain that in the rest frame we have :

$$u(p,1)=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\ u(p,-1)=\begin{pmatrix}0\\1\\0\\0\end{pmatrix},\ v(p,1)=\begin{pmatrix}0\\0\\1\\0\end{pmatrix},\ v(p,-1)=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

Lorentz invariance and basis independence tell us that in general we must have

$\bar{u}(p,s)u(p,s')=\delta_{ss'}$, $\bar{v}(p,s)v(p,s')=-\delta_{ss'}$, (10)

$\bar{u}(p,s)v(p,s')=\bar{v}(p,s')v(p,s)=0$

Furthermore, by Lorentz variance it follows:

$$\sum_s u_\alpha(p,s)\bar{u}_\beta(p,s)=\left(\frac{\not{p}+m}{2m}\right)_{\alpha\beta}$$

$$\sum_s v_\alpha(p,s)\bar{v}_\beta(p,s)=\left(\frac{\not{p}-m}{2m}\right)_{\alpha\beta}$$

The anticommutation relations (7) allow now a quantization of the field operator as

$$\hat{\psi}_\alpha(x)=\int \frac{d^3\vec{p}}{(2\pi)^{3/2}(E_p/m)^{1/2}}\sum_s\left(b(p,s)u_\alpha(p,s)\exp(-ipx)+\right.$$

$$\left.+d^+(p,s)v_\alpha(p,s)\exp(ipx)\right) \qquad (11)$$ where $E_p=\sqrt{\vec{p}^2+m^2}$, $px=p_\mu x^\mu$,

$$\{b(p,s),b^+(p',s')\}=\delta^3(\vec{p}-\vec{p}')\delta_{ss'} \ , \ \{d(p,s),d^+(p',s')\}=\delta^3(\vec{p}-\vec{p}')$$

$$\{b(p,s),b(p',s')\}=\{d(p,s),d(p',s')\}=\{b(p,s),d(p',s')\}=0$$

b,d ; b^+,d^+ are anihilation respective creation operators and depend on $(\vec{p},s)$.

Corresponding to the (6) Lagrangian density, we have a Hamiltonian density

$H=\pi(t,\vec{x})\partial_0\psi(t,\vec{x})-\mathscr{L}(t,\vec{x})=i\overline{\psi}\gamma^0\partial_0\psi-\mathscr{L}$ and so the Hamiltonian is

$$\hat{H}=\int d^3\vec{x}(-i\hat{\overline{\psi}}\gamma^k\partial_k\hat{\psi}+m\hat{\overline{\psi}}\hat{\psi})=\int d^3\vec{x}\, i\hat{\psi}^+\partial_0\hat{\psi}(t,\vec{x})=$$

$$\sum_{s,s'}\int i\,d^3\vec{x}\int d^3\vec{p}\,d^3\vec{p}'\left(\frac{\bar{u}(\vec{p},s)\gamma^0}{E_p^{1/2}}b^+(\vec{p},s)\exp(ipx)+\frac{\bar{v}(\vec{p},s)\gamma^0}{E_p^{1/2}}d(\vec{p},s)\exp(-ipx)\right)$$

$$\frac{m}{(2\pi)^3}(-i)(E_{p'}^{1/2}u(\vec{p}',s')b(\vec{p}',s')\exp(-ip'x)-E_{p'}^{1/2}v(\vec{p}',s')d^+(\vec{p}',s')\exp(ip'x))$$

We have :

$$(\gamma^0p_0+\gamma^kp_k)v(\vec{p},s)=-mv(\vec{p},s)$$

$$\bar{u}(-\vec{p},s')(\gamma^0p_0-\gamma^kp_k)=m\bar{u}(-\vec{p},s') \text{ and so}$$

$$-m^2\bar{u}(-\vec{p},s')\gamma^0v(\vec{p},s)=\bar{u}(-\vec{p},s')\left(\gamma^0p_0\gamma^0\gamma^0p_0-\gamma^kp_k\gamma^0\gamma^0p_0+\gamma^0p_0\gamma^0\gamma^kp_k-\right.$$

$$\left.-\gamma^kp_k\gamma^0\gamma^lp_l\right)v(\vec{p},s)=m^2\bar{u}(-\vec{p},s')\gamma^0v(\vec{p},s) \ .$$

Hence we will obtain

$\bar{u}(-\vec{p},s')\gamma^0v(\vec{p},s)=0$ and by complex conjugation $\bar{v}(\vec{p},s)\gamma^0u(-\vec{p},s')=0$

and therefore the above expression for the Hamiltonian becomes

$$\hat{H}=\sum_{s,s'}\int d^3\vec{p}\,m\left(\bar{u}(\vec{p},s)\gamma^0v(\vec{p},s')b^+(\vec{p},s)b(\vec{p},s')-\right.$$

$$\left.-\bar{v}(\vec{p},s)\gamma^0v(\vec{p},s')d(\vec{p},s)d^+(\vec{p},s')\right) \ .$$

Since u , v are Dirac spinors, it follows that under a restricted Lorentz coordinates transform $(\bar{u}(\vec{p},s)\gamma^\mu u(\vec{p},s'))_\mu$ and $(\bar{v}(\vec{p},s)\gamma^\mu v(\vec{p},s'))$ transform like Lorentz four-vectors. (see Chap. On rotations group and restricted Lorentz group).

Because in the rest frame, $\vec{p}=0$, for the normalized u and v if $s\neq s'$ those Lorentz vectors vanish, it follows in particular that

if $s\neq s'$ then $\bar{u}(\vec{p},s)\gamma^0u(\vec{p},s')=\bar{v}(\vec{p},s)\gamma^0v(\vec{p},s')=0$

and also for $s = s'$, having $\Lambda\in SO^+(3,1)$ with $\Lambda^{-T}\begin{pmatrix}m\\\vec{0}\end{pmatrix}=\begin{pmatrix}p_0\\\vec{p}\end{pmatrix}$

we will have

$(\bar{u}(\vec{p},s)\gamma^{\mu}u(\vec{p},s))_{\mu}=\Lambda\begin{pmatrix}1\\ \vec{0}\end{pmatrix}$ and so $\bar{u}(\vec{p},s)\gamma^{0}u(\vec{p},s)=\frac{p_0}{m}$ and in the same way $\bar{v}(\vec{p},s)\gamma^{0}v(\vec{p},s)=\frac{p_0}{m}$.

Thus, considering also the anticommutation relations it follows:

$\hat{H}=\int d^3\vec{p}\sum_s E_p(b^{+}(\vec{p},s)b(\vec{p},s)+d^{+}(\vec{p},s)d(\vec{p},s))-\delta^3(0)\int d^3\vec{p}\sum_s E_p$ (12)

$b^{+}(\vec{p},s)$ creates a particle and $b(\vec{p},s)$ anihilates a particle with momentum $\vec{p}$ and spin index $s\in\{\pm 1\}$

$d^{+}(\vec{p},s)$ creates an antiparticle and $d(\vec{p},s)$ anihilates an antiparticle with momentum $\vec{p}$ and spin index $s\in\{\pm 1\}$.

If $|0\rangle$ is the ground state of the system, then $b^{+}(\vec{p},s)|0\rangle$ is an E_p+H_0 energy eigenstate of the momentum $\vec{p}$ spin index s particle and $d^{+}(\vec{p},s)|0\rangle$ is an E_p+H_0 energy eigenstate of the momentum $\vec{p}$ spin index s particle.

Since $b^{+}(\vec{p},s)b(\vec{p},s)=d^{+}(\vec{p},s)d(\vec{p},s)=0$, due to anticommutation we can have at most one particle and one antiparticle with the same momentum and spin.

Also, anihilation supposes $b(\vec{p},s)|0\rangle=0$ and $d(\vec{p},s)|0\rangle=0$ for any $\vec{p}$, s .

The first two terms in Hamiltonian expression (12) tell us that each particle and each antiparticle of a given momentum $\vec{p}$ and spin index s has exactly the same energy E_p and since $\delta^3(\vec{0})=\frac{1}{(2\pi)^3}\int d^3\vec{x}=\frac{V}{(2\pi)^3}$, restoring the Planck constant by dimensional analysis, the last term in (12) becomes

$H_0=-\frac{1}{h^3}\int d^3\vec{x}\,d^3\vec{p}\sum_s 2(\frac{1}{2}E_p)$ which is the vacuum energy of $-\frac{1}{2}E_p$ in each unit size phase-space cell $\frac{1}{h^3}d^3\vec{x}\,d^3\vec{p}$ for each spin and for particle and antiparticle separately, precisely the vacuum energy we calculated in Chap. Feynman amplitudes and lattice gauge theory, the analog of the zero point energy $\frac{1}{2}\hbar\omega$ (with a minus sign) of the harmonic oscillator.

Because of the anticommutation relations involving b , b^{+} , d , d^{+} we have :

$\{\hat{\psi}_{\alpha}(x),\hat{\psi}_{\beta}(y)\}=0$, $\{\hat{\bar{\psi}}_{\alpha}(x),\hat{\bar{\psi}}_{\beta}(y)\}=0$

As we proved in Chap. Fermi's golden rule , for large values of $M>0$ we can consider that the following relation, which we will further use, holds :

$\frac{\sin(\tau M)}{\tau}\approx\pi\delta(\tau)$ for any $\tau\in\mathbb{R}$, $\delta(\tau)$ the Dirac distribution function.

Taking $F_M(\tau)=\frac{\sin(\tau M)}{\tau^2}-\frac{M\cos(\tau M)}{\tau}=M^2 f(\tau M)$, $f(\tau)=\frac{\sin(\tau)}{\tau^2}-\frac{\cos(\tau)}{\tau}$

$$g(\tau)=\int_0^{\tau} f(s)\,ds=-\frac{\sin(\tau)}{\tau}+1 \quad \text{, for } \varphi\in C_0^{\infty}(\mathbb{R}) \text{ we have :}$$

$$(F_M,\varphi)=\int f(\tau)\varphi(\tau)\,d\tau=M\int f(\tau)\varphi(\frac{\tau}{M})\,d\tau=-\int g(\tau M)\,M\,\varphi'(\tau)\,d\tau\approx(\pi\delta',\varphi)$$

and therefore for large M we can consider that $F_M(\tau)=\pi\delta'(\tau)$.

Taking $\xi=x-y$, $Q\in SO(3)$ with $(Q_{ij}\,\xi_j)_i=(\|\vec{\xi}\|,0,0)$ we obtain

$$(\{\hat{\psi}_\alpha,\hat{\bar{\psi}}_\beta\})_{\alpha,\beta}=\frac{1}{(2\pi)^3}\int\frac{d^3\vec{p}}{2E_p}((\not{p}+m)\exp(-ip\,\xi)+(\not{p}-m)\exp(ip\,\xi))=$$

$$=\frac{1}{(2\pi)^3}\int d^3\vec{p}\left(\gamma^0\cos(p_0\,\xi^0)\cos(\vec{p}\cdot\vec{\xi})+\frac{\gamma^k p_k}{p_0}\sin(p_0\,\xi^0)\sin(\vec{p}\cdot\vec{\xi})-\right.$$
$$\left.-i\frac{m}{p_0}\sin(p_0\,\xi^0)\cos(\vec{p}\cdot\vec{\xi})\right) \qquad (13)$$

If $\xi=0$ we have $(\{\hat{\psi}_\alpha,\hat{\bar{\psi}}_\beta\})_{\alpha,\beta}=\gamma^0\,\delta^3(\vec{0})$ with the Dirac distribution over $\vec{\xi}$ space.

We assume a momentum range $\|\vec{p}\|=r<M$ and small negligible mass m, $m\to 0$.

In that conditions we have :

$$(\{\hat{\psi}_\alpha,\hat{\bar{\psi}}_\beta\})_{\alpha,\beta}=\frac{1}{(2\pi)^3}\int d^3\vec{p}\,\gamma^0\cos(\|\vec{p}\|\,\xi^0)=\frac{2}{(2\pi)^2}\int_0^{\infty}\gamma^0 r^2\cos(r\,\xi^0)\,dr=$$

$$=-\frac{1}{2\pi}\gamma^0\frac{d^2}{d\,\xi^{02}}\delta(\xi^0)=-\frac{1}{2\pi}\gamma^0\,\delta''(\xi^0) \quad (14)\text{ , if } \vec{\xi}=0 \text{ and if } \vec{\xi}\neq 0 \text{ after some calculus we obtain:}$$

$$(\{\hat{\psi}_\alpha,\hat{\bar{\psi}}_\beta\})_{\alpha,\beta}=\frac{1}{(2\pi)^2}\int_0^{\infty}\int_{-r\|\vec{\xi}\|}^{r\|\vec{\xi}\|}\left(\frac{r}{\|\vec{\xi}\|}\gamma^0\cos(r\,\xi^0)\cos(\tau)+\right.$$
$$\left.+\gamma^k Q_{1k}\frac{1}{\|\vec{\xi}\|^2}\sin(r\,\xi^0)\,\tau\sin(\tau)\right)d\tau\,dr=$$

$$=\frac{1}{(2\pi)^2}\frac{\gamma^0+\gamma^k Q_{1k}}{\|\vec{\xi}\|}F_M(\|\vec{\xi}\|-\xi^0)+\frac{1}{(2\pi)^2}\frac{\gamma^0-\gamma^k Q_{1k}}{\|\vec{\xi}\|}F_M(\|\vec{\xi}\|+\xi^0)+$$
$$+\frac{1}{(2\pi)^2}\gamma^k Q_{1k}\frac{1}{\|\vec{\xi}\|^2}\frac{\sin((\|\vec{\xi}\|-\xi^0)M)}{\|\vec{\xi}\|-\xi^0}-\frac{1}{(2\pi)^2}\gamma^k Q_{1k}\frac{1}{\|\vec{\xi}\|^2}\frac{\sin((\|\vec{\xi}\|+\xi^0)M)}{\|\vec{\xi}\|+\xi^0}$$

$$(\{\hat{\psi}_\alpha,\hat{\bar{\psi}}_\beta\})_{\alpha,\beta}=\frac{1}{4\pi}\left(\frac{\gamma^0+\gamma^k Q_{1k}}{\|\vec{\xi}\|}\delta'(\|\vec{\xi}\|-\xi^0)+\frac{\gamma^0-\gamma^k Q_{1k}}{\|\vec{\xi}\|}\delta'(\|\vec{\xi}\|+\xi^0)+\right.$$
$$\left.+\frac{\gamma^k Q_{1k}}{\|\vec{\xi}\|^2}\delta(\|\vec{\xi}\|-\xi^0)-\frac{\gamma^k Q_{1k}}{\|\vec{\xi}\|^2}\delta(\|\vec{\xi}\|+\xi^0)\right) \qquad (14')$$

Considering now a discretization of the Dirac spinor field in a lattice Λ (as in Chap. Feynman amplitudes and lattice gauge theory), since the path integration variables

$(\hat{\psi}_\alpha(x))_{x\in\Lambda,\alpha}$ and $(\hat{\overline{\psi}}_\alpha(x))_{x\in\Lambda,\alpha}$ are sets of independent anticommuting operators , we can apply Grassmann variables integration and as shown in Chap. Feynman amplitudes and lattice gauge theory we have:

$$Z(\eta,\overline{\eta})=\int D\,\psi D\,\overline{\psi}\exp\left(i\int(\mathscr{L}(\psi,\partial\,\psi)+\overline{\psi}\,\eta+\overline{\eta}\,\psi)d^4x\right)=$$

$$=Z(\eta=0)\exp\left(-i\int\overline{\eta}(x)S(x-y)\,\eta(y)\,d^4x\,d^4y\right)$$ where the propagator is $S=S(x)$

$$S(x)=\int\frac{1}{(2\pi)^4}\exp(-i\,p\,x)\frac{\not{p}+m}{p^2-m^2+i\,\varepsilon}d^4p=$$

$$=-i\frac{1}{(2\pi)^3}\int\frac{1}{2E_p}(\theta(x^0)(\not{p}+m)\exp(-i\,p\,x)-\theta(-x^0)(\not{p}-m)\exp(i\,p\,x))d^3\vec{p}$$

with $E_p=p_0=\sqrt{\vec{p}^2+m^2}$, $Z(\eta=0)=C\det(i\not{\partial}-m)=C\exp(2\,\mathrm{tr}\log(\partial^2+m^2))$

where *C* is a normalization constant and θ is the Heaviside function.

Following Chap. Electromagnetic four-potential . Electromagnetic tensor. Lagrangian of electromagnetism. Energy-momentum tensor of electromagnetic field, the photon particle system can be described by a four-vector boson field $(A^\mu)_\mu=(A^\mu(t,\vec{x}))_\mu$ with a Lagrangian density

$\mathscr{L}(A,\partial A)=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+J^\mu A_\mu$ where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ are the electromagnetic tensor coefficients and $(J^\mu)_\mu$ is the conserved current density of sources

$J^\mu=J^\mu(t,\vec{x})\in\mathbb{R}$, $\partial_\mu J^\mu=0$, $A_\mu=A_\mu(t,\vec{x})\in\mathbb{R}$, $\mu=\overline{0,3}$

We will give now to the photon a hypothetical small mass *M* so that the Lagrangian density becomes that of a massive vector meson :

$$\mathscr{L}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\frac{1}{2}M^2A_\mu A^\mu+J^\mu A_\mu$$

and further for the photon, in physical calculations, we will calculate the outcomes setting where it is possible $M\to 0$.

Integrating by parts , considering that the field becomes small when space-time coordinates go toward infinity we obtain an action

$$S(A)=\int d^4x\,\mathscr{L}=\int d^4x\left(\frac{1}{2}A_\mu((\partial^2+M^2)\,\eta^{\mu\nu}-\partial^\mu\partial^\nu)A_\nu+J^\mu A_\mu\right)\ .$$

The massive boson propagator $(D^{bos}_{\mu\nu}(x))_{\mu,\nu}$ satisfies

$((\partial^2+M^2)\,\eta^{\mu\nu}-\partial^\mu\partial^\nu)D^{bos}_{\nu\lambda}=\delta_{\mu\lambda}\,\delta^4(x)$ and so we find

$D^{bos}_{\nu\lambda}(x)=\int\frac{1}{(2\pi)^4}D^{bos}_{\nu\lambda}(k)\exp(i\,k\,x)d^4k$ where

$D^{bos}_{\nu\lambda}(k)=\left(-\eta_{\nu\lambda}+\frac{k_\nu k_\lambda}{M^2}\right)\frac{1}{k^2-M^2+i\,\varepsilon}$ with $\varepsilon>0$, $\varepsilon\to 0$

As in Chap. Quantum field theory. Path integral formalism… and Feynman amplitudes and lattice gauge theory we obtain
$Z(J)=\int D A \exp(i S(A))=C \exp(i W(J))$ where $C=Z(J=0)$ and

$$W(J)=-\frac{1}{2}\int J^{\mu}(x) D^{bos}_{\mu\nu}(x-y) J^{\nu}(y) d^4x\, d^4y=$$

$$=-\frac{1}{2}\int \frac{1}{(2\pi)^4} J^{\mu *}(k) D^{bos}_{\mu\nu}(k) J^{\nu}(k) d^4k \quad \text{with}$$

$J(k)=\int J(x)\exp(-i k x) d^4x \quad , \; J(x)=\int \frac{1}{(2\pi)^4} J(k)\exp(i k x) d^4k \quad .$

Since current conservation $\partial_{\mu} J^{\mu}(x)=0$ gets translated into momentum space as $k_{\mu} J^{\mu}(k)=0$, we can throw away the $k_{\mu} k_{\nu}$ term from the photon propagator and so

$W(J)=\frac{1}{2}\int \frac{d^4k}{(2\pi)^4} J^{\mu *}(k) \frac{1}{k^2-M^2+i\varepsilon} J_{\mu}(k) \quad .$

Considering two lumps of charges q_1 respective q_2 located at $\vec{x}_1$ respective $\vec{x}_2$ we must have $J=q_1(\delta^3(\vec{x}-\vec{x}_1),0,0,0)+q_2(\delta^3(\vec{x}-\vec{x}_2),0,0,0)=J_1+J_2$ and if we identify E as the potential energy of the two static sources q_1 , q_2 system, we have
$Z(J)=\langle 0|\exp(-i\hat{H}T)|0\rangle=\exp(-iET)=Z(J=0)\exp(iW(J))$

$$W(J)=\frac{1}{2}\int\int dx^0 dy^0 \int \frac{dk_0}{2\pi}\exp(ik_0(x^0-y^0))\left(\int \frac{d^3\vec{k}}{(2\pi)^3}(q_1^2+q_2^2)\left(1-\frac{k_0^2}{M^2}\right)\right.$$

$$\left.\frac{1}{k^2-M^2+i\varepsilon}+\int \frac{d^3\vec{k}}{(2\pi)^3} 2q_1q_2\left(1-\frac{k_0^2}{M^2}\right)\frac{1}{k^2-M^2+i\varepsilon}\exp(i\vec{k}(\vec{x}_1-\vec{x}_2))\right)=$$

$=-E_0(q_1,q_2)T+q_1q_2\int dx^0\int \frac{d^3\vec{k}}{(2\pi)^3}\frac{\exp(i\vec{k}\vec{r})}{-\vec{k}^2-M^2+i\varepsilon}$ with $\vec{r}=\vec{x}_1-\vec{x}_2$, $\int dx^0=T$.

Therefore, to addition with a constant not depending on sources locations the potential energy between the two static sources is

$$E=q_1q_2\int \frac{d^3\vec{k}}{(2\pi)^3}\frac{\exp(i\vec{k}\vec{r})}{\vec{k}^2+M^2}=q_1q_2\int_0^{\infty}\frac{1}{(2\pi)^2}d\rho\int_0^{\pi}\rho^2\sin(\theta)\frac{\exp(i\rho r\cos(\theta))}{\rho^2+M^2}d\theta=$$

$$=\frac{1}{4\pi^2}q_1q_2\int_0^{\infty}d\rho\frac{\rho^2}{\rho^2+M^2}\int_{-1}^{1}\exp(i\rho r t)dt=-\frac{1}{4\pi^2}\frac{q_1q_2}{r}\int_{-\infty}^{\infty}\frac{\rho}{\rho^2+M^2}\exp(i\rho r)d\rho$$

Since $r=\|\vec{r}\|$ is positive, we can close the contour in the upper half plane and pick up the pole at iM obtaining $E=\frac{q_1q_2}{4\pi r}\exp(-Mr)$. The force is $-\nabla_{\vec{r}}E$ and we can see that if $q_1 q_2 > 0$, the force is repelling.

For $M = 0$ we recover as expected the Coulomb potential $V(r)=-\frac{q_1q_2}{4\pi r}$ of the electrostatic field.

To study the spin degrees of freedom of the massive vector meson we should evidently sit in the rest frame of the particle and study how its states respond to rotation.
In the rest frame we have a reference momentum $q = M(1, 0, 0, 0)$ and the Lorentz transformations that leave q invariant form obciously the $SO(3)$ rotations group. $(A^\mu)_\mu$ transforming as a vector, we have a spin j=1 irreducible $SO(3)$ representation with $2j+1=3$ degrees of freedom (considering gauge invariance, we take $\partial_\mu A^\mu = 0$).
In the rest frame the three polarization vectors are $\varepsilon_\mu^a = (0, (\delta_{ka})_{k=\overline{1,3}})$, $a = \overline{1,3}$.
Boosting and rotating those vectors from q four-momentum to the $k = (k_\mu)_{\mu=\overline{0,3}}$ four-momentum, we obtain the polarization vectors $(\varepsilon_\mu^a(k,a))_\mu$, $a = \overline{1,3}$ and the corresponding expressions for the $\hat{A}_\mu(t, \vec{x})$ field operator functions as in Chap. Feynman amplitudes and lattice gauge theory.
But if the particle is massless ($M = 0$) , the best we can do is to transform the particle's four-momentum to the reference momentum $(q^\mu)_\mu = \omega(1, 0, 0, 1)$. The Lorentz transformations that leave q invariant are obviously rotations around the third axis.
Let ψ a momentum eigenstate of the particle in the reference frame with z-axis in the direction of motion and $R = R(\varphi, e_z)$, $e_z = (0,0,1)$ the φ angle rotation around the third axis (notation as in Chap. Representations of the rotation group and of the restricted Lorentz group) and $U = U(R)$ the spin 1 representation of $SO(3)$ acting on the ψ space V. We have obviously $U(R)^{-1} = U(R)^+$. The $(R(\varphi, e_z))_{\varphi\in\mathbb{R}}$ form the $SO(2)$ group and since $\hat{\vec{p}}$ must commute with $U(R)$ it follows

$$\hat{p}_3 U(R)|\psi\rangle = \omega U(R)|\psi\rangle \ , \ \hat{p}_2 U(R)|\psi\rangle = \hat{p}_1 U(R)|\psi\rangle = 0 \ .$$

Therefore $U(R)(V) = V$ and spin 1 representations for a mass zero particle must leave V invariant and are representations of $SO(2)$.
The only representations of $SO(2)$ that are not spin 0 representations and are irreducible spin 1 representations are equivalent to
$U_\pm(R(\varphi, e_z)) = \exp(\pm i\varphi)$ with $V = \mathbb{C}$, $\dim_{\mathbb{R}} V = 2$ or

$$U_\pm(R(\varphi, e_z)) = \exp\left(\varphi \begin{pmatrix} 0 & \pm 1 \\ \mp 1 & 0 \end{pmatrix}\right) \ , \ V = \mathbb{R}^2$$

(Indeed , if $-iJ = \lim_{\varphi\to 0} \frac{\partial U(R)}{\partial \varphi}(\varphi, e_z)$ it follows $U(R) = \exp(-i\varphi J)$, $J = J^+$.
If J has eigenvalue λ for eigenvector u , we have that
$U(R)(\{\mu u | \mu\in\mathbb{C}\}) \subseteq \{\mu u | \mu\in\mathbb{C}\}$ (see Chap. ... Spin representations) .
Thus J must have one single eigenvector and λ = +/- 1 for U to be irreducible spin 1 representation. Moreover , U is equivalent with a real space representation with dimension 2.
Hence the photon has as expected (see Chap. Quantization of an electromagnetic field) two degrees of freedom, the polarization directions which by fixing the gauge can be taken, for a four momentum $(\omega, 0, 0, k)$, $|k| = \omega$, normal to propagation direction as

$(\varepsilon^1_\mu)_\mu=(0,1,0,0)$, $(\varepsilon^2_\mu)_\mu=(0,0,1,0)$ and we have the expressions for the $\hat{A}_\mu(t,\vec{x})$ field operator functions for massless gauge bosons as in Chap. Feynman amplitudes and lattice gauge theory.

The fermion field interacting with an electromagnetic field theory (Q.E.D. , Quantum electrodynamics) involves Dirac spinor fields $\psi=\psi(t,\vec{x})$ gauged with a photon field having a hypothetical mass $M\to 0$, $(A_\mu)_\mu=(A_\mu(t,\vec{x}))_\mu$, replacing in the Dirac Lagrangian density the ∂_μ operator with $\partial_\mu+ie\,A_\mu(t,\vec{x})$ as in the Lagrangian of a charged particle in an electromagnetic field, where e = - $|e|$ for the electron is the particle's electric charge.
The Q.E.D. theory Lagrangian density is

$$\mathscr{L}(\psi,\partial\psi,A,\partial A)=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\frac{1}{2}M^2A_\mu A^\mu+i\overline{\psi}\gamma^\mu(\partial_\mu+ie\,A_\mu)\psi-m\overline{\psi}\psi+$$

$+\overline{\eta}\psi+\overline{\psi}\eta-J^\mu A_\mu$ where $\eta=\eta(t,\vec{x})$ is a Dirac spinor field as a fermion source and $(J^\mu=J^\mu(t,\vec{x}))_\mu$ is a Lorentz four-vector field as a external photon field source.
For this theory we can show, as we did in Chap. Feynman amplitudes and lattice gauge theory, that in computing the amplitudes for various processes which occur in the theory, the $k_\mu\,k_\nu\,/\,M^2$ term in the massive boson propagator disappears, so we can make the hypothetical mass of the photon equal to zero.
Evidently we can use the Feynman rules listed in Chap. Feynman amplitudes and lattice gauge theory and compute the amplitudes for processes which are possible according to the theory.
If we take the boson Lagrangian density for directly a mass of the boson equal to zero, in a discretization of the A field we have the action

$$S(A)=\int\mathscr{L}\,d^4x=\int d^4x\left(\frac{1}{2}A_\mu(\eta^{\mu\nu}\partial^2-\partial^\mu\partial^\nu)A_\nu-J^\mu A_\mu\right)=-\frac{1}{2}A^T\,K\,A+A\cdot J$$ with

$A=(A_\mu(x))_{x\in\Lambda\,,\,\mu=\overline{0,3}}$, $J=(J^\mu(x))_{x\in\Lambda\,,\,\mu=\overline{0,3}}$; Λ the space-time discretization grid.
The formal matrix K is proportional to the discretization of the differential operator $(Q^{\mu\nu})_{\mu,\nu}=(\eta^{\mu\nu}\partial^2-\partial^\mu\partial^\nu)_{\mu,\nu}$. For any $\Phi=\Phi(t,\vec{x})\in\mathbb{R}$, taking $g_\mu=\partial_\mu\Phi$, $g=(g_\mu(x))_{x\in\Lambda,\mu=\overline{0,3}}$ we have $Q^{\mu\nu}g_\nu=(\partial_\lambda\partial^\lambda\partial^\mu-\partial^\mu\partial^\nu\partial_\nu)\Phi=0$ and so formally $K\,g=0$. Thus, since we can take $g\neq 0$ it follows that K has no inverse K^{-1} which could be taken as the boson propagator.
We learned that we must impose an additional constraint on the gauge potential $(A^\mu)_\mu$, procedure known as "fixing the gauge", to solve Maxwell's equation $\partial_\mu F^{\mu\nu}=J^\nu$ (see Chap. Electromagnetic four-potential).
Hence to find a propagator for the massless boson we will use the Fadeev-Popov method as follows.
Suppose we have to do the path integral
$I=\int DA\exp(iS(A))$ and under the transformation $A\to A_g$ we have $S(A)=S(A_g)$ and $DA=DA_g$ so that the transformations g form a group G

having $(A_g)_{g'}=A_{gg'}$ for any $g,g'\in G$ (the G operation in multiplicative notation) .
We would like to write the path integral *I* in the form
$I=\left(\int Dg\right)J$ with J an integral independent of g. Dg is the invariant measure over the group of transformations *G* and $\int Dg$ is the volume of the group.
(for example if G is the plane rotations group and $S(x,y)=S(\sqrt{x^2+y^2})=S(r)$
we have $I=\int dx\,dy\exp(iS(x,y))=\left(\int_0^{2\pi} d\theta\right)J$ with $J=\int dr\exp(iS(r))$)

First we write $1=\Delta(A)\int Dg\,\delta(f(A_g))$. Here *f* is some function of our choice and $\Delta(A)$, known as the Fadeev-Popov determinant depends on *f*.
Notice that $(\Delta(A_{g'}))^{-1}=\int Dg\,\delta(f(A_{g'g}))=\int Dg''\,\delta(f(A_{g''}))=(\Delta(A))^{-1}$
where $g''=g'g$ and we used $Dg''=Dg$.
In other words we showed that $\Delta(A)=\Delta(A_g)$.
Therefore we have the (15) relation :

$$I=\int DA\exp(iS(A))=\int DA\exp(iS(A))\Delta(A)\int Dg\,\delta(f(A_g))=$$
$$=\int Dg\int DA\exp(iS(A))\Delta(A)\,\delta(f(A_g))=\int Dg\int DA\exp(iS(A))\Delta(A)\,\delta(f(A))$$

where in the last identity we changed A to $A_{g^{-1}}$ and used the invariance of DA , $S(A)$ and $\Delta(A)$ under $A\to A_{g^{-1}}$.
We apply the Fadeev-Popov method to electromagnetism. The transformation leaving the action invariant is $A_\mu\to A_\mu-\partial_\mu\Phi$ so g is denoted in the present context by Φ.
We choose $f(A)=\partial A-\sigma$ where $\sigma=\sigma(x)$. We calculate

$$(\Delta(A))^{-1}=\int Dg\,\delta(f(A_g))=\int D\Phi\,\delta(\partial A-\partial^2\Phi-\sigma)\qquad(16)$$

Next we notice that in (15) Δ(*A*) appears multiplied with δ (*f*(*A*)) and so in (16) we can set effectively $f(A)=\partial A-\sigma$ equal to zero. Thus we have

$$I=\left(\int D\Phi\,\delta(\partial^2\Phi)\right)^{-1}\left(\int D\Phi\right)\int DA\exp(iS(A))\,\delta(\partial A-\sigma)=$$
$$=C\int DA\exp(iS(A))\,\delta(\partial A-\sigma)$$

with C a constant not depending on A , σ .
The integral *I* we started with is still independent of *f* in spite of its appearance in (15), and in particular *I* is independent of σ and so we can integrate *I* with an arbitrary functional of σ , in particular $\exp\left(-\frac{i}{2\xi}\int d^4x(\sigma(x))^2\right)$ obtaining an independent of A constant $\widetilde{C}$ such that

$$I=\widetilde{C}\int D\sigma\exp\left(-\frac{i}{2\xi}\int d^4(\sigma(x))^2\right)\int DA\exp(iS(A))\,\delta(\partial A-\sigma)=$$
$$=\widetilde{C}\int DA\exp\left(iS(A)-\frac{i}{2\xi}\int d^4x(\partial A)^2\right)$$

Thus *S* (*A*) can be effectively replaced by

$S_{eff}(A)=\int d^4x\left(\frac{1}{2}A_\mu(\eta^{\mu\nu}\partial^2-\left(1-\frac{1}{\xi}\right)\partial^\mu\partial^\nu)A_\nu-J^\mu A_\mu\right)$ and $Q^{\mu\nu}$ by

$Q^{\mu\nu}_{eff}=\eta^{\mu\nu}\partial^2-\left(1-\frac{1}{\xi}\right)\partial^\mu\partial^\nu$ which does have an inverse whose Fourier transform is

$$D^{bos}_{\nu\lambda}(k)=\left(-\eta_{\nu\lambda}+(1-\xi)\frac{k_\nu k_\lambda}{k^2}\right)\frac{1}{k^2}\ .$$

Hence the photon propagator can be chosen to be

$D^{bos}_{\nu\lambda}(x-y)=\int\frac{d^4k}{(2\pi)^4}\left(-\eta_{\nu\lambda}+(1-\xi)\frac{1}{k^2+i\varepsilon}\right)\frac{1}{k^2+i\varepsilon}\exp(ik(x-y))$

and the effective photon Lagrangian density can be

$\mathcal{L}_{eff}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}-\frac{1}{2\xi}(\partial^\mu A_\mu)^2-J^\mu A_\mu$.

ξ is an arbitrary gauge fixing constant. Taking $\xi = 1$ we obtain the propagator without $k_\mu k_\nu/k^2$ term, the same as in disposing of the $k_\mu k_\nu/M^2$ term for a hypothetical mass of the photon, which we can consider as mentioned above. This is the Feynman-'t Hooft gauge.

The Lorentz gauge for which $\partial^\mu A_\mu=0$ is equivalent to $\xi\to 0$.

For a gauged Lagrangian density $\mathcal{L}((\psi^\alpha,\partial\psi^\alpha)_\alpha,(A^a,\partial A^a)_a)$ involving fermion fields $(\psi,\partial\psi)$ and gauge bosons $(A,\partial A)$, as in Chap. Feynman amplitudes and lattice gauge theory, the passing from a exponential expansion term factor $\overline{\psi}(x_1)\gamma^\mu A_\mu(x_1)\psi(x_1)\overline{\psi}(x_2)\gamma^\nu A_\nu(x_2)\psi(x_2)...\gamma^\lambda A_\lambda(x_r)\psi(x_r)$ (17) corresponding in the path integral during the calculation of a process amplitude , to the respective closed fermion lines cycle of the Feynman diagram amplitude factor $\mathrm{tr}(S(x_r-x_1)\gamma^\mu S(x_1-x_2)\gamma^\nu...S(x_{r-1}-x_r)\gamma^\lambda)$ (where S is the fermion propagator) supposes commuting (17) to $\psi(x_r)\overline{\psi}(x_1)\gamma^\mu A_\mu(x_1)...\gamma^\lambda A_\lambda(x_r)$ (we have suppressed the fermion and boson type indices and Dirac spinor indices).

To consider a proper cycle, the x_1 , x_2 ,..., x_r must have distinct values of x_1^0 , x_2^0 ,..., x_r (integration over $(x_j)_{j=\overline{1,r}}$ variables by excluding $(x_j^0\approx x_k^0\ ,\ j\neq k)$) .

Having the relations (14) and (14') when we neglect the fermion masses, since we can always choose a discretization lattice Λ with time spacing over spatial spacing lattice constants not a square root of a rational number so that on the lattice we have $\|\vec{\xi}\|\neq\pm\xi^0$ for any $x,y\in\Lambda$, $\xi=x-y$, it follows that we can consider that $\hat{\psi}_\alpha(x_r)$ anticommutes with any of the $\overline{\psi}_\beta(x_j)$, $\hat{\overline{\psi}}_\delta(x_j)$, $j=\overline{1,r-1}$, $\alpha,\beta,\delta=\overline{0,3}$.

When we try to anticommute $\hat{\psi}_\alpha(x_r)$ with $\hat{\overline{\psi}}_\beta(x_r)$ we remain with a factor $\overline{\psi}(x_1)\gamma^\mu A_\mu(x_1)...\psi(x_{r-1})\delta^3(\vec{0})\gamma^\lambda_{\alpha\beta}A_\lambda(x_r)\gamma^0_{\beta\alpha}$.

The factor $\gamma^{\lambda}_{\alpha\beta} A_{\lambda}(x_r) \gamma^{0}_{\beta\alpha}$ is multiplied with the coupling boson field $A_{\mu}(y)\gamma^{\mu}$ and the path integration formula through differentiation over source field (Wick contraction process) leads to a term with a factor

$$\gamma^{\mu}\int \gamma^{\lambda}_{\alpha\beta}\gamma^{0}_{\beta\alpha} D^{bos}_{\lambda\mu}(x_r - y)\, d^4 x_r = 4\int \gamma^{\mu} D^{bos}_{0\mu}(x_r - y)\, d^4 x_r =$$

$$= -\frac{4}{(2\pi)^4}\int\int \left(\eta_{0\mu} - \frac{p_0 p_{\mu}}{M^2}\right)\gamma^{\mu}\frac{\exp(i\,p(x_r - y))}{p^2 - M^2 + i\varepsilon} d^4 x_r\, d^4 p = 4\int \frac{\gamma^0}{M^2} d^4 p$$

which is infinite. We choose to ignore the infinite term as a fermion vacuum contribution (the fermion and antifermion fields fluctuating indefinitely with any momentum from the lose boson at x_r) and anticommute $\hat{\psi}(x_r)$ with $\hat{\overline{\psi}}(x_r)$ thus obtaining the (-) minus sign rule for closed fermion cycles in the Feynman diagram. (see Chap. Feynman amplitudes and lattice gauge theory)

Consider now the Fermi theory of weak interaction in a simplified form, with Lagrangian density

$\mathscr{L} = \overline{\psi}(i\,\gamma^{\mu}\partial_{\mu} - m)\,\psi + G(\overline{\psi}\,\psi)^2$ (18) where G is the Fermi coupling constant. The two fermions scattering into two fermions process at order 1 in G approximation corresponds to the Feynman diagram in fig.1 below

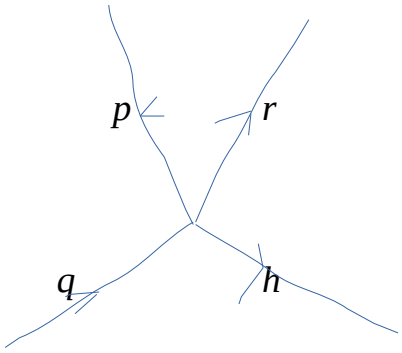


fig.1

and to the Feynman amplitude

$$A_0 = (2\pi)^4 M_0\, \delta^4(p + q - r - h)\ ,$$

$$M_0 = iG \sum_{s1,s2,s3,s4} \left(\overline{u}_{\beta}(r, s_1) u_{\beta}(p, s_2)\overline{u}_{\alpha}(h, s_3) u_{\alpha}(q, s_4) + \right.$$

$$\left. + \overline{u}_{\beta}(r, s_1) u_{\beta}(q, s_2)\overline{u}_{\alpha}(h, s_3) u_{\alpha}(p, s_4)\right)$$

The order 2 in G approximation adds the Feynman diagrams in fig.2 (a) , fig.2 (b) and the Feynman amplitude

$A_1 = (2\pi)^4 M_1\, \delta^4(p + q - r - h)$,

$$A_1=(iG)^2\int\left(\sum_{s1,s2,s3,s4}\left(\bar{u}(r,s_1)\frac{i(\not{l}+m)}{l^2-m^2+i\varepsilon}u(p,s_2)\right)\left(\bar{u}(h,s_3)\frac{i(\not{k}+m)}{k^2-m^2+i\varepsilon}u(q,s_4)\right)+\right.$$

$$\left.+\left(\bar{u}(r,s_1)\frac{i(\not{l}+m)}{l^2-m^2+i\varepsilon}u(q,s_2)\right)\left(\bar{u}(h,s_3)\frac{i(\not{k}+m)}{k^2-m^2+i\varepsilon}u(p,s_4)\right)\right)\delta^4(p+q-l-k)$$

$$\delta^4(r+h-l-k)d^4k\,d^4l\ .$$

We notice that without a cutoff for the four-momentum space integration , $\|k\|_4<\Lambda$ we have $M_1=\infty$. Integrating only on the cutoff we obtain $A=A_0+A_1=(2\pi)^4 M\,\delta^4(p+q-r-h)$ with $M=M_0+M_1\sim G+G^2\Lambda^2$ and the theory is therefore nonrenormalizable. When the allowed energies in the scattering process reach scale $\Lambda \sim (1/G)^{1/2}$ the second term M_1 becomes prevalent and the amplitude can reach order unity and some new physics must take over, just because the cross section is going to violate the unitarity bound from basic quantum mechanics.

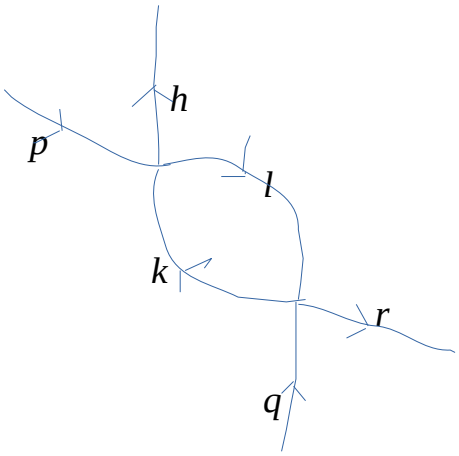


fig.2 (a)

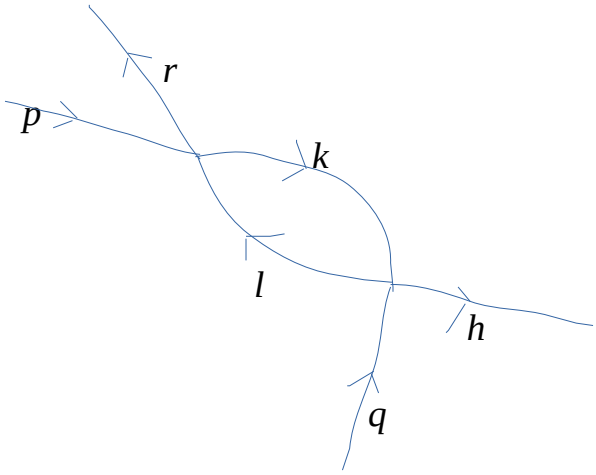


fig.2 (b)

Schematically, consider a theory of a vector boson of mass M coupled to a fermion field via a dimensionless coupling constant g :

$$\mathscr{L}=\bar{\psi}(i\,\gamma^\mu\partial_\mu-m)\,\psi-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\frac{1}{2}M^2A_\mu A^\mu+g\,A_\mu\bar{\psi}\gamma^\mu\psi \qquad (19)$$

The Feynman diagram in fig.3 generates an amplitude $-(ig)^2(\bar{u}\,\gamma^\mu u)\frac{i}{k^2-M^2+i\varepsilon}(\bar{u}\,\gamma_\mu u)$ which when the momentum transfer k is much less than M becomes $i(g^2/M^2)(\bar{u}\,\gamma^\mu u)(\bar{u}\,\gamma_\mu u)$, but this is just as if the fermions are interacting via a Fermi theory with Lagrangian density of the form

$\mathscr{L}=\bar{\psi}(i\,\gamma^\mu\partial_\mu-m)\,\psi+G(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi)$ (20) with $G=g^2/M^2$

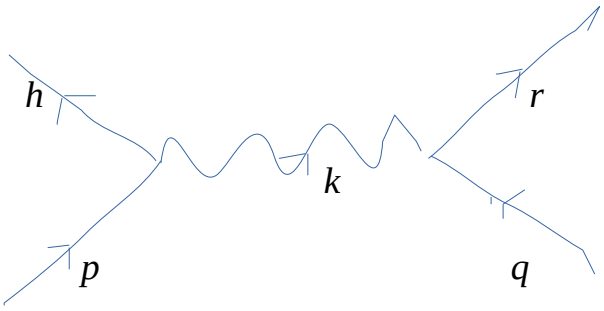


fig.3

If we blithely calculate with the low energy effective theory (20) it cries out that it is going to fail , since the order G^2 amplitude is divergent.
At the energy scale $(1 / G)^{1/2} = M /g$ the vector boson is produced and new physics appears.

Considering in the (19) theory the k four-momentum propagation order 0 respective order 2 in g Feynman diagrams fig.4 and fig.5, for source Dirac spinor fields $\eta = \eta(t, \vec{x})$, the corresponding amplitude of second order in g approximation for the propagation, in a similar way as in Chap. Quantum field theory. Path integral formalism, will be :

$$A = A_0 + A_2 \ , \ A_0 = Z(\eta=0)\left(- \frac{i}{(2\pi)^4} \overline{\eta}(k) D^{fer}(k) \eta(k) \right) d^4 k$$

$$A_2 = Z(\eta=0)\left(\int - \frac{g^2}{(2\pi)^8} \overline{\eta}(k) D^{fer}(k) \gamma^{\mu} D^{fer}(k+r) \gamma^{\lambda} D^{fer}(k) D^{bos}_{\mu\lambda}(r) \eta(k) d^4 r \right) d^4 k$$

where $\eta(k) = \int \eta(x) \exp(i k x) d^4 x$ and D^{fer}, D^{bos} are the fermion respective the boson propagator.

fig.4

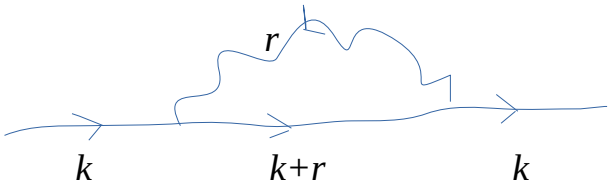


fig.5

As we know , we have

$$\left(\frac{\not{k} + m}{2m} \right)_{\alpha\beta} = u_{\alpha}(k) \overline{u}_{\beta}(k) \ , \ \left(\frac{\not{k} + \not{r} + m}{2m} \right)_{\alpha\beta} = u_{\alpha}(k+r) \overline{u}_{\beta}(k+r)$$

$\bar{u}(k)\not{k}=m\bar{u}(k)$, $(\not{k}+\not{r})u(k+r)=mu(k+r)$
and so we derive
$(\not{k}+m)\gamma^{\mu}r_{\mu}(\not{k}+\not{r}+m)=0$.

Therefore we can dispose of the $\frac{r_{\mu}r_{\lambda}}{M^2}$ term in the boson propagator

$D^{bos}_{\mu\lambda}(r)=\left(-\eta_{\mu\lambda}+\frac{r_{\mu}r_{\lambda}}{M^2}\right)\frac{1}{r^2-M^2+i\varepsilon}$ when we calculate A_2 .

Since even when integrating on a cutoff for the *r* four-momentum the whole amplitude *A* must be finite for a *k* four-momentum particle on mass shell (that is $|k^2-m^2|<\delta$, $\delta\to 0$) if we set the fermion source to produce or remove virtual particles with *k* four-momentum on mass shell, we must have $\eta(k)=-(\not{k}-m)\psi(k)$ where $\psi(k)=\int\psi(x)\exp(ikx)d^4x$, ψ is a Dirac spinor .
The same result can be obtained by Euler-Lagrange equations from variation upon $\delta\overline{\psi}$ in the action $S=\int(\overline{\psi}(i\gamma^{\mu}\partial_{\mu}-m)\psi+\overline{\eta}\psi+\overline{\psi}\eta)d^4x$ which are

$i\gamma^{\mu}\partial_{\mu}\psi(x)-m\psi(x)=-\eta(x)$, leading to $(\gamma^{\mu}k_{\mu}-m)\psi(k)=-\eta(k)$.

Hence with *k* momentum particles on mass shell, we have:

$$iA_0=Z(\eta=0)\frac{1}{(2\pi)^4}\overline{\psi}(k)(\not{k}-m)\psi(k)d^4k$$

$$iA_2=Z(\eta=0)\frac{1}{(2\pi)^8}g^2\overline{\psi}(k)\left(\int d^4r\,\gamma^{\mu}\frac{\not{k}+\not{r}+m}{(k+r)^2-m^2+i\varepsilon}\frac{1}{r^2-M^2+i\varepsilon}\gamma_{\mu}\right)\psi(k)d^4k$$

The integral for A_2 is divergent and therefore we will set for integration over *r* a cutoff Λ so that we have :

$$J(k,\Lambda)=\int^{\Lambda}\frac{\not{k}+\not{r}+m}{(k+r)^2-m^2+i\varepsilon}\frac{1}{r^2-M^2+i\varepsilon}d^4r=$$
$$=\int_0^1\int^{\Lambda}\frac{\not{k}+\not{r}+m}{((r+\alpha k)^2-\alpha(\alpha-1)k^2-(1-\alpha)M^2-\alpha m^2+i\varepsilon)^2}d^4r\,d\alpha=$$
$$=\int_0^1\int_{B_4(0,\Lambda)}\frac{\alpha\not{k}+m}{(q^2-\alpha(\alpha-1)k^2-\alpha M^2-(1-\alpha)m^2+i\varepsilon)^2}d^4q\,d\alpha$$

where $B_{\Lambda}=\{(\alpha,r)\in(0,1)\times\mathbb{R}^4|r\in B_4(\alpha k,\Lambda)\}$, $B_4(z,\Lambda)=\{q\in\mathbb{R}^4|\|q-z\|_4<\Lambda\}$
with $\|\,.\,\|_4$ the euclidean norm of $\mathbb{R}^4$ determines the Λ cutoff.
We proved in the Appendix to Chap. Quantum field theory. Path integral formalism … that

$Q(\Lambda,\mu)=\int\limits_{\|q\|_4<\Lambda}\frac{d^4q}{(q^2-m^2+i\varepsilon)^2}=L+H\log(\frac{\mu^2-i\varepsilon}{\Lambda^2})+O(\frac{\mu^2}{\Lambda^2})$ with L,H independent constants.

Considering the relation that determines A_0 , for the effective, renormalized by second order in g quantum fluctuations, mass m_P we must require, setting the fermion source field to produce or remove virtual particles on effective mass shell (that is $|k^2-m_P^2|<\delta$, $\delta\to 0$, $\eta(k)\propto-(\not{k}-m_P)\psi(k)$) that :

$iA\propto\overline{\psi}(k)(\not{k}-m_P)\psi(k)$ so that we have a constant C such that after some calculus we obtain:

$C(\not{k}-m_P)=\not{k}-m+A(k^2,\Lambda)\not{k}-mB(k^2,\Lambda)$ where

$$A(k^2,\Lambda)=-2i\frac{g^2}{(2\pi)^4}\int_0^1\alpha\left(L+H\log\left(\frac{\alpha M^2+(1-\alpha)m^2+\alpha(\alpha-1)k^2-i\varepsilon}{\Lambda^2}\right)\right)d\alpha$$

$$B(k^2,\Lambda)=-4i\frac{g^2}{(2\pi)^4}\int_0^1\left(L+H\log\left(\frac{\alpha M^2+(1-\alpha)m^2+\alpha(\alpha-1)k^2-i\varepsilon}{\Lambda^2}\right)\right)d\alpha\ .$$

It follows $m_P=\frac{1+B(k^2,\Lambda)}{1+A(k^2,\Lambda)}m$. The mass squared correction by quantum fluctuations for fermions has therefore a superficial degree of divergence in Λ equal to zero (it is bounded in Λ), while for bosons, as explained in Chap. Quantum field theory… Theory renormalization, it has a superficial degree of divergence equal to 2. This so called Weisskopf phenomenon can be understood heuristically in terms of quantum statistics. The “bad” behaviour of bosons has to do with their gregariousness. A fermion would push away the virtual fermions fluctuating in the vacuum thus creating a cavity in the vacuum charge distribution surrounding it. A boson does the opposite.

In the Fermi weak theory with the (18) Lagrangian density, considering a Feynman diagram with F_E external legs , F_I internal lines, V interaction vertices, L loops we compute the amplitude by reducing it to the form $(2\pi)^4\boldsymbol{M}\delta^4(\sum_{i\in A}k_i-\sum_{i\in B}k_i)$ with $(k_i)_{i\in A}$ incoming four-momenta, $(k_i)_{i\in B}$ outgoing four-momenta.

We have for each loop a $\int d^4k$ and for each internal line a $\frac{\not{k}+m}{k^2-m^2+i\varepsilon}$ bringing the powers of momentum down by 1. Hence the superficial degree of divergence is $D=4L-F_I$. The diagram graph brings the relations :

$L = F_I - (V-1)$, $4V = F_E + 2F_I$ and so $D = 4 - \frac{3}{2}F_E + 2V$.

Compared to the corresponding equations for renormalizable theories ($D = 4 - B_E$) derived in Chap. Quantum field theory… Theory renormalization, D now depends on V. Thus if we calculate fermion-fermion scattering ($F_E = 4$) for example, the divergence gets worse and worse as we go to higher and higher order in the perturbation series. For any F_E we would obtain divergent diagrams when V gets sufficiently large so we would have to include an unending stream of counterterms $(\overline{\psi}\psi)^3$, $(\overline{\psi}\psi)^4$, ... , each with an arbitrary coupling constant to be determined by an experimental measurement for an effective field theory. The theory is therefore severely limited in predictive power.

19. Fermion charge and conserved current CPT transformations. Slow and fast electrons Majorana neutrino. Chirality

Fermion charge and conserved current
CPT transformations. Slow and fast electrons
Majorana neutrino. Chirality

We have the Quantum electrodynamics Lagrangian density (see Chap. Dirac spinors … Quantum electrodynamics) :

$$\mathscr{L}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\overline{\psi}(i\gamma^{\mu}(\partial_{\mu}+ieA_{\mu})-m)\psi \ .$$

The Lagrangian density is invariant under a gauge transformation

$\psi(x)\to\exp(i\Lambda(x))\psi(x)$, $A_{\mu}(x)\to A_{\mu}(x)-\frac{1}{e}\partial_{\mu}\Lambda(x)$ where Λ is a real function of $x=(t,\vec{x})$.

(e is the fermion charge , m is the fermion mass, e = - | e | for the electron charge .)

For $\Lambda(x) = \theta$ = constant , this invariance leads according to Noether theorem (see Chap. Lagrangian field theory . Noether theorem) to a conserved curent $J^{\mu}=\overline{\psi}\gamma^{\mu}\psi$ with $\partial_{\mu}J^{\mu}=0$ and a probability density $J^0=\psi^{+}\psi$ so that we have a time independent charge $Q=\int J^0(t,\vec{x})d^3\vec{x}$.

(since we suppose the vanishing of the field $\psi=\psi(t,\vec{x})$ at large distances, $\|\vec{x}\|>R$, $R\to\infty$ we will have $\frac{dQ}{dt}=-\int\partial_k J^k(t,\vec{x})d^3\vec{x}=-\int\limits_{\partial B(\vec{0},R)}J^k n_k d\sigma(\vec{x})=0$)

In Chap. Dirac spinors … Quantum electrodynamics we have proved

$$\widehat{\psi}_{\alpha}(x)=\int\frac{d^3\vec{p}}{(2\pi)^{3/2}(E_p/m)^{1/2}}\sum_s\left(u_{\alpha}(\vec{p},s)b(\vec{p},s)\exp(-ipx)+\right.$$
$$\left.+v_{\alpha}(\vec{p},s)d^{+}(\vec{p},s)\exp(ipx)\right)$$

with $\{b(\vec{p},s),b^{+}(\vec{p}\,',s')\}=\{d(\vec{p},s),d^{+}(\vec{p}\,',s')\}=\delta_{ss'}\delta^3(\vec{p}-\vec{p}\,')$,

$\{b(\vec{p},s),b(\vec{p}\,',s')\}=\{d(\vec{p},s),d(\vec{p}\,',s')\}=\{b(\vec{p},s),d(\vec{p}\,',s')\}=$

$=\{b(\vec{p},s),d^{+}(\vec{p}\,',s')\}=0$, $\bar{u}(-\vec{p},s)\gamma^0 v(\vec{p},s')=\bar{v}(\vec{p},s)\gamma^0 u(-\vec{p},s')=0$,

$$\bar{u}(\vec{p},s)\gamma^0 u(\vec{p},s')=\bar{v}(\vec{p},s)\gamma^0 v(\vec{p},s')=\delta_{ss'}\frac{p_0}{m}$$

and so after some calculus we obtain a charge operator

$$\widehat{Q}=\int\sum_s(b^{+}(p,s)b(p,s)+d(p,s)d^{+}(p,s))d^3\vec{p}=$$
$$=\int\sum(b^{+}(p,s)b(p,s)-d^{+}(p,s)d(p,s))d^3\vec{p}+Q_0$$

where $Q_0=\frac{1}{(2\pi)^3}\int 2\,d^3\vec{x}\,d^3\vec{p}$ is the vacuum charge which turns out to be one unit of charge for each phase-space unit-cell $\frac{d^3\vec{x}\,d^3\vec{p}}{h^3}$ and each spin index.

We have $(\hat{Q}-Q_0)b^+(p,s)|0\rangle=b^+(p,s)|0\rangle$, $b(p,s)|0\rangle=0$

$(\hat{Q}-Q_0)d^+(p,s)|0\rangle=-d^+(p,s)|0\rangle$, $d(p,s)|0\rangle=0$,

where $|0\rangle$ is the ground state of the field theory and we notice that the operator $b^+(p,s)$ creates a particle with $+1$ units of charge, momentum $\vec{p}$, $p_0=\vec{p}^2+m^2$ and spin index s and the operator $d^+(p,s)$ creates the corresponding antiparticle with -1 units of charge, momentum $\vec{p}$, $p_0=\vec{p}^2+m^2$ and spin index s .

For the electron the units of charge are conventionally the negative elementary charge e = - | e | .

The Euler-Lagrange equations derived from the QED Lagrangian density lead to the Dirac equation in presence of an electromagnetic field of potential (A_μ)$_\mu$:

$i\gamma^\mu(\partial_\mu+ieA_\mu)\psi=m\psi$ with $\psi=\psi(t,\vec{x})$ the Dirac spinor field.

Taking $\psi_c=\gamma^2\psi^*$ with ψ^* the complex conjugate field to ψ , we find out that the field ψ_c satisfies the equation $i\gamma^\mu(\partial_\mu-ieA_\mu)\psi_c=m\psi_c$.

Noticing that $\gamma^2\gamma^\mu\gamma^2=\gamma^{\mu*}$ we have that ψ_c is a Dirac spinor field which satisfies the Dirac equation in presence of the electromagnetic field for the opposite charge $-e$ representing therefore the antiparticle to the Dirac spinor ψ particle charged e.

We call the $\psi\rightarrow\psi_c=\gamma^2\psi^*$ transformation the charge conjugation transformation denoted C , associating the matrix $C=\gamma^2\gamma^0$ such that $\overline{\psi}^T=C\psi_c$, $C^2=\boldsymbol{I}$.

We consider also the parity transformation P which corresponds to a coordinates transform $(x^\mu)_\mu\rightarrow(x'^\mu)_\mu=(x^0,-\vec{x})$.

With $\partial'_\mu=\frac{\partial}{\partial x'^\mu}$ we obtain $(i\gamma^\mu\partial'_\mu-m)\gamma^0\psi=0$ if ψsatisfies the Dirac equation.

Therefore under a parity transformation, the Dirac spinor ψ transforms like $\psi(x)\rightarrow\psi'(x')=\eta\gamma^0\psi(x)$ where η is an arbitrary phase factor which we can set 1.

Notice that under parity transformation, $\overline{\psi}\psi$ transforms like a scalar, having $\overline{\psi}(x)\psi(x)=\overline{\psi}'(x')\psi'(x')$ while taking $\gamma^5=i\gamma^0\gamma^1\gamma^2\gamma^3$ we have that $\overline{\psi}\gamma^5\psi$ transforms like a pseudo-scalar with $\overline{\psi}(x)\gamma^5\psi(x)=-\overline{\psi}'(x')\gamma^5\psi'(x')$.

The time reversal transformation we consider T , corresponds to a coordinates transform $(x^\mu)_\mu\rightarrow(x'^\mu)_\mu=(-x^0,\vec{x})$.

Take the Schroedinger equation $i(\partial/\partial t)\psi(t)=\hat{H}\psi(t)$ (for a spinless non-relativistic particle we can take $\hat{H}=-(1/2m)\nabla^2+V(\vec{x})$) and suppose that under T, $t\rightarrow t'=-t$ the wave function transforms as $\psi(t)\rightarrow\psi'(t')=T\psi(t)$ where T is some operator to be determined (up to some arbitrary phase factor η).

Since $\hat{H}$ does not involve time in any way and we want the Schroedinger equation preserved under time reversal , we must have :

$i(\partial/\partial t')\psi'(t')=\hat{H}\psi'(t')$, $T^{-1}\hat{H}=\hat{H}T^{-1}$, $T^{-1}(-i)T(\partial/\partial t)\psi(t)=\hat{H}\psi(t)$.

We are forced to conclude that $T^{-1}(-i)T=i$ (1)
In quantum physics therefore flipping time means flipping i as well.
Let $T=UK$ where K complex conjugates everything to its right. Then (1) holds if $U^{-1}iU=i$ that is if U is just an ordinary unitary operator that does nothing to i .
Acting on a spinless particle we must have $T^2=UKUK=UU^*K^2=+1$.
Next consider a spin ½ non-relativistic particle . Since the spin is proportional to an angular momentum (spin angular momentum) we expect that by time reversal the spin up state becomes the spin down state. Hence we need a non-trivial matrix

$U=\eta\sigma_2$ to flip the spin: $T\begin{pmatrix}1\\0\end{pmatrix}=U\begin{pmatrix}1\\0\end{pmatrix}=i\eta\begin{pmatrix}0\\1\end{pmatrix}$

Thus acting on a spin $\frac{1}{2}$ particle we have $T^2=\eta\sigma_2K\,\eta\sigma_2K=-1$
(since $\eta\eta^*=1$ and $\sigma_2=-\sigma_2^*$).
This leads to the fact that in a system with an odd number of electrons in an electric field each energy level is twofold degenerate. Since the sytem is time reversal invariant , ψ and $T\psi$ have the same energy. Suppose they actually represent the same state. Then $T\psi=\exp(i\alpha)\psi$ and so $T^2\psi=T\exp(i\alpha)\psi=\exp(-i\alpha)T\psi=\psi\neq-\psi$.
So ψ and $T\psi$ must represent two distinct states.
For the Dirac spinor field system we have $\hat{H}=-i\gamma^0\gamma^k\partial_k+\gamma^0 m$ (with the usual convention of greek indexes for indexing from 0 to 3 and latin indexes for indexing from 1 to 3) and we want $i(\partial/\partial t')\psi'(t')=\hat{H}\psi'(t')$.
Once again this happens if $T=UK$ and $T\hat{H}=\hat{H}T$ that is $KU^{-1}\hat{H}UK=\hat{H}$ and so we require $KU^{-1}\gamma^0UK=\gamma^0$ and $KU^{-1}(i\gamma^0\gamma^k)UK=i\gamma^0\gamma^k$ so we have to solve for U such that $U^{-1}\gamma^0U=\gamma^0=\gamma^{0*}$, $U^{-1}\gamma^kU=-\gamma^{k*}$.
γ^2 being the only imaginary gamma matrix, we can take $U=\eta\gamma^1\gamma^3$ with η an arbitrary phase factor and the time reversal transformation is given by

$$\psi(x)\rightarrow\psi'(x')=\eta\gamma^1\gamma^3K\,\psi(x)\ .$$

Thus if we change a Dirac particle to its antiparticle (C transformation) and flip space-time (PT transformation) we obtain
something like $\eta\gamma^5\psi$ with $\gamma^5=i\gamma^0\gamma^1\gamma^2\gamma^3$ and η an arbitrary phase factor, γ^5 appearing as the CPT transformation factor for a Dirac particle.
We notice that acceleration transforms odd under PT and velocity transforms even under PT. Considering the Lorentz force expression we obtain that electric field and magnetic induction field transform odd under PT and therefore the electromagnetic potential transforms even under PT. Thus we can easy verify that the Dirac equation $i\gamma^\mu(\partial_\mu+ieA_\mu)\psi(x)-m\psi(x)=0$ is invariant under CPT transformation if we take $e'=-e$ the CPT conjugated charge.

The general theorem states that any local Lorentz invariant field theory must be invariant under CPT, the combined action of charge conjugation, parity and time reversal.

Consider a Lorentz boost in a fixed direction z , $B(\chi, e_z)$, $\chi \in \mathbb{R}$, $e_z = (0,0,1)$ (see Chap. Representations of the rotation group and of the restricted Lorentz group)
This can be interpreted as a rotation of the time axis into the *z* axis with an imaginary rotation parameter:

(if $\begin{pmatrix} z' \\ t' \end{pmatrix} = \begin{pmatrix} \cosh\chi & \sinh\chi \\ \sinh\chi & \cosh\chi \end{pmatrix} \begin{pmatrix} z \\ t \end{pmatrix}$ then $\begin{pmatrix} z' \\ i\,t' \end{pmatrix} = \begin{pmatrix} \cos(i\chi) & -\sin(i\chi) \\ \sin(i\chi) & \cos(i\chi) \end{pmatrix} \begin{pmatrix} z \\ i\,t \end{pmatrix}$)

If this parameter were real, it would be possible for a 180° rotation to reverse the direction of time and of *z* .
Reversing the direction of one axis is a reflection of space in any number of dimensions. If space has three dimensions it is equivalent to reflecting all the coordinates, because an additional rotation of 180° in the *x*-*y* plane could be included.
This defines a CPT transformation if we adopt the Feynman-Stueckelberg interpretation of antiparticles as the corresponding particles travelling backwards in time. This requires a slight analytic continuation which is well defined under the following assumptions:

1. The theory is Lorentz invariant
2. The vacuum is Lorentz invariant
3. The energy is bounded below

When the above hold, quantum theory can be extended to a Euclidean theory , defined by translating all the operators to imaginary time using the Hamiltonian (see also Chap. Feynman diagrams and lattice gauge theory).
The commutation relations of the Hamiltonian and the Lorentz generators guarantee that Lorentz invariance implies rotational invariance, so that any state can be rotated by 180°.
The implication of CPT is that a “mirror image” of our universe, with all objects having their positions reflected through an arbitrary point (corresponding to position inversion), all momenta reversed (corresponding to a time inversion) and with all matter replaced by antimatter (corresponding to charge inversion) would evolve under exactly our physical laws.

Suppose we want to study a slowly moving electron described by the Dirac spinor $\psi = \psi(t, \vec{x})$ satisfying the Dirac equation $(i\,\gamma^\mu \partial_\mu - m)\,\psi = 0$ (2)

For $\psi(p) = \int \exp(i\,p\,x)\,\psi(x)\,d^4x$ we have $\psi(x) = \frac{1}{(2\pi)^4} \int \exp(-i\,p\,x)\,\psi(p)\,d^4p$

and $(\not{p} - m)\,\psi(p) = 0$ (2’)
(where $\not{p} = \gamma^\mu p_\mu$)

We write $\psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}$ with ϕ,χ two component fields.

Since for an electron at rest, $p=(m,0,0,0)$ from (2') follows $\chi(p)=0$ we expect that for a slowly moving electron $\chi(p)$ to be much smaller than $\phi(p)$.

In contrast, for a fast moving electron, the momentum *p* is much larger than the mass *m* and we can approximate (2') with $\not{p}\,\psi(p)=0$ (3)

We see that if $\psi(p)$ is a solution of (3) then $\gamma^5\,\psi(p)$ is asolution of (3).

We can form two projection operators:

$P_L=\frac{1}{2}(\boldsymbol{I}-\gamma^5)$, $P_R=\frac{1}{2}(\boldsymbol{I}+\gamma^5)$ (since $(\gamma^5)^2=\boldsymbol{I}$ we have $P_L^2=P_L, P_R^2=P_R$, $P_L P_R=P_R P_L=0$) and we define $\psi_L=P_L\,\psi$, $\psi_R=P_R\,\psi$ having $\psi=\psi_L+\psi_R$, ψ_L, ψ_R being linear independent , the left handed respective right handed spinor.

We notice that if instead of the standard gamma matrices we use another set of gamma matrices defined by the transformation $(\gamma^\mu)_\mu\to(W\,\gamma^\mu W^{-1})_\mu$ where W is some 4×4 matrix with an inverse, then (2) is satisfied if we take $\psi\to W\,\psi$

Taking $W=\begin{pmatrix}\boldsymbol{I} & -\boldsymbol{I}\\ \boldsymbol{I} & \boldsymbol{I}\end{pmatrix}$ we obtain $\gamma^k\to\gamma^k$, $\gamma^0\to\begin{pmatrix}0 & \boldsymbol{I}\\ \boldsymbol{I} & 0\end{pmatrix}$, $\gamma^5\to\begin{pmatrix}-\boldsymbol{I} & 0\\ 0 & \boldsymbol{I}\end{pmatrix}$,

$\psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}\to\begin{pmatrix}\phi-\chi\\ \phi+\chi\end{pmatrix}=\widetilde{\psi}=W\,\psi=\begin{pmatrix}\widetilde{\phi}\\ \widetilde{\chi}\end{pmatrix}$, $\psi_L\to\begin{pmatrix}\widetilde{\phi}\\ 0\end{pmatrix}=\widetilde{\psi}_L$, $\psi_R\to\begin{pmatrix}0\\ \widetilde{\chi}\end{pmatrix}=\widetilde{\psi}_R$

If ψ is a Dirac spinor, $\widetilde{\psi}$ is called a Weyl spinor and the corresponding transformed gamma matrices define the Weyl basis of gamma matrices.

In the Weyl basis , relation (3) becomes

$p_0\widetilde{\chi}=-p_k\sigma_k\widetilde{\chi}$, $p_0\widetilde{\phi}=p_k\sigma_k\widetilde{\phi}$ or in terms of the spin operator

$p_0\widetilde{\psi}_R=-2\vec{p}\cdot\vec{S}\,\widetilde{\psi}_R$, $p_0\widetilde{\psi}_L=2\vec{p}\cdot\vec{S}\,\widetilde{\psi}_L$ and since W commutes with γ^k we obtain

$p_0\psi_R=-2\vec{p}\cdot\vec{S}\,\psi_R$, $p_0\psi_L=2\vec{p}\cdot\vec{S}\,\psi_L$ and so because $p_0=\sqrt{\vec{p}^2+m^2}>0$ we have that the left handed spinor spins anticlockwise around the direction of motion (having positive helicity : $\langle\vec{p}\cdot\vec{S}\rangle>0$) and the right handed spinor spins clockwise around the direction of motion (having negative helicity : $\langle\vec{p}\cdot\vec{S}\rangle<0$).

Since ψ_c transforms like a spinor under a Lorentz transformation, Lorentz invariance allows not only the Dirac equation $i\not{\partial}\,\psi=m\,\psi$ but also the Majorana equation,

$i\not{\partial}\,\psi=m\,\psi_c$ (4)

Complex conjugating and multiplying with γ^2 the relation (4) leads to

$i\not{\partial}\,\psi_c=m\,\psi$ (5) and thus $-\partial^2\psi=i\not{\partial}(i\not{\partial})\,\psi=im\not{\partial}\,\psi_c=m^2\psi$ so that *m* is indeed the mass of the particle associated with ψ satisfying (4), known as the Majorana neutrino with Majorana mass *m* .

The Majorana equation can be obtained from the following (6) Lagrangian density upon varying $\overline{\psi}$ for the corresponding stationary action.

$$\mathscr{L}=\overline{\psi} i \partial \!\!\!/ \, \psi-\frac{1}{2} m\left(\psi^T C \, \psi+\overline{\psi} C \, \overline{\psi}^T\right) \qquad (6)$$

where $C^T=\gamma^0 \gamma^2=-C$ and in (6) the $(\psi_\alpha)_\alpha$ and $(\overline{\psi}_\alpha)_\alpha$ variables has to be treated as anticommuting Grassmann numbers as we learned in Chap. Dirac spinors…
Since ψ and ψ_c carry opposite charge the Majorana equation, unlike the Dirac equation can only be applied to electrically neutral fields.
If ψ is left handed then $\partial \!\!\!/ \, \psi$ is right handed and ψ_c is also right handed.
Therefore the Majorana equation preserves handedness. The Majorana equation is taylor made for the neutrino which is considered as a left handed Majorana neutrino.

The Dirac Lagrangian density $\mathscr{L}=\overline{\psi}(i \partial \!\!\!/-m) \psi$ can be written as

$$\mathscr{L}=\overline{\psi}_L i \partial \!\!\!/ \, \psi_L+\overline{\psi}_R i \partial \!\!\!/ \, \psi_R-m\left(\overline{\psi}_L \psi_R+\overline{\psi}_R \psi_L\right)$$

Under the transformations $\psi \rightarrow \exp(i \theta) \psi$ which leave $\mathscr{L}$ invariant and generate according to Noether theorem the conserved current $(J^\mu)_\mu=(\overline{\psi} \gamma^{my} \psi)_\mu$ the left and right handed fields transform in the same way $\psi_L \rightarrow \exp(i \theta) \psi_L$, $\psi_R \rightarrow \exp(i \theta) \psi_R$.
If $m = 0$, the Lagrangian enjoys an additional symmetry under which $\psi \rightarrow \exp(i \theta \gamma^5) \psi$ and in this case, Noethers theorem produces the axial current $(J^{5\mu})_\mu=(\overline{\psi} \gamma^\mu \gamma^5 \psi)_\mu$ and the left and right handed fields transform in opposite way: $\psi_L \rightarrow \exp(-i \theta) \psi_L$, $\psi_R \rightarrow \exp(i \theta) \psi_R$.
Under parity transformation, left handed spinors become right handed and right handed spinors become left handed, since $\gamma^0 \gamma^5=-\gamma^5 \gamma^0$.
Parity violation in weak interactions leaded to the conclusion that a weak interaction Lagrangian occurs only with participation of left handed fields, so in a Fermi weak interaction theory, the interaction terms in the Lagrangian density can only be of the form $G \overline{\psi}_{1L} \gamma^\mu \psi_{2L} \overline{\psi}_{3L} \gamma_\mu \psi_{4L}$ where $\psi_{1,2,3,4}$ denotes four Dirac fields and G is the Fermi coupling.

20. Spin statistics theorem

Spin statistics theorem

Consider two completely identical systems a and b coupled through an interaction energy which is symmetric in the two systems.
If we first consider the two systems together, without including the interaction energy, the systems will have stationary energy eigenstates n, m as eigenfunctions $\Phi_n^a = \Phi_n^a(q^a)$, $\Phi_m^a = \Phi_m^b(q^b)$ and the total energy of the system is $\hat{H} = \hat{H}^a \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \hat{H}^b$ with eigenstates $(\Phi_n^a \otimes \Phi_m^b)_{n,m}$;
$\hat{H}^a \Phi_n^a = H_n^a \Phi_n^a$, $\hat{H}_m^b \Phi_m^b = H_m^b \Phi_m^b$; (q^a) , (q^b) spatial coordinates for a respective b system. The systems being identical we will have
$H_{nm} = H_n^a + H_m^b = H_m^a + H_n^b = H_{mn}$.
The udistorted by interaction total system is degenerated and each eigenstate is a doublet $(\Phi_n^a \otimes \Phi_m^b$, $\Phi_m^a \otimes \Phi_n^b)$ with the exception of that with $m = n$.
In every system distorted by interaction the degeneracy is broken: it corresponds to secular beats in which the energy of the two particle system pulses back and forth and the energy of the distorted system is given in first approximation by the time average of the interaction energy over the undistorted motion which will contain other terms that correspond to the transitions in which the systems a and b exchange places.
Since $(\Phi_n^a \otimes \Phi_m^b)_{n,m}$ is still a basis for the distorted total system Hilbert space, the distorted by interaction Hamiltonian will be:

$$\hat{H} = H^1(nm,nm)\left|\Phi_n^a\right\rangle \otimes \left|\Phi_m^b\right\rangle \left\langle \Phi_n^a\right| \otimes \left\langle \Phi_m^b\right| + H^1(mn,mn)\left|\Phi_m^a\right\rangle \otimes \left|\Phi_n^b\right\rangle \left\langle \Phi_m^a\right| \otimes \left\langle \Phi_n^b\right| +$$
$$H^1(nm,mn)\left|\Phi_n^a\right\rangle \otimes \left|\Phi_m^b\right\rangle \left\langle \Phi_m^a\right| \otimes \left\langle \Phi_m^a\right| \otimes \left\langle \Phi_n^b\right| + H^1(mn,nm)\left|\Phi_m^a\right\rangle \otimes \left|\Phi_n^b\right\rangle \left\langle \Phi_n^a\right| \otimes \left\langle \Phi_n^a\right| \otimes \left\langle \Phi_m^b\right| .$$

because the interaction energy is symmetric in the two systems, we have:
$H^1(nm,nm) = H^1(mn,mn)$, $H^1(nm,mn) = H^1(mn,nm)$ (1)
Considering the (1) relations, diagonalizing $\hat{H}$ we obtain:

$$\hat{H} = (H^1(nm,nm) + H^1(nm,mn))\left|\Phi_{+mn}\right\rangle \left\langle \Phi_{+mn}\right| +$$
$$+ (H^1(nm,nm) - H^1(nm,mn))\left|\Phi_{-mn}\right\rangle \left\langle \Phi_{-mn}\right| \quad \text{where}$$

$$\left|\Phi_{+mn}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\Phi_n^a\right\rangle \otimes \left|\Phi_m^b\right\rangle + \left|\Phi_m^a\right\rangle \otimes \left|\Phi_n^b\right\rangle\right)$$

$$\left|\Phi_{-mn}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\Phi_n^a\right\rangle \otimes \left|\Phi_m^b\right\rangle - \left|\Phi_m^a\right\rangle \otimes \left|\Phi_n^b\right\rangle\right)$$

The eigenstates of $\hat{H}$ are now $\left(\left|\Phi_{+mn}\right\rangle\right)_{m,n}$, $\left(\left|\Phi_{-mn}\right\rangle\right)_{m,n}$ and a perturbation inducing transitions between different eigenstates of $\hat{H}$ can be written as $\hat{H}' = F\exp(-i\,\omega t) + F^+ \exp(i\,\omega t)$ where F and its adjoint operator F^+ are in general functions of $(\hat{p}^a, \hat{q}^a, \hat{p}^b, \hat{q}^b)$ which do not change under the interchange of the two systems and *t* is the time variable.
Then (according to Chap. Fermi's golden rule) the transition probability rate from a state $\left|i\right\rangle = \left|\Phi_{+mn}\right\rangle$ to a state $\left|f\right\rangle = \left|\Phi_{-m'n'}\right\rangle$ is proportional to

$$|\langle f|F|i\rangle|^2=\left|\int \frac{1}{2}(\Phi_m^a(q^a)\Phi_n^b(q^b)+\Phi_n^a(q^a)\Phi_m^b(q^b))F\left(\Phi_{n'}^{a+}(q^a)\Phi_{m'}^{b+}(q^b)-\right.\right.$$
$$\left.\left.-\Phi_{m'}^{a+}(q^a)\Phi_{n'}^{b+}(q^b)\right)dq^a dq^b\right|^2$$

The expression under the integral on the right side of the above relation changes sign when a and b are interchanged and so the integral vanishes and we conclude that transitions between $|\Phi_{+mn}\rangle$ states and $|\Phi_{-m'n'}\rangle$ similar between $|\Phi_{-mn}\rangle$ states and $|\Phi_{+m'n'}\rangle$ states cannot occur.

Thus the level spectrum of the combined, distorted by interaction system can be divided into two spectra which can never combine with one other:

the $(+)$: $|\Phi_m^a\rangle\otimes|\Phi_n^b\rangle+|\Phi_n^a\rangle\otimes|\Phi_m^b\rangle$ symmetric wave functions and

the $(-)$: $|\Phi_m^a\rangle\otimes|\Phi_n^b\rangle-|\Phi_n^a\rangle\otimes|\Phi_m^b\rangle$ antisymmetric wave functions .

The goal of the spin statistics theorem is to establish that only one of the two spectra (+) or (-) is allowed, namely (+) if the individual systems are bosonic (integer spin particles) and (-) if the individual systems are fermionic (half integer spin particles) and so bosons will obey to the Bose-Einstein statistics and fermions will obey to the Fermi-Dirac statistics (see Chap. Quantum statistical ensemble).

Consider now a quantum field particles system described by a particle field operator function $\hat{\Phi}=\hat{\Phi}(x)$, $x=(t,\vec{x})\in\mathbb{R}^4$ acting on a Hilbert space of state vectors containing an unique vacuum state $|0\rangle$ with $\Phi=(\Phi_\lambda)_\lambda$

$$\hat{\Phi}_\lambda(x)=\sum_s\int d^3\vec{k}(u_\lambda(k,s)\hat{b}(k,s)\exp(-ikx)+v_\lambda(k,s)\hat{d}^+(k,s)\exp(ikx)) \quad (2)$$

where $k=(k_0,\vec{k})$, $k_0=\sqrt{\vec{k}^2+m^2}$ and $\hat{b}^+(k,s)$, $\hat{d}^+(k,s)$ / $\hat{b}(k,s)$, $\hat{d}(k,s)$ are creation/anihilation like operators acting on state vectors such that $\hat{b}|0\rangle=\hat{d}|0\rangle=0$ and $\hat{b}^+(k,s)|0\rangle$ is the spin index s and k - four-momentum state vector for the particle and $\hat{d}^+(k,s)|0\rangle$ being the same for the antiparticle.

We have an unitary representation of the inhomogeneous Lorentz group of Poincare transformations $x\to\Lambda x+a$ with $a\in\mathbb{R}^4$, $\Lambda\in SO^+(3,1)$, restricted Lorentz transformation such that:

$$U=U(a,\Lambda)\ ,\ \hat{\Phi}_\lambda(\Lambda x+a)=U(a,\Lambda)\hat{\Phi}_\lambda(x)U^+(a,\Lambda)$$

$U(a_1,\Lambda_1)U(a_2,\Lambda_2)=U(a_1+\Lambda_1 a_2,\Lambda_1\Lambda_2)$, $U(a,\boldsymbol{I})=\exp(i\hat{p}a)$, $U|0\rangle=|0\rangle$ where $\hat{p}$ is the four-momentum operator acting on state vectors

(we have indeed $\hat{\Phi}_\lambda^+(x+a)=\int d^3\vec{k}\,u_\lambda^*(k,s)\exp(ika)\hat{b}^+(k,s)\exp(ikx)|0\rangle=$

$=\int d^3\vec{k}\,u_\lambda^*(k,s)\exp(i\hat{p}a)\hat{b}^+(k,s)\exp(ikx)|0\rangle=U(a,\boldsymbol{I})\hat{\Phi}_\lambda^+(x)U^+(a,\boldsymbol{I})|0\rangle$).

Φ is transforming under some finite dimensional irreducible representation of the restricted Lorentz group : $x\to\Lambda x=x'$ as $\hat{\Phi}_\lambda(x)\to\hat{\Phi}'_\lambda(x')=S_{\lambda\mu}(\Lambda)\hat{\Phi}_\mu(x)$.

We also consider an invariant space of test functions, $f=(f^\mu(x))_\mu$ such that we we have the transformation

$f^{\mu}(x)\rightarrow f^{\mu}_{\Lambda}(x')=f^{\lambda}(x)S_{\lambda\mu}(\Lambda^{-1})$ so that the test field operator defined as

$\hat{\Phi}(f)=\int d^4x f^{\mu}(x)\hat{\Phi}_{\mu}(x)$ is invariant under $x\rightarrow\Lambda x=x'$.

Suppose we want to interchange two space-like separated particles generated by the field at the points x , y in space-time and test the system with test functions $f^{\lambda}(x)$ and $g^{\mu}(y)$. We test therefore the system at the neighbourhoods of two space-like separated points 1 and 2 generated by the field in points *x* respective *y* using arbitrary test functions *f* (*x*) , *g* (*y*). For interchanging the particles we must have a trajectory in space-time, expressing the interchanging process, from *x* to *y*. Since according to relativity no process from a point A to apoint B exist if B is not in the future light-cone of A (or A is in the past light-cone of B) we must therefore perform a measuring process of the vacuum at point *y* applying first to the vacuum state the corresponding test field operator and then we must find a way to conduct the process from *y* to the space-like separated *x*. Because *x* and *y* are space-like separated and we want the time to run forward when we arrive at *x* we must conduct the process from *y* to a point *z* which is in the past light-cone of *y* and in the past light-cone of *x*. Then we conduct the process from *z* to *x*, *x* being in the future light-cone of *z*. Because from *y* to *z* we move backwards in time, for having a field effect of positive energy we must consider the term in exp(*iky*) in the field expression (2) at *y* and since $\hat{b}|0\rangle=\hat{d}|0\rangle=0$ we must take at y the effect of $g^{\mu*}(y)\hat{\Phi}^{+}_{\mu}(y)$ as correspondng test field operator on the vacuum state $|0\rangle$. Φ^{+} is the antiparticle field, which according to interpretation is the particle moving backwards in time, that is the field creates, moving from the future proximity of *y* (where the particle 2 is supposed to be) a particle with positive energy. Now we can conduct further the measuring process by applying the field operator $f^{\lambda}(x)\hat{\Phi}_{\lambda}(x)$ on $g^{\mu*}(y)\hat{\Phi}^{+}_{\mu}(y)|0\rangle$, that is the field anihilates moving from the past proximity of *x* (where the particle 1 is supposed to disappear) a particle with positive energy.

The required expectation value of the measuring process is therefore $\langle 0|f^{\lambda}(x)\hat{\Phi}_{\lambda}(x)\hat{\Phi}^{+}_{\mu}(y)g^{\mu*}(y)|0\rangle$.

If we switch now particles and test first at *x* and then at *y* we move from *x* to a point *z'* in the future light-cone of *x* and in the future light cone of y and from *z'* , which is in the past light-cone of *y* , getting the expectation value $\langle 0|g^{\mu*}(y)\hat{\Phi}^{+}_{\mu}(y)\hat{\Phi}_{\lambda}(x)f^{\lambda}(x)|0\rangle$.

For $\xi=y-x$ we have $\langle 0|\hat{\Phi}^{+}_{\mu}(y)\hat{\Phi}_{\lambda}(x)|0\rangle=$

$=\langle 0|U(y,\boldsymbol{I})\hat{\Phi}^{+}_{\mu}(0)U^{+}(y,\boldsymbol{I})U(y,\boldsymbol{I})\hat{\Phi}_{\lambda}(x-y)U^{+}(y,\boldsymbol{I})|0\rangle=$

$=\langle 0|\hat{\Phi}^{+}_{\mu}(0)\hat{\Phi}_{\lambda}(-\xi)|0\rangle=H_{\mu\lambda}(\xi)=\langle 0|\hat{\Phi}^{+}_{\mu}(0)\exp(-i\hat{p}\,\xi)\hat{\Phi}_{\lambda}(0)|0\rangle.$

Let $K_{\mu\lambda}(p)=\int d^4\xi\exp(i\,p\,\xi)\langle 0|\hat{\Phi}^{+}_{\mu}(0)\exp(-i\,\hat{p}\,\xi)\hat{\Phi}_{\lambda}(0)|0\rangle.$

We can always take a complete orthonormate system of four-momentum state vectors $(|\psi\rangle)_{\psi}$ with $\hat{p}|\psi\rangle=p_{\psi}|\psi\rangle$, $\sum_{\psi}|\psi\rangle\langle\psi|=\boldsymbol{I}$ and $p_{\psi 0}\geq 0$, $p^2_{\psi}\geq 0$ for any permissible state vector $|\psi\rangle$ and we will have:

$$K_{\mu\lambda}(p)=\sum_{\psi}\int d^4\xi\exp(i\,p\,\xi)\langle 0|\hat{\Phi}^{+}_{\mu}(0)\exp(-i\,\hat{p}\,\xi)|\psi\rangle\langle\psi|\hat{\Phi}_{\lambda}(0)|0\rangle=$$
$$=\sum_{\psi}(2\pi)^4\delta^4(p-p_{\psi})\langle\psi|\hat{\Phi}_{\lambda}(0)|0\rangle\langle 0|\hat{\Phi}^{+}_{\mu}(0)|\psi\rangle$$
$$H_{\mu\lambda}(\xi)=\int\frac{1}{(2\pi)^4}\exp(-i\,p\,\xi)K_{\mu\lambda}(p)d^4p=$$
$$=\sum_{\psi}\exp(-i\,p_{\psi}\xi)\langle\psi|\hat{\Phi}_{\lambda}(0)|0\rangle\langle 0|\hat{\Phi}^{+}_{\mu}(0)|\psi\rangle\qquad(3).$$

For $\hat{\Phi}_{\lambda}(0)|0\rangle=\sum_{\psi}c_{\psi}|\psi\rangle$, $\langle 0|\hat{\Phi}^{+}_{\mu}(0)=\sum_{\psi}d_{\psi}\langle\psi|$ since $(|\psi\rangle)_{\psi}$ is a complete orthonormal system we have
$\sum_{\psi}|c_{\psi}||d_{\psi}|\le(\langle 0|\hat{\Phi}^{+}_{\mu}(0)\hat{\Phi}_{\mu}(0)|0\rangle\langle 0|\hat{\Phi}^{+}_{\lambda}\hat{\Phi}_{\lambda}(0)|0\rangle)<\infty$ and so the series on the right side of (3) is absolute convergent and uniform absolute convergent with respect to $z\in\{\xi-i\,\eta\in\mathbb{C}^4|\eta_0\ge 0\}$ (z on the place of ξ variable in (3)) .
Hence $H_{\mu\lambda}(\xi)=\lim_{\eta\to 0\ ,\ \eta 0\ge 0}H_{\mu\lambda}(\xi-i\,\eta)$ and for $\alpha=(\alpha_0,\alpha_1,\alpha_2,\alpha_3)\in\mathbb{N}^4$ $\alpha!=\alpha_0!\,\alpha_1!\,\alpha_2!\,\alpha_3!$ we have if $\eta_0>0$ that $p_{\psi}\eta\ge 0$ and so:
$$\sum_{\alpha}\sum_{\psi}\frac{|(p_{\psi})^{\alpha}|}{\alpha!}|\exp(-i\,p_{\psi}(\xi-i\,\eta))||\zeta^{\alpha}|\left|\langle\psi|\hat{\Phi}_{\lambda}(0)|0\rangle\langle 0|\hat{\Phi}^{+}_{\mu}(0)|\psi\rangle\right|\le$$
$$\le\exp(4\,p_{\psi 0}\|\zeta\|)\sum_{\psi}|c_{\psi}||d_{\psi}|\quad\text{for any }\zeta\in\mathbb{C}^4.$$
Therfore we have an analytic function on $D=\{\xi-i\,\eta\in\mathbb{C}^4|\eta_0>0\}\cap\{z\in\mathbb{C}^4|z^2\ne 0\}$ with $z=(z_0,z_1,z_2,z_3)$, $z^2=z_0^2-z_1^2-z_2^2-z_3^2$, $H_{\mu\lambda}(z)=\sum_{\psi}\exp(-i\,p_{\psi}z)c_{\psi}d_{\psi}$ and $H_{\mu\lambda}(\xi)$ is the boundary value of an analytic function on *D*.
We have for any $\Lambda\in SO^{+}(3,1)$ that $H_{\mu\lambda}(\Lambda\,\xi)=\langle 0|\hat{\Phi}^{+}_{\mu}(\Lambda\,0)\hat{\Phi}_{\lambda}(-\Lambda\,\xi)|0\rangle=$
$=\langle 0|U\,\hat{\Phi}^{+}_{\mu}(0)U^{+}\,U\,\hat{\Phi}_{\lambda}(-\xi)U^{+}|0\rangle=H_{\mu\lambda}(\xi)$ where $U=U(0,\Lambda)$.
Hence for any $\Lambda\in SO^{+}(3,1)$, $z\in D$ we have $H_{\mu\lambda}(\Lambda\,z)=H_{\mu\lambda}(z)$(because if $z\in D$ then $\Lambda\,z\in D$.

Let $(J_k,K_k)_{k=\overline{1,3}}$ the generators of $SO^{+}(3,1)$ (see Chap. Representations of the restricted Lorentz group). It is easy to see that for any $\chi\in\mathbb{C}$, $z\in D$, if $\Lambda=\exp(\chi K_3)$ satisfies $\Lambda\,z\in D$ then exists a continuous path $\gamma:[0,1]\to\mathbb{C}$ with $\gamma(0)=0$, $\gamma(1)=\chi$ such that for $\Lambda_t=\exp(\gamma(t)K_3)$ we have $\Lambda_t\,z\in D$ for any $t\in[0,1]$ and therefore, by analytic continuation we obtain
$$H_{\mu\lambda}(\Lambda\,z)=H_{\mu\lambda}(z)\text{ for }\Lambda=\exp(\chi K_3)\ ,\ z\in D\ ,\ \Lambda\,z\in D\ .$$
Consider $Q=\{\exp(\theta_1J_1+\theta_2J_2+\theta_3J_3)|\theta_i\in\mathbb{C}\ ,\ i=\overline{1,3}\}=S.$
Obviously $Q\,z\in D$ for any $z\in D$ and by analytic continuation $H_{\mu\lambda}(Q\,z)=H_{\mu\lambda}(z).$

Thus for given $z=(z_0,z_1,z_2,z_3)\in D$ we find $Q\in S$ with $Qz=z'=(z'_0,0,0,z'_3)$ $z'^2=z^2$, $z'\in D$ and we can choose $\chi\in\mathbb{C}$ such that for $\Lambda=\exp(\chi K_3)$ we have $\Lambda z'=(\sqrt{z^2},0,0,0)$ where the square root $\sqrt{z^2}$ is taken with positive imaginary part. We will have $H_{\mu\lambda}(\Lambda z')=H_{\mu\lambda}(z')=H_{\mu\lambda}(Qz)=H_{\mu\lambda}(z)$ and so $H_{\mu\lambda}(z)=H_{\mu\lambda}(\sqrt{z^2},0,0,0)$ and since we can verify that $\{z^2|z\in D\}\supset\mathbb{C}\setminus\mathbb{R}_+$ and so $H_{\mu\lambda}$ can be analytically continuated on $B=\{\zeta\in\mathbb{C}^4|\zeta^2\in\mathbb{C}\setminus\mathbb{R}_+\}$.

Since $\langle 0|\hat{\Phi}^+_\mu(y)\hat{\Phi}_\lambda(x)|0\rangle$ must be Lorentz invariant it follows that for any $\Lambda\in SO^+(3,1)$, $U=U(0,\Lambda)$ we have $H_{\mu\lambda}(\Lambda\xi)=S^*_{\mu\mu'}(\Lambda)S_{\lambda\lambda'}(\Lambda)H_{\mu'\lambda'}(\xi)$ (4) where S^* is the complex conjugate of S.

According to Chap. Representations of the restricted Lorentz group (final) we have that *S* is an irreducible (j_1 , j_2) representation so that

$$j_1,j_2\in\frac{1}{2}\mathbb{N}\ ,\ \Lambda=\exp\left((-i\vec{\theta}-\vec{\chi})\frac{1}{2}(i\vec{J}-\vec{K})\right)\exp\left((-i\theta+\vec{\chi})\frac{1}{2}(i\vec{J}+\vec{K})\right)$$

$$S(\Lambda)=\exp\left((-i\vec{\theta}-\vec{\chi})\vec{M}_+\right)\exp\left((-i\vec{\theta}+\vec{\chi})\vec{M}_-\right)\ ,\ M_{+3}=\frac{1}{2}H_+\ ,\ M_{-3}=\frac{1}{2}H_-$$

H_+ having the spectrum $(-2j_1,-2j_1+2,...,2j_1)$ and
H_- having the spectrum $(-2j_2,-2j_2+2,...,2j_2)$.

Because for any $\Lambda=\exp\left((-i\theta-\chi)\frac{1}{2}(iJ_3-K_3)\right)\exp\left((-i\theta+\chi)\frac{1}{2}(iJ_3+K_3)\right);\theta,\chi\in\mathbb{C}$

we have $(\Lambda z)^2=z^2$,by analytic continuation on θ,χ variables, we can take in (4)

$$\Lambda=\exp(-i\pi(iJ_3-K_3))\ ,\ S(\Lambda)=\exp(-i\pi H_+)\ ,\ S^*(\Lambda)=\exp(i\pi H^*_-).$$

iJ_3-K_3 has eigenvalues ±1 and is diagonalizable and so $\Lambda=-\boldsymbol{I}$. H_+ and H^*_- are also diagonalizable (see Chap. Repres. of the restricted Lorentz group (final)) and so $\exp(-i\pi H_+)=\exp(2j_1i\pi)\boldsymbol{I}$, $\exp(i\pi H^*_-)=\exp(2j_2i\pi)\boldsymbol{I}$.

Hence $H_{\mu\lambda}(-\xi)=\exp(2(j_1+j_2)i\pi)H_{\mu\lambda}(\xi)$ for any space-like ξ because for $\xi^2<0$ we have $\xi\in B$. Thus for bosons $j_1+j_2\in\mathbb{N}$ and we have $H_{\mu\lambda}(-\xi)=H_{\mu\lambda}(\xi)$ and for fermions $j_1+j_2\in\frac{1}{2}+\mathbb{N}$ and we have $H_{\mu\lambda}(-\xi)=-H_{\mu\lambda}(\xi)$.

Testing the interchanging of particles in space-like separated points *x* , *y* with $f^{\lambda'}(x')\to\delta^4(x'-x)\delta_{\lambda\lambda'}$, $g^{\mu'}(y')\to\delta^4(y'-y)\delta_{\mu\mu'}$ with x' , y' variable and $\to$ convergence in distributions space, since we have already proven the splitting of the level spectrum in (+) and (-) spectra with no transitions between them, we will have for the expectation values, considering the commuting/anticommuting for the individual wave functions of the respective spectra (+)/(-), one of the relations: $\langle 0|\hat{\Phi}^+_\mu(y)\hat{\Phi}_\lambda(x)|0\rangle=\pm\langle 0|\hat{\Phi}_\lambda(x)\hat{\Phi}^+_\mu(y)|0\rangle$.

Proving the spin statistics theorem is therefore reduced to verify that “wrong” commutation relations cannot take place.

Taking $F_{\mu\lambda}(-\xi)=\langle 0|\hat{\Phi}_\mu(x)\hat{\Phi}^+_\lambda(y)|0\rangle=\langle 0|\hat{\Phi}_\mu(0)\hat{\Phi}^+_\lambda(\xi)|0\rangle$ the 'wrong' commutation relation is for both bosonic and fermionic case

$F_{\lambda\mu}(\xi)+H_{\mu\lambda}(\xi)=0$ for $\xi^2<0$ (5)

(because $H_{\mu\lambda}(-\xi)=(-1)^{2(j1+j2)}H_{\mu\lambda}(\xi)$ for a (j_1,j_2) representation if $\xi^2<0$.

Let for $f=f(x)$, $\bar{f}=f(-x)$ and we will have:

$\|\hat{\Phi}(f)|0\rangle\|^2=\int f^{\mu*}(y)\langle 0|\hat{\Phi}^+_\mu(y)\hat{\Phi}_\lambda(x)|0\rangle f^\lambda(x)d^4x\,d^4y=$

$=\int f^{\mu*}(y)H_{\mu\lambda}(y-x)f^\lambda(x)d^4x\,d^4y$

$\|\hat{\Phi}^+(\bar{f})|0\rangle\|=\int f^\mu(-y)\langle 0|\hat{\Phi}_\mu(y)\hat{\Phi}^+_\lambda(x)|0\rangle f^{\lambda*}(-x)d^4x\,d^4y=$

$=\int f^\mu(y)\langle 0|\hat{\Phi}_\mu(x)\hat{\Phi}^+_\lambda(y)|0\rangle f^{\lambda*}(x)=\int f^{\mu*}(y)F_{\lambda\mu}(y-x)f^\lambda(x)d^4x\,d^4y$

where for the last equality we have taken the complex conjugate of the integrand considering the fact that the left side is real , being a squared norm.

Taking for $y-x=\xi$, $\xi^2<0$: $f^\lambda(x')=\alpha_\lambda\delta^4(x'-x)+\beta_\lambda\delta^4(x'-y)$ with arbitrary α_λ , β_λ , from (5) follows now $\|\hat{\Phi}(f)|0\rangle\|=\|\hat{\Phi}^+(\bar{f})|0\rangle\|=0$ and so, α,β being arbitrary we obtain $\hat{\Phi}_\lambda(x)|0\rangle=\hat{\Phi}^+_\lambda(x)|0\rangle=0$ for any $\lambda,x,$ which leads, considering (2) to the conclusion that $\hat{\Phi}=0$ and thus the 'wrong' commutation relations cannot take place or the field vanishes, which proves the spin statistics theorem.

(indeed, multiplying for example $\hat{\Phi}^+_\lambda(x)|0\rangle=0$ with $\exp(-ikx)$ for given k and integrating over $x\in\mathbb{R}^4$ it follows $\sum_s \delta(k_0-\sqrt{\vec{k}^2+m^2})u^*_\lambda(k,s)\hat{b}^+(k,s)|0\rangle=0$ (6)

so that applying to (6) $\hat{b}(k,s')$, since $\hat{b},\hat{b}^+$ are anihilation/creation like operators and satisfy an commutation/anticommutation rule

$\hat{b}(k,s)\hat{b}^+(k',s')\pm\hat{b}^+(k',s')\hat{b}(k,s)=\delta^3(\vec{k}'-\vec{k})\,\delta_{ss'}$

we obtain $u^*_\lambda(k,s)=0$ for any λ,k,s with $k_0=\sqrt{\vec{k}^2+m^2}$)

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21. Quantum statistical ensemble Bose-Einstein and Fermi-Dirac statistics

Quantum statistical ensemble

A quantum statistical ensemble describes a macrostate of a quantum system through thermodynamically macroscopically equivalent microstates of a quantum system having a Hilbert space H_S of wave functions satisfying all the Schroedinger equation $i\hbar\partial_t\psi=\widehat{H}\psi$, $\psi=\psi(t,\vec{x})$, $t\in\mathbb{R}$, $\vec{x}\in\mathbb{R}^3$, $\psi(t)=\psi(t,\cdot)\in H_S$ and $\widehat{H}$ is the Hamiltonian operator acting on H_S .

A microstate of the statistical ensemble at time moment *t* can be one of orthonormal $n\in\mathbb{N}$ states $(\psi_s(t))_{s=\overline{1,n}}$, $\psi_s(t)\in H_S$ such that for the system prepared in the macrostate, there is a probability $p_s\geq 0$ for a microstate to be $\psi_s(t)$ with $s=\overline{1,n}$ $\sum_1^n p_s=1$. Thus we define a density operator of the given macrostate by

$$\rho=\rho(t)=\sum_{s=1}^{n} p_s|\psi_s(t)\rangle\langle\psi_s(t)|$$

It follows that $\rho(t)$ is a continuous linear compact self-adjoint trace operator on H_S having the trace equal to one.

(for a trace operator A if $(|m\rangle)_m$ is a complete orthonormal system then the trace defined by $\mathrm{tr}\,A=\sum_m\langle m|A|m\rangle$ not depends on the chosen complete orthonormal system $(|m\rangle)_m$ and for the density operator we have

$\mathrm{tr}\,\rho=\sum_m\langle m|\rho|m\rangle=\sum_{s=1}^{n}\sum_m p_s\langle m|\psi_s\rangle\langle\psi_s|m\rangle=\sum_s p_s\sum_m\langle\psi_s|m\rangle\langle m|\psi_s\rangle=1$ since $\langle\psi_s|\psi_s\rangle=1$ and $\sum_m|m\rangle\langle m|=\boldsymbol{I}_{H_s}$)

Also, considering the Schroedinger equation, we have:

$$\partial_t(|\psi_s(t)\rangle\langle\psi_s(t)|)=|\partial_t\psi_s(t)\rangle\langle\psi_s(t)|+|\psi_s(t)\rangle\langle\partial_t\psi_s(t)|=$$

$=\frac{1}{i\hbar}(\widehat{H}|\psi_s(t)\rangle\langle\psi_s(t)|-|\psi_s(t)\rangle\langle\widehat{H}\psi_s(t)|)=\frac{1}{i\hbar}[\widehat{H},|\psi_s(t)\rangle\langle\psi_s(t)|]$ and so we derived

$\partial_t\rho=\frac{1}{i\hbar}[\widehat{H},\rho]$, the von Neumann equation.

For an observable *A* (as we mentioned in Chap. Quantum mechanics formalism, by discretization we can consider that A is a compact self-adjoint (and obviously linear continuous) operator on H_S) we define

$\sigma(A)=\{a\in\mathbb{R}|$ exists $v\in H_S$ such that $Av=av\}$ the spectrum of A and $S_a=\{v\in H_S|Av=av\}$ the eigenspace of eigenvalue a for A and we have:

$A=\sum_{a\in\sigma(A)} aP_a$ where P_a is the projector of H_S on the closed subspace S_a .

For A compact and self-adjoint, $a\neq 0$ we have that S_a is finite dimensional.

We have also $P_a\psi=\sum_i |a,i\rangle\langle a,i|\psi\rangle$ where $(|a,i\rangle)_i$ is an orthonormal complete sytem in S_a and $\langle\psi_s|P_a|\psi_s\rangle$ is the transition probability from the state ψ_s to one of the $|a,i\rangle$ states.

$\mathrm{tr}(\rho P_a)=\mathrm{tr}(P_a\rho)=\sum_m\langle m|P_a\sum_{s=1}^n p_s|\psi_s\rangle\langle\psi_s|m\rangle=\sum_{s=1}^n p_s\langle\psi_s|P_a|\psi_s\rangle$

$\mathrm{tr}(\rho P_a)$ can be interpreted as the probability that a measurement of observable A, performed on the system prepared in the macrostate with density operator ρ leads to the result a (Born rule).

$\mathrm{tr}(\rho A)=\mathrm{tr}(A\rho)=\sum_{s=1}^n p_s\langle\psi_s|A|\psi_s\rangle$ can be interpreted as the expectation value of the observable A on a system prepared in the macrostate with density operator ρ (at time moment t) : $\langle A\rangle_t=\mathrm{tr}(\rho(t)A(t))$.

The thermodynamical parameters are described as expectation values of observables on the system.

According to von Neumann equation, for an observable A we have:

$$\frac{d}{dt}\langle A\rangle_t=\frac{d}{dt}\mathrm{tr}(\rho A)=\mathrm{tr}((\partial_t\rho)A)+\mathrm{tr}(\rho(\partial_t A))=\frac{1}{i\hbar}\mathrm{tr}([\hat{H},\rho]A)+\langle\partial_t A\rangle_t$$

Since any compact self-adjoint operator has a complete orthonormal system of eigenvectors we derive that if A is compact self-adjoint and AB is a trace operator with A,B linear continuous operator on H_S then $\mathrm{tr}(AB)=\mathrm{tr}(BA)$.

Therefore $\mathrm{tr}([\hat{H},\rho]A)=\mathrm{tr}([A,\hat{H}]\rho)$ and so we obtain:

$$\frac{d}{dt}\langle A\rangle_t=\frac{1}{i\hbar}\langle[A,\hat{H}]\rangle_t+\langle\partial_t A\rangle_t \qquad (1)$$

If f is a polynomial and A , B are compact self-adjoint linear continuous operators with $[A,B]=\pm i\hbar$ then we obtain without difficulties that $[A,f(B)]=\pm i\hbar f'(B)$ and so for any class C^1 function $g:[-M,M]\to\mathbb{R}$ where $M=\|B\|=\sup_{\langle\varphi|\varphi\rangle=1}\langle\varphi|B|\varphi\rangle$ we have $[A,g(B)]=\pm i\hbar g'(B)$

(For example , for $\hat{H}=\frac{\hat{p}^2}{2m}+V(x)$ we will have $\frac{d\langle\hat{x}\rangle_t}{dt}=\frac{1}{i\hbar}\langle[\hat{x},\hat{H}]\rangle_t=\frac{\langle\hat{p}\rangle_t}{m}$

$\frac{d\langle v\rangle_t}{dt}=\frac{1}{m}\frac{d\langle\hat{p}\rangle_t}{dt}=\frac{1}{i\hbar}\langle\hat{p},\hat{H}\rangle_t=-\left\langle\frac{\partial V(x)}{\partial x}\right\rangle_t$, relation corresponding to the classical equation of motion for a mass m particle).

Since in general the Hamiltonian can be seen as a continuous differentiable function of position and momentum operators , having the relations

$\hat{H}=\hat{H}(\hat{X},\hat{P})$, $[\hat{X}_j,\hat{P}_k]=i\delta_{ik}\hbar$ and so $[\hat{X}_j,\hat{H}]=i\hbar\partial_{P_j}\hat{H}$, $[\hat{P}_j,\hat{H}]=-i\hbar\partial_{X_j}\hat{H}$

$\hat{X}$, $\hat{P}$ not depending explicite on time $\partial_t\hat{X}=0$, $\partial_t\hat{P}=0$ the relation (1) leads to

$$\frac{d\langle \hat{X}_j \rangle_t}{dt} = \langle \partial_{P_j} \hat{H}(\hat{X}, \hat{P}) \rangle_t \qquad (2)$$

$$\frac{d\langle P_j \rangle_t}{dt} = -\langle \partial_{X_j} \hat{H}(\hat{X}, \hat{P}) \rangle_t \qquad (3)$$

Relations (2) and (3) are the corresponding form for quantum systems to the Hamilton-Jacobi relations from classical mechanics.

Consider now a system of identical quantum particles. The Hilbert space *S* of wave functions of the system can be considered the direct sum of the Hilbert spaces of *N* factors tensorial products of the same one particle system Hilbert space *V*.

$S = \underset{N \in \mathbb{N}^*}{\oplus} \left(\overset{N}{\underset{i=1}{\otimes}} V \right)$ and the Hamiltonian operator of the sytem is $\hat{H} = \underset{N \in \mathbb{N}^*}{\oplus} \hat{H}_N$ where

$$S_N = \overset{N}{\underset{i=1}{\otimes}} V \ , \ \hat{H}_N : S_N \to S_N \text{ with}$$

$$\hat{H}_N(\psi_1 \otimes \psi_2 ... \otimes \psi_N) = (\hat{H}_1 \psi_1) \otimes \psi_2 ... \otimes \psi_N + \psi_1 \otimes (\hat{H}_1 \psi_2) ... \otimes \psi_N + ...$$
$$... + \psi_1 \otimes \psi_2 ... \otimes (\hat{H}_1 \psi_N)$$

for any $\psi_i \in V$, $i = \overline{1, N}$, $N \in \mathbb{N}^*$; $\hat{H}_1 : V \to V$ the one particle system Hamiltonian.

According to spin-statistics theorem, if the particles are bosons (integer spin particles), the energy eigenstates of the statistical ensemble we will consider to determine a macrostate of the multiparticle system will be symmetrical tensorial products of the states $(|\varepsilon_s\rangle)_{s \in \mathbb{N}}$ and if the particles are fermions (half integer spin particles) the energy eigenstates of the statistical ensemble will be antisymmetrical tensorial products of the states $(|\varepsilon_s\rangle)_{s \in \mathbb{N}}$, where $(|\varepsilon_s\rangle)_{s \in \mathbb{N}}$ is a complete orthonormal system of eigenstates for the one particle system Hamiltonian operator.

We denote $\hat{H}_1 |\varepsilon_s\rangle = \varepsilon_s |\varepsilon_s\rangle$, $\varepsilon_s \in \mathbb{R}$ for any $s \in \mathbb{N}$.

The eigenstates are

$\varepsilon_{n0n1...ns...} = \frac{1}{N!} \sum_{\sigma} \overset{N}{\underset{i=1}{\otimes}} |\varepsilon_{s\sigma i}\rangle$ for bosons and $\varepsilon_{n0n1...ns...} = \frac{1}{N!} \sum_{\sigma} \varepsilon(\sigma) \overset{N}{\underset{i=1}{\otimes}} |\varepsilon_{s\sigma i}\rangle$ for fermions where $N \in \mathbb{N}^*$, $s_1, s_2, ..., s_N \in \mathbb{N}$, σ is a permutation of $\{1, 2, ..., N\}$, $\varepsilon(\sigma)$ is the signature of σ and $n_s = \text{card}\{i \in \mathbb{N}^* | s_i = s\}$ for any $s \in \mathbb{N}$

If $\sum_s n_s = N$ we will have $\varepsilon_{n0n1...ns...} \in S_N$, $\hat{H}_N |\varepsilon_{n0n1...ns...}\rangle = (\sum_s n_s \varepsilon_s) |\varepsilon_{n0n1...ns...}\rangle$.

If the particles are fermions we have $\varepsilon_{n0n1...ns...} = 0$ if exists s such that $n_s > 1$ and so we take $n_s = 0, 1$ for any $s \in \mathbb{N}$ for fermions (Pauli exclusion principle).

The density operator will be :

$\rho = \sum_{n0, n1, ..., ns, ...} p_{n0n1...ns...} |\varepsilon_{n0n1...ns...}\rangle \langle \varepsilon_{n0n1...ns...}| = \underset{N}{\oplus} \rho_N$ with $\rho_N : S_N \to S_N$,

$\rho_N = \sum_{\substack{n0, ..., ns... \\ \sum_s ns = N}} p_{n0n1...ns...} |\varepsilon_{n0n1...ns...}\rangle \langle \varepsilon_{n0n1...ns...}|$, $p_{n0n1...ns...} \in [0, 1]$.

$\mathrm{tr}\,\rho=1$ leads to $\sum_{n0,n1,\ldots ns\ldots} p_{n0n1\ldots ns\ldots}=1$, $\sum_{N\in\mathbb{N}^*}\mathrm{tr}\,\rho_N=1$.

By analogy with the relations for classical statistical ensemble, for a quantum multiparticle system prepared in a macrostate at equilibrium with a reservoir having temperature T and chemical potential μ we must have

$$p_{n0n1\ldots ns\ldots}=\exp\left(\frac{\Omega-\sum_s n_s\varepsilon_s+\mu N}{k_BT}\right) \quad \text{where} \quad N=\sum_s n_s \ , \ \frac{1}{Z}=\exp\left(\frac{\Omega}{k_BT}\right) \ ,$$

$$Z=\sum_{n0}\sum_{n1}\ldots\sum_{ns}\ldots\exp\left(\frac{(\mu-\varepsilon_0)n_0}{k_BT}\right)\ldots\exp\left(\frac{(\mu-\varepsilon_s)n_s}{k_BT}\right)\ldots$$

(k_B is the Boltzmann constant).

If the particles are bosons we obtain the Bose-Einstein distribution with n_s passing all values in $\mathbb{N}$: $Z_{BE}=\prod_s Z_{BE}^{(s)}$, $p_{n0n1\ldots ns\ldots}=\frac{1}{Z_{BE}}\prod_s\exp\left(\frac{(\mu-\varepsilon_s)n_s}{k_BT}\right)$ where

$$Z_{BE}^{(s)}=\frac{1}{1-\exp\left((\mu-\varepsilon_s)/(k_BT)\right)} \quad \text{and we must have} \quad \mu<\varepsilon_s \ \text{for any} \ s \ .$$

The probability that n_s particles belong to the one particle state determined by $|\varepsilon_s\rangle$ is $P_{sBE}(n_s)=\frac{1}{Z_{BE}^{(s)}}\exp\left(\frac{(\mu-\varepsilon_s)n_s}{k_BT}\right)$ and so the averaged occupation number of the state $|\varepsilon_s\rangle$ is

$$f_{BE}(\varepsilon_s)=\langle n_s\rangle_{BE}=\sum_{ns=0}^{\infty} n_s P_{sBE}(n_s)=\frac{1}{\exp\left((\varepsilon_s-\mu)/(k_BT)\right)-1} \quad (4)$$

If the particles are fermions we obtain the Fermi-Dirac distribution with n_s = 0,1 :

$$Z_{FD}=\prod_s Z_{FD}^{(s)} \ , \ p_{n0n1\ldots ns\ldots}=\frac{1}{Z_{FD}}\prod_s\exp\left(\frac{(\mu-\varepsilon_s)n_s}{k_BT}\right) \text{ where}$$

$$Z_{FD}^{(s)}=1+\exp\left((\mu-\varepsilon_s)/(k_BT)\right) \ .$$

The probability that n_s particles (n_s = 0,1) belong to the one particle state determined by $|\varepsilon_s\rangle$ is $P_{sFD}(n_s)=\frac{1}{Z_{FD}^{(s)}}\exp\left(\frac{(\mu-\varepsilon_s)n_s}{k_BT}\right)$ and the averaged occupation number of the state $|\varepsilon_s\rangle$ is

$$f_{FD}(\varepsilon_s)=\langle n_s\rangle_{FD}=\frac{1}{\exp\left((\varepsilon_s-\mu)/(k_BT)\right)+1} \quad (5)$$

We notice that for a specified value of $\varepsilon_s=\varepsilon$ we can have one or more indicices s such that $\varepsilon_s=\varepsilon$. We can have a degeneracy of the eigenvalue energy level , $g_s=\mathrm{card}\{s'\in\mathbb{N}\,|\,\varepsilon_{s'}=\varepsilon_s\}$ and so in fact the averaged number of particles which belong to an energy state with energy eigenvalue $\varepsilon=\varepsilon_s$ is therefore equal to

$\frac{g_s}{\exp\left((\varepsilon_s-\mu)/(k_BT)\right)-1}$ (6) for bosons and $\frac{g_s}{\exp\left((\varepsilon_s-\mu)/(k_BT)\right)+1}$ (7) for fermions , g_s being the degeneracy of the energy level ε_s.

Therefore at equilibrium with the macrostate at temperature T and chemical potential μ we will have

$$\rho=\bigoplus_N \rho_N \ , \ \rho_N=\exp\left((\Omega-\hat{H}_N+\mu N)/(k_B T)\right) \ , \ \exp\left(\Omega/(k_B T)\right)=1/Z$$

$$Z=\sum_N \operatorname{tr}\exp\left((-\hat{H}_N+\mu N)/(k_B T)\right)$$

The entropy is $S=-k_B \operatorname{tr}(\rho\log\rho)=-k_B\sum_N \operatorname{tr}(\rho_N\log\rho_N)=$

$$=-k_B\sum_{n0,\dots ns\dots} p_{n0\dots ns\dots}\log p_{n0\dots ns\dots}=-k_B\sum_N \operatorname{tr}\left(\rho_N(\Omega-\hat{H}_N+\mu N)/(k_B T)\right)$$

$$S=-\frac{\Omega}{T}+\frac{1}{T}\sum_N \operatorname{tr}(\rho_N\hat{H}_N)-\frac{\mu}{T}\sum_N \operatorname{tr}(\rho_N N)$$

The thermodynamical parameters U and N_t are

$U=\sum_N \operatorname{tr}(\rho_N\hat{H}_N)$, $N_t=\sum_N \operatorname{tr}(N\rho_N)$ and so we have confirmed the relation for macroscopic thermodynamical parameters :

$U=\Omega+T S+\mu N_t$ with $\Omega-$macrocanonical potential , $S-$entropy ,

$U-$internal energy, N_t-averaged particle number.

In a similar way, for a canonical statistical ensemble of systems in a macrostate at eqilibrium with a reservoir at temperature T (the system not changes particles with the reservoir and we have a determined particles number N) we have a Hamiltonian $\hat{H}=\hat{H}_N$ which has a complete orthonormate system of eigenstates $\left(\left(\left|E_n,i\right\rangle\right)_{i=\overline{1,gn}}\right)_n$ in a way that we have $\left(\left|E_n,i\right\rangle\right)_{i=\overline{1,gn}}=\left(\left|\varepsilon_{n0\dots ns\dots}\right\rangle\right)_{\substack{\sum_s n_s=N \\ \sum_s n_s\varepsilon_s=E_n}}$

$$\rho=\rho_N=\exp\left(\frac{F-\hat{H}}{k_B T}\right)=\frac{1}{Z}\exp\left(-\frac{\hat{H}}{k_B T}\right) \ , \ \log Z=-\frac{F}{k_B T}$$

$$Z=\operatorname{tr}\exp\left(-\hat{H}/(k_B T)\right)=\sum_n g_n\exp\left(-E_n/(k_B T)\right)$$

$$\rho=\sum_n\sum_{i=1}^{g_n} p_{ni}\left|E_n,i\right\rangle\left\langle E_n,i\right| \ , \ p_{ni}=\frac{1}{Z}\exp\left(-E_n/(k_B T)\right) \ , \ \sum_n\sum_{i=1}^{g_n} p_{ni}=\operatorname{tr}\rho=1$$

$$S=-k_B\sum_n\sum_{i=1}^{g_n} p_{ni}\log p_{ni}=-k_B\operatorname{tr}(\rho\log\rho)$$

It follows

$$U=\sum_n\sum_{i=1}^{g_n} p_{ni}E_n=\operatorname{tr}(\rho\hat{H})$$

$$S=-k_B\operatorname{tr}\left(\rho(-\hat{H}/(k_B T)-\log Z)\right)=\frac{1}{T}U-\frac{1}{T}F$$

Therefore $U=T S+F$ and F is the free energy potential.

Hence in the case of a canonical statistical ensemble at equilibrium we have:

$$p_{ni}=\exp\left(\frac{F-E_n}{k_BT}\right)=\exp\left(-\frac{S}{k_B}\right)\exp\left(\frac{U-E_n}{k_BT}\right) \ .$$

Let $E_n>E_0$ for $n\neq 0$ and it follows:

$$\frac{U-E_n}{k_BT}=\frac{\langle\widehat{H}\rangle_t-E_0}{k_BT}+\frac{E_0-E_n}{k_BT} \ , \ \lim_{T\to 0}\exp\left(\frac{E_0-E_n}{k_BT}\right)=\delta_{n0} \text{ for any } n \text{ and so}$$

$$\lim_{T\to 0}p_{ni}=p_{ni}^{(0)}=C\,\delta_{n0} \text{ with } C=\lim_{T\to 0}\exp\left(-\frac{S}{k_B}\right)\exp\left(\frac{\langle\widehat{H}\rangle_t-E_0}{k_BT}\right)$$

For $\rho^{(0)}=\lim_{T\to 0}\rho$ we must have

$$1=\mathrm{tr}\,\rho^{(0)}=\sum_n\sum_{i=1}^{g_n}p_{ni}^{(0)}=\sum_{i=1}^{g_0}C=C\,g_0 \ , \ C=\frac{1}{g_0} \ ,$$

$$\rho^{(0)}=\sum_n\sum_{i=1}^{g_n}p_{ni}^{(0)}|E_n,i\rangle\langle E_n,i|=\sum_{i=1}^{g_0}\frac{1}{g_0}|E_0,i\rangle\langle E_0,i|=\frac{1}{g_0}P_{E_0} \text{ where } P_{E_0} \text{ is the projector}$$

on the E_0 eigenspace.

Also we derive

$$\lim_{T\to 0}\langle\widehat{H}\rangle_t=\mathrm{tr}\left(\widehat{H}\,\rho^{(0)}\right)=\sum_n\sum_{i=1}^{g_n}E_n p_{ni}^{(0)}=\sum_n\sum_{i=1}^{g_n}E_n\frac{1}{g_0}\delta_{n0}=E_0 \ ,$$

$$\lim_{T\to 0}S=-k_B\,\mathrm{tr}\left(\rho^{(0)}\log\rho^{(0)}\right)=k_B\log g_0$$

If g_0 not depends on extensive parameters , it follows that

$\lim_{T\to 0}S\left(T,(X_j)_j\right)=S(0)=k_B\log g_0=\text{const.}$, where $(X_j)_j$ are the extensive parameters.

The entropy at 0 absolute temperature is constant not depending on extensive parameters. If $g_0=1$ (non-degeneracy on the fundamental energy level E_0) we have $\lim_{T\to 0}S=0$ (Nernst-Planck theorem) as we expected according to the third principle of thermodynamics.

We notice that as the absolute temperature approaches zero the system condensates in the fundamental states at energy level E_0. The known condensate quantum systems (crystal lattices, quantum gases) have non-degeneracy on the fundamental energy level.

We can consider a system of identical quantum particles in a way that the particles are in states corresponding to energy levels ε_s, each energy level having a degeneracy g_s , $s\in S$, S the set of energy states indices (there are g_s posibilities for a particle to be in a state of energy level ε_s at index $s\in S$) . Let N_s the population number of particles which are in a state with the same energy level ε_s indexed at $s\in S$. If the particles are fermions, they satisfy Pauli exclusion principle and so at most one particle can occupe a state and we have $N_s\leq g_s$. The number of distinct microscopic states for level ε_s generating the same macroscopic state (if we permute states within the same energy level indexed s , the macrostate do not changes) is the

combinations number of g_s elements taken N_s times, which is equal to $\frac{g_s!}{N_s!(g_s-N_s)!}$ and the total number of microscopic states which are compatible to a macroscopic state defined by the occupation numbers $(N_s)_s$ will be

$$W^{FD}=\prod_s \frac{g_s!}{N_s!(g_s-N_s)!} \ .$$

If the particles are bosons, they can pile up in the same state and the number of distinct microstates for level ε_s , generating the same macrostate is the combinations number of g_s elements taken N_s times with repetition, which is equal to $\frac{(N_s+g_s-1)!}{(g_s-1)!N_s!}$ and the total number of microscopic states which are compatible to a macroscopic state defined by occupation numbers $(N_s)_s$ is

$$W^{BE}=\prod_s \frac{(N_s+g_s-1)!}{(g_s-1)!N_s!} \ .$$

We consider that only the occupation numbers vary as the system approaches equilibrium .

The entropy is therefore $S=S((N_s)_s)=k_B \log W^{\substack{FD \\ BE}}$ and at thermodynamical equilibrium we have $S=\max\{S((N_s)_s)\Big|\sum_s N_s=N \ , \ \sum_s \varepsilon_s N_s=U\}$.

Taking additional to $(N_s)_s$ variables the Lagrange coefficients α,β we must have $d\sum_s(\log(g_s!)-\log(N_s!)-\log((g_s-N_s)!)+\alpha N_s+\beta\varepsilon_s N_s)=0$ which leads to $-\log(N_s+1)+\log(g_s-N_s)+\alpha+\beta\varepsilon_s=0$ for any s in the fermionic case at and $d\sum_s(\log((N_s+g_s-1)!)-\log((g_s-1)!)-\log(N_s!)+\alpha N_s+\beta\varepsilon_s N_s)=0$ which leads to

$$\log(N_s+g_s)-\log(N_s+1)+\alpha+\beta\varepsilon=0 \text{ for any } s \text{ in the bosonic case.}$$

Since we consider $N_s \gg 1$ we obtain $N_s=\frac{g_s}{\exp(-\alpha-\beta\varepsilon_s)\pm 1}$ at equilibrium with

$(+)$ sign for fermions and $(-)$ sign for bosons .

At thermodynamical equilibrium we must therefore have

$$dS=k_B\sum_s(\log(g_s\pm N_s)-\log N_s)dN_s=-k_B\sum_s \alpha d N_s+\beta\varepsilon_s d N_s$$

$dS=-k_B\alpha d N-k_B\beta d U$ and so we have $\alpha=\frac{\mu}{k_B T}$, $\beta=-\frac{1}{k_B T}$

since other extensive parameters as the volume are considered constant,

and the occupation numbers at equilibrium are $N_s=\frac{g_s}{\exp((\varepsilon_s-\mu)/(k_B T)\pm 1)}$

as we expected from (6) and (7) .

We have obtained also :

$$N=\sum_s \frac{g_s}{\exp\left(\frac{\varepsilon_s-\mu}{k_B T}\right)\pm 1} \quad , \quad U=\sum_s \frac{g_s\,\varepsilon_s}{\exp\left(\frac{\varepsilon_s-\mu}{k_B T}\right)\pm 1} \quad .$$

22. Decoherence. Choi-Kraus theorem No-communication theorem

Decoherence, Choi-Kraus theorem, No-communication theorem

Consider a system *S* and environment (bath) *B* which are closed and can be treated quantum-mechanically. Let H_S and H_B be the system's and bath's Hilbert spaces of state functions respectively. Then the combined system and bath system has the Hilbert space of states the tensor product space $H_{SB}=H_S\otimes H_B$ and we consider that states of the combined system have an unitary evolution in time , which (according to Chap. Quantum mechanics formalism) is of the form $\psi(t)=\widehat{U}(t)\,\psi(0)$ where t is the time variable and $\widehat{U}=\exp(-i\,\widehat{H}\,t/\hbar)$, $\widehat{H}$ is the Hamiltonian operator of the combined SB system. $\widehat{H}$ can be considered a self-adjoint compact operator on H_{SB} ($\widehat{U}$ is therefore an unitary operator on H_{SB}). Thus the density operator ρ_{SB} = $\rho_{SB}(t)$ of the combined system has a time evolution given by $\rho_{SB}(t)=\widehat{U}(t)\,\rho_{SB}(0)\,\widehat{U}^{+}(t)$ (1) . (see Chap. Quantum statistical ensemble)

To give a description of the system *S* alone, we perform a partial trace over the bath and ρ_{SB} obtaining the system reduced density matrix ρ_S = $\mathrm{tr}_B\,\rho_{SB}$

(if $(|m\rangle)_m$ is an orthonormal complete system of H_B there is an obvious isometric isomorphism $\bigoplus_m (H_S\otimes \mathbb{C}\,m)\to H_S\otimes H_B$ (with $\oplus$ direct sum of Hilbert spaces) and so any continuous linear operator $T\in L(H_S\otimes H_B)$ can be written as $T=\sum_{k.l} T^{(kl)}\otimes(|k\rangle\langle l|)$ with $(|k\rangle)_k=(|l\rangle)_l=(|m\rangle)_m$, $T^{(kl)}\in L(H_S)$, $T(|h\rangle\otimes|k\rangle)=\sum_l T^{(lk)}(|h\rangle)\otimes|l\rangle$.

If T is a non-negative operator and the series $\sum_j T^{(jj)}$ converges in the strong operator topology of $L(H_S)$ then it is independent of the chosen basis of H_B and we take $\mathrm{tr}_B T=\sum_j T^{(jj)}\in L(H_S)$)

Thus the transition probability of the system S into a state $|\varphi\rangle=|\varphi(t)\rangle$ is at time *t* given by $\langle\varphi(t)|\rho_S(t)|\varphi(t)\rangle$.

If the states of the system *S* cannot be described independently of the environment *B* states, the system and bath are entangled and a pure state of the combined *SB* system $|\psi\rangle\in H_{SB}$ cannot be written as a product $|\psi\rangle=|\psi_S\rangle\otimes|\psi_B\rangle$.

However we assume that initially system and bath are not entangled and so we can write $\rho_{SB}(0)=\rho_S(0)\otimes\rho_B(0)$ (2) .

Decoherence can be viewed as the loss of information from a system into the environment, since every system is loosely coupled with the energetic state of its surroundings. Viewed in isolation, the system's dynamics are non-unitary (although the combined system plus environment evolves in an unitary fashion) and so the loss of information occurs .

(in the entropy formula $S(\rho)=-\mathrm{tr}(\rho\log\rho)$ if ρ evolves unitary, $\rho(t)=U(t)\rho(0)U^{+}(t)$ with $UU^{+}=\boldsymbol{I}$ we have $S(\rho(t))=S(\rho(0))$ and so no loss of information)

The original system's wave function can be expanded as a sum of elements in a quantum superposition, corresponding to a projection of the wave vector onto a basis. We will choose an expansion where the resulting basis elements interact with the environment in an element specific way. Such elements will – with overwhelming probability – be rapidly separated from each other by their natural unitary time evolution along their own independent paths. After a very short interaction there is almost no chance of any further interference. The process is effectively irreversible. The different elements become "lost" from each other in the expanded phase space created by coupling with the environment. The original elements are said to have decohered. The environment has effectively selected out those expansions or decompositions of the original state vector that decohere with each other. This is called "environmentally induced superselection" or einselection.

Let the system S be initially in state $|\psi\rangle=\sum_i |i\rangle\langle i|\psi\rangle$ where $(|i\rangle)_i$ is an orthonormal einselected basis of H_S.

Thus before any interaction between the two subsystems, the joint state can be written as $|b_f\rangle=\sum_i |i\rangle|\epsilon\rangle\langle i|\psi\rangle$ if we let $|\epsilon\rangle$ be the environment's initially state and we use the notation $|i\rangle|\epsilon\rangle=|i\rangle\otimes|\epsilon\rangle\in H_{SB}$.

If the environment absorbs the system, each element of the system's basis interacts with the environment such that $|i\rangle|\epsilon\rangle$ evolves into $|\epsilon_i\rangle\in H_{SB}$ and so $|b_f\rangle$ evolves into $|a_f\rangle=\sum_i |\epsilon_i\rangle\langle i|\psi\rangle$. The unitarity of time evolution of the combined system demands that the total state basis remains orthonormal and so we have $\delta_{ij}=\langle\epsilon_i|\epsilon_j\rangle$. This orthonormality of the environment states is the defining characteristic required for einselection.

In an idealized measurement, the system disturbs the environment, but is itself undisturbed by the environment. In this case, each element of the basis interacts with the environment such that $|i\rangle|\epsilon\rangle$ evolves into $|i,\epsilon_i\rangle=|i\rangle|\epsilon_i\rangle$ and so $|b_f\rangle$ evolves into $|a_f\rangle=\sum_i |i,\epsilon_i\rangle\langle i|\psi\rangle$. In this case unitarity demands

$\delta_{ij}=\langle\epsilon|\langle i|j\rangle|\epsilon\rangle=\langle i,\epsilon_i|j,\epsilon_j\rangle=\langle i|j\rangle\langle\epsilon_i|\epsilon_j\rangle$, $\langle\epsilon_i|\epsilon_i\rangle=1$

Additionally, for decoherence to become einselection by virtue of the large number of hidden degrees of freedom, it requires the einselection condition $\langle\epsilon_i|\epsilon_j\rangle\approx\delta_{ij}$.

Initially the density matrix of the combined system is $\rho(0)=|b_f\rangle\langle b_f|=|\psi\rangle\langle\psi|\otimes|\epsilon\rangle\langle\epsilon|$ and the reduced density matrix of the system before interaction is

$\rho_S(0)=\mathrm{tr}_B(\rho(0))=|\psi\rangle\langle\psi|\langle\epsilon|\epsilon\rangle^2=|\psi\rangle\langle\psi|$.

Taking $\varphi=\sum_i |i\rangle\langle i|\varphi\rangle$, $\psi_i=\langle i|\psi\rangle$, $\varphi_i=\langle i|\varphi\rangle$ the transition probability of the to the state φ is $P^{before}_{\psi\to\varphi}=\langle\varphi|\rho_S|\varphi\rangle=|\langle\varphi|\psi\rangle|^2=\sum_i|\psi_i^*\,\varphi_i|^2+\sum_{i,j\,,\,i\neq j}\psi_j^*\,\psi_i\,\varphi_j\,\varphi_i^*$.

As we notice , the terms that involve $i\neq j$ can be thought as representing interference between the different basis elements or quantum alternatives which is a purely quantum effect and represents the non-additivity of the probabilities of quantum alternatives.

The density matrix after the interaction is $\rho=|a_f\rangle\langle a_f|=\sum_{i,j}\psi_j^*\,\psi_i|i,\epsilon_i\rangle\langle j,\epsilon_j|=\sum_{i,j}\psi_i\,\psi_j^*|i\rangle\langle j|\otimes|\epsilon_i\rangle\langle\epsilon_j|$ and the reduced density matrix is $\rho_S=\mathrm{tr}_B(\sum_{i,j}\psi_i\,\psi_j^*|i\rangle\langle j|\otimes|\epsilon_i\rangle\langle\epsilon_j|)=\sum_i|\psi_i|^2|i\rangle\langle i|$ where we used the einselection condition $\langle\epsilon_i|\epsilon_j\rangle=\delta_{ij}$.

The transition probability to the state $\varphi=\sum_i\varphi_i|i\rangle$ after the interaction will be

$$P^{after}_{\psi\to\varphi}=\langle\varphi|\rho_S|\varphi\rangle=\sum_{k,l,i}\varphi_k^*|\psi_i|^2\varphi_l\langle k|i\rangle\langle i|l\rangle=\sum_i|\psi_i^*\,\varphi_i|^2$$

which has no contribution of the interference terms.

The loss of interference effects corresponds to the diagonalization of the "environmentally traced over" density matrix, so the decoherence has irreversibly converted quantum behaviour (additive probability amplitudes) to classical behaviour (additive probabilities).

As a consequence, the system behaves as a classical statistical ensemble of the different elements rather than as a single coherent quantum superposition of them. From the perspective of each ensemble member's measuring device (any measuring device or apparatus acts as an environment), the systems appears to have irreversibly collapsed onto a state with a precise value for the measured attributes, relative to that element. And this provided one explains how the Born rule coefficients effectively act as probabilities, as per the measurement postulate , constitutes a solution to the quantum measurement problem.

Further the Hamiltonian for the combined system can be written as $\hat{H}=\hat{H}_S\otimes\boldsymbol{I_B}+\boldsymbol{I_S}\otimes\hat{H}_B+\hat{H}_I$, where $\hat{H}_S$, $\hat{H}_B$ are the system and bath Hamiltonians respectively, $\hat{H}_I$ is the interaction between system and bath Hamiltonian and $\boldsymbol{I_S},\boldsymbol{I_B}$ are the identity operators on the H_S , H_B Hilbert spaces.

Considering (1) and (2) relations, the evolution of the combined system becomes $\rho_{SB}(t)=\hat{U}(t)(\rho_S(0)\otimes\rho_B(0))\hat{U}^+(t)$.

The interaction Hamiltonian can be written as $\hat{H}_I=\sum_i\hat{S}_i\otimes\hat{B}_i$ where $\hat{S}_i,\hat{B}_i$ are operators that act on system and bath respectively .

We can take $(|j\rangle)_j$ an orthonormal complete system in H_B such that $\rho_B(0)=\sum_j a_j|j\rangle\langle j|$ and let $(|k\rangle)_k=(|l\rangle)_l=(|m\rangle)_m=(|n\rangle)_n=(|j\rangle)_j$ so that we have

$$\hat{U}=\sum_{k,l} U^{kl}\otimes|k\rangle\langle l| \quad , \quad \hat{U}^+=\sum_{m,n} U^{mn+}\otimes|n\rangle\langle m|$$

Thus after some calculus we obtain

$$\rho_S(t)=\mathrm{tr}_B\hat{U}(t)(\rho_S(0)\otimes\rho_B(0))\hat{U}^+(t)=$$

$$=\sum_{s,k,l,m,n,j} U^{kl}(t)\rho_S(0)U^{mn+}(t)a_j\langle s|k\rangle\langle l|j\rangle\langle j|n\rangle\langle m|s\rangle=\sum_{m,j} A_{mj}(t)\rho_S(0)A_{mj}^+(t)$$

where $A_{mj}(t)=\langle m|\hat{U}(t)|j\rangle\sqrt{a_j}$ are the so called Kraus operators acting on H_S. For an arbitrary $\rho_S(0)=\sum_q p_q|q\rangle\langle q|$ with $\sum_q p_q=1$, $p_q>0$ (the general form of a density operator), the condition $\mathrm{tr}\,\rho_S(t)=1$, taking $l=mj$ as the combined index and $(|r\rangle)_r$ a complete orthonormal system in H_S, leads to:

$$1=\sum_l\sum_q\sum_r p_q\langle r|A_l|q\rangle\langle q|A_l^+|r\rangle=\sum_{l,q} p_q\langle q|A_l^+\sum_r|r\rangle\langle r|A_l|q\rangle=$$

$$=\sum_q p_q\langle q|\sum_l A_l^+A_l|q\rangle \text{ and so } \sum_q p_q\langle q|\sum_l(A_l^+A_l-\boldsymbol{I_S})|q\rangle=0 \qquad (3)$$

for arbitrary p_q, $(|q\rangle)_q$ with $\sum_q p_q=1$, $p_q\geq 0$ and therefore from (3) follows $\sum_l A_l^+A_l=\boldsymbol{I_S}$ the condition satisfied by the Kraus operators.

We have the operator sum representation

$\rho_S(t)=\sum_l A_l\rho_S(0)A_l^+$ (4) with $\sum_l A_l^+A_l=\boldsymbol{I_S}$, $A_l=A_l(t)$ (5)

In particular, if there is more than one term present in the (4) sum for ρ_S, then the dynamics of the system will be non-unitary and hence decoherence will take place. As we noticed, any measurement device acts as an environment. Measurements are made on observables. Repeated measurements made on a statistical ensemble of systems with wave functions Hilbert space *H* and prepared in a macrostate with density matrix ρ results in a probability distribution over the eigenvalue spectrum of the measuring observable which is a discrete probability distribution $p(a)=\mathrm{tr}(\rho P_a)$, $a\in\sigma(A)=\{a'\in\mathbb{R}|$ exists $u\in H$ such that $Au=a'u\}$ where the observable $A:H\to H$ is a compact continuous linear self-adjoint operator on H and P_a is the projector of H on the eigenspace of eigenvalue a for A. We have obviously $A=\sum_a aP_a$ and the $(P_a)_a$ is a family of pairwise orthogonal projectors, $\bigoplus_a P_a=\boldsymbol{I_H}$ (6), $P_a=P_a^+$, $P_a^2=P_a$ (7)

Immediately after measurement, the statistical state is a classical distribution over the eigenspaces associated with the possible eigenvalues *a* of the observable.

After measurement the density matrix becomes

$\rho\to\sum_a P_a\rho P_a=\rho_m$ and so with t time moment immediately after measurement,

taking $(P_a)_a=(A_l(t))_l$, $\rho=\rho_S(0)$, $\rho_m=\rho_S(t)$ and considering (6), (7) we recognize (4) , (5) .

We conclude that if we have H a Hilbert space with quantum states density matrices $\rho\in L(H)$ (as defined density matrix, ρ is a compact self-adjoint non-negative operator $\langle x|\rho|x\rangle\geq 0$ for any $x\in H$, $\mathrm{tr}\,\rho=1$), any interaction with an environment of quantum statistical ensembles represented on H defines a quantum operation Φ upon density matrices $\rho\in L(H)$, $\Phi(\rho)=\sum_l A_l\rho A_l^+$ (8) where $(A_l)_l$ is a sequence of continuous linear operators $A_l\in L(H)$ satisfying

$$\sum_l A_l^+ A_l=\boldsymbol{I}_{\boldsymbol{H}}$$

By a discretization with a bounded lattice grid of the spatial coordinates domain we will restrict ourselves to using finite dimensional Hilbert spaces H .
A correlated system with the H Hilbert space system defines a quantum states combined Hilbert space $H\otimes H_C$ and density matrices $\widetilde{\rho}=\sum_{k,m} T^{(km)}\otimes|k\rangle\langle m|\in L(H\otimes H_C)$ where $(|k\rangle)_k=(|m\rangle)_m$ is an orthonormal basis of the (considered finite dimensional) environment Hilbert space H_C and $T^{(km)}\in L(H)$

A linear map $\Phi: L(H)\to L(H)$ induces a map $\widetilde{\Phi}: L(H\otimes H_C)\to L(H\otimes H_C)$ $\widetilde{\Phi}(\widetilde{\rho})=\sum_{k,m}\Phi(T^{(km)})\otimes|k\rangle\langle m|$ which acts like $\Phi\otimes\mathrm{id}$; $\widetilde{\Phi}=\Phi\otimes\mathrm{id}$ where $\mathrm{id}: L(H_C)\to L(H_C)$, $\mathrm{id}(M)=M$ for any $M\in L(H_C)$, $\widetilde{\rho}=\sum_{k,m} T^{(km)}\otimes|k\rangle\langle m|$

To be a quantum operation, a map $\Phi: L(H)\to L(H)$ should therefore satisfy three properties:
1. It should be linear
2. It should be completely positive (that is for any (finite dimensional) H_C if $\widetilde{\rho}\in L(H\otimes H_C)$ is non-negative then $\widetilde{\Phi}(\widetilde{\rho})$ is non-negative) so that it takes quantum states to quantum states (even for sytems correlated with the one which the map is acting on) .
3. It should satisfy $\Phi(A^+)=\Phi(A)^+$ and be trace preserving (again that it takes quantum states to quantum states).

We will prove the following Choi-Kraus theorem:

A map $\Phi: L(H) \to L(H)$ with H a finite dimensional Hilbert space is linear , completely positive, trace preserving and satisfies $\Phi(A^+)=\Phi(A)^+$ for any $A\in L(H)$ if and only if exist $(V_l)_{l=\overline{1,d}}$ such that $\sum_1^d V_l^+ V_l = \boldsymbol{I}_{\boldsymbol{H}}$ and $\Phi(X)=\sum_1^d V_l X V_l^+$ for any $X\in L(H)$

Also it will follow $d \le (\dim H)^2$

Proof of Choi-Kraus theorem

Let $\Phi(X)=\sum_1^d V_l X V_l^+$ for $X\in L(H)$ with $V_l \in L(H)$, $\sum_1^d V_l^+ V_l = \boldsymbol{I}_{\boldsymbol{H}}$.

We have $\operatorname{tr}\Phi(X)=\sum_1^d \operatorname{tr}(V_l X V_l^+)=\sum_1^d \operatorname{tr}((\sum_1^d V_l^+ V_l)X)=\operatorname{tr} X$ and also

$\Phi(X^+)=\Phi(X)^+$ is obvious.

For $H_C=\mathbb{C}^n$, $\widetilde{X}\in L(H\otimes H_C)$ we have $(\Phi\otimes \mathrm{id}_n)(\widetilde{X})=\sum_1^d (V_l\otimes \boldsymbol{I}_{\boldsymbol{n}})\widetilde{X}(V_l\otimes \boldsymbol{I}_{\boldsymbol{n}})^+$

Obviously if $\widetilde{X}\ge 0$ ($\langle x|\widetilde{X}|x\rangle \ge 0$ for any $x\in H\otimes H_C$) it follows $(V_l\otimes \boldsymbol{I}_{\boldsymbol{n}})\widetilde{X}(V_l\otimes \boldsymbol{I}_{\boldsymbol{n}})\ge 0$ and so $\widetilde{\Phi}(\widetilde{X})\ge 0$ if $\widetilde{X}\ge 0$.

Let now $\Phi: L(H)\to L(H)$ linear , trace preserving and completely positive and satisfying $\Phi(A^+)=\Phi(A)^+$ for any $A\in L(H)$.

We can take an orthonormal basis $(|i\rangle)_{i=\overline{1,n}}$ of H ($\dim H=n$) and an orthonormal basis $(|i\rangle_C)_{i=\overline{1,n}}$ of $H_C=\mathbb{C}^n$ and consider

$$\widetilde{\Phi}=\sum_{i,j}\Phi(|i\rangle\langle j|)\otimes|i\rangle_C\,{}_C\langle j| \in L(H\otimes H_C)$$

Since $(|i\rangle\langle j|)^+=|j\rangle\langle i|$ and for $A=\sum_{i,j}|i\rangle\langle j|\otimes|i\rangle_C\,{}_C\langle j|$, for any $\varphi=\sum_{i,j}\alpha_{ij}|i\rangle\otimes|j\rangle_C$ we have $\langle\varphi|A|\varphi\rangle=\sum_{p,q,r,s,i,j}\alpha_{pq}^*\alpha_{rs}\delta_{pi}\delta_{qi}\delta_{jr}\delta_{js}=\left|\sum_i \alpha_{ii}\right|^2\ge 0$, it follows from the assumptions we made on Φ that the above defined operator $\widetilde{\Phi}$ is self-adjoint and positive semi-definite. Therefore we can diagonalize $\widetilde{\Phi}$ as

$$\widetilde{\Phi}=\sum_1^d |\varphi_l\rangle\langle\varphi_l| \text{ with } d\le n^2 \ , \ \varphi_l=\sum_{i,j}\alpha_{ij}^l|i\rangle\otimes|j\rangle_C \ , \ \alpha_{ij}^l\in\mathbb{C} \ .$$

Let $V_l=\sum_{i,j}\alpha_{ij}^l|i\rangle\langle j|$ and we will have :

$$\Phi(|m\rangle\langle q|)=(\boldsymbol{I}_{\boldsymbol{H}}\otimes {}_C\langle m|)\widetilde{\Phi}(\boldsymbol{I}_{\boldsymbol{H}}\otimes|q\rangle_C)=\sum_{l,i,k}\alpha_{im}^l\alpha_{kq}^{l*}|i\rangle\langle k| \qquad (9)$$

$$\sum_l V_l|m\rangle\langle q|V_l^+=\sum_{l,i.j,k,r}\alpha_{ij}^l|i\rangle\langle j|m\rangle\langle q|\alpha_{kr}^{l*}|r\rangle\langle k|=\sum_{l,ik}\alpha_{im}^l\alpha_{kq}^{l*}|i\rangle\langle k| \qquad (10)$$

Since $(|m\rangle\langle q|)_{m,q}$ is a basis in $L(H)$ from (9) and (10) follows

$\Phi(X)=\sum_1^d V_l X V_l^+$ for any $X\in L(H)$.

Because Φ is trace preserving we have for any $|q\rangle\in H$ that

$$1=\mathrm{tr}(\Phi(|q\rangle\langle q|))=\sum_{l,m}\langle m|V_l|q\rangle\langle q|V_l^+|m\rangle=\sum_l\langle q|V_l^+(\sum_m|m\rangle\langle m|)V_l|q\rangle=$$

$=\langle q|\sum_l V_l^+ V_l|q\rangle$ and so $\sum_l V_l^+ V_l=\boldsymbol{I}_{\boldsymbol{H}}$ closing the proof of Choi-Kraus theorem.

The no-communication theorem states that, within the context of quantum mechanics, it is not possible to transmit bits of information by means of carefully prepared mixed or pure states.

Suppose Alice and Bob perform measurements on system *S* whose underlying Hilbert space is $H=H_A\otimes H_B$. Alice performs a local measurement on her part of the system (the Hilbert space H_A). If the density operator of the system is σ, Alice's measurement effect is described by a quantum operation on the system state, which according to Choi-Kraus theorem, on the whole system density operator acts like

$P(\sigma)=\sum_l(V_l\otimes\boldsymbol{I}_{\boldsymbol{H_B}})\sigma(V_l\otimes\boldsymbol{I}_{\boldsymbol{H_B}})^+$ (11) where $V_l\in L(H_A)$ are the Kraus matrices satisfying $\sum_l V_l^+ V_l=\boldsymbol{I}_{\boldsymbol{H_A}}$.

The factor $\boldsymbol{I}_{\boldsymbol{H_B}}$ from the (11) expression means that Alice's measurement apparatus not interract with Bob’s subsytem.

The relative state of Bob’s system is given by the partial trace of the overall state with respect to Alice's system, $\mathrm{tr}_{H_A}(P(\sigma))$.

We have $\sigma=\sum_i T_i\otimes S_i$ with $T_i\in L(H_A)$, $S_i\in L(H_B)$,

$$\mathrm{tr}_{H_A}(P(\sigma))=\mathrm{tr}_{H_A}(\sum_l\sum_i V_l T_i V_l^+\otimes S_i)=\sum_i\sum_l(\mathrm{tr}(V_l T_i V_l^+))S_i=\sum_i(\mathrm{tr}\,T_i)S_i=\mathrm{tr}_{H_A}(\sigma)$$

and so $\mathrm{tr}_{H_A}(P(\sigma))=\mathrm{tr}_{H_A}(\sigma)$.

Therefore statistically, assuming that all measurable properties of Bob’s system can be calculated from its reduced density matrix, which is true given the Born rule for calculating the probability of making various measurements, Bob cannot tell the difference between what alice did and a random measurement (or whether she did anything at all) and that is clearly the statement of the no-communication theorem.

23. Entanglement. Bell inequalities
Tsirelson’s bound. Applications of entanglement

Entanglement . Bell inequalities. Tsirelson bound . Applications of entanglement

Quantum entanglement occurs when a group of particles are generated , interact or share spatial proximity in a way such that the quantum state of each particle of the group cannot be described independently of the state of the others, including when the particles are separated by a large distance. Measurements of physical properties such as position, momentum, spin and polarization performed on entangled particles can in some cases be found to be perfectly correlated. Any measurement of a particle's properties results in an apparent and irresversible wave function collapse of that particle and changes the original quantum state. With entangled particles, such measurement affects the entangled system as a whole.

Consider two arbitrary quantum sytems *A* and *B* with the respective Hilbert spaces of states H_A and H_B . The Hilbert space for the composite sytem is the tensor product $H_A \otimes H_B$. Let $(|i\rangle_A)_i$ an orthonormal complete sytem for H_A and $(|j\rangle_B)_j$ an orthonormal complete system for H_B . The most general state in $H_A \otimes H_B$ is $|\psi\rangle_{AB} = \sum_{i,j} c_{ij} |i\rangle_A \otimes |j\rangle_B$. This state is called separable if there exist $(c_i^A)_i$, $(c_j^B)_j$ such that $c_{ij} = c_i^A c_j^B$ yielding $|\psi\rangle_A = \sum_i c_i^A |i\rangle_A$, $|\psi\rangle_B = \sum_j c_j^B |j\rangle_B$, $|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B$.

A state $|\psi\rangle_{AB}$ that is not separable(i.e.it cannot be represented as $|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B$) will be called an entangled state.

For example, given two basis vectors $(|0\rangle_A, |1\rangle_A)$ of H_A and two basis vectors $(|0\rangle_B, |1\rangle_B)$ of H_B ($|0\rangle_{A,B}, |1\rangle_{A,B}$ can be the polarization or spin eigenstates of photons or respective electrons forming a possible entangled pair of photons respective electrons in a *AB* composite system) the following state is an entangled state: $\frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B)$.

Now suppose Alice is an observer for sytem *A* and Bob is an observer for sytem *B*. If in the entangled state given above Alice makes a measurement in the $(|0\rangle, |1\rangle)$ eigenbasis of A, there are two possible outcomes, occuring with equal probability:

1. Alice measures 0 and the system collapses to $|0\rangle_A \otimes |1\rangle_B$.
2. Alice measures 1 and the system collapses to $|1\rangle_A \otimes |0\rangle_B$.

Then any subsequent measurement performed by Bob in the same basis will always return 1 if the former occurs and will always return 0 with certainity if the latter occurs. This remains true even if the systems *A* and *B* are spatially separated and thus the system *B* has been altered by the Alice performing a local measurement on system *A* .

If Bob's measurement is in another basis $(|x(\theta)\rangle_B, |y(\theta)\rangle_B)$, we say another linear polarization in the *x y* plane along any axis, we will have :

$|1\rangle_B=\langle 1|x(\theta)\rangle_B|x(\theta)\rangle_B+\langle 1|y(\theta)\rangle|y(\theta)\rangle_B$
$|0\rangle_B=\langle 0|x(\theta)\rangle_B|x(\theta)\rangle_B+\langle 0|y(\theta)\rangle_B|y(\theta)\rangle_B$
$|x(\theta)\rangle=\begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}$, $|y(\theta)\rangle=\begin{pmatrix}-\sin\theta\\ \cos\theta\end{pmatrix}$, $|0\rangle=\begin{pmatrix}1\\0\end{pmatrix}$, $|1\rangle=\begin{pmatrix}0\\1\end{pmatrix}$
$|0\rangle=\cos\theta|x(\theta)\rangle-\sin\theta|y(\theta)\rangle$, $|1\rangle=\sin\theta|x(\theta)\rangle+\cos\theta|y(\theta)\rangle$
and therefore the outcome will be $|x(\theta)\rangle_B$ with probability $\sin^2\theta$ and $|y(\theta)\rangle_B$ with probability $\cos^2\theta$ in the former case and $|x(\theta)\rangle_B$ with probability $\cos^2\theta$ and $|y(\theta)\rangle_B$ with probability $\sin^2\theta$ in the latter case.

Hence the quantum mechanical result by Heisenberg's uncertainity principle that polarization states cannot be simultaneously determined with certainity for two different polarization axes can be confirmed. The same result will be valid, by similar reasons, for spin states measured along different axes (the spin states are eigenstates $\vec{n}\cdot\vec{\sigma}$ with $\vec{n}$ versor of the direction along the spin is measured, $\vec{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$,

$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $\sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ the Pauli matrices).

Thus the EPR (Einstein-Podolski-Rosen) paradox (Bohm's variant) regarding the non-violation of Heisenberg's principle in quantum mechanics is resolved.
(the paradox arises in the way that since Alice measures her particle's polarization in the (0,1) basis, Bob would automatically know his particle's polarization in the (0,1) basis, because of the entanglement and could also measure the polarization of his particle in a different basis thus knowing the polarizations in the two different bases simultaneously with certainity. In fact, Alice's measurement action affects the whole combined system of entangled particles altering Bob's result.)

For a quantum ensemble we have the system described by a density operator
$\rho=\sum_i p_i|\psi_i\rangle\langle\psi_i|$, $p_i\in[0,1]$, $\sum_i p_i=1$ (see Chap. Quantum statistical ensemble)
A bipartite composite system has density matrices, representing states of a quantum ensemble, having the general form
$\rho=\sum_i p_i(\sum_j c^*_{ij}(|\alpha_{ij}\rangle_A\otimes|\beta_{ij}\rangle_B))(\sum_k c_{ik\ A}\langle\alpha_{ik}|\otimes_B\langle\beta_{ik}|)$ with $p_i\in[0,1]$, $\sum_i p_i=1$,
$\sum_j|c_j|^2=1$, c^*_{ij} the complex conjugate of c_{ij}
A mixed state ρ (a trace class and positive semi-definite operator on) $H_A\otimes H_B$ is valled separable if it can be written as $\rho=\sum_i w_i\rho_i^A\otimes\rho_i^B$ with ρ_i^A , ρ_i^B density operators on H_A rspective H_B .
By writing the density matrices ρ_i^A,ρ_i^B as sums of pure ensembles,
(of the form $\rho=|\psi\rangle\langle\psi|$) we may assume without loss of generality that ρ_i^A,ρ_i^B are themselves pure ensembles.
A mixed state which is not separble is called an entangled state.

For a pure state $|\psi\rangle$ on $H_A\otimes H_B$ we have :

$$\rho=|\psi\rangle\langle\psi|=c_{ij}c_{kl}^{*}|i\rangle_{A\,A}\langle k|\otimes|j\rangle_{B\,B}\langle l| \text{ with } \sum_{i,j}|c_{ij}|^2=1 \quad \text{and}$$

$\rho_A=\mathrm{tr}_B\rho=c_{is}c_{ks}^{*}|i\rangle_{A\,A}\langle k|$, $\rho_B=\mathrm{tr}_A\rho=c_{sj}c_{sl}^{*}|j\rangle_{B\,B}\langle l|$ where we used Einstein summation convention for the *s* index.

It follows $\mathrm{tr}\,\rho_A=\mathrm{tr}\,\rho_B$ and that ρ_A,ρ_B are positive semi-definite since they are of the form CC^{+} and respective $C^{+}C$ where $C=(c_{ij})_{ij}$ and so ρ_A,ρ_B are the partial density matrices for subsystems A respective B .

If ρ is a pure separable state we will have:

$\rho=|\psi\rangle\langle\psi|$ with $|\psi\rangle=c_i^A c_j^B|i\rangle_A\otimes|j\rangle_B$, $\sum_i|c_i^A|^2=\sum_j|c_j^B|^2=1$

$$\rho=c_i^A c_k^{A*}c_j^B c_l^{B*}|i\rangle_{A\,A}\langle k|\otimes|j\rangle_{B\,B}\langle l| \quad , \quad \rho_A=c_i^A c_k^{A*}|i\rangle_{A\,A}\langle k|$$

We can take an unitary operator U on H_A such that $UU^{+}=\boldsymbol{I}_{H_A}$, $U|i\rangle_A=U_{ij}|j\rangle_A$, $U_{ij}c_i^A=\delta_{1j}$ and so $U\rho_A U^{+}=|1\rangle_{A\,A}\langle 1|$ and for the von Neumann entropy follows $S(\rho_A)=S(U\rho_A U^{+})=-\mathrm{tr}(\rho_A\log\rho_A)=0$. In the same way we obtain $S(\rho_B)=0$.

The von Neumann entropy can be taken as a entanglement measure for pure bipartite states.

A pure bipartite state $\rho=|\psi\rangle\langle\psi|$ on $H_A\otimes H_B$ for $\dim H_A=\dim H_B=n$ will be maximal entangled if the reduced states of each subsystem, ρ_A , ρ_B are $\rho_A=\frac{1}{n}\boldsymbol{I}_{H_A}$ respective $\rho_B=\frac{1}{n}\boldsymbol{I}_{H_B}$ (because as we know the Shannon entropy achieves its maximum at and only at the uniform probability distribution).

For $\dim H_A=\dim H_B=2$ the functions

$$|\varphi^{\pm}\rangle=\frac{1}{\sqrt{2}}(|0\rangle_A\otimes|0\rangle_B\pm|1\rangle_A\otimes|1\rangle_B) \quad ,$$

$$|\psi^{\pm}\rangle=\frac{1}{\sqrt{2}}(|0\rangle_A\otimes|1\rangle_B\pm|1\rangle_A\otimes|0\rangle_B)$$

define four maximal entangled pure states called the Bell states and they form a complete orthonormal system in $H_A\otimes H_B$.

For ρ a general density matrix on $H_A\otimes H_B$ we have

$\rho=\sum_{i,j,k,l}p_{kl}^{ij}|i\rangle_{A\,A}\langle j|\otimes|k\rangle_{B\,B}\langle l|$ and we define the partial transpose

$$\rho^{TB}=(\boldsymbol{I}\otimes T)(\rho)=\sum_{i,j,k,l}p_{lk}^{ij}|i\rangle_{A\,A}\langle j|\otimes|k\rangle_{B\,B}\langle l| \quad \text{where}$$

$$T(\sum_{k,l}c_{kl}|k\rangle\langle l|)=\sum_{k,l}c_{lk}|k\rangle\langle l| \quad .$$

If ρ is separable we have

$\rho=\sum_i p_i\rho_i^A\otimes\rho_i^B$ with ρ_i^A,ρ_i^B density matrices on H_A respective H_B , $\sum_i p_i=1$,

$$p_i\in[0,1] \quad \text{following} \quad \rho^{TB}=\sum_i p_i\rho_i^A\otimes(\rho_i^B)^T$$

As the transposition preserves eigenvalues, the spectrum of $(\rho_i^B)^{\mathrm{T}}$ is the same as the spectrum of ρ_i^B and in paticular $(\rho_i^B)^{\mathrm{T}}$ must still be positive semi-definite. Thus ρ^{TB} must be positive semi-definite and the fact that the partial transpose ρ^{TB} is positive semi-definite is a necesar condition for ρ to be separable.
Therefore if the partial transpose of a density matrix has a negative eigenvalue, then that density matrix is an entangled state. (Peres-Horodecki or PPT positive partial transpose criterion)
The Peres-Horodecki criterion is a necesar and sufficient condition for entanglement if and only if the product space $H_A \otimes H_B$ has the dimension 2×2 or 2×3 .
The result is independent of the part that was transposed since $\rho^{TA} = (\rho^{TB})^{\mathrm{T}}$.

Quantum information processing is the study of information processing tasks that can be accomplished (only) using quantum mechanical systems. What we refer to, are tasks that can be possible only if the laws of quantum mechanics apply to the system used for processing the information or that are accomplished in a more efficient way if performed by a quantum system (in terms of time or material resources).
The power of quantum computation seems to come from two main ingredients: quantum superposition (in the form of parallelism that allows to compute all the possible solutions of a problem at once) and interference (that leads to algorithms that select a constructive interference for the correct solution, so that we obtain the right answer with high probability once we measure the quantum system and collapse the superposition state).
In the same way as classical computers are physical systems, circuits made of wires and gates, a quantum computer is also composed of wires and gates. The wires are used to carry information arround, while the gates perform operations, manipulate the information. Quantum gates however have the properties of being linear and invertible, as they represent the unitary evolution of a quantum system (a collection of two level sytems or qubits (of polarization or spin ½ states)).
We thus define a composite Hilbert space of dimension $N = 2^n$, where n is the number of qubits, as the tensor product of the Hilbert spaces for each qubit :
$H=\bigotimes_{i=1}^{n} H_i$ with H_i the Hilbert space for each qubit, having elements of the form $\alpha|0\rangle+\beta|1\rangle$ with $\alpha,\beta\in\mathbb{C}$, $(|0\rangle,|1\rangle)$ an orthonormal basis of H_i . A normalized qubit has $|\alpha|^2+|\beta|^2=1$. The operators space is the product operators space (also called Pauli operators space). The elements of a basis of this product operators space are defined as $P_l=\bigotimes_{j=1}^{n} P_l^{(j)}$ where each $P_l^{(j)}$ is either a Pauli matrix $\{\sigma_x,\sigma_y,\sigma_z\}$ or the identity $\boldsymbol{I}$ operator on the H_j space of the qubit j .
We notice that $P_l=P_l^{+}$ and $\mathrm{tr}(P_l P_{l'})=N\,\delta_{ll'}$ so the basis is orthogonal but not normalized.
A basis for a two-qubit system is given by the four states
$|00\rangle=|0\rangle_A\otimes|0\rangle_B$, $|01\rangle=|0\rangle_A\otimes|1\rangle$, $|10\rangle=|1\rangle_A\otimes|0\rangle_B$, $|11\rangle=|1\rangle_A\otimes|1\rangle_B$.

The action of a Pauli matrix on the vectors of its own Hilbert space is as usual (e.g. $\sigma_x^A|0\rangle_A=|1\rangle_A$, $\sigma_x^A|1\rangle_A=|0\rangle_A$ with $|0\rangle=\begin{pmatrix}1\\0\end{pmatrix}$, $|1\rangle=\begin{pmatrix}0\\1\end{pmatrix}$).
But operators of the *A* Hilbert space do not act on the vectors of the other Hilbert space so we make a contextual identification in notations (e.g. $\sigma_x^A\otimes \boldsymbol{I}_B=\sigma_x^A$).
There are several operators which are normally used in quantum computation and that describe the possible evolution of the system:
$\text{Not}^A=\sigma_x^A\otimes \boldsymbol{I}_B$, $\text{Not}^B=\boldsymbol{I}_A\otimes\sigma_x^B$,
Hadamard gate $H=(\sigma_x+\sigma_z)\frac{1}{\sqrt{2}}$,
Controlled not gate : rotate B conditionally on the state in the space A as
$C^A\text{NOT}^B=E_A^+\otimes \boldsymbol{I}_B+E_A^-\otimes\sigma_x^B$ where $E^+=|0\rangle\langle 0|$, $E^-=|1\rangle\langle 1|$.
At the end of a circuit, the qubits are measured. Usually it is implicit that the qubits are measured in their computational basis $(|0\rangle,|1\rangle)$.
$|0\rangle,|1\rangle$ are the eigenvectors of σ_z . The eigenvectors of σ_x form an equivalent basis denoted $(|+\rangle,|-\rangle)$ with $|+\rangle=\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$, $|-\rangle=\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)$
The operator that performs the change of frame is therefore the Hadamard matrix:
For $|\psi\rangle_z=a|0\rangle+b|1\rangle$, $|\psi\rangle_x=a|+\rangle+b|-\rangle$ we have $|\psi\rangle_x=H|\psi\rangle_z$.
We can also just have general single qubit gates *U* that describe any general rotation on a single qubit.
If we combine this single qubit rotations with the C NOT gates on any pair of qubits we are able to build any possible algorithm (or computation) on the system. That also means that we are able to enforce any possible evolution of the system, by letting it evolve under these two types of gates.

The so called No-cloning theorem states that “It is impossible to make a perfect copy of an unknown, pure state by an unitary operation”. Suppose we want to copy an arbitrary state $|\psi\rangle=a|0\rangle+b|1\rangle$ on the blank initial state $|i\rangle$. Therefore we have an unitary operator *U* defined on the tensor product space such that for any state which is to copy we have $U|\psi,i\rangle=|\psi,\psi\rangle$ where we use notation $|\psi,\varphi\rangle=|\psi\rangle\otimes|\varphi\rangle$ for any states $|\psi\rangle,|\varphi\rangle$.
If we assume to be able to copy any arbitrary state, we can assume that we can copy at least another state $|\varphi\rangle$ which is not the state $|\psi\rangle$ and is not orthogonal to it.
For this second state we have also :
$U|\varphi,i\rangle=|\varphi,\varphi\rangle$, $U^+U=\boldsymbol{I}$ and so $\langle\varphi|\psi\rangle=\langle\varphi,i|U^+U|\psi,i\rangle=\langle\varphi,\varphi|\psi,\psi\rangle=\langle\varphi|\psi\rangle^2$.
This equation is satisfied only if $\langle\varphi|\psi\rangle=1$ or $\langle\varphi|\psi\rangle=0$. In the first case , the two states are in effect the same state (up to a normalization factor or a global phase which are not important). In the second case the two states are orthogonal, in contradiction with the hypothesis.

A unitary operator cannot copy an arbitrary state . If we find an operator that clone one state, it can only copy that state and states which are orthogonal to it, but it cannot clone all other states. In a Hilbert space it is therefore possible to define an operator that clone the basis states, but not an arbitrary superposition of them.
The No-communication theorem (see Chap. Decoherence … No-communication theorem) implies the No-cloning theorem. That is , cloning is a sufficient condition for the communication of classical information to occur. To see this, suppose that quantum states could be cloned. Assume parts of a maximally entangled Bell state of a 2-qubit system are distributed to Alice and Bob. Alice could send bits to Bob in the following way:
If Alice wishes to transmit “0” , she measures the spin of her electron in the z-direction, collapsing Bob’s state to either $|z+\rangle_B$ or $|z-\rangle_B$ (the eigenstates of σ_z^B). To transmit “1” , Alice does noting to the qubit. Bob creates many copies of his electron’s state and measures the spin of each copy in the z-direction. Bob will know that Alice has transmitted a “0” if all his measurements wil produce the same result; otherwise his measurements will have outcomes $|z+\rangle_B$ or $|z-\rangle_B$ with equal probability. This would allow Alice and Bob to communicate classical bits each other (possibly across space-like separations violating causality).

We can transform the $(|00\rangle,|01\rangle,|10\rangle,|11\rangle)$ basis of the two-qubit system in the Bell states basis applying a Hadamard gate and a $C^A\mathrm{NOT}^B$ gate as follows :

$$|00\rangle \overset{H_A}{\rightarrow} \frac{1}{\sqrt{2}}(|10\rangle+|00\rangle) \overset{C^A\mathrm{NOT}^B}{\rightarrow} |\varphi^+\rangle$$

$$|01\rangle \overset{H_A}{\rightarrow} \frac{1}{\sqrt{2}}(|11\rangle+|01\rangle) \overset{C^A\mathrm{NOT}^B}{\rightarrow} |\psi^+\rangle$$

$$|10\rangle \overset{H_A}{\rightarrow} \frac{1}{\sqrt{2}}(|00\rangle-|10\rangle) \overset{C^A\mathrm{NOT}^B}{\rightarrow} |\varphi^-\rangle$$

$$|11\rangle \overset{H_A}{\rightarrow} \frac{1}{\sqrt{2}}(|01\rangle-|11\rangle) \overset{C^A\mathrm{NOT}^B}{\rightarrow} |\psi^-\rangle$$

Measuring $C^A\mathrm{NOT}^B$ in the incoming $(|00\rangle,|01\rangle,|10\rangle,|11\rangle)$ basis is called a Bell measurement.
Notice that for $a,b=0,1$ we have $C^A\mathrm{NOT}^B|a\,b\rangle=|a\,a\oplus b\rangle$ where $\oplus$ means addition modulo 2 .

EPR Quantum key distribution

The problem in question is that Alice needs to send a highly private message to Bob such that Eve is unable to gain any information when she tries to listen in.
If Alice and Bob share a private key (a string of random bits known only to them), then Alice can convert her message to ASCII (a string of bits no longer than the key) add (modulo 2) each bit of her message to the corresponding bit of the key and send the result to Bob . Receiving this string, Bob adds the key to it, to extract Alice's message.
Alice and Bob need to establish therefore a shared random key and they must ensure that Eve can't know the key, and they can do that exploiting quantum information (and specifically entanglement).
Let's suppose that Alice and Bob share a supply of entangled pairs prepared in the state $|\psi^-\rangle$. For each qubit in her/his possession, Alice and Bob decide to measure either σ_1 or σ_3. The decision is pseudo-random, each choice occuring with probability ½ . Then , after the measurements are performed both Alice and Bob publicly announce what observables they measured but do not reveal the outcomes they obtained. For those cases, about half in which they measured their qubits along different axes , their results are discarded (as Alice and Bob obtained uncorrelated outcomes). For those cases in which they measured along the same axis, their results, though random, are perfectly (anti-)correlated. Hence they established a shared random key.
However, Eve might have clandestinely tampered with the pairs at some time in the past, to find out the key. Then the pairs that Alice and Bob possess might be (unbeknownst to Alice and Bob) not perfect $|\psi^-\rangle$ but rather pairs that are entangled with qubits in Eve's possession. Eve can then wait until Alice and Bob make their public announcements and proceed to measure her qubits in a manner designed to acquire maximal information about the results that Alice and Bob obtained.
If Eve has indeed tampered with Alice's and Bob's pairs, then the most general possible state for an *AB* pair and a set of *E* qubits has the form :
$|\gamma\rangle_{ABE}=|00\rangle_{AB}|e_{00}\rangle_E+|01\rangle_{AB}|e_{01}\rangle_E+|10\rangle_{AB}|e_{10}\rangle_E+|11\rangle_{AB}|e_{11}\rangle_E$.
The defining property of $|\psi^-\rangle$ is that it is an eigenstate with eigenvalue -1 of both $\sigma_1^A\sigma_1^B$ and $\sigma_3^A\sigma_3^B$.
Suppose that *A* and *B* are able to verify that the pairs in their possession have this property.
To satisfy $\sigma_3^A\sigma_3^B=-1$ we must have $|\gamma\rangle_{ABE}=|01\rangle_{AB}|e_{01}\rangle_E+|10\rangle_{AB}|e_{10}\rangle_E$
and to satisfy $\sigma_1^A\sigma_1^B=-1$ we must have $|\gamma\rangle_{ABE}=\frac{1}{\sqrt{2}}(|01\rangle_{AB}-|10\rangle_{AB})|e\rangle_E=|\psi^-\rangle|e\rangle$.
We see that it is possible for the *A B* pairs to be eigenstates with eigenvalue -1 of $\sigma_1^A\sigma_1^B$ and $\sigma_3^A\sigma_3^B$ only if they are completely unentangled with Eve's qubits.
Therefore, Eve will not be able to learn anything about Alice's and Bob's measurement results by measuring her qubits. The random key is secure.

To verify the properties $\sigma_1^A \sigma_1^B = -1 = \sigma_3^A \sigma_3^B$, Alice and Bob can sacrifice a portion of their shared key and publicly compare their measurement outcomes. They should find that their results are indeed perfectly correlated. If so, they will have high statistical confidence that Eve is unable to intercept the key. If not, they have detected Eve's nefarious activity, may then discard the key and make a fresh attempt to establish a secure key.
Another variation of this key distribution scheme is "the time-reversed EPR" scheme. Here both Alice and Bob prepare one of the four states $|z+\rangle, |z-\rangle, |x+\rangle, |x-\rangle$ and they both send their qubits to Charlie. Then Charlie performs a Bell measurement on the pair projecting out one of $|\varphi^{\pm}\rangle, |\psi^{\pm}\rangle$ and he publicly announces the result. Since all four of these states are simultaneous eigenstates of $\sigma_1^A \sigma_1^B$ and $\sigma_3^A \sigma_3^B$, when Alice and Bob both prepared their spins along the same axis (as they do about half the time), they share a single bit.
Of course, Charlie could be allied with Eve, but Alice and Bob can verify that Charlie has acquired no information as before, by comparing a portion of their key.
This scheme has the advantage that Charlie could operate a central switching station by storing qubits received from many parties, and then perform his Bell measurement when two of the parties request a secure communication link. A secure key can be established even if the quantum communication line is down temporarily, as long as both parties had the foresight to send their qubits to Charlie on an earlier occasion (when the quantum channel was open).

Dense coding

Alice and Bob are linked to a quantum channel and Alice wants to send messages to Bob.
She might send classical bits , preparing a qubit in one of the states $|0\rangle = |z+\rangle$, $|1\rangle = |z-\rangle$ (spin states in direction z of an electron for example), send the qubit to Bob who can measure the qubit along the *z* direction for spin to infer the choice Alice made.
But we can suppose that Alice and Bob share an entangled pair of qubits in the state $|\varphi^+\rangle_{AB}$, one qubit was shipped to Alice and the other to Bob, anticipating the later use of entanglement. Now Alice can use the entanglement as a resource to send Bob two classical bits of information in the following way.
Alice can perform on her member of the entangled pair one of four possible unitary transformations:
1) $\boldsymbol{I}$ (she does nothing)
2) σ_1
3) σ_2
4) σ_3
By doing so, she transforms $|\varphi_{AB}^+\rangle$ to one of four mutually orthogonal states:

1) $|\varphi^+\rangle_{AB}$
2) $|\psi^+\rangle_{AB}$
3) $|\psi^-\rangle_{AB}$
4) $|\varphi^-\rangle_{AB}$

Now she sends her qubit to Bob who receives it and then performs an orthogonal collective measurement on the pair that projects onto the maximally entangled basis. The measurement outcome unambiguosly distinguishes the four possible actions that Alice could have performed. Therefore the single qubit sent from Alice to Bob carried 2 bits of classical information. Hence this procedure is called “dense coding”.
If the message is highly confidential Alice need not worry that her message might be intercepted and deciphered. The transmitted qubit has density matrix $\rho_A=\frac{1}{2}\boldsymbol{I}_{\boldsymbol{A}}$ and so carries no information at all. All the information is in the correlation between qubits *A* and *B* and this information is inaccessible unless the adversary is able to obtain both members of the entangled pair . (Of course, the adversary can jam the channel, preventing the information but reaching Bob).Alice and Bob really did need to use the channel twice to exchange two bits of information – a qubit had to be transmitted for them to establish their entangled pair in the first place. But the first transmission could have taken place a long time ago. The point is that when an emergency arose and two bits had to sent immediately while only use of the channel was possible, Alice and Bob could exploit the pre-existing entanglement to communicate efficiently.

Quantum teleportation

The teleportation consists in Alice sending an unknown qubit $|\psi\rangle_C$ she has, to Bob that shares an entangled pair in state $|\varphi^+\rangle_{AB}$ with Alice, using entanglement as a resource and transmitting information only through a classical channel.
First Alice unites the unknown qubit she wants to send to Bob, $|\psi\rangle_C=a|0\rangle_C+b|1\rangle_C$ with her member of $|\varphi^+\rangle_{AB}$. On these two qubits she performs a Bell measurement, projecting onto one of the four states $|\varphi^\pm\rangle_{CA},|\psi^\pm\rangle_{CA}$.
After some calculus we obtain:

$$|\psi\rangle_C|\varphi^+\rangle_{AB}=\frac{1}{2}|\varphi^+\rangle_{CA}|\psi\rangle_B+\frac{1}{2}|\psi^+\rangle_{CA}\sigma_1|\psi\rangle_B-\frac{i}{2}|\psi^-\rangle_{CA}\sigma_2|\psi\rangle_B+\frac{1}{2}|\varphi^-\rangle_{CA}\sigma_3|\psi\rangle_B$$

Alice sends then her measurement outcome (two bits of classical information) through the classical channel to Bob who receiving this information performs in dependence on it one of four operations on his qubit:

$|\varphi^+\rangle_{CA}\rightarrow \boldsymbol{I}_{\boldsymbol{B}}$
$|\psi^+\rangle_{CA}\rightarrow \sigma_1^B$
$|\psi^-\rangle_{CA}\rightarrow \sigma_2^B$
$|\varphi^-\rangle_{CA}\rightarrow \sigma_3^B$

Considering the above calculus result, this action transforms his qubit into a perfect copy of $|\psi\rangle_C$: $|\psi\rangle_B = a|0\rangle_B + b|1\rangle_B$.

As we exposed above, performing measurements on an entangled pair of particles the outcomes show a correlation between the two particles and the particles must be considered as parts of one sytstem, even the particles are space-like separated by a great distance. However, according to special relativity, information cannot travel faster than light so we must assume that a measurement performed on one of the particles affects the whole system of two particles since the creation of the entanglement relation when the particles shared spatial proximity.

As we noticed in discussion of the EPR paradox , entanglement not violates Heisenberg's uncertainity principle of quantum mechanics.
Also we will show that if the rules of quantum mechanics apply and there is no (faster than light) action at distance (locality assumption), then we must assume that the correlation between measurements on entangled particles cannot be determined by hidden variables (which hidden determination would be resulting from the incompletness of the theory) that set the evolution of the measured properties once for all at the beginning of entanglement relation (realism assumption). Therefore quantum mechanics entanglement is incompatible with local realism.

Let us suppose we are capable of making a state $|\psi^-\rangle_{AB} = \frac{1}{\sqrt{2}}(|01\rangle_{AB} - |10\rangle_{AB})$ of two identical spin $1/2$ particles with H_A Hilbert space for Alice's particle, H_B Hilbert space for Bob's particle, $H_A \otimes H_B$ Hilbert space for the whole two-particles system, $\dim H_A = \dim H_B = 2$
Then for $\vec{n} = (n_1, n_2, n_3)$, $\vec{n}^2 = 1$ the operators $\vec{n}\cdot\vec{\sigma}^A = n_j \sigma_j^A$, $\vec{n}\cdot\vec{\sigma}^B = n_j \sigma_j^B$ measure the spin orientation ± 1 along the $\vec{n}$ direction for Alice's respective Bob's particle of the entangled system. (where $\sigma_j^A = \sigma_j \otimes \boldsymbol{I_B}$, $\sigma_j^B = \boldsymbol{I_A} \otimes \sigma_j$)
We expect that if Bob or Alice measures the spin of his/her particle along a direction, that affects the whole system of two particles and so if Alice measures the spin of her particle along a direction *n* after Bob measured his particle's spin along a direction *m*, the results will be correlated.
As we know from statistics, if *X* and *Y* are independent random variables, for the expectation values $\langle X\rangle, \langle Y\rangle, \langle XY\rangle$ we will have $\langle X\rangle\langle Y\rangle - \langle XY\rangle = 0$.
Therefore considering correlations between measuring *B* spin along *m* and measuring *A* spin along *n* we need to evaluate the expectation value
$\langle(\vec{n}\cdot\vec{\sigma}^A)(\vec{m}\cdot\vec{\sigma}^B)\rangle = \langle\psi^-|(\vec{n}\cdot\vec{\sigma}^A)(\vec{m}\cdot\vec{\sigma}^B)|\psi^-\rangle$.
We can verify that $(\vec{\sigma}^A + \vec{\sigma}^B)|\psi^-\rangle = 0$ and therefore we have:

$$\langle(\vec{n}\cdot\vec{\sigma}^A)(\vec{m}\cdot\vec{\sigma}^B)\rangle=-\langle(\vec{n}\cdot\vec{\sigma}^A)(\vec{m}\cdot\vec{\sigma}^A)\rangle=-n_i m_j \mathrm{tr}(\sigma_j^A|\psi^-\rangle\langle\psi^-|\sigma_i^A)=$$
$$=-n_i m_j \mathrm{tr}(\mathrm{tr}_B(\sigma_j^A|\psi^-|\langle\psi^-|\sigma_i^A))=-n_i m_j\frac{1}{2}\mathrm{tr}(\sigma_j|0\rangle_{A\,A}\langle 0|\sigma_i+\sigma_j|1\rangle_{A\,A}\langle 1|\sigma_i)=$$
$$=-\vec{n}\cdot\vec{m}=-\cos\theta \text{ where } \theta \text{ is the angle between } n \text{ and } m \text{ directions.}$$

Consider now two directions *a* , *a'* along Alice can measure the spin of her particle. Consider also two directions *b* , *b'* along Bob can measure the spin of his particle. The locality implies that Bob measuring along *b* or *b'* not affects the result of Alice measuring along *a* or *a'*.

Let $\sigma_a^A, \sigma_{a'}^A$ the possible outcomes of Alice's measurement in spin measuring experiments along directions a respective a' and $\sigma_b^B, \sigma_{b'}^B$ the possible outcomes outcomes of Bob's measurement in spin measuring experiments along directions b respective b'.

$\sigma_b^B, \sigma_{b'}^B, \sigma_a^A, \sigma_{a'}^A$ are measured at each k-th experiment and are values of random variables $\sigma_b^B, \sigma_{b'}^B, \sigma_a^A, \sigma_{a'}^A$.

Realism implies that we have $\sigma_{bk}^B, \sigma_{b'k}^B, \sigma_{ak}^A, \sigma_{a'k}^A \in\{-1,1\}$ well defined random values at each k-th experiment and so the expectation value $\langle S\rangle=\langle\sigma_a^A\sigma_b^B\rangle+\langle\sigma_{a'}^A\sigma_{b'}^B\rangle+\langle\sigma_a^A\sigma_{b'}^B\rangle-\langle\sigma_{a'}^A\sigma_b^B\rangle$ according to local realism must be

$$\langle S\rangle=\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^{N}S_k \text{ where } S_k=\sigma_{ak}^A(\sigma_{bk}^B+\sigma_{b'k}^B)-\sigma_{a'k}^A(\sigma_{bk}^B-\sigma_{b'k}^B)$$

We have that $\sigma_{bk}^B+\sigma_{b'k}^B, \sigma_{bk}^B-\sigma_{b'k}^B\in\{2,-2,0\}$ and

$\sigma_{bk}^B+\sigma_{b'k}^B=\pm 2$ if and only if $\sigma_{bk}^B-\sigma_{b'k}^B=0$.

Therefore we can derive $S_k\in\{\pm 2\}$ for any $k\in\mathbb{N}^*$ and so $-2\le\langle S\rangle\le 2$ (*) if local realism applies.

But as we proved, in assumption of quantum mechanics rules we must have

$$\langle S\rangle=\langle(\vec{a}\cdot\vec{\sigma}^A)(\vec{b}\cdot\vec{\sigma}^B)\rangle+\langle(\vec{a}'\cdot\vec{\sigma}^A)(\vec{b}'\cdot\vec{\sigma}^B)\rangle+\langle(\vec{a}\cdot\vec{\sigma}^A)(\vec{b}'\cdot\vec{\sigma}^B)\rangle-\langle(\vec{a}'\cdot\vec{\sigma}^A)(\vec{b}\cdot\vec{\sigma}^B)\rangle=$$
$$=-(\vec{a}\cdot\vec{b}+\vec{a}'\cdot\vec{b}'+\vec{a}\cdot\vec{b}'-\vec{a}'\cdot\vec{b}) \ .$$

Taking $\vec{a}=(0,0,1), \vec{a}'=(1,0,0), \vec{b}=\frac{1}{\sqrt{2}}(-1,0,1), \vec{b}'=\frac{1}{\sqrt{2}}(1,0,1)$ we obtain $\langle S\rangle=-2\sqrt{2}<2$ which is in contradiction with (*).

If we take $\vec{a}=(0,0,-1), \vec{a}'=(-1,0,0)$ and leave $\vec{b}, \vec{b}'$ the same as above we obtain $\langle S\rangle=2\sqrt{2}>2$.

Hence local realism is violated by quantum mechanical entanglement. No hidden variables theory completion is possible, confirming so the non-classical interpretation of quantum mechanics.

We can test the violation of local realism also considering other quantitative properties of the correlations between measurement outcomes obtained by Bob and Alice that violate properly chosen Bell inequalities.

We can verify that the projection operator onto the spin up (+) / spin down (-) along direction *n* states is :

$E(\vec{n},\pm)=\frac{1}{2}(\boldsymbol{I}\pm\vec{n}\cdot\vec{\sigma})$.

If $\vec{n}\cdot\vec{m}=\cos\theta$ we have:

$\langle\psi^-|E^A(\vec{n},-)E^B(\vec{m},-)|\psi^-\rangle=\langle\psi^-|E^A(\vec{n},+)E^B(\vec{m},+)|\psi^-\rangle=\frac{1}{4}(1-\cos\theta)$

$\langle\psi^-|E^A(\vec{n},+)E^B(\vec{m},-)|\psi^-\rangle=\langle\psi^-|E^A(\vec{n},-)E^B(\vec{m},+)|\psi^-\rangle=\frac{1}{4}(1+\cos\theta)$.

Thus when Alice measures spin along *n* and Bob measure spin along *m* the probability that the outcomes are the same is $\frac{1}{2}(1-\cos\theta)$ and the probability that the outcomes are opposite is $\frac{1}{2}(1+\cos\theta)$.

Now sppose Alice will measure her spin along one of three axes in the *x*-*z* plane

$\vec{m}=(0,0,1),\vec{n}=(\frac{\sqrt{3}}{2},0,-\frac{1}{2}),\vec{p}=(-\frac{\sqrt{3}}{2},0,-\frac{1}{2}).$

If Bob measures along $-\vec{n}$ and sends the result to Alice, then Alice knows what would have happened if she had measured along $\vec{n}$, the results being perfectly correlated if we assume that Alice shares with Bob the state $|\psi^-\rangle$. Now Alice can go ahead and measure along $\vec{m}$. The probability that the outcomes are the same according to quantum mechanics is $\frac{1}{2}(1+\vec{m}\cdot\vec{n})$ (Bob measures along $-\vec{n}$ to obtain Alice's result for measuring along $\vec{n}$) In the same way Alice and Bob can work together to determine outcomes for the measurement of Alice's spin along any of two of the axes $\vec{m},\vec{n},\vec{p}$.

Supposing that there are actually local hidden variables that provide a complete description of the system and the quantum correlations arise from a probability distribution governing the hidden variables, then we have a Bell inequality statement true: $P_{same}(m,n)+P_{same}(n,p)+P_{same}(p,m)\geq 1$ where $P_{same}(a,b)$ denotes the probability that the outcomes for directions $\vec{a}$ and $\vec{b}$ are the same.

But in quantum mechanics we derive

$P_{same}(m,n)+P_{same}(n,p)+P_{same}(p,m)=\frac{1}{2}(1+\vec{m}\cdot\vec{n})+\frac{1}{2}(1+\vec{n}\cdot\vec{p})+\frac{1}{2}(1+\vec{p}\cdot\vec{m})=\frac{3}{4}<1$,

violating the Bell inequality.

Thus we have some kind of local game played by Alice and Bob:

1. Alice and Bob share an entangled state $|\psi^-\rangle$.
2. For each pair of directions $(a,b)\in\{(m,n),(n,p),(p,m)\}=M$ Bob measures the spin of his particle along $-\vec{b}$ and Alice measures the spin of her particle along $\vec{a}$ and they compare results.
3. Alice and Bob win the game if they obtain the same outcome for at least one of the pairs chosen in doing 2.

Hidden variable theory implies that Alice and Bob must win anytime but quantum mechanics rules allow directions *m,n,p* for which the winning probability is less than ¾ .

For photons travelling in *z*-direction the linear polarization states for θ oriented frame $|x(\theta)\rangle=\begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}$, $|y(\theta)\rangle=\begin{pmatrix}-\sin\theta\\ \cos\theta\end{pmatrix}$ and they are the eigenstates with eigenvalues

$+1$ respective -1 of the operator

$\tau(\theta)=|x(\theta)\rangle\langle x(\theta)|-|y(\theta)\rangle\langle y(\theta)|$ which is similar to $\vec{n}\cdot\vec{\sigma}$ for spin $\frac{1}{2}$ states along direction $\vec{n}$.

Suppose Alice and Bob share a Bell state $|\psi^-\rangle=\frac{1}{\sqrt{2}}(|01\rangle_{AB}-|10\rangle_{AB})$

with $|0\rangle=|x(0)\rangle$, $|1\rangle=|y(0)\rangle$.

Obviously we have $\rho_A=\frac{1}{2}|0\rangle_{A\,A}\langle 0|+\frac{1}{2}|1\rangle_{A\,A}\langle 1|$, $\rho_B=\frac{1}{2}|0\rangle_{B\,B}\langle 0|+\frac{1}{2}|1\rangle_{B\,B}\langle 1|$ and so both of the entangled photon beams carry unpolarized light.

Alice chooses randomly j =1,2,3 a polarization filter which allows complete passing of the $x(\theta_j)$ polarization direction states and deflects the $y(\theta_j)$ polarization direction states of her beam part of the entangled photons system.

Bob does the same with his beam part of the entangled photons system.

Measuring the intensity of the filtered beam versus the incoming beam, Alice and Bob can determine the $W(a_i, b_j)$ probability that Alice's photons get through the filter with θ_i orientation and not get through the filter with θ_j orientation (since the polarizations of the entangled photons are anti-correlated).

Hence according to quantum mechanics rules we have

$$W(a_i,b_j)=\langle\psi^-|(x(\theta_i)\otimes x(\theta_j))\rangle^2 \quad .$$

After some calculus we obtain

$|\psi^-\rangle=\frac{1}{\sqrt{2}}\sin(\theta_j-\theta_i)(|x(\theta_i)\rangle_A|x(\theta_j)\rangle_B+|y(\theta_i)\rangle_A|y(\theta_j)\rangle_B)+$

$+\frac{1}{\sqrt{2}}\cos(\theta_j-\theta_i)(|x(\theta_i)\rangle_A|y(\theta_j)\rangle_B-|y(\theta_i)\rangle_A|x(\theta_j)\rangle_B)$ and so in quantum mechanics

$$W(a_i,b_j)=\frac{1}{2}\sin^2(\theta_i-\theta_j)$$

Assuming local realism, the property that a photon passes or not through the filter must be well established(by hidden variables as we assume) and the filterings which are space-like separated satisfy locality being independent each of other.

Taking with this assumptions M_j the set of Alice's photons that pass through the j=1,2,3 polarization filter , since for any sets M_1, M_2, M_3 we have $(M_1\setminus M_2)\cup(M_2\setminus M_3)\supset M_1\setminus M_3$ we derive that local realism provides the Bell

inequality $W(a_1,b_2)+W(a_2,b_3)-W(a_1,b_3)\geq 0$ (**)
Taking $\theta_1=0$, $\theta_2=\theta$, $\theta_3=2\theta$ the relation (**) is equivalent to
$1\geq 2\cos^2\theta$ which is violated for $\theta\in\left(0,\frac{\pi}{4}\right)$ leading to the same conclusion as above,
that local realism is violated by quantum mechanics entanglement.

For a bipartite quantum system having Hilbert space $H_A\otimes H_B$ with H_A, H_B the subsystem *A* respective *B* corresponding Hilbert spaces , we can consider sets of measurement settings S_A , S_B , sets of measurement outcomes K_A , K_B and corresponding observables in two distinct models of entanglement:
i) $A_a^x: H_A\rightarrow H_A$, $B_b^y: H_B\rightarrow H_B$, $(a,b)\in S_A\times S_B$, $(x,y)\in K_A\times K_B$
tensor product model of entanglement
(A_a^x, B_b^y belong usually to the set of observables (liniar continuous compact self-adjoint operators for example) which have spectrum x respective y)
ii) $A_a^x, B_b^y: H\rightarrow H$, $H=H_A\otimes H_B$, $(a,b)\in S_A\times S_B$, $(x,y)\in K_A\times K_B$ such that $[A_a^x, B_b^y]=0$ for any $A_a^x\in M_A$, $B_b^y\in M_B$ and any $(a,b,x,y)\in S_A\times S_B\times K_A\times K_B$
commuting operators model of entanglement

Then entanglement in a state $\psi\in H_A\otimes H_B$ can be described through correlations between observables $A_a^x\in M_A$ and oservables $B_b^y\in M_B$ (involving expectation values $\langle\psi|A_a^x\otimes B_b^y|\psi\rangle$ in the i) case of tensor product model and expectation values $\langle\psi|A_a^x B_b^y|\psi\rangle$ in the ii) case of commuting operators model).
We notice that, since $[A_a^x\otimes \boldsymbol{I_B}, \boldsymbol{I_A}\otimes B_b^y]=0$ a tensor product model is a commuting operators model.
The entangled spin ½ particles system we presented above with dimH_A=dimH_B=2 $\psi=|\psi^-\rangle_{AB}$ outcomes $x=y=\{1,-1\}$ settings given by $S_A=\{a,a'\}$, $S_B=\{b,b'\}$ $M_A=M_B=M=\{C\in M_{2\times 2}(\mathbb{C})|A=A^+ , A^2=\boldsymbol{I}\}$ with a,a',b,b' considered as labels for arbitrary settings like directions along we measure spin orientation, revealed the quantum nature of its correlations in the upper bounding of the Bell expression $\langle S\rangle=\langle A_a B_b\rangle+\langle A_{a'} B_{b'}\rangle+\langle A_a B_{b'}\rangle-\langle A_{a'} B_b\rangle$.
As showed above, choosing the right directions $\vec{a},\vec{a}',\vec{b},\vec{b}'$ we obtain $\langle S\rangle=2\sqrt{2}$ while for the clasical hidden variables assumption we obtained $\langle S\rangle\in[-2,2]$.
In the quantum case , taking
$S=A_a B_b+A_{a'} B_{b'}+A_a B_{b'}-A_{a'} B_b$ (1) , from the entanglement model assumptions we have $A_a^2=A_{a'}^2=B_b^2=B_{b'}^2=\boldsymbol{I}$ and also after some calculus we obtain
$S^2=4\boldsymbol{I}+[A_a,A_{a'}][B_b,B_{b'}]$ (2) (Obviously in writing (1) we identified $A_\alpha=A_\alpha\otimes\boldsymbol{I_B}$, $B_\beta=\boldsymbol{I_A}\otimes B_\beta$ for $\alpha=a,a'$ and $\beta=b,b'$)

We have also $|||[A_a, A_{a'}]|||\leq 2||A_a||||A_{a'}||\leq 2$, $|||[B_b, B_{b'}]|||\leq 2$ and so it follows $\langle S\rangle^2\leq\langle S^2\rangle\leq 8$, $\langle S\rangle\leq 2\sqrt{2}$.
Hence the upper bound of $\langle S\rangle$ in the quantum case is $2\sqrt{2}$. In the classical case we would have $[A_a, A_{a'}]=[B_b, B_{b'}]=0$ and so from (2) we obtain the the upper bound for $\langle S\rangle$ equal to 2 .

Therefore in the general entanglement model, if are given some real values $(\mu_{abxy})_{a\in S_A, b\in S_B, x\in K_A, y\in K_B}$, we can consider general Bell expressions
$B_t=\sum_{a,b,x,y}\mu_{abxy}\langle\psi|A_a^x\otimes B_b^y|\psi\rangle$ in the tensor product model and
$B_c=\sum_{a,b,x,y}\mu_{abxy}\langle\psi|A_a^x B_b^y|\psi\rangle$ in the commuting operators model and the corresponding so called Tsirelson bounds

$$T_t=\sup_{\psi\in H_A\otimes H_B, A_a^x, B_b^y} B_t \quad \text{in the tensor product model and}$$

$$T_c=\sup_{\psi\in H_A\otimes H_B, A_a^x, B_b^y} B_c \quad \text{in the commuting operators model.}$$

Since tensor product algebras in particular commute we have $T_t\leq T_c$.
In finite dimensions, commuting algebras are always isomorphic to (direct sums of) tensor product algebras so only for for infinite dimensions it is possible $T_t\neq T_c$.
Tsirelson's problem of the question whether for all Bell expressions $T_t=T_c$, has been shown to be equivalent to Conne's embedding problem. This happens because the Conne's embedding conjecture implies that it should be possible to approximate many infinite-dimensional matrices with finite dimensional ones and the tensor product model uses finite dimensional matrices, while the commuting operators model uses a more general object that functions like a matrix with an infinite number of rows and columns.
Tsirelson's problem has been solved with a negative answer using arguments from the computational complexity theory for provers that share entangled particles.
When two provers that are entangled quantum computers propose solutions to the same problem one can verify a solution by playing a non-local game putting them questions related to the problem, cross-check the answers, and the provers win the game if their responses align most of the time to convince you that the solution is correct.
Researchers showed that by interogating two provers separately about their answers, you can quickly verify solutions to an even larger class of problems than you can when you only have one prover to interogate, since entanglement makes it possible for the provers to come up with the questions themselves (The verifier computer doesn't have to compute the questions. The verifier forces the provers to compute the questions for them). You can verify fast a much larger class of problems than you can without entanglement.

It has been proved that the class of problems that can be verified (in polynomial time) through interaction with entangled provers, a class called MIP^* is exactly equal to the class of problems that are no harder than the halting problem, a class called RE.
Let hand a program to a pair of entangled provers. You ask them to tell you whether it halt. You're prepared to verify their answer through a kind of non-local game: The provers generate questions and win based on the coordination between their answers. If the program does in fact halt, the provers should be able to win this game 100% of the time. If it doesn't halt , the provers should only win by chance 50% of the time. Therefore determination of the maximum-winning probability for a specific instance of this non-local game requires solving the halting problem, which means that calculating the approximate maximum-winning probability for non-local games is undecidable, just like the halting problem.
An algorithm that uses the tensor product model of the entanglement establishes a floor, or minimum value, on the approximate maximum-winning probability for all non-local games. Another algorithm, which uses the commuting operators model of entanglement establishes a ceiling. These algorithms produce more precise answers the longer they run. If the answer to Tsirelson's problem is true and the two models of entanglement really are equivalent, the floor and the ceiling should keep pinching closer together, narrowing in on a single value for the approximate maximum-winning percentage, which makes the calculation of this number decidable.
Hence the answer to Tsirelson's problem is negative.

The Tsirelson's problem has been solved through this way of computational complexity problems by co-authors of the proofs Henry Yuen, Zhengfeng Ji, Anand Natarajan, Thomas Vidick and John Wright.

24. Feynman amplitudes and lattice gauge theory

Feynman amplitudes and lattice gauge theory

We consider, (by suitable choosing of length, time and charge units) that the reduced Planck constant and the speed of light in vacuum constant are equal to 1.

$\hbar=1$, $c=1$

For a quantum field system described by field operator functions

$\hat{\varphi}=\hat{\varphi}(t,\vec{x})$ $(x=(t,\vec{x})=(x_\alpha)_{\alpha=\overline{0,3}}$ space-time coordinates $)$ in the Minkowski space with signature (+ , - , - , -) , $\eta=(\eta^{\alpha\beta})_{\alpha,\beta=\overline{0,3}}$ Minkowski metric coefficients and a Lagrangian density

$\mathscr{L}=\mathscr{L}(\varphi,\partial\varphi)$ with $\varphi=(\varphi_i)_i$ the action is

$S(\varphi)=\int \mathscr{L}(\varphi,\partial\varphi)d^4x$ and we can have $S(\varphi)=\int\left(\frac{1}{2}\varphi_i M_{ij}\varphi_j-V(\varphi)\right)d^4x$

where M_{ij} is a differential operator and we use Einstein summation convention.

We can make a discretization of the quantum field in the form

$q(t)=(q^k(t))_{k=\overline{1,M}}=(\varphi(t,an_1,an_2,an_3))_{n1,n2,n3\in\mathbb{Z}}$

The momentum field operator function is

$\hat{\pi}=\frac{\partial\widehat{\mathscr{L}}}{\partial(\partial_0\varphi)}$ and corresponds in discretization to the momentum coordinates

$p(t)=(\pi(t,an_1,an_2,an_3))_{n1,n2,n3\in\mathbb{Z}}$ of a discretized phase space evolution $(p(t),q(t))$ with a Hamiltonian operator given by the discretized correspondent of the expression

$\hat{H}(t)=\int(\hat{\pi}(t,\vec{x})\partial_0\hat{\varphi}(t,\vec{x})-\mathscr{L}(\hat{\varphi},\partial\hat{\varphi})(t,\vec{x}))d^3\vec{x}$ which we denote

$\hat{H}=\hat{H}(\hat{p},\hat{q})$.

As we know, (see Chap. Quantum statistical ensemble) for any observable $A = A(t)$ for the expectation value $\langle A\rangle_t=\mathrm{tr}(\rho A)$ $(\rho$ the density operator $)$ we have an evolution equation

$\frac{d}{dt}\langle A\rangle_t=i\langle[\hat{H},A]\rangle_t+\langle\partial_0 A\rangle_t$ $([\hat{H},A]=\hat{H}A-A\hat{H}$ the commutator $)$

Since $\hat{p}$, $\hat{q}$ not depend explicitly on time we can consider evolution equations for $\hat{p}$, $\hat{q}$ observables functions $A(\hat{p})$, $A(\hat{q})$ like

$\frac{d}{dt}A(\hat{p})(t)=i[\hat{H},A(\hat{p})](t)$; $\frac{d}{dt}A(\hat{q})(t)=i[\hat{H},A(\hat{q})](t)$

and so $A(\hat{p})$, $A(\hat{q})$ evolve like

$$A(\hat{q})(t)=\exp(i\hat{H}t)A(\hat{q})(0)\exp(-i\hat{H}t)\ ;\quad A(\hat{p})(t)=\exp(i\hat{\hat{H}}t)A(\hat{p})(0)\exp(-i\hat{H}t) \tag{1}$$

Therefore in the continuum limit of the discretization $(a\to 0)$ we have an evolution of operators :

$A(\hat{\varphi})(t)=\exp(i\hat{H}t)A(\hat{\varphi})(0)\exp(-i\hat{H}t)$

Given the final and initial states $\varphi_F=\varphi_F(\vec{x})$, $\varphi_I=\varphi_I(\vec{x})$ corresponding in the discretization to q_F respective q_I we have the transition amplitude for the system

from state φ_I at $t=0$ to state φ_F at $t=T$: $\langle\varphi_F|\exp(-i\hat{H}t)|\varphi_I\rangle=A$ (do not confuse with the observable A)

$|A|^2$ is the probability for the system to be in state φ_F at time $t=T$ if at time $t=0$ it was measured in state φ_I , since from state φ_I the system evolves according to Schroedinger equation like

$\exp(-i\hat{H}t)\left|\varphi_I\right\rangle$

Considering a normalization of *p* and *q* states in which

$\langle q'|q\rangle=\delta(q'-q)$, $\langle q|p\rangle=\exp(ipq)$ and

$$\int|q\rangle\langle q|\,d^Mq=\boldsymbol{I} \text{ and } \int|p\rangle\langle p|\frac{d^Mp}{(2\pi)^M}=\boldsymbol{I}$$

and taking $\delta t=\frac{T}{N}$ we have for $t_1\in[I\,\delta t,(I+1)\delta t]$, if we consider that

$\hat{H}=\frac{\hat{p}^2}{2m}+V(\hat{q})$ the following relations :

$$\langle q_F|\exp(-i\hat{H}t)A(\hat{q})(t_1)|q_I\rangle=\left(\prod_{j=1}^{N-1}\int dq^j\right)\langle q_F|\exp(-i\hat{H}\delta t)|q_{N-1}\rangle\langle q_{N-1}|$$

$$\exp(-\hat{H}\delta t|q_{N-2})\rangle...\langle q_{I+1}|\exp(-i\hat{H}\delta t)A(\hat{q})(0)|q_I\rangle...\langle q_1|\exp(-i\hat{H}\delta t)|q_I\rangle$$

$$\langle q_{I+1}|\exp(-i((\hat{p}^2/2m)+V(\hat{q}))\delta t)|A(\hat{q})(0)|q_I\rangle=$$

$$\frac{\int d^Mp}{(2\pi)^M}\exp(-i\,\delta t((p^2/2m)+V(q_I)))A(q_I)\langle q_{I+1}|p\rangle\langle p|q_I\rangle=$$

$\left(\frac{-im}{2\pi\delta t}\right)^{M/2}A(q_I)\exp((im(q_{I+1}-q_I)^2/2\delta t)-iV(q_I)\delta t)$ and so

$$\langle q_F|\exp(-i\hat{H}T)A(\hat{q})(t_1)|q_I\rangle=$$

$$\left(\frac{-im}{2\pi\delta t}\right)^{MN/2}\left(\prod_{k=1}^{N-1}dq_k\right)\exp(i\,\delta t(\sum_{j=0}^{N}(m/2)((q_{j+1}-q_j)/\delta t)^2)-V(q_j))A(q_I)= \tag{2}$$

$$C\int Dq(t)\exp(i\int_0^T((1/2)m\dot{q}^2-V(q))dt)A(q(t_1))=$$

$$C\int Dq(t)\exp(iS(q))A(q(t_1))$$

where $Dq(t)$ stands for integration over all paths $q=q(t)$ with $q(0)=q_I$, $q(T)=q_F$

(In deriving (2) we used the Fresnel integrals :

$\int_0^\infty\cos(x^2)dx=\int_0^\infty\sin(x^2)dx=\frac{1}{2}\sqrt{\frac{\pi}{2}}$)

Therefore in the same way, for

$A_i=A_i(\hat{\varphi})$, $i=\overline{1,n}$ operatorial functions, we will have :

$$\langle\varphi_F|\exp(-i\hat{H}T)T(A_1(t_1,\vec{x}_1)...A_n(t_n,\vec{x}_n))|\varphi_I\rangle=$$

$$C\int D\varphi\exp(iS(\varphi))T(A_1(\varphi(t_1,\vec{x}_1))...A_n(\varphi(t_n,\vec{x}_n))) \tag{3}$$

where *C* is a (discretization dependent) constant and $D\varphi$ stands for integration

over all paths $\varphi=\varphi(t)$ with $\varphi(0)=\varphi_I$ and $\varphi(T)=\varphi_F$, $\varphi(t)=\varphi(t,.)$ and if $(q^i)_{i=\overline{1,M}}=(\varphi(an_0,an_1,an_2,an_3))_{n_0,n_1,n_2,n_3\in\mathbb{Z}}$ is a discretization of the field, we define :

$\int D\varphi...=\int\prod_{i=1}^{M}dq^i...$ and also:

$$T(A_1(\hat{\varphi}(t_1,\vec{x}_1))...A_n(\hat{\varphi}(t_n,\vec{x}_n)))=$$

$$\sum_{\sigma\in Sn}\left(\prod_{j=1}^{n-1}\theta(t_{\sigma(j)}-t_{\sigma(j+1)})\right)A_1(\hat{\varphi}(t_{\sigma(1)},\vec{x_{\sigma(1)}}))...A_n(\hat{\varphi}(t_{\sigma(n)},\vec{x_{\sigma(n)}}))$$

with θ the Heaviside function $\theta(t)=\begin{cases}1 & \text{for } t>0\\ 0 & \text{for } t<0\end{cases}$

In the formula above, we take the 0 argument value of the Heaviside function to be 1 and divide the right side of the identity for every case of k times occurrence of the same value of t_j by k! .

The Euler – Lagrange equations

$d_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi)}-\frac{\partial\mathcal{L}}{\partial\varphi}=0$ and the commutation rules $[\hat{p}^k,\hat{q}^j]=i\delta_{jk}$

which commutation rules translated to the continuum limit become

$[\hat{\pi}^k(t,\vec{x}),\hat{\varphi}^j(t,\vec{x})]=\delta^3(\vec{x})\delta_{kj}$ with $\hat{\pi}^k=\frac{\widehat{\partial\mathcal{L}}}{\partial(\partial_0\varphi)}$ lead to:

a) $$\hat{\varphi}(t,\vec{x})=\frac{1}{(2\pi)^{3/2}}\int\frac{1}{(2\omega_k)^{1/2}}\left(a(\vec{k})\exp(-i(\omega_k t-\vec{k}\,\vec{x}))+b^+(\vec{k})\exp(i(\omega_k t-\vec{k}\,\vec{x}))\right)d^3\vec{k} \quad (4a)$$

for a complex boson free field theory with :

$\mathcal{L}(\varphi,\partial\varphi)=(\partial\varphi^+)(\partial\varphi)-m^2\varphi^+\varphi$, $\omega_k=\sqrt{\vec{k}^2+m^2}$; a,a^+ and b,b^+ annihilation and creation operators for the particle respective the antiparticle of the field satisfying commutation relations :

$[a(\vec{k}),a^+(\vec{k}')]=[b(\vec{k}),b^+(\vec{k}')]=\delta^3(\vec{k}-\vec{k}')$, $[a(\vec{k}),b(\vec{k}')]=0$

b) $$\widehat{A_\mu}(t,\vec{x})=\sum_s\frac{1}{(2\pi)^{3/2}}\int\frac{1}{(2\omega_k)^{1/2}}\left(\varepsilon_\mu(\vec{k},s)a(\vec{k},s)\exp(-i(\omega_k t-\vec{k}\,\vec{x}))+\varepsilon_\mu(\vec{k},s)a^+(\vec{k},s)\exp(i(\omega_k t-\vec{k}\,\vec{x}))\right)d^3\vec{k} \quad (4b)$$

where $(\varepsilon_\mu(\vec{k},s))_\mu$ are the polarization vectors $s=\overline{1,3}$ for $m\neq0$ and $s=1,2$ for $m=0$. Also we have $[a(\vec{k},s),a^+(\vec{k}',s')]=\delta^3(\vec{k}-\vec{k}')\delta_{ss'}$

For $m\neq0$ in the rest frame $k=(m,0,0,0)$ we have $\varepsilon(\vec{0},s)=(0,(\delta_{is})_i)$

By Lorentz invariance it follows that :

$k^\mu\varepsilon_\mu=0$, $\varepsilon^\mu(\vec{k},s)\varepsilon_\mu(\vec{k},s')=-\delta_{ss'}$ and $\sum_s\varepsilon_\mu(\vec{k},s)\varepsilon_\lambda(\vec{k},s)=K_{\mu\lambda}$ with (4)

$$K_{\mu\lambda}=-\eta_{\mu\lambda}+(k_\mu k_\lambda/m^2) \text{ if } m\neq 0$$

If $m=0$, for $K_{\mu\lambda}$ to be well determined by k we give to the massless bosons a hypothetical mass and compute with tending to 0 mass value.

The b) case is the case of a gauge vector boson free field theory

The gauge bosons free field Lagrangian density is (see Chap. Non-abelian gauge theory) given by :

$$\mathscr{L}((A^a_\mu,\partial A^a_\mu)_{a,\mu})=-\frac{1}{4}(\partial_\mu A^a_\nu-\partial_\nu A^a_\mu)(\partial^\mu A^{a\nu}-\partial^\nu A^{a\mu})-$$

$$-\frac{1}{2}g(\partial_\mu A^a_\nu-\partial_\nu A^a_\mu)f^{abc}A^{b\mu}A^{c\nu}-$$

$$-\frac{1}{4}g^2 f^{abc}f^{ade}A^b_\mu A^c_\nu A^{d\mu}A^{e\nu}+\frac{1}{2}M_a^2 A^a_\mu A^{a\mu}$$

M_a are the gauge bosons masses and f^{abc} are the structure coefficients of the gauge group Lie algebra , having normalized generators $(T^a)_a$ with $[T^b,T^c]=if^{abc}T^a$, $\mathrm{tr}(T^aT^b)=\frac{1}{2}\delta_{ab}$ and T^a hermitian traceless.

c) For spin ½ fermions in a free field theory the Lagrangian density is the Dirac Lagrangian density :

$\mathscr{L}(\psi,\partial\psi)=\overline{\psi}(i\gamma^\mu\partial_\mu-m)\psi$ with γ^μ the gamma matrices, $\overline{\psi}=\psi^+\gamma^0$

$\psi=(\psi_\alpha)_{\alpha=\overline{0,3}}(t,\vec{x})$ Dirac spinor field.

$$\widehat{\psi}_\alpha(t,\vec{x})=\frac{1}{(2\pi)^{3/2}}\int\frac{1}{(E_p/m)^{1/2}}\Big(\sum_s u_\alpha(p,s)b(p,s)\exp(-ipx)+ \quad (4c)$$

$$v_\alpha(p,s)d^+(p,s)\exp(ipx)\Big)d^3\vec{p}$$

where $s=1,2$ and $p=(p_\mu)_{\mu=\overline{0,3}}=(p_0,\vec{p})$, $px=p_\mu x^\mu$, $E_p=p_0=\sqrt{\vec{p}^2+m^2}$

$(i\gamma^\mu\partial_\mu-m)\psi=0$ and $(\not{p}-m)u(p,s)=0$, $(\not{p}+m)v(p,s)=0$ (4')

since by Euler – Lagrange equations , the spinor field satisfies the Dirac equations with $\not{p}=\gamma^\mu p_\mu$

The annihilation and creation operators for particles respective antiparticles b,b^+ respective d,d^+ satisfy anti-commutation relations :

$\{b(p,s),b^+(p',s')\}=\{d(p,s),d^+(p',s')\}=\delta_{ss'}\delta^3(\vec{p}-\vec{p}')$ (4'')

$\{b(p,s),d(p',s')\}=\{b(p,s),b(p',s')\}=\{d(p,s),d(p',s')\}=0$ (4'')

with $\{A,B\}=AB+BA$, the anti-commutator

The normalized *u* and *v* functions are so that in the rest frame

$p=(m,0,0,0),u(p,1)=(1,0,0,0),u(p,2)=(0,1,0,0),v(p,1)=(0,0,1,0)$

$v(p,2)=(0,0,0,1)$ as column vectors and by Lorentz invariance we will have:

$\overline{u}(p,s)u(p,s')=\delta_{ss'}$, $\overline{v}(p,s)v(p,s')=-\delta_{ss'}$

$\overline{u}(p,s)v(p,s')=\overline{v}(p,s)u(p,s')=0$

and $\sum_s u_\alpha(p,s)\overline{u_\beta}(p,s)=\left(\frac{\not p+m}{2m}\right)_{\alpha\beta}$ (4''')

and $\sum_s v_\alpha(p,s)\overline{v_\beta}(p,s)=\left(\frac{\not p-m}{2m}\right)_{\alpha\beta}$ (4''')

Considering a perturbed by sources $J=J(t,\vec{x})$ Lagrangian density $\mathscr{L}=\mathscr{L}(\varphi,\partial\varphi)+J\varphi$, in the discretization we may have $S(\varphi)=\int\left(\frac{1}{2}\varphi_i M_{ij}\varphi_j+J_i\varphi_i\right)d^4x=\frac{1}{2}q^T A q+J^T q$ with A a symmetric real non-singular matrix.

$\frac{1}{2}q^T A q+J^T q=\frac{1}{2}(q^T+J^T A^{-1})A(q+A^{-1}J)-\frac{1}{2}J^T A^{-1}J$ (5) and so

$Z(J)=\int D\varphi\exp(iS(\varphi))=C(\int d^M q\exp((i/2)q^T Aq))\exp(-(i/2)J^T A^{-1}J).$

Diagonalizing A and considering the already mentioned Fresnel integrals we obtain

$\int d^M q\exp((i/2)q^T Aq)=\left(\frac{(2\pi i)^M}{\det A}\right)^{1/2}$

A^{-1} corresponds to the propagator $D=D(x-y)$ which in the continuum limit satisfies $M_{ij}D_{jk}(x)=\delta_{ik}\delta^4(x)$ (6)

and we have $Z(J)=Z(J=0)\exp((-i/2)\int J_j(x)D_{jk}(x-y)J_k(y)d^4x\,d^4y)$

The ground state corresponds to the state with lowest energy possible , no perturbations in the field (only vacuum fluctuations) : $\varphi\equiv 0$ and we denote it $|0\rangle$. Taking $\varphi_F=\varphi_I=|0\rangle$, according to (3) we will have:

$$\langle 0|\exp(-i\hat{H}T)\mathbf{T}(\varphi(x_1)\ldots\varphi(x_n))|0\rangle=$$

$$C\int D\varphi\exp(i\int\mathscr{L}(\varphi,\partial\varphi)d^4x)\varphi(x_1)\ldots\varphi(x_n)=$$

$$\left(\frac{\delta^n}{\delta iJ(x_1)\ldots\delta iJ(x_n)}C\int D\varphi\exp(i\int\mathscr{L}(\varphi,\partial\varphi)+J\varphi d^4x)\right)\Bigg|_{J=0}=Z(J=0)$$

$$\left(\frac{\delta^n}{\delta iJ(x_1)\ldots\delta iJ(x_n)}\exp((-i/2)\int J_k(x)D_{kl}(x-y)J_l(y)d^4x\,d^4y)\right)\Bigg|_{J=0}$$

where $\frac{\delta}{\delta iJ(x_k)}$ must be understood as a partial derivative with respect to

$iJ(x_k)d^4x.$

In the case of fermion fields Lagrangian density $\mathscr{L}=\mathscr{L}(\psi,\partial\psi)$, because the spinor fields are complex we have ψ and $\overline{\psi}$ as independent integration variables and a perturbed Lagrangian density form by spinor sources η and $\overline{\eta}$ as below:

$\mathscr{L}(\psi,\partial\psi)+\overline{\psi}\eta+\overline{\eta}\psi$ and the path integral:

$$Z(\eta,\overline{\eta})=\int D\psi D\overline{\psi}\exp(i\int(\mathscr{L}(\psi,\partial\psi)+\overline{\psi}\eta+\overline{\eta}\psi)d^4x) \quad (7)$$

We have: $\mathscr{L}(\psi,\partial\psi)=\overline{\psi}K\psi$, $K=i\partial\!\!\!/-m$

$$\mathscr{L}(\psi,\partial\psi)+\overline{\eta}\psi+\overline{\psi}\eta=(\overline{\psi}+\overline{\eta}K^{-1})K(\psi+K^{-1}\eta)-\overline{\eta}K^{-1}\eta \quad (8)$$

The propagator $S=(i\partial\!\!\!/-m)^{-1}$, $S=(S_{\alpha\beta}(x))_{\alpha,\beta=\overline{0,3}}$

$S = D^{fer}$,fermion propagator,

satisfies $(i\partial\!\!\!/-m)S(x)=\delta^4(x)$

and we have therefore $S(x)=\int\frac{1}{(2\pi)^4}\exp(-ipx)\frac{p\!\!\!/+m}{p^2-m^2+i\varepsilon}d^4p$ (8')

with $\varepsilon>0$, $\varepsilon\to 0$. Using residues theorem in the integration above over p_0 integration variable we obtain :

$$iS(x)=\frac{1}{(2\pi)^3}\int(2E_p)^{-1}\left(\theta(x^0)(p\!\!\!/+m)\exp(-ipx)-\right.$$

$$\left.-\theta(-x^0)(p\!\!\!/-m)\exp(ipx)\right)d^3\vec{p} \quad (8'')$$

where in the above expression we take $E_p=p_0=\sqrt{\vec{p}^2+m^2}$

Considering the (4'') anti-commutation relations we can take therefore the $(\overline{\psi}_\alpha(x))_{\alpha,x}$ and $(\psi_\alpha(x))_{\alpha,x}$ integration variables as two sets of independent Grassmann integration variables. Grassmann numbers are defined such that if η and ξ belong to the same set of Grassmann numbers then $\eta\xi=-\xi\eta$.

Therefore the most general function of a Grassmann number is $f=f(\eta)=a+b\eta$ with a , b ordinary numbers .

Since for η , ξ Grassmann variables we must have $\int d\eta f(\eta+\xi)=\int d\eta f(\eta)$ and so $\int d\eta b\xi=0$ for any ξ and we have $\int d\eta=0$ for η Grassmann integration variable.

Since given three Grassmann variables χ,η,ξ we have $\chi(\eta\xi)=(\eta\xi)\chi$ we conclude that the product of two Grassmann numbers must be an ordinary number and thus the integral $\int\eta d\eta$ is an ordinary number which is taken to be equal to a normalization constant.

Therefore, if $\eta=(\eta_1,\ldots,\eta_N)$ and $\overline{\eta}=(\overline{\eta}_1,\ldots,\overline{\eta}_N)$ are sets of independent Grassmann variables and $s=(s_1,\ldots s_N),r=(r_1,\ldots,r_N)$ not depend on η , $\overline{\eta}$, A is a N x N matrix then we can derive

$\int d\eta d\overline{\eta}\exp((\overline{\eta}+s)A(\eta+r))=\int d\eta d\overline{\eta}\exp(\overline{\eta}A\eta)=C\det A$ with C a normalization constant. (8''')

Hence, considering (8) the relation (7) becomes

$$Z(\eta,\overline{\eta})=Z(\eta=0)\exp(-i\int\overline{\eta_\alpha}(x)S_{\alpha\beta}(x-y)\eta_\beta(y)d^4xd^4y)$$

and we have $Z(\eta=0)=C\det(i\partial\!\!\!/-m)$,

with $\gamma^5=i\gamma^0\gamma^1\gamma^2\gamma^3$ we will have also:

$\det(i\partial\!\!\!/-m)=\exp(\mathrm{tr}\ln(i\partial\!\!\!/-m))$

$\mathrm{tr}\ln(i\partial\!\!\!/-m)=\mathrm{tr}\ln(\gamma^5(i\partial\!\!\!/-m)\gamma^5)=\mathrm{tr}\ln(-i\partial\!\!\!/-m)=(1/2)4\,\mathrm{tr}\ln(\partial^2+m^2)$

The factor of 4 appears because at the left member we have the trace of a 4x4 matrix.

Recall that $Z(\eta=0)=\int D\psi D\overline{\psi}\exp(i\int\mathscr{L}(\psi,\partial\psi)d^4x)=\langle 0|\exp(-i\hat{H}T)|0\rangle$ (9)

(with $T\to\infty$ understood so that we integrate over all of spacetime in (9))

and so if $E=\langle 0|\hat{H}|0\rangle$ is the energy of the vacuum we will have:

$$iET=-2\,\mathrm{tr}\ln(\partial^2+m^2)+AVT=-2\int d^4x\langle x|\ln(\partial^2+m^2)|x\rangle+AVT=$$

$$-2\int d^4x\int\frac{d^4k}{(2\pi)^4}\int\frac{d^4q}{(2\pi)^4}\langle x|k\rangle\langle k|\ln(\partial^2+m^2)|q\rangle\langle q|x\rangle+AVT$$

Since in the momentum space normalization $\langle k|q\rangle=(2\pi)^4\delta^4(k-q)=VT$ (V space volume , T time interval of the considered field domain) we obtain

$i\frac{E}{V}=-2\int\frac{d^4k}{(2\pi)^4}\ln(k^2-m^2+i\varepsilon)+A'$ where A , A' are infinite constants corresponding to the multiplicative factor C (and changing the sign under the logarithm)

Let $\frac{A'}{2}=\int\frac{d^4k}{(2\pi)^4}\ln(k^2-m'^2+i\varepsilon)$ and we will have

$$\frac{E}{V}=2i\int\frac{d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega}{2\pi}\ln\left(\frac{\omega^2-\omega_k^2+i\varepsilon}{\omega^2-\omega'^2_k+i\varepsilon}\right)$$

We treat the (convergent) integral over ω by integrating by parts and then by residues theorem, obtaining:

$$\frac{E}{V}=-2i\int\frac{d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega}{2\pi}\left(\frac{2\omega_k^2}{\omega^2-\omega_k^2+i\varepsilon}-\frac{2\omega'^2_k}{\omega^2-\omega'^2_k+i\varepsilon}\right)=$$

$$=\int\frac{d^3\vec{k}}{(2\pi)^3}(-2(\omega_k-\omega'_k))$$

(where we defined $\omega_k=\sqrt{\vec{k}^2+m^2}$, $\omega'^2_k=\sqrt{\vec{k}^2+m'^2}$)

Restoring the Planck constant through dimensional analysis we have

$E_0=-\int\frac{d^3\vec{x}\,d^3\vec{p}}{h}\sum_s 2\left(\frac{1}{2}E_p\right)$ with $E_p=\sqrt{\vec{p}^2c^2+m^2c^4}$

The infinite additive term E_0 is precisely the analogue of the zero point energy of the quantum harmonic oscillator but for the Dirac field , as we see , comes with a peculiar minus sign. For each spin and for the electron and positron separately (hence the factor of 2) we have an energy (- 1 / 2) E_p in each unit-size phase-space cell (1 / h^3) $d^3x\,d^3p$.

To compute a Feynman amplitude for all modulo time ordering equivalence classes of Feynman diagrams with

$(x_i^a)_{i=\overline{1,s}}$ outgoing legs end vertices and

$(x_i^b)_{i=\overline{1,n}}$ incoming legs end vertices and

$(x_i)_{i=\overline{1,m}}$ interaction vertices, $(p_i)_{i=\overline{1,s}}$ outgoing momenta and

$(q_i)_{i=\overline{1,n}}$ incoming momenta, considering that $\hat{H}|0\rangle = V_0|0\rangle$

with V_0 constant vacuum energy, which by measuring energy at this level can be considered to be equal to 0, we have to compute

$$\int P((x^a),(x),(x^b))(\prod_{j=1}^{s}\exp(i p_j x_j^a)d^4x_j^a)(\prod_{k=1}^{n}\exp(-i q_k x_k^b)d^4x_k^b)(\prod_{l=1}^{m}d^4x_l)$$

where $P((x^a),(x),(x^b)) = \langle 0|T((\prod_{j=1}^{s}\hat{\varphi}(x_j^a))(\prod_l \hat{\varphi}(x_l))(\prod_{k=1}^{n}\hat{\varphi}(x_k^b)))|0\rangle$

and "amputate" the external legs ,(i . e. multiply with

$(\prod_{j=1}^{s}(p_j^2 - m^2 + i\varepsilon))(\prod_{k=1}^{n}(q_k^2 - m^2 + i\varepsilon))$, the incoming and respective outgoing particles being considered on mass shell).

Notice that the interaction vertices must not be all distinct and so we will integrate over the set of distinct x_l , $l = \overline{1,m}$ and $\prod_l \hat{\varphi}(x_l)$ represents the product of a exponential expansion coefficient and the taken interaction vertices terms from the expression of the interaction Lagrangian density

$\tilde{\mathcal{L}}(\varphi,\partial\varphi) = \mathcal{L}(\varphi,\partial\varphi) +$ interaction terms

As we derived above , for

$P((x^a),(x),(x^b))$ we have a Wick contraction computation from the expression

$$\tilde{C}\left(\frac{\delta^{n+s+m}}{\delta i J(x_1^a)\ldots\delta i J(x_l)\ldots\delta i J(x_n^b)}\exp((\frac{-i}{2})\int J(x)D(x-y)J(y)d^4x\,d^4y)\right)\Big|_{J=0}$$

with $\tilde{C} = Z(J=0)$ constant . (9')

For a Lagrangian density of fermion fields (quarks and leptons) interacting with gauge boson fields we have :

$$\begin{aligned}\tilde{\mathcal{L}}((\psi^\alpha,\partial\psi^\alpha)_\alpha,(A^a,\partial A^a)_a) &= \overline{\psi}^\alpha(i\delta_{\alpha\beta}\gamma^\mu\partial_\mu - m_\alpha\delta_{\alpha\beta})\psi^\beta + \\ +\sum_g\Big(g\overline{\psi}^\alpha\gamma^\mu A_\mu^a T_{\alpha\beta}^a\psi^\beta &- (1/4)(\partial_\mu A_\nu^a - \partial_\nu A_\mu^a)(\partial^\mu A^{a\nu} - \partial^\nu A^{a\mu}) - \\ &- (1/2)g(\partial_\mu A_\nu^a - \partial_\nu A_\mu^a)f^{abc}A^{b\mu}A^{c\nu} - \\ &- (1/4)g^2 f^{abc}f^{ade}A_\mu^b A_\nu^c A^{d\mu}A^{e\nu} + (1/2)M_a^2 A_\mu^a A^{a\mu}\Big)\end{aligned} \quad (10)$$

In the electroweak SU(2)xU(1) or in the unified electroweak+chromodynamics SU(3)xSU(2)xU(1) theory for any g coupling we have a corresponding set of gauge bosons and respective gauge group generators defined coefficients :

$((A_\mu^a)_\mu,(T_{\alpha\beta}^a)_{\alpha\beta})_a$ with μ - Lorentz index

α,β - colour, flavour , lepton sort index

In quantum chromodynamics SU(3) or in the grand unified SU(5) theory we have an unique coupling constant g with the set of gauge bosons and gauge group generators.

We have following Feynman rules to compute Feynman amplitudes of fermion and gauge boson (gluon) particle transition processes for a perturbation theory approach (which is relevant in the case of a weak couplings like in electroweak theory or asymptotic freedom of quantum chromodynamics):
(The considered process has $q_1,\ldots,q_n$ incoming fermions momenta, $p_1,\ldots,p_s$ outgoing fermions momenta and $k_1,\ldots,k_h$ outgoing bosons momenta and the Feynman diagram is with

$x_1^a,\ldots,x_s^a$ outgoing fermions legs end vertices,
$x_1^b,\ldots,x_n^b$ incoming fermions legs end vertices,
$x_1,\ldots,x_r$ fermion interaction vertices,
$y_1,\ldots,y_k$ cubic gluon interaction vertices,
$z_1,\ldots,z_q$ quartic gluon interaction vertices,
$y_1^a,\ldots,y_h^a$ outgoing boson legs end vertices,
$(x_{1l},x_{2l})_{l=\overline{1,m}}$ internal lines).

1. For each interaction vertex write $(2\pi)^4\delta^4(\sum_{k\in A}k-\sum_{k\in B}k)$

(where A is the set of incoming to the vertex momenta and B is the set of outgoing from the vertex momenta)
and write the coupling: a) $ig\gamma^\mu$ for x_l vertices;
b) $gf^{abc}(\eta^{\mu\nu}(r_1-r_2)^\lambda+\eta^{\nu\lambda}(r_2-r_3)^\mu+\eta^{\lambda\mu}(r_3-r_1)^\nu)$ where r_1,r_2,r_3 label the incoming to the cubic gluon interaction vertex respective a,b,c gluon momenta (do not confuse the gluon indices a , b, c with the notations with a , b upper index for outgoing respective incoming legs) for y_l vertices.
c) $-ig^2\left(f^{abc}f^{ade}(\eta^{\mu\lambda}\eta^{\nu\epsilon}-\eta^{\mu\epsilon}\eta^{\nu\lambda})+f^{adc}f^{abe}(\eta^{\mu\lambda}\eta^{\nu\epsilon}-\eta^{\lambda\epsilon}\eta^{\mu\nu})+\right.$
$\left.+f^{abd}f^{ace}(\eta^{\nu\mu}\eta^{\lambda\epsilon}-\eta^{\nu\epsilon}\eta^{\mu\lambda})\right)$ for z_l vertices.

2. For each internal line write the propagator :

a) $\frac{i(\not{p}+m)}{p^2-m^2+i\varepsilon}$ for a mass m fermion line labeled with p momentum

b)

$i\left(-\eta_{\mu\nu}+\frac{k_\mu k_\nu}{M^2}\right)\frac{1}{k^2-M^2+i\varepsilon}$ for a mass M boson line labeled with k momentum.

c)For massless bosons we will consider a hypothetical tending to 0 non-vanishing mass in computations that are confronted with lattice method computations which will be further presented. In that case, the $k_\mu k_\nu/M^2$ term in the propagator disappears in computations because the masses of the two fermions linked in the amplitude expression to the propagator of a massless boson as the photon or the SU(3) bosons in SU(3)xSU(2)xU(1) theory or in quantum chromodynamics are

equal (flavour changing occurs only through the W bosons which are massive) and we can use (4') , (8') , (4'''). Otherwise we can have an additional ghost action by Fadeev-Popov method with gauge parameter leading to a propagator $i(-\eta_{\mu\nu}+(1-\xi)(k_\mu k_\nu/k^2))/k^2$ where we can take the gauge parameter $\xi=1$.

For example we have in an amplitude expression the factor

$$iD^{fer}_{\alpha\beta}(p)\gamma^\mu_{\beta\epsilon}iD^{bos}_{\mu\nu}(r)iD^{fer}_{\epsilon\delta}(q)\delta^4(p-q-r)$$ which contains

$$\bar{u}(p)\gamma^\mu u(q)(-\eta_{\mu\nu}+(r_\mu r_\nu)/M^2)\delta^4(p-q-r)=$$

$$=(-\bar{u}(p)\gamma_\nu u(q)+((p-q)_\nu(m-m)\bar{u}(p)u(q)/M^2))\delta^4(p-q-r)$$

and as we can see the term containing the hypothetical mass disappears since the involved fermions masses are equal.

3. Write $\bar{u}(p_j,s)$ for outgoing fermions, $u(q_j,s)$ for incoming fermions, write $\bar{v}(q_j,s)$ for incoming antifermions, $v(p_j,s)$ for outgoing antifermions, write $\varepsilon_\mu(k_j,s)$ for outgoing or incoming bosons.

4. Multiply the written factors and multiply the result with a (-1) factor for each closed fermion cycle.

5. Momenta k associated with internal lines are to be integrated over with $\frac{d^4k}{(2\pi)^4}$ measure.

6. The external legs are "amputated" since according to rule 2. we write the propagators only for internal lines. The particles are on mass shell (i.e. we have $p_j^2-m^2=0$, $q_j^2-m^2=0$, $k_j^2-M^2=0$ where m and M take the respective values of the corresponding particles).

The amplitude has the form $(2\pi)^4\boldsymbol{M}\delta^4(\sum_{j=1}^{s}p_j+\sum_{j=1}^{h}k_j-\sum_{j=1}^{n}q_j)$ with $\boldsymbol{M}$ an invariant Feynman amplitude.

Since the fermion field operators anti-commute, for a set $(\hat{\varphi}_i)_{i=\overline{1,m}}$ of operators in which $\hat{\varphi}_{i1},\ldots,\hat{\varphi}_{ir}$ with $i_1<i_2<\ldots<i_r$ anti-commute each with other and the remaining $\{1,\ldots,m\}\setminus\{i_1,\ldots,i_r\}\ni i,\hat{\varphi}_i$ operators commute with any of the operators in the set we define :

$$T(\prod_{i=1}^{m}\hat{\varphi}_i(x_i))=\sum_{\sigma\in Sm}\varepsilon(\tilde{\sigma})(\prod_{i=1}^{m-1}\theta(x^0_{\sigma(i)}-x^0_{\sigma(i+1)}))(\prod_{i=1}^{m}\hat{\varphi}_{\sigma(i)}(x_{\sigma(i)}))$$ where

$$\tilde{\sigma}=\sigma|_{\{i1,\ldots,ir\}}$$ and $$\varepsilon(\tilde{\sigma})=\mathrm{sgn}\prod_{1\le k<l\le r}(\sigma(i_l)-\sigma(i_k))$$

In the above definition for T we take $\theta(0)=1$ and divide rhe right member by $k!$ for every k times occurence of the same value of x_i^0.

Also, considering that for a fermion lines closed cycle with (x_1 , … , x_{r+1}) , $x_1=x_{r+1}$ interaction vertices , from

$\overline{\psi}(x_1)\gamma^{\mu}A_{\mu}(x_1)\psi(x_1)\overline{\psi}(x_2)\gamma^{\nu}A_{\nu}(x_2)\psi(x_2)...\gamma^{\lambda}A_{\lambda}(x_r)\psi(x_r)$, in order to obtain the proper r vertices fermion cycle factor of the amplitude,

$\mathrm{tr}\left(S(x_r-x_1)\gamma^{\mu}S(x_1-x_2)\gamma^{\nu}...S(x_{r-1}-x_r)\gamma^{\lambda}\right)$ we must anti-commute to

$\psi_l(x_r)\overline{\psi}(x_1)\gamma^{\mu}...\gamma^{\lambda}A_{\lambda}(x_r)$ (for the d^{+} of $\hat{\psi}(x_r)$ meet the d of $\hat{\overline{\psi}}(x_1)$)

(The x_i variables are obviously to be integrated over in the final amplitude expression). Thus we will have the extra (-) sign for each closed fermion cycle of the Feynman diagram and on the cycle we must have an anti-fermion propagating backwards in time.

To compute the total amplitude for the Feynman diagrams with the given outgoing and incoming momenta of fermions / anti-fermions and bosons and given numbers of fermion interaction vertices, cubic and quartic gluon interaction vertices we have to deal with the expression of amplitude *A* as follows :

$$A=cf\int\frac{1}{s!h!n!}\left\langle 0\left|\left(\sum_{\sigma\in Ss}\varepsilon(\sigma)\prod_{i=1}^{s}\tilde{b}(p_{\sigma(i)})\right)\sum_{\sigma\in Sh}\prod_{j=1}^{h}\tilde{a}(k_{\sigma(j)})T\left(R((x),(y),(z))\right)\right.\right.$$
$$\left.\left.\left(\sum_{\sigma\in Sn}\varepsilon(\sigma)\prod_{l=1}^{n}\tilde{b}^{+}(q_{\sigma(l)})\right)\right|0\right\rangle\left(\prod_{i=1}^{r}d^4x_i\right)\left(\prod_{i=1}^{k}d^4y_i\right)\left(\prod_{i=1}^{q}d^4z_i\right)$$

where *cf* is a coefficient from the exponential expansion carried by the interaction terms product we consider in the Feynman diagram and $R((x),(y),(z))$ has the form :

$\left(\prod_{l=1}^{r}\hat{\overline{\psi}}^{\alpha}(x_l)igT^{a}_{\alpha\beta}\gamma^{\mu}\hat{A}^{a}_{\mu}(x_l)\hat{\psi}^{\beta}\right)\left(\prod_{j=1}^{k}i\hat{K}_c(y_j)\right)\left(\prod_{j=1}^{q}i\hat{K}_q(z_j)\right)$, where

$K_c(y_j)=-(1/2)gf^{abd}\left(\partial_{\mu}A^{a}_{\nu}-\partial_{\nu}A^{a}_{\mu}\right)A^{b\mu}A^{d\nu}(y_j)$ and

$K_q(z_j)=-(1/4)g^2f^{abc}f^{ade}A^{b}_{\mu}A^{c}_{\nu}A^{d\mu}A^{e\nu}(z_j).$

and for normalization we have taken :

$$(\tilde{a},\tilde{b},\tilde{d})=\left(\frac{(2\pi)^3}{V}\right)^{1/2}(a,b,d)$$

Suppressing the spin and polarization indices in $u(p,s),u(q,s)$ and $\varepsilon(k,s)$, considering summation over them, we have:

$$A=cf\int\left\langle 0\left|T\left(\left(\prod_{j=1}^{s}\exp(ip_jx^{a}_{j})\overline{u}(p_j)\hat{\psi}(x^{a}_{j})\right)\left(\prod_{j=1}^{h}\exp(ik_jy^{a}_{j})(-\varepsilon^{\lambda}(k_j))\right)\right.\right.$$
$$\left.\left.\hat{A}_{\lambda}(y^{a}_{j})\right)R((x),(y),(z))T\left(\prod_{j=1}^{n}\exp(-iq_jx^{b}_{j})u(q_j)\hat{\overline{\psi}}(x^{b}_{j})\right)\right|0\right\rangle \qquad (11)$$
$$V^{-(s+h+n)/2}\left(\prod_{j=1}^{s}(E_{pj}/m)^{1/2}\right)\left(\prod_{j=1}^{h}(2\omega_{kj})^{1/2}\right)\left(\prod_{j=1}^{n}(E_{qj}/m)^{1/2}\right)$$
$$\left(\prod_{j=1}^{s}d^3\vec{x}^{a}_{j}\right)\left(\prod_{j=1}^{h}d^3\vec{y}^{a}_{j}\right)\left(\prod_{j=1}^{n}d^3\vec{x}^{b}_{j}\right)\left(\prod_{j=1}^{r}d^4x_j\right)\left(\prod_{j=1}^{k}d^4y_j\right)\left(\prod_{j=1}^{q}d^4z_j\right)$$

In (11) we have taken $x_i^{a0}=y_j^{a0}=T\,;x_l^{b0}=0$ and any space or time integration is on $[0,T]$ time interval and a volume V spatial domain.

We understand also that the incoming and outgoing fermions or bosons can have different boson sort or flavour indices which we have suppressed in the above expression.

The $\hat{\psi}$ and $\hat{A}$ operator functions in (10) are the same as given in (4c) and (4b) because we consider in the perturbation theory approach of Feynman diagrams the relations of type (3) with the not gauged free theory Lagrangian density from (10) (having g = 0).

Considering type (3) and (9') relations we will have (12) :

$$A=\sum_{\text{diagrams}}\widetilde{C}S_F V^{-(s+h+n)/2}\int((\prod_{j=1}^{s}(E_{pj}/m)^{1/2}\exp(ip_jx_j^a)\bar{u}(p_j)iD^{fer}(x_j^a-x_{1lj}))$$
$$(\prod_{j=1}^{h}(2\omega_{kj})^{1/2}\exp(ik_jy_j^a)(-\varepsilon(k_j))iD^{bos}(y_j^a-y_{lj}))$$
$$(\prod_{j=1}^{n}(E_{qj}/m)^{1/2}\exp(-iq_jx_j^b)iD^{fer}(x_{2lj}-x_j^b)u(q_j))$$
$$(\prod(\text{internal lines propagators and couplings}))$$
$$(\prod_{j=1}^{r}d^4x_j)(\prod_{j=1}^{k}d^4y_j)(\prod_{j=1}^{q}d^4z_j)(\prod_{j=1}^{s}d^3\vec{x}_j^a)(\prod_{j=1}^{h}d^3\vec{y}_j^a)(\prod_{j=1}^{n}d^3\vec{x}_j^b)$$

with $\widetilde{C}=Z(\eta=0,g=0)$ and S_F a symmetry factor.

As established, we integrate over $0<x_{1lj}^0<T=x_j^{a0}$ in the diagrams of the (12) sum and considering (4''') and (8'') we have:

$$\int(E_{pj}/m)^{1/2}\exp(ip_jx_j^a)\bar{u}(p_j)D^{fer}(x_j^a-x_{1lj})d^3\vec{x}_j^a= \quad (13)$$
$$=(E_{pj}/m)^{-1/2}\bar{u}(p_j)\exp(ip_jx_{1lj})$$

and similar :

$$\int(E_{qj}/m)^{1/2}\exp(-iq_jx_j^b)iD^{fer}(x_{2lj}-x_j^b)u(q_j)d^3\vec{x}_j^b= \quad (14)$$
$$=\exp(-iq_jx_{2lj})u(q_j)(E_{qj})^{-1/2}$$

and also we will have :

$$\int(2\omega_{kj})^{1/2}\exp(ik_jy_j^a)(-\varepsilon(k_j))iD^{bos}(y_j^a-y_{lj})d^3\vec{y}_j^a= \quad (15)$$
$$=(2\omega_{kj})^{-1/2}\varepsilon(k_j)\exp(ik_jy_{lj})$$

To prove (15) we integrate over k^0 using the residues theorem in the boson propagator expression

$\int\exp(-ik(y_j^a-y_{lj}))\dfrac{-\eta_{\mu\lambda}+(k_\mu k_\lambda/M^2)}{k^2-M^2+i\varepsilon}d^4k$ and for that the integral over the semicircle $\{k^0=R\exp(i\theta)\}$, $\theta\in[-\pi,0]$ must be considered. The only case in which the integral not vanishes for $R\to\infty$ is when $\lambda=\mu=0$ and the remaining not vanishing term is (with $y=y_j^a-y_{lj}$) :

$$\lim_{R\to\infty}\int_{-\pi}^{0}\frac{\exp(-iR\,e^{i\theta}y^0+i\vec{k}\,\vec{y})R^3\cos(3\theta)}{R^2e^{2i\theta}-\vec{k}^2-M^2+i\varepsilon}d\theta$$

Since $\cos(3\theta)=\cos(\theta)(1-2\sin^2(\theta))-2\sin^2(\theta)\cos(\theta)$ we will have the only not vanishing remaining term (after some calculus) :

$$B=\int_0^R\frac{\exp(-iR\sqrt{1-(x/R)^2}\,y^0+i\vec{k}\,\vec{y}-xy^0)}{R^2(1-2(x/R)^2)+2iRx\sqrt{1-(x/R)^2}-\vec{k}^2-M^2+i\varepsilon}R^2dx+$$
$$+\int_R^0\frac{\exp(iR\sqrt{1-(x/R)^2}\,y^0+\vec{k}\,\vec{y}-xy^0)}{R^2(1-2(x/R)^2)-2iRx\sqrt{1-(x/R)^2}-\vec{k}^2-M^2+i\varepsilon}R^2dx \qquad (16)$$

The integrands in (16) are dominated by the absolutely integrable function $\exp(-xy^0)$ for $x\in(0,\infty)$ and so taking a cut-off for integration over k with $|k^0|<R$ and large R we have $B=-2i\frac{\sin(Ry^0)}{y^0}\exp(i\vec{k}\,\vec{y})=P(y^0)\exp(i\vec{k}\,\vec{y})$ which integrated over $\vec{k}$ leads to $P(y^0)(2\pi)^3\delta^3(\vec{y}_j^{\,a}-\vec{y}_{lj})$.

In order to have external legs for the gauge bosons , we integrate the $\vec{y}_j^{\,a}$ and $\vec{y}_{lj}$ variables on a set $\|\vec{y}_j^{\,a}-\vec{y}_{lj}\|\geq\varepsilon$ and so,after $d^3\vec{y}_j^{\,a}d^4y_{lj}$ integration, the non-vanishing term left by applying the residues theorem on the boson propagator expression disappears and we can use (15) in the computation of the amplitude.

Note that for an outgoing anti-particle with momentum p_j we must take $\exp(ip_jx_j^a)\hat{\bar{\psi}}(x_j^a)v(p_j)$ instead of $\exp(ip_jx_j^a)\bar{u}(p_j)\hat{\psi}(x_j^a)$ and for an incoming antiparticle with momentum q_j we take $\exp(-iq_jx_j^b)\bar{v}(q_j)\hat{\psi}(x_j^b)$ instead of $\exp(-iq_jx_j^b)\hat{\bar{\psi}}(x_j^b)u(q_j)$ in the (11) expression.

The final and initial states of the considered process, which are $\langle 0|\tilde{b}(p_1)...\tilde{b}(p_s)\tilde{a}(k_1)...\tilde{a}(k_h)|=\langle 0|\psi_F$ and $\tilde{b}^+(q_1)...\tilde{b}^+(q_n)|0\rangle=|\psi_I\rangle$ have to be normalized for computing the effective process amplitude *A* and the transition probability $|A|^2$ such that $\langle\psi_F|\psi_F\rangle=\langle\psi_I|\psi_I\rangle=1$.

We can prove that if $[R,\tilde{a}(q)]=0$ then $\langle 0|R\tilde{a}^l(q)\tilde{a}^{l+}(q)R^+|0\rangle=l!\langle 0|RR^+|0\rangle$. Using this , and the fact that a state of many fermions of the same sort vanishes if there are two fermions with the same momentum (this is in fact the Pauli exclusion principle and follows from the anti-commutation relations) it follows that we must normalize with a factor of $1/\sqrt{l!}$ for each occurrence of l identical bosons with the same momentum and the corresponding transition probability will be adjusted by a statistical factor (eliminating double counting of events)

$S=\prod_i\frac{1}{l_i!}$ with l_i the number of occurrences of a boson with the same momentum.

Considering the way we calculate Feynman amplitudes (amputating external legs), the relations (12) , (13), (14), (15) and the symmetry factor that comes out to be the same from the many ways in which we can associate a Feynman diagram to an (11) expression we can conclude that the relation between the transition amplitude and the total amplitude for all Feynman diagrams of a given couplings order and given outgoing and incoming momenta of given respective fermions and respective bosons is :

$A=V^{-(s+h+n)/2}(\prod_{j=1}^{s}\left(\frac{E_{pj}}{m}\right)^{-1/2})(\prod_{j=1}^{n}\left(\frac{E_{qj}}{m}\right)^{-1/2})(\prod_{j=1}^{h}(2\omega_{kj})^{-1/2})A_F$ where

$A_F=(2\pi)^4 \boldsymbol{M}\,\delta^4(\sum_1^s p_j+\sum_1^h k_i-\sum_1^n q_l)$ is the total Feynman amplitude.

The $u(p,s)$, $v(p,s)$, $\varepsilon(p,s)$ which are needed in the amplitude computation are determined by theirs normalization values in the rest frame.

For a decay process we have $n=1$ and since

$(\delta^4(q_1-\sum_1^h k_i-\sum_1^s p_j))^2=\frac{\delta^4(q_1-\sum_1^h k_i-\sum_1^s p_j)VT}{(2\pi)^4}$ and momentum space $d^3\vec{p}$ contains $\frac{V}{(2\pi)^3}d^3\vec{p}$ states, we can compute a differential decay rate $\frac{|A|^2}{T}$,

$$d\Gamma=\frac{(2\pi)^4 m}{E_{q1}}\left(\prod_{j=1}^{h}\frac{d^3\vec{k}_j}{(2\pi)^3 2\omega_{kj}}\right)\left(\prod_{j=1}^{s}\frac{m d^3\vec{p}_j}{(2\pi)^3 E_{pj}}\right)|\boldsymbol{M}|^2\delta^4(q_1-\sum_1^h k_i-\sum_1^s p_j)$$

For a two fermion scattering process we have $n=2$, $\vec{v}_1$, $\vec{v}_2$ velocities of the incoming particles, $\mathrm{n}=1/V$ concentration of a incoming particle, we compute a differential effective cross section $\frac{|A|^2}{T\,\mathrm{n}\,|\vec{v}_1-\vec{v}_2|}$, $d\sigma=$ (*)

$$\frac{(2\pi)^4 m_1 m_2}{|\vec{v}_1-\vec{v}_2|E_{q1}E_{q2}}\left(\prod_{j=1}^{h}\frac{d^3\vec{k}_j}{(2\pi)^3 2\omega_{kj}}\right)\left(\prod_{j=1}^{s}\frac{m d^3\vec{p}_j}{(2\pi)^3 E_{pj}}\right)|\boldsymbol{M}|^2\delta^4(\sum_1^2 q_l-\sum_1^h k_i-\sum_1^s p_j)$$

Obviously we have

$((2\pi)^4\delta^4(p-p'))^2=(2\pi)^4\delta^4(p-p')\int\exp(-i(p-p')x)d^4x=$

$=(2\pi)^4\delta^4(p-p')VT$ and so taking in discretization $\delta^4(p-p')=C\,\delta_{pp'}$ we obtain $\delta^4(p-p')=\frac{VT}{(2\pi)^4}\delta_{pp'}$

In the same way we have:

$\delta^3(\vec{p}-\vec{p}')=\frac{V}{(2\pi)^3}\delta_{\vec{p}\vec{p}'}$ and $((2\pi)^3\delta^3(\vec{p}-\vec{p}'))^2=(2\pi)^3\delta^3(\vec{p}-\vec{p}')V$

Also , to be able to count states, we enclose our system in a box, say a cube with length L on each side with L much larger than the characteristic size of our system, having $V = L^3$. With periodic boundary conditions , the allowed plane wave states $\exp(i\vec{p}\vec{x})$ carry momentum $\vec{p}=\frac{2\pi}{L}(n_1,n_2,n_3)$ where $n_i\in\mathbb{Z}.$

The allowed values of momentum form a lattice of points with spacing $2\pi/L$ between points. Experimentalists measure momentum with finite resolution, small but much larger than $2\pi/L$. Thus an infinitesimal volume $d^3\vec{p}$ in momentum space contains $d^3\vec{p}/(2\pi/L)^3=V\,d^3\vec{p}/(2\pi)^3$ states.

In some cases we can split a process in small distance effects, as scattering $q_1,...,q_n$ incoming fermions momenta into $k_1,...,k_h$ outgoing bosons momenta and $p_1,...,p_s,q_{n+1},...,q_{n+r}$ outgoing fermions momenta, with $q_{n+1},...,q_{n+r}$ internal fermion lines momenta which in the large distance effects decay respective into external k_{h+i} boson momenta and p_{s+i} fermion momenta $(i=\overline{1,r})$

Since the $D^{fer}_{\alpha\beta}(q_{n+i})$ Fourier transform of the fermion propagator can be written as $\frac{2m\,u_\alpha(q_{n+i})\bar{u}_\beta(q_{n+i})}{q_{n+i}^2-m^2+i\varepsilon}$ and in the amplitude computation we must take $q_{n+i}=k_{h+i}+p_{s+i}$ we have the process amplitude factorization:

$$A_F(q,\widetilde{k},\widetilde{p})=A_F(q,k,\overline{p})\prod_{j=1}^{r}\frac{2mi}{(k_{h+j}+p_{s+j})^2-m^2+i\varepsilon}\boldsymbol{M}(k_{h+j}+p_{s+j},k_{h+j},p_{s+j})$$

where $q=(q_i)_{i=\overline{1,n}}$, $\widetilde{k}=(k_i)_{i=\overline{1,h+r}}$, $\widetilde{p}=(p_i)_{i=\overline{1,s+r}}$ and $\overline{p}=(p_1,...,p_s,k_{h+1}+p_{s+1},...,k_{h+r}+p_{s+r})$ and $A_F(a,b,c)$ is the Feynman amplitude for a incoming fermions, b outgoing bosons, c outgoing fermions momenta and $A_F=(2\pi)^4\boldsymbol{M}\,\delta^4((\sum a)-(\sum b)-(\sum c))$

We notice that the amplitude has a pike when the $k_{h+j}+p_{s+j}=q_{n+j}$ are on mass shell and so we can describe the transition probability of the process by the transition probability derived from the squared absolute value of the small distance effects amplitude which corresponds to an $(a,b,c)=(q,k,\overline{p})$ process.

In the case of quantum electrodynamics *U*(1) or electroweak *SU*(2)x*U*(1) theory, the renormalized couplings *g*, in a range of momentum are relatively small and so the higher order terms in *g* from the expansion of $\exp(i\int\mathcal{L}(\psi,\partial\psi,A,\partial A)d^4x)$ can be neglected, allowing a perturbation theory approach of the $q_1,...,q_n,k_1,...,k_h,p_1,...,p_s$ transition process, in which we take in consideration only the low order Feynman diagrams for the process.

In the case of quantum chromodynamics *SU*(3) , or unified *SU*(3)x*SU*(2)x*U*(1) or grand unified *SU*(5) theories the renormalized couplings go to zero when the momentum range goes to infinity and so we can have a perturbation theory approach

only for a high momentum range (asymptotic freedom). For a lower momentum range we must take the amplitudes defined by following relation (17):

$$A=V^{-(s+h+n)/2}\int\left((\prod_{j=1}^{s}(E_{pj}/m)^{1/2}\exp(ip_jx_j^a))(\prod_{j=1}^{h}(2\omega_{kj})^{1/2}\exp(ik_jy_j^a))\right.$$
$$\left.(\prod_{j=1}^{n}(E_{qj}/m)^{1/2}\exp(-iq_jx_j^b))S((x^a),(y^a),(x^b))\right)(\prod_{j=1}^{s}d^3\vec{x}^a)(\prod_{j=1}^{h}d^3\vec{y}^a)(\prod_{j=1}^{n}d^3\vec{x}^b)$$

where

$$S((x^a),(y^a),(x^b))=\left\langle 0\left|T\left((\prod_{j=1}^{s}\overline{u}_\alpha(p_j)\hat{\psi}_\alpha(x_j^a))(\prod_{j=1}^{h}(-\varepsilon^\lambda(k_j))\hat{A}_\lambda(y_j^a))\right.\right.\right.$$
$$\left.\left.\left.(\prod_{j=1}^{n}\hat{\overline{\psi}}_\beta(x_j^b)u_\beta(q_j))\right)\right|0\right\rangle=(\prod_{j=1}^{s}\overline{u}_\alpha(p_j))(\prod_{j=1}^{h}(-\varepsilon^\lambda(k_j)))(\prod_{j=1}^{n}u_\beta(q_j))C\int DA\,D\psi\,D\overline{\psi}$$
$$\exp(i\int\mathscr{L}(\psi,\partial\psi,A,\partial A)d^4x)(\prod_{j=1}^{s}\psi_\alpha(x_j^a))(\prod_{j=1}^{h}A_\lambda(y_j^a))(\prod_{j=1}^{n}\overline{\psi}_\beta(x_j^b))$$

considering $\mathscr{L}(\psi,\partial\psi,A,\partial A)$ as in (10) with all interaction terms within and according to a type (3) relation C is a discretisation dependent constant.

Also we take $x_j^a=T, y_j^a=T, x_j^b=0$ with $[0,T]$ the interaction process time interval and V, the space volume for the fields interaction process.

Notice that the $\hat{\psi}$, $\hat{A}$ operators are no more defined by (4c), (4b) relations, because we consider all Feynman diagrams associated with the process and take therefore all interaction terms products, which means that we consider the type (3) relation with the whole gauged Lagrangian density from (10).

Since the high order Feynman diagrams count (due to strong couplings), we expect that the quarks participate in interactions in groups (confinement) and so we have to consider that hadrons (groups of quarks and antiquarks of various colour indexes confined by gluon fields) will be forming.

The colour charge of a quark/antiquark defined by $(\psi_i)_{i=\overline{1,3}}$ with i colour index, ψ_i Dirac spinors,is defined by:

$\rho^a=\overline{\psi}_i\frac{1}{2}\lambda_{ij}^a\psi_j$ and there are 8 colour charges, one for each $(\lambda_{ij}^a)_{i,j}$ self-adjoint traceless 3x3 Gell-Mann matrix of the SU(3) colour gauge group generators:

$$\lambda^1=\begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix},\ \lambda^2=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix},\ \lambda^3=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&0\end{pmatrix},\ \lambda^4=\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix},$$
$$\lambda^5=\begin{pmatrix}0&0&-i\\0&0&0\\i&0&0\end{pmatrix},\ \lambda^6=\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix},\ \lambda^7=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix},\ \lambda^8=\frac{1}{\sqrt{3}}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-2\end{pmatrix}.$$

The $\hat{\rho}^a$ observables with $\langle \varphi|\hat{\rho}^a|\psi\rangle=(1/2)\lambda^a_{ij}\langle\overline{\varphi}_i|\psi_j\rangle$ are hermitean but not commute, so we choose a maximal subset of commuting colour charge operators which is

$\{(1/2)\lambda_3,(1/2)\lambda_8\}$,to define a colour charge observable: $\hat{\rho}^3\vec{e}_3+\hat{\rho}^8\vec{e}_8$.

For $a=3,8$,if $\psi_c=\gamma^2\psi^*$ with ψ^* the complex conjugate of ψ , corresponds to the antiparticle to ψ we have: $\overline{\psi}_{ci}\lambda^a_{ij}\psi_{cj}=\psi_i^{\mathrm{T}}\gamma^{2+}\gamma^0\lambda^a_{ij}\gamma^2\psi^*_j=-\overline{\psi}_i\lambda^a_{ij}\psi_j$, because

$\lambda^{aT}=\lambda^a$ for $a=3,8.$

Therefore the antiquarks carry the opposite colour charges to the quarks colour charges.

The forming hadrons must be colour charge singlets and so they can be the tensorial products of wave functions as mesons (quark- antiquark pairs) :

$\psi_M(t,x_1,x_2)=\sum_{i=1}^{3}\frac{1}{\sqrt{3}}\psi_{ci}(t,x_1)\psi_i(t,x_2)$ or as three quark/antiquark baryons:

$$\psi_B(t,x_1,x_2,x_3)=\sum\frac{1}{\sqrt{6}}\epsilon_{ijk}\psi_i(t,x_1)\psi_j(t,x_2)\psi_k(t,x_3)$$

$$\psi_{cB}(t,x_1,x_2,x_3)=\sum\frac{1}{\sqrt{6}}\epsilon_{ijk}\psi_{ci}(t,x_1)\psi_{cj}(t,x_2)\psi_{ck}(t,x_3)$$

In the amplitude expressions they appear as

$\sum\overline{\psi}_i\gamma^\mu\psi_i=\psi^\mu_M$ vector meson,

$\sum\overline{\psi}_i\psi_i=\psi_M$ scalar meson,

$(\sum\epsilon_{ijk}\psi_{i\alpha}\psi_{j\beta}\psi_{k\gamma})=(\psi_B^{\alpha\beta\gamma})$ baryon,

$(\sum\epsilon_{ijk}\overline{\psi}_{i\alpha}\overline{\psi}_{j\beta}\overline{\psi}_{k\gamma})=(\psi_{\overline{B}}^{\alpha\beta\gamma})$ antibaryon

The common eigenvectors (colour eigenstates) of $\hat{\rho}^3$, $\hat{\rho}^8$ are

$\psi_r=\begin{pmatrix}1\\0\\0\end{pmatrix}\otimes\psi=\vec{r}\otimes\psi$; $\psi_g=\begin{pmatrix}0\\1\\0\end{pmatrix}\otimes\psi=\vec{g}\otimes\psi$; $\psi_b=\begin{pmatrix}0\\0\\1\end{pmatrix}\otimes\psi=\vec{b}\otimes\psi$ with ψ a Dirac spinor function ,having colour charges respectively

$\vec{q}_r=\frac{1}{2}\vec{e}_3+\frac{1}{2\sqrt{3}}\vec{e}_8$; $\vec{q}_g=-\frac{1}{2}\vec{e}_3+\frac{1}{2\sqrt{3}}\vec{e}_8$; $\vec{q}_b=-\frac{1}{\sqrt{3}}\vec{e}_8$.

We have $\vec{q}_r+\vec{q}_g+\vec{q}_b=0.$ The mesons and baryons have neutral colour charge.

The mesons are integer spin particles (0 – scalar , 1 – vector) and the baryons are half integer spin particles.

For example the proton is $\sum\frac{1}{\sqrt{6}}\epsilon_{abc}u^a u^b d^c$ with a,b,c colour indices

u up-quark, d down-quark, where two of the quarks u^a,u^b,d^c carry opposite secondary spin quantum numbers (if the u^a , u^b , d^c are spin eigenvectors). The proton is a spin ½ particle. The same way spin ½ combination *udd* gives the other nucleon, known as the neutron.

For a three quark baryon for example, with $\hat{\psi}^1, \hat{\psi}^2, \hat{\psi}^3$ respective the three quark operator functions, the process with p_1, p_2, p_3 outgoing four-momenta and q_1, q_2, q_3 incoming four-momenta, having $p_i = q_i, i = \overline{1,3}$ on mass shell will have an amplitude defined by the following relation (18):

$$A(\vec{p}_1, \vec{p}_2, \vec{p}_3) = \int \frac{1}{6} V^{-3} \left(\prod_{l=1}^{3} \exp(i p_l (x_l^a - x_l^b)) \bar{u}^l_{i l \alpha l}(p_l) u^l_{j l \beta l}(p_l) (E_{pl}/m_l)\right)$$
$$\epsilon_{i1i2i3} \epsilon_{j1j2j3} \langle 0 | \hat{\psi}^1_{i1\alpha1}(x_1^a) \hat{\psi}^2_{i2\alpha2}(x_2^a) \hat{\psi}^3_{i3\alpha3}(x_3^a) \hat{\bar{\psi}}^1_{j1\beta1}(x_1^b) \hat{\bar{\psi}}^2_{j2\beta2}(x_2^b) \hat{\bar{\psi}}^3_{j3\beta3}(x_3^b) | 0 \rangle$$
$$\prod_{k=1}^{3} d^3 \vec{x}_k^a d^3 \vec{x}_k^b$$

where we use Einstein summation convention for $il, jl, \alpha l, \beta l$ indices and take $x_l^{a0} = T, x_l^{b0} = 0$, $p_l^0 = E_{pl} = \sqrt{\vec{p}_l^2 + m_l^2}$

il, jl are colour indices from 1 to 3 and $\alpha l, \beta l$ are Dirac indices from 0 to 3 .

Therefore, a energy eigenstate wave function $\psi_{0B} = \psi_{0B}(\vec{x}_1, \vec{x}_2, \vec{x}_3)$ for the baryon can be derived, taking

$\psi_{0B} = \int (1/(2\pi)^9) \exp(i \vec{p}_l \vec{x}_l) A(\vec{p}_1, \vec{p}_2, \vec{p}_3) d^3 \vec{p}_1 d^3 \vec{p}_2 d^3 \vec{p}_3$ (19).

As we mentioned , for an antiparticle occurring instead of a particle in the composition of the baryon in the $A(p_1, p_2, p_3)$ expression we will take

$v_\alpha(p) \hat{\bar{\psi}}_\alpha(x^a)$ instead of $\bar{u}_\alpha(p) \hat{\psi}_\alpha(x^a)$ and

$\bar{v}_\beta(p) \hat{\psi}_\beta(x^b)$ instead of $u_\beta(p) \hat{\bar{\psi}}_\beta(x^b)$

Also we have:

$$\langle 0 | \hat{\psi}^1_\alpha(x_1^a) \hat{\psi}^2_\beta(x_2^a) \hat{\psi}^3_\gamma(x_3^a) \hat{\bar{\psi}}^1_\delta(x_1^b) \hat{\bar{\psi}}^2_\varepsilon(x_2^b) \hat{\bar{\psi}}^3_\varphi(x_3^b) | 0 \rangle =$$
$$= C \int D A D \psi D \bar{\psi} \Big(\exp\left(i \int \mathcal{L}(\psi, \partial\psi, A, \partial A) d^4 x\right) \quad (18')$$
$$\psi^1_\alpha(x_1^a) \psi^2_\beta(x_2^a) \psi^3_\gamma(x_3^a) \bar{\psi}^1_\delta(x_1^b) \bar{\psi}^2_\varepsilon(x_2^b) \bar{\psi}^3_\varphi(x_3^b) \Big)$$

It follows that for making computed theoretical predictions and comparisons of different processes , we must be able to compute (by making a suitable discretization) path integrals of the form

$\int D A D \psi D \bar{\psi} \exp(\mathcal{L}(\psi, \partial\psi, A, \partial A) d^4 x) O(A, \psi, \bar{\psi})$

where O is a function operator depending on the fields $A, \psi, \bar{\psi}$ and can be for example :

$$O(A, \psi, \bar{\psi}) = \int \Bigg(\left(\prod_{j=1}^{s} \exp(i p_j x_j^a)\right) \left(\prod_{j=1}^{h} \exp(i k_j y_j^a)\right) \left(\prod_{j=1}^{n} \exp(-i q_j x_j^b)\right) \quad (18'')$$
$$\left(\prod_{j=1}^{s} \psi^{\alpha j}_{\mu j}(x_j^a)\right) \left(\prod_{j=1}^{h} A^{aj}_{\lambda j}(y_j^a)\right) \left(\prod_{j=1}^{n} \bar{\psi}^{\beta j}_{\nu j}(x_j^b)\right) \Bigg) \left(\prod_{j=1}^{s} d^3 \vec{x}_j^a\right) \left(\prod_{j=1}^{h} d^3 \vec{y}_j^a\right) \left(\prod_{j=1}^{n} d^3 \vec{x}_j^b\right)$$

where $\alpha j, \beta j, a j$ are quark/lepton/gluon sort and colour indices and $\mu j, \nu j$ respective λj are Dirac and Lorentz indices.

Consider now a hadron with momentum $k=(k^0,\vec{k})$ and the light-cone coordinates $x^+=(x^0+\vec{x}\cdot\mathrm{vers}\,\vec{k})/\sqrt{2}$, $x^-=(x^0-\vec{x}\cdot\mathrm{vers}\,\vec{k})/\sqrt{2}$

$\vec{x}_\perp=\vec{x}-(\vec{x}\cdot\mathrm{vers}\,\vec{k})\,\mathrm{vers}\,\vec{k}$, $\vec{x}_\parallel=(\vec{x}\cdot\mathrm{vers}\,\vec{k})\,\mathrm{vers}\,\vec{k}$.

The quark constituents of the hadron have momenta k_j (j = 1 , 2 for mesons and j = 1 , 2 , 3 for baryons) with fractions x_j and relations

$k_j^+=x_j k^+$, $\sum x_j=1$, $\sum \vec{k}_{j\perp}=0$, $2k_j^+k_j^--\vec{k}_{j\perp}^2=m_j^2$, $\vec{k}_{j\perp}\cdot\mathrm{vers}\,k=0$

$x_j\in[0,1]$, $k_j^0=\frac{1}{\sqrt{2}}\left(x_jk^++\frac{\vec{k}_{j\perp}^2+m_j^2}{2x_jk^+}\right)$

$k^+k^-=M^2$ where M is the effective mass of the hadron,

$k^0=\frac{1}{\sqrt{2}}\left(k^++\frac{M^2}{2k^+}\right)$, $\vec{k}_j=\vec{k}_{j\perp}+\frac{1}{\sqrt{2}}\left(x_jk^+-\frac{\vec{k}_{j\perp}^2+m_j^2}{2x_jk^+}\right)\mathrm{vers}\,\vec{k}$.

Thus we have a functional dependence $k_j=k_j(x_j,\vec{k}_{j\perp},\vec{k})$ (20).

With the constituents momenta $(k_j)_j$ in the place of $(p_j)_j$ momenta in $(18),(19)$ like relations, we can change the variables $(k_j)_j$ to variables

$$((x_j)_{j=\overline{1,m-1}},(k_{j\perp}^1,k_{j\perp}^2)_{j=\overline{1,m-1}},\vec{k})=(\tilde{x},\tilde{k}_\perp,\vec{k})$$

where $k_{j\perp}^l=\vec{k}_{j\perp}\cdot e_l$, $e_l\cdot e_i=\delta_{il}$, $e_i\cdot\vec{k}=0$; $i,l=1,2$

and m is the hadron's number of quark constituents and so we have the hadron momentum space wave function and the hadron energy eigenstate wave function computable according to (18) , (18') respective (19) like relations in the form

$A((k_j)_{j=\overline{1,m}})=\widetilde{DA}(\tilde{x},\tilde{k}_\perp,\vec{k})$

$\psi_{0H}((\vec{x}_j)_{j=\overline{1,m}})=\int B(\tilde{x},\tilde{k}_\perp,\vec{k},(\vec{x}_j)_{j=\overline{1,m}})\,d^{m-1}\tilde{x}\,d^{2m-2}\tilde{k}_\perp\,d^3\vec{k}$ (21).

The distribution amplitude us defined as :

$DA(\tilde{x},\vec{k})=\int\widetilde{DA}(\tilde{x},\tilde{k}_\perp,\vec{k})\,d^{2m-2}\tilde{k}_\perp$ and taking $W=\int|DA(\tilde{x},\vec{k})|^2\,d^{m-1}\tilde{x}$

we have that $\frac{1}{W}|DA(\tilde{x},\vec{k})|^2\,d^{m-1}\tilde{x}$ describes the probability of finding the constituents in state of $(x_j)_{j=\overline{1,m}}$ fraction values of k^+ at hadron momentum $\vec{k}$.

(The location variables in (21), $\vec{x}_j$ and the momentum fractions x_j should obviously not be mixed up!)

With the relations (20), an amplitude for a process of (p_1 , … , p_s) outgoing fermions momenta, which are grouping themselves as outgoing hadrons (k_1 , … , k_m) having fraction values for constituents respectively

$((x_{il})_{l=\overline{1,mi}})_{i=\overline{1,m}}$ taking $\tilde{x}_i=(x_{il})_{l=\overline{1,mi-1}}$, $\tilde{x}=(\tilde{x}_i)_{i=\overline{1,m}}$,

(q_1 , … , q_n) incoming fermions momenta, which are grouping themselves as incoming hadrons(k'_1 , … , $k'_{m'}$) having fraction values for constituents respectively

$((x'_{il})_{l=\overline{1,m'i}})$ taking $\tilde{x}'_i=(x'_{il})_{l=\overline{1,m'i-1}}$, $\tilde{x}'=(\tilde{x}'_i)_{i=\overline{1,m'}}$,

(r_1 , … , r_h) outgoing bosons momenta , can be described as a function of the constituents fractions and normal momentum components for the hadrons , and of the momenta of the hadrons:

$A(q,r,p)=A_H(\widetilde{x},\widetilde{k}_\perp,\widetilde{x}',\widetilde{k}'_\perp,\vec{k},\vec{k}',r)$.

To compute decay rates or cross sections we need the transition probabilities $|A|^2$.

Integrating $|A_H|^2$ over the $\widetilde{x},\widetilde{k}_\perp,\widetilde{x}'$, $\widetilde{k}'_\perp$ variables with the weight $\left(\prod_{i=1}^{m}\frac{|\widetilde{DA}_i(\widetilde{x}_i,\widetilde{k}_{i\perp},\vec{k}_i)|^2}{W_i}\right)\left(\prod_{i=1}^{m'}\frac{|\widetilde{DA}'_i(\widetilde{x}'_i,\widetilde{k}'_{i\perp},\vec{k}'_i)|^2}{W'_i}\right)$, where

$W_i=\int|\widetilde{DA}_i(\widetilde{x}_i,\widetilde{k}_{i\perp},\vec{k}_i)|^2 d^{mi-1}\widetilde{x}_i d^{2mi-2}\widetilde{k}_{i\perp}$

$W'_i=\int|\widetilde{DA}'_i(\widetilde{x}'_i,\widetilde{k}'_{i\perp},\vec{k}_i)|^2 d^{m'i-1}\widetilde{x}'_i d^{2m'i-2}\widetilde{k}'_{i\perp}$,

we obtain a transition probability in terms of the momenta of the hadrons:

$|\widetilde{A}_H|^2=|\widetilde{A}_H|^2(\vec{k},\vec{k}',r)$.

Let for $i=\overline{1,m}$, $q^i=(q^i_l)_{l=\overline{1,mi}}$ the momenta of the quarks/antiquarks which are constituents of the outgoing hadron with four-momentum k_i .

As we noticed we have the bijective correspondence $(q^i_l)_l=(q^i_l)_l(\widetilde{x}_i,\widetilde{k}_{i\perp},\vec{k}_i)$.

The number of q^i states (on mass shell) corresponding to a hyper-volume $dw=d^{mi-1}\widetilde{x}_i d^{2mi-2}\widetilde{k}_{i\perp}d^3\vec{k}_i$ located at $(\widetilde{x}_i,\widetilde{k}_{i\perp},\vec{k}_i)$ is

$$dw=\left(\frac{V}{(2\pi)^3}\right)^{mi}\left|\det\frac{D((q^i_l)_l)}{D(\widetilde{x}_i,\widetilde{k}_{i\perp},\vec{k}_i)}\right|d^{mi-1}\widetilde{x}_i d^{2mi-2}\widetilde{k}_{i\perp}d^3\vec{k}_i$$

and therefore the number of k_i states (on mass shell) corresponding to a volume $d^3\vec{k}_i$ located at $\vec{k}_i$ is $\left(\frac{V}{(2\pi)^3}\right)^{mi}\widetilde{W}_i(\vec{k}_i)d^3\vec{k}_i$ where

$$\widetilde{W}_i(\vec{k}_i)=\int\left|\det\frac{D((q^i_l)_l)}{D(\widetilde{x}_i,\widetilde{k}_{i\perp},\vec{k}_i)}\right|d^{mi-1}\widetilde{x}_i d^{2mi-2}\widetilde{k}_{i\perp}$$

with integration on [0,1] for the momentum fractions variables and a certain bounded range of momentum for the normal momenta variables.

Thus we obtain computable differential decay rates and differential cross sections for a hadron decay or a two hadrons scattering to a number of outgoing hadrons processes:

$$d\Gamma=\frac{|\widetilde{A}_H|^2}{T}\prod_{i=1}^{m}\left(\frac{V}{(2\pi)^3}\right)^{mi}\widetilde{W}_i(\vec{k}_i)d^3\vec{k}_i \qquad (22)$$

$$d\sigma=\frac{|\widetilde{A}_H|^2}{|\vec{v}_1-\vec{v}_2|}\frac{V}{T}\prod_{i=1}^{m}\left(\frac{V}{(2\pi)^3}\right)^{mi}\widetilde{W}_i(\vec{k}_i)d^3\vec{k}_i \qquad (23)$$

where $|A_H|^2=|A_H|^2((\vec{k}_i)_{i=\overline{1,m}},\vec{k}'_1)$ for a hadron decay and $|A_H|^2=|A_H|^2((\vec{k}_i)_{i=\overline{1,m}},\vec{k}'_1,\vec{k}'_2)$ for a two hadrons scattering .

Obviously , also leptons or bosons can appear as outgoing particles. We simply include their momenta in the outgoing momenta list and do the calculations as they have no constituents as well and so if such a particle is listed under index j and so the list of its constituents is void and m_j= 0.

k_i are the outgoing momenta, k'_i are the incoming momenta and $\vec{v}_1, \vec{v}_2$ are the velocities of the scattering hadrons V, T are spatial volume and respective time interval for the process action.
V, T are constants part of the lattice simulation we consider and the discretization and fermion Grassmann variables normalization constants which appear as coefficients in a lattice simulation computation are to be setup by measurements performed in one of any known physical process from the computing of which we can extract the coefficient and it will have the same value for any other process we further consider for computation.

Consider now the scattering process corresponding to the Feynman diagram in fig.1

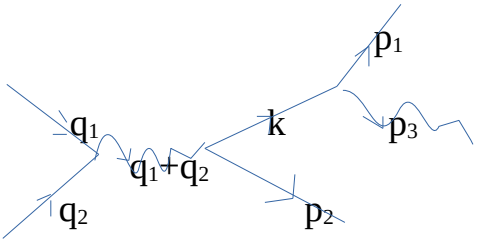


fig.1

q_1 , q_2 are the incoming fermions, p_1 , p_2 are outgoing fermions , p_3 is an outgoing boson four-momentum end legs lines labels and $q_1 + q_2$ labels as four-momentum an internal boson line, k labels as four-momentum an internal fermion line.
As we shown above we can factorize the fig.1 process through the decay of the k particle to p_1 and p_3 particles obtaining for the Feynman amplitudes the relation:

$$\widetilde{A}_F = A_F((q_1,q_2),(p_3),(p_1,p_2)) =$$
$$= A_F((q_1,q_2),\phi,(p_2,p_1+p_3))\frac{2mi}{(p_1+p_3)^2 - m^2 + i\varepsilon}\boldsymbol{M}((p_1+p_3),(p_3),(p_1)) \quad (24)$$

where ϕ stands for an empty list of bosons four-momenta.
In the mass centre frame of the incoming particles (which are supposed to be on mass shell) we can consider
$\vec{q}_1 = (q,0,0)$, $\vec{q}_2 = (-q,0,0)$ and also $\vec{q}_i^{\,2} = q_i^{02}$, $q_i^0 = q$ because we neglect the incoming fermions masses.
Momentum conservation leads to
$k = p_1 + p_3$, $\sum_i p_i^0 = 2q$, $\sum_i \vec{p}_i = \vec{q}_1 + \vec{q}_2 = 0$ and we take the fractions relations:
$p_i^0 = x_i q$, $\sum_i x_i = 2$ and neglecting fermion and boson masses we have also
$\|\vec{p}_i\| = x_i q$ since the particles are supposed to be on mass shell.
Let $\frac{\vec{p}_i \cdot \vec{p}_j}{\|\vec{p}_i\| \, \|\vec{p}_j\|} = \cos(\theta_{ij})$.

From the momentum conservation follows now

$2(1-x_1)=x_2x_3(1-\cos(\theta_{23}))$

$2(1-x_2)=x_1x_3(1-\cos(\theta_{13}))$

$2(1-x_3)=x_1x_2(1-\cos(\theta_{12}))$

Using Feynman rules with the convention that Greek indices are Dirac spinor indices and Latin indices are fermion / boson designating indices , (24) becomes:

$$\widetilde{A}_F=-(2\pi)^4\frac{2m_cg^2}{4q^2(1-x_2)}\bar{u}^c_\alpha(p_1+p_3)T^a_{cd}\gamma^\mu_{\alpha\beta}v^d_\beta(p_2)\frac{1}{r^2}\left(\eta^{\mu\lambda}-\frac{r_\mu r_\lambda}{M_a^2}\right)\gamma^\lambda_{\rho\varepsilon}\bar{v}^{c'}_\rho(q_1) \quad (25)$$

$$u^{d'}_\varepsilon(q_2)T^a_{c'd'}u^c_\beta(p_1+p_3)\gamma^\nu_{\delta\beta}\bar{u}^e_\delta(p_1)T^{a'}_{ec}\varepsilon^{a'}_\nu(p_3)\delta^4(p_1+p_2+p_3-q_1-q_2)$$

where $r=q_1+q_2$.

Considering the (4') relations we have

$\bar{v}^{c'}_\rho(q_1)\gamma^\lambda_{\rho\varepsilon}(q_1+q_2)_\lambda u^{d'}_\varepsilon(q_2)=(-m_{c'}+m_{d'})\bar{v}^{c'}_\varepsilon(q_1)u^{d'}_\varepsilon$ and since we have taken

$m_{c'}\approx m_{d'}\approx 0$ we can drop the $\frac{r_\mu r_\lambda}{M_a^2}$ term in (25) .

Taking $\widetilde{A}_F=(2\pi)^4\widetilde{\boldsymbol{M}}\,\delta^4(p_1+p_2+p_3-q_1-q_2)$ and considering (4) , (4''') relations, with summation over (averaged) spin polarizations, we will have

$$\text{a}\quad |\widetilde{\boldsymbol{M}}|^2=\frac{g^4}{16q^4(1-x_2)^2}\left|T^{a'}_{ec}T^a_{cd}T^a_{c'd'}\right|^2 4m_c^2\,\text{tr}\left(\frac{\not p_1+\not p_3+m_c}{2m_c}\gamma^\mu\frac{\not p_2-m_d}{2m_d}\gamma^{\mu'}\right)$$

$$\text{tr}\left(\frac{\not q_1-m_{c'}}{2m_{c'}}\gamma^\lambda\frac{\not q_2+m_{d'}}{2m_{d'}}\gamma^{\lambda'}\right)\frac{\eta^{\mu\lambda}\eta^{\mu'\lambda'}}{((q_1+q_2)^2)^2}\,\text{tr}\left(\frac{\not p_1+m_e}{2m_e}\gamma^\nu\frac{\not p_1+\not p_3+m_c}{2m_c}\gamma^{\nu'}\right)$$

$$\left(-\eta^{\nu\nu'}+\frac{p_{3\nu}p_{3\nu'}}{M^2_{a'}}\right) \qquad (26)$$

We have

$$\text{tr}\left(\frac{\not p_1+m_e}{2m_e}\gamma^\nu\frac{\not p_1+\not p_3+m_c}{2m_c}\gamma^{\nu'}\right)p_{3\nu}p_{3\nu'}=$$

$=u^e_\alpha(p_1)\bar{u}^e_\beta(p_1)\not p_{3\beta\gamma}u^c_\gamma(p_1+p_3)\bar{u}^c_\delta(p_1+p_3)\not p_{3\delta\alpha}$ and

$\bar{u}^e(p_1)\not p_3u^c(p_1+p_3)=(-m_e+m_c)\bar{u}^e(p_1)u^c(p_1+p_3)\approx 0$

(since we take $m_e\approx m_c\approx 0$) .

Therefore we can drop the $\frac{p_{3\nu}p_{3\nu'}}{M^2_{a'}}$ term in the (26) expression for $|\widetilde{\boldsymbol{M}}|^2$.

We can verify that

$\text{tr}\,\gamma^\nu\gamma^\mu=4\eta^{\mu\nu}$, $\text{tr}\,\gamma^\mu\gamma^\nu\gamma^\lambda\gamma^\sigma=4(\eta^{\mu\nu}\eta^{\lambda\sigma}-\eta^{\mu\lambda}\eta^{\nu\sigma}+\eta^{\mu\sigma}\eta^{\nu\lambda})$ and that the traces of a product of an odd number of gamma matrices vanish.

It follows :

$$\mathrm{tr}\left((\not r_1+m_1)\gamma^\mu(\not r_2+m_2)\gamma^\nu\right)=4\left(r_1^\mu r_2^\nu+r^\nu r_2^\mu-\eta^{\mu\nu}r_1\cdot r_2+\eta^{\mu\nu}m_1m_2\right)$$

and so for $B_{\lambda\lambda'}=\mathrm{tr}\left(\frac{\not q_1-m_{c'}}{2m_{c'}}\gamma^\lambda\frac{\not q_2+m_{d'}}{2m_{d'}}\gamma^{\lambda'}\right)$ we obtain

$$B_{\lambda\lambda'}=\begin{cases}\eta^{\lambda\lambda'}\left(1-\frac{2q^2}{m_{c'}m_{d'}}\right) & \text{for } \lambda,\lambda'\neq 0,1\\ 0 & \text{for } \{\lambda,\lambda'\}=\{0,1\}\\ \eta^{\lambda\lambda'} & \text{for } \lambda=\lambda'\in\{0,1\}\end{cases} \qquad (27)$$

and also, after some calculus:

$$\mathrm{tr}\left(\frac{\not p_1+m_e}{2m_e}\gamma^\nu\frac{\not q_1+\not p_3+m_c}{2m_c}\gamma^{\nu'}\right)\eta^{\nu\nu'}=4\left(1-\frac{q^2}{m_em_c}(1-x_2)\right) \qquad (28)$$

In the cross section expression we have , according to a (*) relation ,we will have a partial factor $\frac{m_{c'}m_{d'}}{q^2}$ and since we approximate $m_{c'}\approx m_{d'}\approx 0$, from the (27) factor, in the cross section expression we must keep only $-2\eta^{\lambda\lambda'}q^2$ with $\lambda,\lambda'=2,3$ having further:

$$\mathrm{tr}\left(\frac{\not p_1+\not p_3+m_c}{2m_c}\gamma^\mu\frac{\not p_2-m_d}{2m_d}\gamma^{\mu'}\right)(-2\eta^{\lambda\lambda'})\eta^{\mu\lambda}\eta^{\mu'\lambda'}=$$

$$=-2-\frac{1}{m_cm_d}(2p_{21}^2+2(2-x_2)x_2q^2) \qquad (29)$$

Since in the cross section expression we have also a partial factor $\frac{m_dm_e}{x_1x_2q^2}$ and we approximate $m_d\approx m_e\approx 0$ we must keep from the (28) factor only $-\frac{4}{m_c}(1-x_2)q^2$ and from the (29) factor, only $-2(p_{21}^2+(2-x_2)x_2q^2)$.

Thus the differential cross section is , after some calculus

$$d\sigma=\frac{f}{q^9}\frac{p_{21}^2+(2-x_2)x_2q^2}{(1-x_2)x_1x_2x_3}d^3\vec p_1d^3\vec p_2d^3\vec p_3\delta^4(q_1+q_2-p_1-p_2-p_3)=$$

$$=\frac{f}{q^7}\frac{x_2^2\cos^2(\theta_2)+(2-x_2)x_2}{(1-x_2)x_1x_2x_3}\sin(\theta_1)\sin(\theta_2)x_1^2x_2^2q^6dx_1dx_2d\theta_1d\theta_2d\varphi_1d\varphi_2$$

$$\delta(2q-q(x_1+x_2+x_3))d^3\vec p_3\delta^3(\vec q_1+\vec q_2-\vec p_1-\vec p_2-\vec p_3)$$

where $f=\left|T^{a'}_{ec}T^a_{cd}T^a_{c'd'}\right|^2\frac{1}{8(2\pi)^9}\frac{g^4}{|\vec v_1-\vec v_2|}$ (in the mass centre of the incoming particles frame).

Integrating over $(\theta_i,\varphi_i)\in(0,\pi)\times(0,2\pi)$, $i=1,2$ and $\vec p_3$ we obtain

$$d\sigma = \frac{32}{3} f \pi^2 \frac{x_1 x_2^2 (3-x_2)}{q(1-x_2)(2-x-1-x_2)} \delta(2q - q(x_1+x_2+x_3)) =$$

$$= F \frac{2x_2^2(3-x_2)}{x_3^2(1-\cos(\theta_{13}))} dx_1 dx_2$$

where $F = \frac{16}{3}\frac{fT}{q}\pi$ and T is the process time interval .

(the Dirac distribution factor is over the 0 component of the four momentum, which is conjugated to time variable and we have therefore $\delta(q'-q'') = \frac{T}{2\pi}\delta_{q'q''}$)

The differential cross section has a pike at $x_3 = 0$ and at $\cos(\theta_{13}) = 1$.

In both cases it follows $x_2 = 1$ and $(p_1+p_3)^2 = q^2((2-x_2)^2 - x_2^2) = 4q^2(1-x_2) = 0.$

Therefore, since we neglected the fermion mass, the *k* = p_1+p_3 fermion can be considered on mass shell and $\vec{p}_1$, $\vec{p}_3$ are collinear.

Let us choose the x^3 axis close to the direction $\vec{k} = \vec{p}_1 + \vec{p}_3$ and with orientation opposite to $\vec{p}_2$ orientation, so that the light-cone frame coordinates are

$$x^+ = (x^3 + x^0)/\sqrt{2} \ , \ x^- = (x^0 - x^3)/\sqrt{2} \ , \ \vec{x}_\perp = (x_1, x_2, 0)$$

Then $\vec{k}_\perp \approx \vec{0}$, $k^+ = (p_1^0 + p_3^0 + \|\vec{p}_2\|)/\sqrt{2} = ((2-x_2)q + x_2 q)/\sqrt{2} = \sqrt{2}q$.

In the scattering experiments, 2 *q* is very large (it is the energy at which the particles collide in the mass centre frame).

Since the *k* particle is on mass shell when the cross section reaches the piked significant value, we have $k^- = (\vec{k}_\perp^2 + m_c^2)/(2k^+)$.

Therefore, since $\vec{k}_{\perp,} \approx \vec{0}$, $m_c \approx 0$ and k^+ is very large, k^- must be very small and so $k^3 = (k^+ - k^-)/\sqrt{2}$ is also very large.

The *k* particle on mass shell propagates from the q_1+q_2 boson decay location $\vec{0}$ to the location $\vec{x}$ where decays into the p_1 fermion and the p_3 boson and because $\vec{k}_\perp \approx \vec{0}$ we can assume $\vec{x}_\perp \approx \vec{0}$

We have $\vec{k} = \frac{m_c \vec{v}}{\sqrt{1-\vec{v}^2}}$, the propagation time is $T = x^0$

and Lorentz invariance leads to $kx = m_c T\sqrt{1-\vec{v}^2}$. Also because $\vec{v}T = \vec{x}$

and $k^0 = \frac{m_c}{\sqrt{1-\vec{v}^2}}$ we obtain $k^0 x^3 \approx k^3 x^0$, $k^+ x^- \approx k^- x^+$.

Hence $kx = k^+ x^- + k^- x^+ - \vec{k}_\perp \vec{x}_\perp \approx 2k^+ x^- \approx 2k^- x^+$.

Because k^+ is very large and k^- is very small (obviously as an absolute value) it follows that $\vec{x} \approx (0,0,x^3)$ must be very large as an absolute value.

The scattering cross section goes to infinity when

$p_0^3 \approx 0$ ($x_3 = 0$) and so we can call the fig.1 diagram not infrared safe.

Since x^3 is very large, the decay of the *k* emergent particle into a p_1 fermion and a p_3 boson occurs at a large distance from the q_1,q_2 fermions scattering point and

therefore we can reduce a scattering process through factorization, as exposed, to the small distance effects (in the fig.1 case the scattering to *k* and p_2 fermions on mass shell) which will be infrared safe.

Consider now a quark-antiquark meson. The constituents quark and antiquark constantly change colour due to strong interaction such that when a colour α quark is at location $\vec{r}_1$ an anticolour α antiquark is at location $\vec{r}_2$ with $\alpha\in\{\text{r,g,b}\}$. For the quark-gluon-antiquark interaction within the meson, the gluon fields change much faster than the quark and antiquark fields an so we can consider a potential energy of the quark-antiquark pair which is $V(\vec{r})=E(r)$ where $\vec{r}=\vec{r}_1-\vec{r}_2$, $r=\|\vec{r}\|$ and $E(r)$ is the energy of the gluons intermediating the quark-antiquark interaction.

During the gluon fields interaction time *T*, while the quark and antiquark are respectively at location $\vec{r}_1$ and $\vec{r}_2$ we have a quark colour charge current $J_1^{a\mu}(t,\vec{x})=g\,\psi^{\alpha T}T^a_{\alpha\beta}\psi^{\beta}\overline{\psi}_1\gamma^{\mu}\psi_1(t,\vec{x})$ and an antiquark colour charge current $J_2^{a\mu}(t,\vec{x})=-g\,\psi^{\alpha T}T^a_{\alpha\beta}\psi^{\beta}\overline{\psi}_{2c}\gamma^{\mu}\psi_{2c}(t,\vec{x})$, where we have a minus sign since the quark and antiquark carry opposite colour charges and the notations correspond to :

$T^a=\frac{1}{2}\lambda^a$, the ψ^{α} is one of the three colour charge eigenvectors $(1,0,0)$, $(0,1,0)$, $(0,0,1)$ and $\psi_c=\gamma^2\psi^*$ noticing that $\overline{\psi}_c\gamma^{\mu}\psi_c=\overline{\psi}\gamma^{\mu}\psi$ with ψ_i a Dirac spinor.

Considering the location of the quark and antiquark during the faster changing gluon fields intermediated interaction we can take $(\overline{\psi}_1\gamma^{\mu}\psi_1)_{\mu}=(\delta^3(\vec{x}-\vec{r}_1),0,0,0)$ and $(\overline{\psi}_2\gamma^{\mu}\psi_2)_{\mu}=(\delta^3(\vec{x}-\vec{r}_2),0,0,0)$.

Not considering the cubic and quartic gluon interactions the gluon fields Lagrangian density is :

$$\mathcal{L}((A^a,\partial A^a)_a)=-\frac{1}{4}(\partial_{\mu}A^a_{\nu}-\partial_{\nu}A^a_{\mu})(\partial^{\mu}A^{a\nu}-\partial^{\nu}A^{a\mu})+\frac{1}{2}M_a^2A^a_{\mu}A^{a\mu}+(J_1^{a\mu}+J_2^{a\mu})A^a_{\mu}$$

We have :

$$Z(J)=\exp(-iE(r)T)=Z(J=0)\exp\left(-(i/2)\int J^a(x)D^a(x-y)J^a(y)d^4x\,d^4y\right)$$

where $D^a_{\mu\nu}(x-y)=\int-\frac{1}{(2\pi)^4}\frac{\exp(-ik(x-y))}{k^2-M_a^2+i\varepsilon}\left(\eta^{\mu\nu}-\frac{k_{\mu}k_{\nu}}{M_a^2}\right)d^4k$ is the gluon propagator.

Excluding the vacuum energy (that is excluding $Z(J=0)$) we can take

$$E(r)T=\int\left(\frac{1}{2}(J_1^a(x)D^a(x-y)J_1^a(y)+J_2^a(x)D^a(x-y)J_2^a(y))+\right.$$

$$\left.+J_1^aD^a(x-y)J_2^a(y)\right)d^4x\,d^4y=\int d^4k\int dx^0dy^0\exp(-ik^0(x^0-y^0)) \quad (30)$$

$$\frac{-1+k^{02}/M_a^2}{k^2-M_a^2+i\varepsilon}S_{\alpha a}\frac{g^2}{(2\pi)^4}(1-\exp(\vec{k}\vec{r}))=T\frac{g^2}{(2\pi)^3}S_{\alpha a}\int\left(\frac{1-\exp(i\vec{k}\vec{r})}{\vec{k}^2+M_a^2}\right)d^3\vec{k}$$

where $S_{\alpha a}=0$ for $a\notin\{3,8\}$, $S_{\alpha 3}=\frac{1}{4}$, $S_{\alpha 8}=\frac{1}{12}$ for $\alpha\in\{\mathrm{r,g}\}$, $S_{b3}=0$, $S_{b8}=\frac{1}{3}$

and in (30) we take the summation over *a* index.

Taking $M_3=M_8=0$ we have:

$$E(r)=E_0-\frac{g^2}{3(2\pi)^3}\int\frac{\exp(i\vec{k}\vec{r})}{\vec{k}^2}d^3\vec{k}$$

$$\int\frac{\exp(i\vec{k}\vec{r})}{\vec{k}^2}d^3\vec{k}=2\pi\int_0^{\pi}\int^{\infty}\exp(ikr\cos(\theta))\sin(\theta)\,d\theta\,dk=4\pi\int_0^{\infty}\frac{\sin(kr)}{kr}dk$$

We integrate over a range of momentum $k=\|\vec{k}\|$ for which $kr\ll 1$ so that we have quark confinement (the SU(3) chromodynamics coupling is strong at low energy).

Let $\|\vec{k}\|<a$. Hence with $ar\ll 1$ we will have:

$$E(r)=E_0-\frac{g^2}{3(2\pi)^3}4\pi\int_0^{ar}\frac{1}{r\tau}\sin(\tau)d\tau\approx$$

$$\approx E_0-\frac{g^2}{6\pi^2 r}\int_0^{ar}\left(1-\frac{1}{6}\tau^2\right)d\tau=E_0-g^2\frac{a}{6\pi^2}+Br^2$$

where $B=\frac{g^2a^3}{108\pi^2}$ and we take $V(\vec{r})=Br^2$ the potential energy of the quark-antiquark system.

The wave function of the meson, $\psi(t,\vec{r}_1,\vec{r}_2)=\exp(-i\hat{H}t)\,\psi_M(\vec{r}_1,\vec{r}_2)$

taking m as the effective mass of the meson, satisfies the time-independent Schroedinger equation :

$$E\,\psi_M(\vec{r}_1,\vec{r}_2)=-\frac{1}{2m}\nabla^2_{\vec{r}_1,\vec{r}_2}\psi_M(\vec{r}_1,\vec{r}_2)+V(\vec{r})\,\psi_M(\vec{r}_1,\vec{r}_2)\qquad(31)$$

where E is the energy level of the meson.

Searching for $\psi_M(\vec{r}_1,\vec{r}_2)=\frac{1}{m}x^{-3/4}F(x)$, $G(x)=F(bx)$, $x=\|\vec{r}_1-\vec{r}_2\|^2$

te equation (31) becomes $\frac{d^2G}{dx^2}(x)+\left(-\frac{mBb^2}{4}+\frac{mbE}{4x}+\frac{3}{16x^2}\right)G(x)=0$ (32)

We choose b such that $mBb^2=1$ and take $\kappa=\frac{mbE}{4}$, $\mu=\frac{1}{4}$ and so

the (32) equation for G is the Whittaker function equation

$$\frac{d^2G}{dx^2}+\left(-\frac{1}{4}+\frac{\kappa}{x}+\frac{1/4-\mu^2}{x^2}\right)G=0\qquad(33).$$

The equation (33) , with parameters

κ , μ has a fundamental system of solutions $M_{\kappa,\mu}$, $W_{\kappa,\mu}$

$$M_{\kappa,\mu}(z)=z^{\frac{1}{2}+\mu}\exp(-\frac{1}{2}z)\left(1+\sum_{p=1}^{\infty}\frac{\left(\frac{1}{2}+\mu-\kappa\right)...\left(\frac{1}{2}+\mu-\kappa+p-1\right)}{p!(2\mu+1)...(2\mu+p)}z^p\right)$$

$$W_{\kappa,\mu}(z)=\frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-\kappa)}M_{\kappa,\mu}(z)+\frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-\kappa)}M_{\kappa,-\mu}(z)$$

For $\kappa=\mu-\frac{1}{2}+n$, $n\in\mathbb{N}^*$ we have that $M_{\kappa,\mu}(z)=z^{\frac{1}{2}}\exp(-\frac{1}{2}z)P(z)$ where P is a polynomial of degree $n-1$.

Therefore, for energy levels E_n , $E_n=(4n-1)\sqrt{\frac{B}{m}}$, $n\in\mathbb{N}^*$ the energy eigenstates are polynomial defined by the relations :

$$\psi_{Mn}(\vec{r}_1,\vec{r}_2)=\frac{1}{m}x^{-3/4}M_{\kappa n,1/4}(x/b)=$$

$$=\frac{b^{-3/4}}{m}\exp(-\frac{x}{2b})\left(1+\sum_{p=1}^{n-1}(-1)^p\frac{(n-1)...(n-p)}{p!\,1\cdot3...(2p+1)}2^p\left(\frac{x}{b}\right)^p\right) \qquad (34)$$

$$\kappa_n=n-\frac{1}{4}\ ,\ x=\|\vec{r}_1-\vec{r}_2\|\ ,\ b=(mB)^{-1/2}$$

Since a wave function $\psi_{0M}(\vec{r}_1,\vec{r}_2)$ is computable for the meson in a lattice simulation (as in (19) for the baryon example) equating this function with the (34) relation function we should be able to determine the constants B , b , g^2a^3 in the range of momentum given by a.

Consider now a three quark baryon consisting of three quarks with masses m_1, m_2 , m_3 and having different colours at a time.
As above , in this case we will have three colour charge currents

$$J_1^{a\mu}(t,\vec{x})=g\,\delta_{r\alpha}\frac{1}{2}\lambda^a_{\alpha\beta}\delta_{r\beta}\delta^3(\vec{x}-\vec{r}_1)\delta_{\mu0}$$

$$J_2^{a\mu}(t,\vec{x})=g\,\delta_{g\alpha}\frac{1}{2}\lambda^a_{\alpha\beta}\delta_{g\beta}\delta^3(\vec{x}-\vec{r}_2)\delta_{\mu0}$$

$$J_3^{a\mu}(t,\vec{x})=g\,\delta_{b\alpha}\frac{1}{2}\lambda^a_{\alpha\beta}\delta_{b\beta}\delta^3(\vec{x}-\vec{r}_3)\delta_{\mu0}$$

where $\vec{r}_1,\vec{r}_2,\vec{r}_3$ are the position vectors of the three quarks during the faster changing gluon fields intermediated interaction in which we must consider all possible permutation of colour index values over the 1 , 2 , 3 positions in the interaction time interval of length T.

For $d_1=\|\vec{r}_2-\vec{r}_3\|$, $d_2=\|\vec{r}_3-\vec{r}_1\|$, $d_3=\|\vec{r}_1-\vec{r}_2\|$, the potential energy of the three quark system is $V(\vec{r}_1,\vec{r}_2,\vec{r}_3)=E(d_1,d_2,d_3)$ and satisfies:

$$E\,T=E_0{}'T+\sum_a\int\left(J_1^a(x)D^a(x-y)J_2^a(y)+J_2^a(x)D^a(x-y)J_3^a(y)+\right.$$

$$\left.+J_3^a(x)D^a(x-y)J_1^a(y)\right)d^4x\,d^4y$$

where in the sum over a we consider an average over all permutations of the colour index values over the 1 , 2, 3 positions.

Following steps as in the calculation for the meson case it follows that we can take

$V(\vec{r}_1,\vec{r}_2,\vec{r}_3)=B\sum_{i=1}^3 d_i^2$ with $B=\frac{g^2a^3}{216\,\pi^2}$ for $a\,d_i\ll 1$, a the range of momentum.

The energy eigenstates of the baryon system satisfy the time independent Schroedinger equation :

$$E\,\psi_B(\vec{r}_1,\vec{r}_2,\vec{r}_3)=V(\vec{r}_1,\vec{r}_2,\vec{r}_3)\,\psi_B(\vec{r}_1,\vec{r}_2,\vec{r}_3)+\sum_{i=1}^3-\frac{1}{2m_i}\nabla_{\vec{r}_i}^2\,\psi_B(\vec{r}_1,\vec{r}_2,\vec{r}_3)$$

which for $x_i=d_i^2$, $i=\overline{1,3}$, $\psi_B(\vec{r}_1,\vec{r}_2,\vec{r}_3)=\psi(x_1,x_2,x_3)$ becomes:

$$E\,\psi=(x_1+x_2+x_3)B\,\psi+\sum\frac{1}{m_1}\left(2\frac{\partial^2\psi}{\partial x_2^2}x_2+2\frac{\partial^2\psi}{\partial x_3^2}x_3+3\frac{\partial\psi}{\partial x_2}+3\frac{\partial\psi}{\partial x_3}\right)$$

where the sum is taken over all circular permutations of (1 , 2 , 3).

We have solutions in the form $\psi(x_1,x_2,x_3)=\psi_1(x_1)\,\psi_2(x_2)\,\psi_3(x_3)$,

$$E=E_1+E_2+E_3 \text{ with } E_i\,\psi_i(x)=-\frac{1}{\overline{m}_i}(2\,\psi''(x)\,x+3\,\psi_i(x))+B\,\psi_i(x)\,x \quad (35)$$

where $\frac{1}{\overline{m}_1}=\frac{1}{m_2}+\frac{1}{m_3}$ with circular permutations over (1, 2, 3)

In the same way as for the meson wave function we obtain polynomial defined solutions

$$\psi_{in}(x)=\frac{b_i^{-3/4}}{\overline{m}_i}\exp(-\frac{x}{2b_i})\left(1+\sum_{p=1}^{n-1}(-1)^p\frac{(n-1)...(n-p)}{p!\,1\cdot3...\cdot(2p+1)}2^p\left(\frac{x}{b_i}\right)^p\right)$$

with $b_i=(2\overline{m}_iB)^{-1/2}$ for partial energy level $E_{in}=(4n-1)\sqrt{\frac{B}{2\overline{m}_i}}$.

The corresponding energy levels are $E_{n1n2n3}=E_{1n1}+E_{2n2}+E_{3n3}$ with eigenstates defined by $\psi_{n1n2n3}(x_1,x_2,x_3)=\psi_{n1}(x_1)\,\psi_{n2}(x_2)\,\psi_{n3}(x_3)$, $n_i\in\mathbb{N}^*$, $i=\overline{1,3}$.

So we have the (lowest level) eigenstate ψ_{0B} and with (19) we can recover the hadron momentum space wave function, needed in distribution amplitude calculations, by a Fourier transform.

As we mentioned we must be able to compute path integrals having the form

$\int D\,A\,D\,\psi\,D\,\overline{\psi}\exp(i\int\tilde{\mathcal{L}}(\psi,\partial\,\psi,A,\partial\,A)d^4x)O(\psi,\overline{\psi})$ (36)

where $O(\psi,\overline{\psi})$ can have for example the expression:

$$O(\psi,\overline{\psi})=(\prod_{i=1}^s\psi_{\beta i}^{\alpha i}(x_i))(\prod_{j=1}^n\overline{\psi}_{\delta j}^{\gamma j}(x_j{}'))\text{ with}$$

αi , γj colour and fermion sort indices and βi , δj Dirac spinor indices.

Since the Lagrangian density $\tilde{\mathcal{L}}$ has a expression like in (10) , the path integral over $D\,\psi D\,\overline{\psi}$, where $\psi,\overline{\psi}$ can be considered independent sets of Grassmann

variables, can be computed as a sum of Wick contraction terms, as shown for the (9') relation (with $\eta, \overline{\eta}$ variables conjugated to $\overline{\psi}$ respective ψ on the sides of the propagator, which is *D* (*x*-*y*) in the (9') relation) and so for the (36) integral not vanish ,we must have *s* = *n* .

To compute (36) we perform first a Wick rotation to imaginary time $t \to it = t_E$ and formulate the theory on a hyper-cubic lattice in 4-dimensional (Wick rotated Minkowski space-time $(t, \vec{x}) \to (t_E, \vec{x})$) Euclidean space-time, $\Lambda = \{(n_\mu a)_\mu\}_{n\mu \in \mathbb{Z},\ \mu=\overline{0,3}}$, $\psi(t, \vec{x}) = 0$ if $|t| > T$ or exists $k \in \{1, 2, 3\}$ such that $|x^k| > L$.

As the lattice spacing *a* goes to 0, we expect to recover 4-dimensional rotational invariance and (by Wick rotation) Lorentz invariance.

The relativistic relation

$E^2/c^2 - \vec{p}^2 = m^2 c^2$ with E energy, $\vec{p}$ momentum, m rest mass becomes by Wick rotation to imaginary time:

$$E'^2/c'^2 - \vec{p}'^2 = m^2 c'^2 \text{ with } c' = -ic.$$

For $\hbar = 1$, $c = 1$ and $E' = i\frac{\partial}{\partial it}$, $p'_k = -i\frac{\partial}{\partial x^k}$ as translation generators,

we will have $-\partial^2/\partial t_E^2 - \partial_k \partial_k = m^2$.

Therefore the corresponding Dirac equation for the Wick rotated space-time must be $\left(\gamma^0 \frac{\partial}{\partial t_E} + i\gamma^k \partial_k - im\right)\psi = 0$ and the Euclidean Lagrangian for a free fermion theory is

$\mathcal{L}_E(\psi, \partial\psi) = \overline{\psi}\left(i\gamma^0 \frac{\partial}{\partial t_E} + \gamma_k \partial_k + m\right)\psi$ and so $\exp(i\int \mathcal{L}(\psi, \partial\psi) d^4x)$ which occurs in the theory path integral formalism, becomes in the Wick rotated space-time

$\exp(i\int \mathcal{L}_E(\psi, \partial\psi) dit\, d^3\vec{x}) = \exp(-S_E(\psi, \overline{\psi}))$ where

$S_E(\psi, \overline{\psi}) = \int \overline{\psi}\left(i\gamma^0 \frac{\partial}{\partial it} + \gamma_k \partial_k + m\right)\psi dt\, d^3\vec{x} = \int \overline{\psi}(\gamma_\mu \partial_\mu + m)\psi dt\, d^3\vec{x}$ is the euclidean action.

On each link, say the one going from $x \in \Lambda$ to one of its nearest neighbours $x + a\hat{\mu} \in \Lambda$ where $\hat{\mu} = (\delta_{\alpha\mu})_{\alpha=\overline{0,3}}$ we associate an *N* by *N* unitary simple matrix, parallel transporter $U_\mu(x) \in SU(N)$ with N the number of colour x flavour/ lepton sort indices:

$$U_\mu(x) = \exp(-i \int_x^{x+a\hat{\mu}} \sum_g g A_\mu^b T^b dx^\mu)$$

the T^b are $N \times N$ hermitian traceless matrices, $(A_\mu^b)_b$ are real gauge boson fields which we can normalize such that $\mathrm{tr}(T^c T^b) = \frac{1}{2}\delta_{cb}$, $\mathrm{tr}\, T^b = 0$.

the $(T^b)_b$ are the generators of the gauge group representation. For each g coupling we have a set $(A^a, T^a)_a$ of gauge bosons and generators .

We have $U_\mu(x) = \boldsymbol{I} - i\sum_g a g A_\mu^b(x) T^b + O(a^2)$

Obviously we used Einstein summation convention for the *b* index.
Considering the form of the euclidean free fermion theory in a fermions interacting gauged theory we will take a discretized euclidean fermion action

$$S_F(\psi,\overline{\psi})=a^4\sum_{x\in\Lambda}\overline{\psi}(x)(\not{D}+m)\psi(x)$$

where $\psi=(\psi^{\alpha})_{\alpha}$, ψ^{α} Dirac spinor, $m=\mathrm{diag}(m_{\alpha})_{\alpha}$, α colour x flavour/lepton sort index , m_{α} mass of the α fermion ,

$$\not{D}=\gamma_{\mu}(\partial_{\mu}-i\sum_{g}g\,A_{\mu}^{b}(x)T^{b})$$

(where obviously we used the discretization of the ∂_{μ} operator)

$$\partial_{\mu}f(x)=\frac{f(x+a\hat{\mu})-f(x)}{a}\ .$$

We have also the gluon fields discretized euclidean action $S_G(U)$ we must establish.
Consider the square $P(x)$, known as a plaquette, bounded b the corners
x , $x+a\hat{\mu}$, $x+a\hat{\mu}+a\hat{\nu}$, $x+a\hat{\nu}$ with $x\in\Lambda$.
For each plaquette $P(x)$ we consider the expression:

$$P_{\mu\nu}(x)=U_{\mu}(x)U_{\nu}(x+a\hat{\mu})U_{\mu}^{+}(x+a\hat{\nu})U_{\nu}^{+}(x)\ .$$

Since $[T^b,T^c]=if^{dbc}T^d$, $\mathrm{tr}(T^bT^c)=\frac{1}{2}\delta_{bc}$, $\mathrm{tr}\,T^b=0$ we have :

$$\mathrm{tr}\,P_{\mu\nu}=\mathrm{tr}\exp(-ia^2\sum_{g}F_{\mu\nu}^{b}T^{b}+O(a^3))$$

where $F_{\mu\nu}^{b}=g(\partial_{\mu}A_{\nu}^{b}-\partial_{\nu}A_{\mu}^{b})+g^2f^{bcd}A_{\mu}^{c}A_{\nu}^{d}$
Under a gauge transformation $\psi(x)\to\Omega(x)\psi(x)$, $\Omega(x)\in SU(N)$,
the U_{μ} fields transform like $U_{\mu}(x)\to\Omega(x)U_{\mu}(x)\Omega^{+}(x+a\hat{\mu})$
We take the lattice plaquette gauge invariant euclidean action

$$S(P)=\sum_{g}\sum_{\mu\nu}(1/g^2)\Re\,\mathrm{tr}(\mathbf{I}-P_{\mu\nu})=(1/4)\sum_{g}(a^4/g^2)\Re\,\mathrm{tr}(F_{\mu\nu}^{b}F_{\mu\nu}^{b})+O(a^6)$$

The lattice euclidean gluon fields discretized action will be:

$$S_G[U]=\sum_{x\in\Lambda}(S(P)(x)+a^4\sum_{\mu,b}M_b^2A_{\mu}^{b2}(x))$$, where

M_b is the mass of the b boson and $A_{\mu}^{b}(x)=(2/(g\,a))\mathrm{tr}(i(U_{\mu}(x)-\mathbf{I})T^{b})$.

Further we will take $\nabla_{\mu}^{s}\psi(x)=\frac{U_{\mu}(x)\psi(x+a\hat{\mu})-U_{\mu}^{+}(x)\psi(x-a\hat{\mu})}{2a}$
and under a gauge transformation $\psi(x)\to\Omega(x)\psi(x)$ it will folow

$$\nabla_{\mu}^{s}\psi(x)\to\Omega(x)\nabla_{\mu}^{s}\psi(x)+O(a)\ .$$

We have also :

$$\nabla_{\mu}^{s}\psi(x)=\frac{U_{\mu}(x)+U_{\mu}^{+}}{2}\partial_{\mu}\psi(x)+\frac{U_{\mu}(x)-U_{\mu}^{+}(x)}{2a}\psi(x)=$$
$$=(\partial_{\mu}-i\sum_{g}g\,A_{\mu}^{b}(x)T^{b})\psi(x)+O(a)$$

Taking $S_F[U](\psi,\overline{\psi})=a^4\sum_{x\in\Lambda}\overline{\psi}(x)(\gamma_\mu\nabla^s_\mu+m)\psi(x)$ it follows that in the $a\to 0$ continuum limit, $S_F[U]$ is gauge invariant and equal to the lattice euclidean fermion action.

Therefore, the (36) path integral can be computed by Wick rotation as

$$\int DAD\psi D\overline{\psi}\exp(-\int\mathscr{L}_E(\psi,\partial\psi,A,\partial A)dtd^3\vec{x})O(\psi,\overline{\psi})= \\ =\int DA\exp(-S_G[U])\int D\psi D\overline{\psi}\exp(-S_F[U](\psi,\overline{\psi}))O(\psi,\overline{\psi}) \quad (37)$$

We can write $-S_F[U](\psi,\overline{\psi})=\overline{\psi}D_W[U]\psi$ where $D_W[U]$ is a matrix acting on the $(\psi(x))_{x\in\Lambda}$ space.

Since ψ , $\overline{\psi}$ can be considered as independent sets of Grassmann variables, with (8) , (8''') relations, we have:

$$Z(\eta,\overline{\eta})=\int D\psi D\overline{\psi}\exp(-S_F[U](\psi,\overline{\psi})+\overline{\eta}\psi+\overline{\psi}\eta)= \\ =C\det(D_W[U])\exp(-\overline{\eta}D_W^{-1}[U]\eta)$$

with C a normalization, discretization dependent constant and so we can compute:

$$\int D\psi D\overline{\psi}\exp(-S_F[U](\psi,\overline{\psi}))O(\psi,\overline{\psi})= \\ =C\det(D_W[U])\frac{\partial^{s+n}}{(\prod_{i=1}^{s}\partial\overline{\eta}^{\alpha i}_{\beta i}(x_i))(\prod_{j=1}^{n}\eta^{\gamma j}_{\delta j}(x'_j))}\exp(-\overline{\eta}D_W^{-1}[U]\eta)\Big|_{\eta=\overline{\eta}=0}= \quad (37')$$

$$=C\langle O\rangle_F[U]\left|\det(D_W[U])\right|$$

If,as in (18") the $O(\psi,\overline{\psi})$ requires integration over $(\vec{x}_i)_i$, $(\vec{x}'_j)_j$ we can include that in the $\langle O\rangle_F[U]$ factor.

Therefore the calculation of (36), (37) integral reduces to computation of $C\int D[U]\langle O\rangle_F[U]\exp(-S_G[U])\left|\det(D_W[U])\right|$ where $\int D[U]...$ means integration over the $(A^b_\mu(x))_{x\in\Lambda,b,\mu}$ variables, with C a normalization , discretization dependent constant.

For the free theory, $(U_\mu(x)=\mathbf{I})$ the ∇^s_μ operator becomes ∂^s_μ ,

$\partial^s_\mu f(x)=\frac{f(x+a\hat{\mu})-f(x-a\hat{\mu})}{2a}$ and so

$-S_F[U](\psi,\overline{\psi})=-\int\overline{\psi}(\gamma_\mu\partial^s_\mu+m)\psi d^4x$

The Fourier transform on the momentum space of $-(\gamma_\mu\partial^s_\mu+m)\psi$ is

$-\left(\frac{i}{a}\gamma_\mu\sin(ap_\mu)+m\right)\mathscr{F}\psi$ and the propagator D_W^{-1} satisfies

$-(\gamma_\mu \partial^s_\mu + m) D_W^{-1}(x) = \delta^4(x)$ and so on the momentum space we have

$$\mathcal{F}\, D_W^{-1}(p) = \frac{i a^{-1} \gamma_\mu \sin(a p_\mu) - m}{m^2 + a^{-2}(\sin^2(a p_0) - \sum_j \sin^2(a p_\mu))}$$

The momentum space propagator has a pole at $p^2 = -m^2$ when $a \to 0$ but has more poles, known as doublers , when $\sin^2(a p_0) - \sum_j \sin^2(a p_j) = m^2 a^2$.

Doublers can interact with each other via loop corrections and in computations we remove them by perturbing slightly the $\gamma_\mu \nabla^s_\mu + m$ operator, taking

$$S_F[U](\psi, \overline{\psi}) = -\overline{\psi} D_W[U] \psi = a^4 \sum_{x \in \Lambda} \overline{\psi} \left(\gamma_\mu \nabla^s_\mu + m - \frac{a}{2} \nabla^{s+}_\mu \nabla^s_\mu \right) \psi \ .$$

Monte-Carlo sampling method

Let $P : [0, L]^M \to \mathbb{R}_+$ with P continuous and $\int P(x) d^M x = W < \infty$

Then we have a probability on $[0, L]^M$ given by

$\overline{P}(A) = \int_A \frac{P(x)}{W} d^M x$ for any measurable set in $[0, L]^M$.

For $n = (n_i)_i \in \{0, ..., q-1\}^M$ we denote $C_n = \prod_{i=1}^M [n_i L/q, (n_i + 1) L/q]$

and take a sample $(x_k)_{k = \overline{1, S}}$, $x_k \in [0, L]^M$, $S = q^{M+1}$ such that:

$\text{card}\{k = \overline{1, S} | x_k \in C_n\} = [S \overline{P}(C_n)]$

We consider also the measures on $[0, L]^M$ defined by:

$$\varepsilon_k(A) = \begin{cases} 1 & \text{if } x_k \in A \\ 0 & \text{else} \end{cases} \ , \ \mu_S = \frac{1}{S} \sum_{k=1}^S \varepsilon_k$$

Then for any Borel set A of $[0 , L]^M$ with $\overline{P}(\partial A) = 0$ we can show that $(*)$:

$\lim_{q \to \infty} \mu_S(A) = \overline{P}(A)$ and so for any continuous $F : [0, L]^M \to \mathbb{R}$ we have

$$\int F(x) P(x) d^M x = W \int F \, d\overline{P}(x) = \lim_{q \to \infty} W \int F \, d\mu_S(x) = \lim_{q \to \infty} \frac{W}{S} \sum_{k=1}^S F(x_k)$$

Now we demonstrate $(*)$:

By compactness of $\overline{A} = A \cup \partial A$, measure definition and density of rational fractions, for large enough $q \in \mathbb{N}$ we find $(n j)_j$, $n j \in \{0, ..., q-1\}^M$, $n j \neq n l$ for $j \neq l$ such that $\left| \overline{P}(\bigcup_j C_{n j}) - \overline{P}(A) \right| < \varepsilon$,

$$\left| \overline{P}(\bigcup_j C_{n j}) - \mu_S(\bigcup_j C_{n j}) \right| < \frac{q^M}{S} \leq \frac{1}{q}$$

$\left| \mu_S(\bigcup_j C_{n j}) - \mu_S(A) \right| < \varepsilon$ with arbitrary positive ε and the result follows.

In a lattice simulation we do the space-time integrations on a bounded hypercube of time interval length T and space volume V so that we can consider that Λ is a finite set of lattice points. We can use Monte-Carlo sampling method to compute the (37) integral.

Let M be the dimension of the $(A_\mu^b(x))_{x\in\Lambda,b,\mu}$ space,

taking $A=(A_\mu^b(x))_{x\in\Lambda,b,\mu}\in[-L/2,L/2]^M$,

$C_n=\prod_{i=1}^{M}[n_i\delta-L/2,(n_i+1)\delta]$ for $n=(n_i)_i\in\{0,...,q-1\}^M$, $\delta=L/q$.

Then we take samples:

$A^{(k)}\in[-L/2,L/2]^M$, $k=\overline{1,S}$, $S=q^{M+1}$, $U_\mu^{(k)}(x)=\mathbf{I}-i\sum_g a g A_\mu^{(k)b}(x)T^b$

such that for any multi-index n we have

$\text{card}\{k=\overline{1,S}|A^{(k)}\in C_n\}=\lfloor S\overline{P}(C_n)\rfloor$; $\overline{P}$ is a probability on $[-L/2,L/2]^M$ space

defined by the density $\frac{1}{W}\exp(-S_G[U])\left|\det(D_W[U])\right|$

with $W=\int\exp(-S_G[U])\left|\det(D_W[U])\right|d^M A$

According to above considerations , the (37) integral can be determined as

$C\lim_{q\to\infty}\frac{W}{S}\sum_{k=1}^{S}\langle O\rangle_F[U^{(k)}]$.

Meson and baryon masses

A scalar meson appears as a combination $\psi_M(x_1,x_2)=\overline{\psi}^a(x_1)\psi^a(x_2)$ with no summation over the colour index $a=\overline{1,3}$ since at a location $\vec{x}$ the quark and antiquark have one colour (anti-colour), taking $x_i=(t,\vec{x}_i)=(t,\vec{x})$ for $i=1,2$.

For the scalar meson we consider an equivalent scalar field of a spin 0 particle having an effective mass m , $\hat{\varphi}=\hat{\varphi}(t,\vec{x})$ as in (4a) and the equivalent propagator from $(0,\vec{x})$ to $(t,\vec{x})$, $t>0$ which is $-i\langle 0|\hat{\varphi}(t,\vec{x})\hat{\varphi}^+(0,\vec{x})|0\rangle$.(38)

Therefore , taking $\hat{F}(t)=\hat{\psi}_M((t,\vec{x}),(t,\vec{x}))$ for a given location $\vec{x}$, the (38) propagator must be similar to Lorentz invariant $-i\langle 0|\hat{F}(t)\hat{F}(0)|0\rangle$.

After some calculus, according to above established results we derive

$$C(t)=\int D[U]\langle O\rangle_F[U]\exp(-S_G[U])\left|\det(D_W[U])\right|=K\int\frac{\exp(-\sqrt{\vec{k}^2+m^2}\,t)}{\sqrt{\vec{k}^2+m^2}}d^3\vec{k}$$

with K a t , m independent constant and

$O(\psi,\overline{\psi})=(\overline{\psi}^a(t,\vec{x})\psi^a(t,\vec{x}))(\overline{\psi}^a(0,\vec{x})\psi^a(0,\vec{x}))$

A baryon appears as $\psi_B(x_1,x_2,x_3)=(\psi_\alpha^a(x_1)\psi_\beta^b(x_2)\psi_\gamma^c(x_3))_{\alpha\beta\gamma}$, $a\neq b\neq c\neq a$ colour indices, taking $x_i=(t,\vec{x}_i)=(t,\vec{x})$, $i=\overline{1,3}$ at given location $\vec{x}$.

We consider for a spin ½ baryon an equivalent Dirac spinor field having an effective mass m , $\hat{\psi}=\hat{\psi}(t,\vec{x})$ as in (4c) and the equivalent propagator trace from $(0,\vec{x})$ to $(t,\vec{x})$: $-i\langle 0|\hat{\psi}_\alpha(t,\vec{x})\,\hat{\overline{\psi}}_\alpha(0,\vec{x})|0\rangle$.

Thus similar to above we derive

$$C(t)=\int D[U]\langle O\rangle_F[U]\exp(-S_G[U])\left|\det D_W[U]\right|=K m\int\frac{\exp(-\sqrt{\vec{k}^2+m^2}\,t)}{\sqrt{\vec{k}^2+m^2}}d^3\vec{k}$$

with K a t,m independent constant and the Lorentz invariant

$$O(\psi,\overline{\psi})=\psi^a_\alpha(t,\vec{x})\,\psi^b_\beta(t,\vec{x})\,\psi^c_\gamma(t,\vec{x})\,\overline{\psi}^a_\alpha(0,\vec{x})\,\overline{\psi}^b_\beta(0,\vec{x})\,\overline{\psi}^c_\gamma(0,\vec{x})$$

Focussing on the baryon case, integrating in spherical coordinates and then by parts we obtain, after a variable changing:

$C(t)=\frac{4\pi K m}{t^2}\int_0^\infty\exp(-\sqrt{k^2+m^2t^2})dk$ and so for $G(t)=tC(t)$ we have

$G(t)=4\pi K m^2P(mt)$ where $P(z)=\frac{1}{z}\int_0^\infty\exp(-\sqrt{k^2+z^2})$, $z=mt$,

$G'(t)=4\pi K m^3P'(z)$, $\frac{G'(t)}{G(t)}=m\frac{P'(z)}{P(z)}=-m\left(\frac{1}{z}+H(z)\right)$ with

$$H(z)=\left(\int_0^\infty\frac{z\exp(-\sqrt{k^2+z^2})}{\sqrt{k^2+z^2}}dk\right)\left(\int_0^\infty\exp(-\sqrt{k^2+z^2})dk\right)^{-1}=$$

$$=\left(\int_0^\infty\frac{u\exp(-\sqrt{1+k^2}/u)}{\sqrt{1+k^2}}dk\right)\left(\int_0^\infty u\exp(-\sqrt{1+k^2}/u)dk\right)^{-1}\text{ with }z=\frac{1}{u}$$

Variable changing to $s=\exp(-\sqrt{1+k^2}/u)$ leads to

$$\int_0^\infty u\exp(-\sqrt{1+k^2}/u)dk=\int_1^\infty\exp(-\tau/u)\,\tau/\sqrt{\tau^2-1}\,d\tau=$$

$$=\int_1^\infty u\sqrt{\tau^2-1}\exp(-\tau/u)\,d\tau=\int_0^h u\sqrt{u^2\ln^2(s)-1}\,ds$$

$$\int_0^\infty\frac{u\exp(-\sqrt{1+k^2}/u)}{\sqrt{1+k^2}}dk=\int_0^h\frac{u^2}{\sqrt{u^2\ln^2(s)-1}}ds\text{ where }h=\exp(-z)\ .$$

Hence after some calculus we obtain:

$$H(z)=\left(\int_0^1\frac{|\ln(h)|^{1/2}}{(\ln^2(s)+2\ln(s)\ln(h))^{1/2}}ds\right)\left(\int_0^1\frac{(\ln^2(s)+2\ln(s)\ln(h))^{1/2}}{|\ln(h)|^{1/2}}ds\right)^{-1}\ .$$

We can verify that for $s\in(0,1)$ we have:

$$\frac{|\ln(h)|^{1/2}}{(\ln^2(s)+2\ln(s)\ln(h))^{1/2}}<\frac{1}{\sqrt{2|\ln(s)|}}\ ,$$

$\int_0^1\frac{1}{\sqrt{|\ln(s)|}}ds=\int_0^\infty\tau^{-1/2}\exp(-\tau)\,d\tau=\Gamma(1/2)$ and for $z>1$ also

$$\frac{(\ln^2(s)+2\ln(s)\ln(h))^{1/2}}{|\ln(h)|^{1/2}}<(1+\sqrt{2})|\ln(s)|\ ,$$

$\int_0^1 |\ln(s)|ds=\int_0^\infty \tau\exp(-\tau)d\tau<\infty$ and so by dominated convergenge for $z\to\infty$,

it follows that

$$\lim_{z\to\infty} H(z)=\left(\int_0^1 (2|\ln(s)|)^{-1/2}ds\right)\left(\int_0^1 (2|\ln(s)|)^{1/2}ds\right)^{-1}=$$

$$=\frac{1}{2}\left(\int_0^\infty s^{-1/2}\exp(-s)ds\right)\left(\int_0^\infty s^{1/2}\exp(-s)ds\right)^{-1}=(1/2)\Gamma(1/2)(\Gamma(3/2))^{-1}=1\ .$$

Therefore $\lim_{t\to\infty} -\frac{G'(t)}{G(t)}=m$ and so for large t we can consider that

$$\frac{\ln C(t)-\ln C(t+a)}{a}=m\ ,\ ma=\ln\left(\frac{C(t)}{C(t+a)}\right) \qquad (39)$$

In the same way , the (39) relation results valid also for the meson case.
Notice that in the ψ_M , ψ_B expressions we have supressed flavour differences between the various ψ factors, so that we can have mesons made from an up-quark and a down-antiquark for example or baryons made from two up-quarks and one down-quark like the proton for example. Also we make the location variables $\vec{x}_i$ equal to the same $\vec{x}$ only after computing $\langle O\rangle_F[U]$ according to (37') Wick contraction relation, since otherwise, because we consider the quark fields variables as Grassmann variables in the integration, we would have a vanishing $O(\psi,\overline{\psi})$ operator value due to appearing of squared Grassmann variables in the expression of $O(\psi,\overline{\psi})$. The locations of the quarks / antiquarks in a many-quark system as a meson or a baryon can be considered to be approximatively the same (due to quark confinement), but however not identically the same.

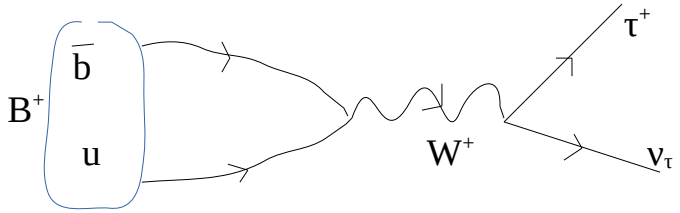
Consider the SU(3) quantum chromodynamics theory with two degenerate quark flavours , the up-quark and the down-quark with equal masses $m = m_u = m_d$. The boson masses are vanishing , $M_a = 0$.
The lattice action depends on two free parameters:
- the quark mass m;
- the value of the strong interaction coupling *g* (which can be absorbed into the *A* integration variable).
Then we can compute (in dependence of m) , for a lattice spacing *a* the masses of the π meson (made of an up-quark and a down-antiquark) and the proton p (made of two up-quarks and a down-quark): only the dimensionless quantities am_π and am_p can be computed, according to (39).
From experiments we can determine the fraction $(m_\pi/m_p)_{exp}$ and so we can tune the quark mass m such that the lattice simulation computed $(m_\pi/m_p)_{lat}$ matches the experimental $(m_\pi/m_p)_{exp}$. Then we determine the spacing *a* in physical units from $(am_\pi)_{lat}$ and m_π^{phys} .

The continuum limit must be taken using the constant line of physics m_π , $m_p << a^{-1}$ while keeping $(m_\pi/m_p)_{lat}$ constant.

With relations (39) we are able to compute effective masses of mesons , baryons and even atomic nuclei which are made of nucleons which are protons (two up- and one down- quark) and neutrons (two down- and one up- quark) and can be considered as a system of many quarks hold together by the strong interaction. The most part of their particles masses are then given by the gluon intermediated interaction energy. The strong interaction, intermediated by the SU(3) gluons (in the unified SU(3)xSU(2)xU(1) theory) has a positive contribution to the nucleon binding energy in an atomic nucleus while the weak and electromagnetic interaction , intermediated by the SU(2)xU(1) gluons which for positive electric charged protons turns out to be a repelling (Coulombian) force has a negative contribution to the nucleon binding energy. Thus for large (heavy) atomic nuclei the negative binding energy (as an absolute value) can exceed the positive binding energy, because the weak and electromagnetic interaction becomes more significant as the dimension of the nucleus increases. Therefore the fusion of two light nuclei to another light nucleus happens with energy emission and the fission of a heavy atomic nucleus happens also with an emission of energy. The energy gain per fission event ΔE can be computed as $\Delta E = \Delta m c^2$,where Δm is the difference between the sum of effective masses of the outgoing from the fission particles (atomic nuclei and other hadrons) and the sum of incoming in the fission interaction particles (atomic nucleus to be fissioned and the fission event producing particle which can be for example a neutron) effective masses.

To allow transitions between different flavours of quarks for decays like

$$B^+ = \bar{b}u \xrightarrow{W^+} \tau^+ + \bar{\nu}_\tau \quad (40)$$



where the notations are:
b – for the bottom-quark , u – for the up-quark,
W^+ for the combination of $W^1 + i\, W^2$ first two weak SU(2) bosons,
τ^+ - for the tau-antimuon , ν_τ - for the tau-neutrino,
B^+ - for the b – meson in which a bottom-antiquark and an up-quark are confined by the strong interaction,
we add to the SU(3)xSU(2)xU(1) theory Lagrangian density, weak interaction terms like

$g\,\overline{\psi}^{b\alpha}\gamma^{\mu}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)W_{\mu}^{+}\,\psi^{u\alpha}$, with b,u flavours , α colour index and

$\gamma^5=i\,\gamma^0\gamma^1\gamma^2\gamma^3$ or equivalently we add $-ig\,\overline{\psi}^{b\alpha}\gamma_{\mu}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)W_{\mu}^{+}\,\psi^{u\alpha}$ to the euclidean Lagrangian density.

Obviously in the lattice simulation we have

$W_{\mu}^{+}=(2i/(ag))\,\mathrm{tr}\,(U_{\mu}-\mathbf{I})(T^1+iT^2)$ where $2T^1$ and $2T^2$ correspond to the σ_1 respective σ_2 Pauli matrices , from the generators of SU(2) and *g* is the weak coupling constant.

Since it is a weak coupling we can have a perturbative approach and for the decay transition (40) we have to compute expressions for an operator

$$O(\psi,\overline{\psi},U)=\int\left(\overline{\psi}_i^{\tau}(x_1)\,\psi_j^{\nu}(x_2)(-ig)\,\overline{\psi}^{b\alpha}(x)\,\gamma_{\mu}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)W_{\mu}^{+}(x)\right.$$
$$\left.\psi^{u\alpha}(x)\,\psi_k^{b\alpha}(y_1)\,\overline{\psi}_l^{u\alpha}(y_2)\right)d^4x$$

and with $x_s=(T,\vec{x}_s)$, $y_s=(0,\vec{y}_s)$, $s=1,2$ we take for $i,j,k,l=\overline{0,3}$:

$$A_{lat}^{ijkl}(\vec{x}_1,\vec{x}_2,\vec{y}_1,\vec{y}_2)=\int D[U]\langle O\rangle_F[U]\exp(-S_G[U])\left|\det D_W[U]\right| \quad (41)$$

On the other hand, in the electroweak interaction theory, inter-flavour transitions can be allowed by considering mixed down-type weak interaction partners (d' , s' , b') to the (u , c , t) up-type quarks given by unitary Cabibo-Kobayashi-Maskawa matrix

$$V_{CKM}=\begin{pmatrix}V_{ud}&V_{us}&V_{ub}\\V_{cd}&V_{cs}&V_{cb}\\V_{td}&V_{ts}&V_{tb}\end{pmatrix}\quad\text{with}\quad\begin{pmatrix}d'\\s'\\b'\end{pmatrix}=V_{CKM}\begin{pmatrix}d\\s\\b\end{pmatrix}$$

$|V_{ij}|^2$ is the transition probability from a flavour j quark to a flavour i quark so that the significant changed part of the electroweak Lagrangian density will be

$$\mathscr{L}_{W^{\pm}}=g\,(\overline{u}\;\;\overline{c}\;\;\overline{t})\,\gamma^{\mu}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)V_{CKM}\begin{pmatrix}d\\s\\b\end{pmatrix}W_{\mu}^{-}+g\,(\overline{d}\;\;\overline{s}\;\;\overline{b})\,V_{CKM}^{+}\gamma^{\mu}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)\begin{pmatrix}u\\c\\t\end{pmatrix}W_{\mu}^{+}$$

(The $\frac{\mathbf{I}-\gamma^5}{2}$ appearing since only the left-handed fields participate in the weak interaction.

An equivalent to A_{lat}^{ijkl} in the modified electroweak theory according to $\mathscr{L}_{W^{\pm}}$ is

$$A_W^{ijkl}(\vec{x}_1,\vec{x}_2,\vec{y}_1,\vec{y}_2)=V_{ub}^{*}\int\left\langle 0\left|\hat{\overline{\psi}}_i^{\tau}(x_1)\,\hat{\psi}_j^{\nu}(x_2)\,\hat{\overline{\psi}}^{\nu}(y)\,\gamma^{\mu}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)\hat{\psi}^{\tau}(y)\right.\right.$$
$$\left.\left.\widehat{W}_{\mu}^{-}(y)\widehat{W}_{\lambda}^{+}(y')\,\hat{\overline{\psi}}^{b\alpha}(y')\,\gamma^{\lambda}\left(\frac{\mathbf{I}-\gamma^5}{2}\right)\hat{\psi}^{u\alpha}(y')\,\hat{\psi}_k^{b\alpha}(y_1)\,\hat{\overline{\psi}}_l^{\mu\alpha}(y_2)\right|0\right\rangle d^4y\,d^4y'=$$

$$=CV_{ub}^{*}\int\left((D^{\nu}(x_2-y)\gamma^{\mu}(\mathbf{I}-\gamma^5)D^{\tau}(y-x_1))_{ji}D_{\mu\lambda}^{bos}(y-y')\right.$$
$$\left.(D^{b}(y_1-y')\gamma^{\lambda}(\mathbf{I}-\gamma^5)D^{u}(y'-y_2))_{kl}\right)d^4y\,d^4y' \quad (42)$$

where C is a constant.

Corresponding to the A^{ijkl} we have the momentum dependent amplitude:

$$B(p,q,s,h)=\int\left(\exp(ipx_2)\bar{u}_j^{\nu}(p)(E_p/m_{\nu})^{1/2}\exp(iqx_1)v_i^{\tau}(q)(E_q/m_{\tau})^{1/2}\right.$$
$$\exp(-isy_1)\bar{v}_k^{b}(s)(E_s/m_b)^{1/2}\exp(-ihy_2)u_l^{u}(h)(E_h/m_u)^{1/2}$$
$$\left.A^{ijkl}(\vec{x}_1,\vec{x}_2,\vec{y}_1,\vec{y}_2)\right)d^3\vec{x}_1d^3\vec{x}_2d^3\vec{y}_1d^3\vec{y}_2$$

After some calculations, considering (42) and (13) , (14) type relations we can derive:

$$B_W(p,q,s,h)=CV_{ub}^{*}\left(\frac{m_{\nu}m_{\tau}m_bm_u}{E_pE_qE_sE_h}\right)^{1/2}(\bar{v}^{b}(s)\gamma^{\lambda}(\mathbf{I}-\gamma^5)u^{u}(h))$$
$$(\bar{u}^{\nu}(p)\gamma^{\mu}(\mathbf{I}-\gamma^5)v^{\tau}(q))\left(-\eta^{\mu\lambda}+\frac{(p+q)_{\lambda}(p+q)_{\mu}}{M^2}\right)\frac{1}{(p+q)^2-M^2}$$

where C is a constant which can depend on the interaction time interval T and the interaction space volume, since we consider momentum conservation and incoming and outgoing momenta on mass shell , having therefore

$p+q=s+h$, $\delta^4(p+q-s-h)=\frac{VT}{(2\pi)^4}$ and M is the W-boson mass.

Notice that for a given quark or lepton and given four-momentum p on mass shell, the $u(p)$, $v(p)$ Dirac spinors are defined by their normalization values in the rest frame , where $\vec{p}=0$ and spin index variable 1 ,2 is supposed to be understood.

Therefore we have a constant C' depending on V, T, g and discretization and normalization of Grassmann variables of the lattice simulation, such that

$B_W(p,q,s,h)=C'B_{lat}(p,q,s,h)$ where we take $p+q=s+h$ and the four-momenta p,q,s,h are on mass shell. (43)

From (43) we can extract in some momentum range a value CV_{ub}^{*} where C is a lattice simulation dependent constant and similarly CV_{ud}^{*} and CV_{us}^{*} with the same constant.

Requiring that V_{CKM} is an unitary matrix and so $|V_{ub}|^2+|V_{ud}|^2+|V_{us}|^2=1$, we obtain the values of V_{ub} , V_{us} , V_{ud} and in the same way the whole V_{CKM} to multiplication with global phase factors which can be absorbed into the quark field functions.

As we know, SU(N) requires a basis of $N^2 - 1$ hermitean traceless matrices as generators, and so a matrix $U\in SU(N)$ requires N^2-1 real parameters. Adding one real parameter to determine the determinant of absolute value 1, we obtain that an unitary CKM NxN matrix requires N^2 real parameters. 2 N – 1 of these parameters are not physically significant because one phase factor can be absorbed into each quark field (both of the mass eigenstates and the weak primed eigenstates of the N

down-type flavours) but the matrix is independent of a common phase. Hence the total number of free variables independent of the choice of the phases of basis vectors is $N^2 - (2N - 1) = (N - 1)^2$.

Splitting suitable chosen generators of SU(N), which are complex hermitian traceless matrices into real and pure imaginary generators we show without difficulties that an unitary matrix V can be expressed as $V = \exp(A + iB)$ where A is a real antisymmetric matrix having all diagonal elements equal to zero and *B* is a real symmetric matrix. Therefore from the $(N - 1)^2$ free real variables which remained to define the CKM matrix, $N(N - 1)/2$ are rotation angles (the *A* matrix above) which are the so called quark mixing angles .

The remaining $(N - 1)(N - 2)/2$ are imaginary phase variables which cause CP-violation as we will show.

For N = 2 we have no complex phase factors an one quark mixing angle. For N = 3 there are three mixing angles and one CP- violating complex phase. For CP- violation to occur we must have at least three families of quarks.

To create an imbalance of matter and antimatter, for the Universe to exist, from an initial condition of balance, a necessary condition is the existence of CP- violation, or equivalent, considering the CPT theorem, the existence of time reversal T- violation, so at least three families of quarks exist in nature.

The reason why a complex phase factor in $(V_{ij})_{i,j}$ causes CP- violation can be seen as follows:

Consider any given particles (or sets of particles) a and b and their antiparticles $\bar{a}$ and $\bar{b}$. Now consider the processes $a \to b$ and the corresponding antiparticle processes $\bar{a} \to \bar{b}$ under CP transformation,denote their amplitudes M respectively $\bar{M}$. Before CP- violation, these terms must be the same complex number $M = \bar{M}$.

Let $M = |M| \exp(i\theta)$. If a phase factor is introduced (from the CKM matrix), denote it $\exp(i\varphi)$.

$\bar{M}$ contains the conjugate matrix to M , so it picks up a phase factor $\exp(-i\varphi)$.

Now we have : $M = |M| \exp(i\theta) \exp(i\varphi)$, $\bar{M} = |M| \exp(i\theta) \exp(-i\varphi)$.

Physically measurable reaction rates are proportional to $|M|^2 = |\bar{M}|^2$.

However, consider that are two different routes $a \overset{1}{\to} b$ and $a \overset{2}{\to} b$, or equivalently

two unrelated intermediate states $a \to 1 \to b$ and $a \to 2 \to b$ and we have:

$$M = |M_1| \exp(i\theta_1) \exp(i\varphi_1) + |M_2| \exp(i\theta_2) \exp(i\varphi_2)$$

$$\bar{M} = |M_1| \exp(i\theta_1) \exp(-i\varphi_1) + |M_2| \exp(i\theta_2) \exp(-i\varphi_2) \text{ and so}$$

$$|M|^2 - |\bar{M}|^2 = -4|M_1||M_2| \sin(\theta_1 - \theta_2) \sin(\varphi_1 - \varphi_2).$$

Thus we see that a complex phase factor gives rise to processes that proceed at different rates for particles and antiparticles and CP is violated.

There can be considered also a lepton mixing matrix or neutrino mixing matrix, which contains information on the mismatch of quantum states of the three flavours of neutrinos ν_e , ν_τ , ν_μ in the charged current weak interaction with the lepton partners e , τ , μ . That matrix is an unitary matrix, called the

Pontecorvo-Maki-Nakagawa-Sakata matrix, PMNS.

Random walk, mean free path and critical mass of a fissile material

A random walk is a random process that describes a path that consists of a succession of random steps on some mathematical space.
A lattice random walk is a random walk on a regular lattice where at each step the location jumps to another site according to some probability distribution.
In a simple symmetric random walk the location can jump only to neighbouring sites of the lattice forming a lattice path and the probabilities of the location jumping to each one of its immediate neighbours are the same.
Consider a tridimensional lattice $\Lambda=\{(n_i a)_{i=\overline{1,3}} | n_i\in\mathbb{Z}\ ,\ i=\overline{1,3}\}$.
To define the random walk we consider the product probability space of succession of steps:

$S=(\prod_{i\in\mathbb{N}^*}\{-1,1\}^3$, $\hat{P}=\bigotimes_{i\in\mathbb{N}^*}(\bigotimes_1^3 P))$ with $P(\{-1\})=P(\{1\})=\frac{1}{2}$ and the independent random variables $Z_{i\alpha}: S\to\{-a,a\}$ with $Z_{i\alpha}((x_j^\beta)_{j\in\mathbb{N}^*\ ,\ \beta=\overline{1,3}})=x_i^\alpha a$.

We have $E(Z_{i\alpha})=\int Z_{i\alpha}d\hat{P}=0$ and we take $\vec{Z}_i=(Z_{i\alpha})_{\alpha=\overline{1,3}}$, $\vec{S}_n=\sum_{i=1}^n \vec{Z}_i$.

In order for $S_{n\alpha}$ to be $k_\alpha a$ it is necessary and sufficient that the number of +1 steps in α direction excceds the number of -1 steps taken in α direction of the n steps defined tridimensional walk. Therefore, for the α direction, $+1$ step must be taken $(n+k_\alpha)/2$ times from a total of n steps . The total number of *n* steps considered tridimensional walks is 2^{3n}. Therefore we can derive

$$\hat{P}\circ\vec{S}_n^{-1}(\{(k_1 a,k_2 a,k_3 a)\})=\prod_{\alpha=1}^3\left(\binom{n}{(n+k_\alpha)/2}\frac{1}{2^n}\right)$$ which implies $n\equiv k_\alpha \pmod 2$

for the probability not be equal to 0.
Using the Stirling formula : $\lim_{n\to\infty}\frac{\sqrt{2\pi n}(n/\mathrm{e})^n}{n!}=1$ after some calculus we obtain

$$\ln\left(\binom{n}{(n+k_\alpha)/2}\frac{1}{2^n}\right)\approx\frac{k_\alpha^2}{2n}-\frac{1}{2}\ln n+\ln\sqrt{\frac{2}{\pi}}$$ for large n.

Therefore the asymptotic probability distribution for the defined tridimensional random walk as the number of steps increases when the step length is constant for each step is a function of the radius from the origin $\rho=\rho(r)$ having

$$\hat{P}\circ\vec{S}_n^{-1}(A)\simeq\int_A\rho(r)\,dr\,d\Omega=\int_A\left(\frac{2}{n\pi}\right)^{3/2}r^2\exp\left(\frac{r^2}{2n}\right)dr\,d\Omega$$

$d\Omega$ - solid angle , $\rho(r)=\left(\frac{2}{n\pi}\right)^{3/2}r^2\exp\left(\frac{r^2}{2n}\right)$

Also we can compute :

$$E(|S_{2n\alpha}|)=\int |S_{2n\alpha}|d\hat{P}=a\sum_{k=0}^{n}2k\binom{2n}{n+k}\frac{1}{2^{2n}}=$$

$$=\frac{a}{2^{2n}}\sum_{k=0}^{n}\left((n+k)\binom{2n}{n+k}-(n-k)\binom{2n}{n-k}\right)=$$

$$=\frac{a}{2^{2n}}\left(n\binom{2n}{n}+\sum_{k=0}^{2n}k\binom{2n}{k}-2\sum_{k=0}^{n}k\binom{2n}{k}\right)$$

We have:

$$k\binom{2n}{k}=2n\binom{2n-1}{k-1}$$

$$\sum_{k=1}^{n}\binom{2n-1}{k-1}=\sum_{k=0}^{n-1}\binom{2n-1}{k}=\sum_{k=n}^{2n-1}\binom{2n-1}{k}=\sum_{k=n+1}^{2n}\binom{2n-1}{k-1}$$

and therefore we obtain

$E(|S_{2n\alpha}|)=\frac{a}{2^{2n}}n\binom{2n}{n}$ and using the Stirling formula it follows

$E(|S_{2n\alpha}|)\simeq\frac{a}{\sqrt{2\pi}}\sqrt{2n}$ for large $n.$ The net distance travelled in a lattice simple random walk is proportional to the square root of the number of steps.

The mean free path is the average distance over which a moving particle (such as an atom, molecule , photon or neutron), travels before substantially changing its direction or energy, typically as a result of one or more successive collisions with other particles.

Imagine a beam o particles being shot through a target and consider an infinitesimally thin slab of the target. The area of the slab is L^2 (L is the width and height of the slab) and its volume is L^2 dx (dx is the thickness of the infinitesimal slab). The concentration of the atoms in the slab is n. The typical number of stopping atoms in the slab is then n L^2 dx . If *l* is the mean free path, then the probability of stopping within the distance *l* must be equal to 1: $\wp(\text{stopping within } l)=1$.

The probability that a beam particle will be stopped in the slab of thickness dx is the net area of the stopping atoms (which is the scattering cross section times the number of stopping atoms in the slab) divided by the total area of the slab:

$$\wp(\text{stopping within } dx)=\frac{\sigma n L^2 dx}{L^2}=n\sigma dx \quad .$$

Hence the mean free path is $l=(n\sigma)^{-1}$ where σ is the scattering cross section.

Consider now a fissile material of atoms in which fission events are produced by an existent neutron population. A neutron can scatter on atoms of the material, changing its momentum, or produce a fission event on an atom releasing other neutrons which can cause further fission events, leading to a chain reaction. If the effective neutron multiplication factor *k*, the average number of neutrons released per fission event that

go on to cause another fission event rather than being absorbed or leaving the material, is equal to 1 ($k = 1$) the mass is critical and the chain reaction is self sustaining.

Most interactions of neutrons with the material are scattering events, so that a given neutron obeys a random walk until it either escapes from the medium or causes a fission reaction. If $k = 1$ we can consider that we have the same neutron travelling a random walk of $n_s + n_f$ steps experiencing n_s scattering events and n_f fission events and during the fission event steps the neutron travels a net distance corresponding to a mean scattering free path l, while the total net distance travelled during both fission event steps and scattering event steps together will be R_c, the radius of a spherical critical mass.

Since the number of steps squared is proportional to the distance travelled in a random walk we have: $\frac{R_c}{l}=\sqrt{s}$ with $s=1+\frac{n_s}{n_f}$.

Also, if σ is the neutrons on atoms scattering process effective cross section and n is the nuclear number density of atoms we have $l=(\sigma n)^{-1}$ and so $R_c\simeq\frac{\sqrt{s}}{\sigma n}$. If M is the critical mass, ρ is the density of the material and m is the mass of one atom of the material, we will have:

$$M=\rho\frac{4}{3}\pi R_c^3\ ,\ n=\frac{3}{4\pi}\frac{M}{m}\frac{1}{R_c^3}\ ,\ R_c\simeq\frac{\sqrt{s}}{\sigma}\frac{m}{M}R_c^3\frac{3}{4\pi}$$ and generally

$1\simeq\frac{f\sigma}{m\sqrt{s}}\rho^{2/3}M^{1/3}$ where f is a factor which takes into account geometrical and other effects. The critical mass depends inversely on the square of density.

In a theory with neutrons and atomic kernels as confined quarks, we should be able to compute in lattice gauge simulation, according to (23) relations the differential cross section for scattering of neutrons on atomic kernels $d\sigma$ and the differential cross section for the fission event process $d\sigma_f$ taking $|\vec{v}_1-\vec{v}_2|=|\vec{v}|=v$ as the absolute value of the neutrons velocity by its thermodynamic average

$v=\sqrt{\frac{2\langle\varepsilon\rangle}{m_0}}=\sqrt{\frac{3k_bT}{m_0}}$ with k_b Boltzmann constant ,

T temperature, m_0 neutron mass.

Then we can determine $\sigma=\int d\sigma$, $\sigma_f=\int d\sigma_f$, $s=1+\frac{\sigma}{\sigma_f}$.

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25. Fermi’s golden rule
Spontaneous and stimulated emission

Fermi's golden rule
Sponataneous and stimulated emission

Consider a quantum system described by an unperturbed Hamiltonian operator H_0 having the eigenstates $|n\rangle$ for eigenvalues E_n : $H_0|n\rangle = E_n|n\rangle$ for any $|n\rangle$, $(|n\rangle)_{n\in S}$ being a complete orthonormal set of energy eigenstates.
The system evolves under a weak perturbation of H_0 so that the effective Hamiltonian operator of the system is considered to be
$H = H_0 + \widetilde{H}(t)$ with $t \in \mathbb{R}$ the time variable and the general state of the system (belonging to the system Hilbert space of wavefunctions) $|\psi\rangle = |\psi(t)\rangle$ satisfies the Schroedinger equation $i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = (H_0 + \widetilde{H}(t))|\psi(t)\rangle$ (1) .
We can expand $|\psi(t)\rangle$ in the form $|\psi(t)\rangle = \sum_n a_n(t)\exp(-i E_n t/\hbar)|n\rangle$ (2)
with $a_n = a_n(t)$ being unknown functions and $|a_n(t)|^2$ being the transition probability at time t into the state $|n\rangle$.
We assume that at time $t = 0$ the system is in an initial state $|i\rangle$: $|\psi(0)\rangle = |i\rangle$ and so $a_n(0) = \delta_{ni}$ for any $n \in S$.
For a measured final state $|f\rangle$ at time t we have that $w_{fi} = |a_f(t)|^2$ is the transition probability after a transition time t from the initial state $|i\rangle$ to the final state $|f\rangle$.
Plugging (2) into (1) we obtain :

$$i\hbar \frac{d\, a_k(t)}{dt} = \sum_n \langle k|\widetilde{H}(t)|n\rangle a_n(t)\exp(i\, t(E_k - E_n)/\hbar) \qquad (3)$$

For $\widetilde{H} = 0$ it is evident that $a_k(t) = a_k(0) = \delta_{ki}$ and so in the zero-th order form of (3), since $\widetilde{H}$ is weak, we can take $a_n(t) \approx \delta_{ni}$ and we have

$$i\hbar \frac{d\, a_f(t)}{dt} = \langle f|\widetilde{H}(t)|i\rangle \exp(i\,\omega_{fi}) \qquad (4) \text{ where } \omega_{fi} = \frac{1}{\hbar}(E_f - E_i)$$

$$i\hbar\, a_f(t) = \int_0^t \langle f|\widetilde{H}(t')|i\rangle \exp(i\,\omega_{fi} t')\, dt'$$

Suppose $\widetilde{H}$ is a periodic perturbation with ω pulsation. Since $\widetilde{H}$ is self-adjoint we must have $\widetilde{H}(t) = F\exp(-i\,\omega t) + F^+ \exp(i\,\omega t)$ and from (4) follows

$$a_f(t) = -\langle f|F|i\rangle \frac{\exp(i(\omega_{fi} - \omega)t) - 1}{\hbar(\omega_{fi} - \omega)} - \langle f|F^+|i\rangle \frac{\exp(i(\omega_{fi} + \omega)t) - 1}{\hbar(\omega_{fi} + \omega)} \qquad (5) .$$

We have resonance values of ω_{fi} at $\pm\omega$.
If $E_f > E_i$ we have a resonant absorption of energy at $\omega = \omega_{fi}$.
If $E_f < E_i$ we have resonant emission of energy at $\omega = -\omega_{fi}$.
For $\omega = \omega_{fI} > 0$ it is therefore sufficient to keep the first term of (5) and for $\omega = -\omega_{fI} > 0$ it is sufficient to keep the second term of (5) .

Hence in the case of emission $\omega = \omega_{if}$ we have

$$|a_f|^2 = 4|\langle f|F^+|i\rangle|^2 \frac{\sin^2(\frac{1}{2}(\omega_{if}-\omega)t)}{\hbar^2(\omega_{if}-\omega)^2}$$

$$\frac{dw_{fi}}{dt} = \frac{2}{\hbar^2}|\langle f|F^+|i\rangle|^2 \frac{\sin((\omega_{if}-\omega)t)}{\omega_{if}-\omega} \qquad (6)$$

For $f_a(x) = \frac{\sin(\frac{\pi}{a}x)}{\pi x}$ with $a>0$,

$$\text{rect}(a\xi) = \begin{cases} 1 & \text{for } \xi \in (-\frac{1}{2a}, \frac{1}{2a}) \\ \frac{1}{2} & \text{for } \xi \in \{-\frac{1}{2a}, \frac{1}{2a}\} \\ 0 & \text{for } \xi \in \mathbb{R}\setminus[-\frac{1}{2a}, \frac{1}{2a}] \end{cases}$$

taking the inverse Fourier transformation $\mathcal{F}$ on temperate distributions

space $S'(\mathbb{R})$ we have $\mathcal{F}(\text{rect}(a\xi))(x) = \int_{-\frac{1}{2a}}^{\frac{1}{2a}} \exp(-2\pi i \xi x)\, dx = f_a(x)$

$\lim_{a\to 0} \text{rect}(a\xi) = 1$, $\lim_{a\to 0} \mathcal{F}(\text{rect}(a\xi)) = \lim_{a\to 0} f_a(x) = \lim_{a\to 0} \mathcal{F}(1) = \delta(x)$

Therefore , for large $t > 0$ we can consider

$\frac{\sin((\omega_{if}-\omega)t)}{\omega_{if}-\omega} = \pi\delta(\omega_{if}-\omega) = \pi\hbar\,\delta(E_i - E_f - \hbar\omega)$ and so for large t we have

$\frac{dw_{fi}}{dt} = \frac{2\pi}{\hbar}|\langle f|F^+|i\rangle|^2 \delta(E_i - E_f - \hbar\omega)$ for resonant emission (7)

and in a similar way for resonant absorption, for large t we have

$\frac{dw_{fi}}{dt} = \frac{2\pi}{\hbar}|\langle f|F|i\rangle|^2 \delta(E_f - E_i - \hbar\omega)$ (8) .

If $\Gamma_{i\to f} = \frac{dw_{fi}}{dt}$ is the $|i\rangle$ to $|f\rangle$ transition probability rate and N_f, N_i are the are the occupancy numbers of $|f\rangle$ respective $|i\rangle$ at a time moment t then

$\frac{dN_i}{dt} = -\Gamma_{i\to f} N_i$, $N_i(t) = N_i(0)\exp(-\Gamma_{i\to f} t)$.

Suppose $|i\rangle$ are excited states and $i \to f$ transitions occur by spontaneous emission.

Then considering $P(t) = \frac{N_i(t)}{\int_0^\infty N_i(t')\,dt'} = \Gamma_{i\to f}\exp(-\Gamma_{i\to f} t)$ the mean lifetime of an excited state is $\tau = \int_0^\infty t\,P(t)\,dt = \frac{1}{\Gamma_{i\to f}}$.

An electron in an atomic system (one atom system of a gas or a crystal lattice system, a semiconductor crystal system with conduction band and valence band) can jump from one energy level to another energy level if the system Hamiltonian is perturbed by an electromagnetic wave having vector potential

$A=(0,\vec{A}),\vec{A}=\left(\frac{\hbar}{2\varepsilon\omega V}\right)^{1/2}(a_{\vec{k}}\exp(i\vec{k}\cdot\vec{x})\exp(-i\omega t)+a_{\vec{k}}^{+}\exp(-i\vec{k}\cdot\vec{x})\exp(i\omega t))\epsilon$

with $A=A(t,\vec{x})$, $\vec{x}\in\mathbb{R}^3$, $A_0=0$, ϵ -polarization versor

V volume of the spatial box where the system is confined , $\omega=kc$,

ε -electric permittivity of vacuum, $k=\|\vec{k}\|$ -wave number, c - vacuum light speed (see Chap. Quantization of electromagnetic field)

If the unperturbed Hamiltonian for the electron is

$H_0=\frac{p^2}{2m}+V(\vec{x})$ with $p=-i\hbar\nabla_{\vec{x}}$ the momentum operator, then according to Chap. Lagrangian of electromagnetic field the Hamiltonian perturbation from the electromagnetic wave will be

$\widetilde{H}=\frac{(p+e\vec{A})^2}{2m}+V-\frac{p^2}{2m}-V$ with e -electron charge ,m -mass of electron .

$\widetilde{H}=\frac{e}{2m}(p\cdot\vec{A}+\vec{A}\cdot p)+\frac{e^2\vec{A}^2}{2m}$.

Since we consider $\widetilde{H}$ a weak perturbation we neglect the $\vec{A}^2$ term and also, because $\epsilon\cdot\vec{k}=0$ we have $p\cdot\vec{A}=\vec{A}\cdot p$ and so

$\widetilde{H}=F\exp(-i\omega t)+F^{+}\exp(i\omega t)$ where $F=\left(\frac{\hbar}{2\varepsilon\omega V}\right)^{1/2}\frac{e}{m}a_{\vec{k}}\exp(i\vec{k}\cdot\vec{x})\epsilon\cdot p$.

The electron can jump from state $|\psi_\alpha\rangle$ to state $|\psi_\beta\rangle$ which are eigenstates of H_0 with eigenvalues E_α respective E_β , $\alpha,\beta\in\{1,2\}$, $\alpha\neq\beta$, $E_2>E_1$.

If the initial state is $|i\rangle=|\psi_2\rangle$ and the final state is $|f\rangle=|\psi_1\rangle$ a photon $\hbar\omega$ is emitted and if the initial state is $|i\rangle=|\psi_1\rangle$ and the final state is $|f\rangle=|\psi_2\rangle$ a photon $\hbar\omega$ is absorbed and this occurs at (or near to) resonance values $\hbar\omega=E_2-E_1$, $\omega=2\pi\nu$, ν -the freqequency of the perturbing electromagnetic wave .

The perturbing field can be a electromagnetic wave at frequency near to the resonance value $\frac{E_2-E_1}{h}$ which produces a stimulated emission or a environmental single photon (or a vacuum fluctuation) at the same resonance frequency , in which case we have a spontaneous emission. We can have also absorption in the presence of a perturbing electromagnetic field with frequency near to $\frac{E_2-E_1}{h}$.

According to (7) in the case of stimulated emission we can estimate the probability rate of the event as

$\frac{dw_{21}}{dt}=\frac{e^2}{m^2}\frac{\pi}{\varepsilon\omega V}|\langle f|\epsilon\cdot p|i\rangle|^2\langle a_{\vec{k}}^{+}a_{\vec{k}}\rangle\,\delta(E_2-E_1-\hbar\omega)$ where $\langle a_{\vec{k}}^{+}a_{\vec{k}}\rangle$ corresponds to $n_{\vec{k}}$ -the number of photons with wave vector $\vec{k}$ and polarization versor ϵ (see Chap. Quantization of a electromagnetic field).

We have $[\widehat{H}_0,\hat{x}_i]=[\frac{\hat{p}^2}{2m},\hat{x}_i]=\frac{1}{2m}(\hat{p}\cdot[\hat{p},\hat{x}_i]+[\hat{p},\hat{x}_i]\cdot\hat{p})=-i\frac{\hbar}{m}\hat{p}_i$

$\langle f|[\widehat{H}_0,\hat{x}_j]|i\rangle=(E_f-E_i)\langle f|\hat{x}_j|i\rangle$ and so

$\langle f|\epsilon\cdot p|i\rangle=\frac{i}{\hbar}\frac{m}{e}(E_f-E_i)\,\epsilon\cdot p_e$ where $p_e=\langle f|e\hat{\vec{x}}|i\rangle$ is the transition dipole moment.

The final state $|f\rangle=|\psi_1\rangle$ can have a degeneracy g_1 (the number of independent H_0 eigenstates which correspond to the same eigenvalue as $|f\rangle$) and the transition can occur from the state $|i\rangle$ to any of the g_1 degeneracy states $|f\rangle$ and therefore

$\frac{dw_{21}}{dt}=\frac{\pi}{\varepsilon V}g_1|\epsilon\cdot p_e|^2 n_{\vec{k}}\,\omega\,\delta(E_2-E_1-\hbar\omega)$ (9) for stimulated emission .

In the same way, for absorption we will have a transition probability rate

$\frac{dw_{12}}{dt}=\frac{\pi}{\varepsilon V}g_2|\epsilon\cdot p_e|^2 n_{\vec{k}}\,\omega\,\delta(E_2-E_1-\hbar\omega)$ (10) where g_2 is the degeneracy of the $|\psi_2\rangle$ state.

For the spontaneous emission we will have a perturbing field with $n_{\vec{k}}=1$ interacting with the system and so a transition probability rate

$\frac{d\overline{w}_{21}}{dt}=\frac{\pi}{\varepsilon V}g_1|\epsilon\cdot p_e|^2\,\omega\,\delta(E_2-E_1-\hbar\omega)$ (11)

To obtain the effective transition probability rate we must take in consideration all values of the wave vector $\vec{k}$ with the versor in a solid angle $\Delta\Omega$ and corresponding energy $\hbar k c$ in an interval $(E,E+dE)$. Therefore we must integrate over the volume element in the $\vec{k}$ -space $d^3\vec{k}$ multiplying with $\frac{V}{(2\pi)^3}$ which is the number of $\vec{k}$ states in a unit volume element $dk_1dk_2dk_3$ (according to Chap. Canonical quantization of a scalar field).

Therefore the transition probability rates are :

$\frac{dW_{21}}{dt}=\int\frac{\pi}{\varepsilon V}g_1|\epsilon\cdot p_e|^2 n_{\vec{k}}\,\omega\,\delta(E_2-E_1-\hbar\omega)\frac{V}{(2\pi)^3}d^3\vec{k}$

$\frac{dW_{21}}{dt}=\frac{\pi}{\hbar\varepsilon c^3}g_1|\epsilon\cdot p_e|^2\,\nu^3 n_{\vec{k}}\Delta\Omega$ with $\nu=\frac{1}{h}(E_2-E_1)$ (12)

$\frac{dW_{12}}{dt}=\frac{\pi}{\hbar\varepsilon c^3}g_2|\epsilon\cdot p_e|^2\,\nu^3 n_{\vec{k}}\Delta\Omega$ (13)

In the case of stimulated emission the emitted photons have the same wave vector and the same polarization and phase as the perturbing photons, therefore the stimulated emission radiation is coherent.

For the spontaneous emission, the direction of $\vec{k}$ is undetermined ($\Delta\Omega=4\pi$) and the perturbation is a random electromagnetic fluctuation of the medium.

Hence $\frac{d\overline{W}_{21}}{dt}=\frac{\pi}{\hbar\varepsilon c^3}g_1\left|\epsilon\cdot p_e\right|^2 4\pi\nu^3$ (14)

We have the following emission (absorption) Einstein coefficients :

$B_{21}=\frac{\pi}{\hbar\varepsilon c^3}g_1\left|\epsilon\cdot p_e\right|^2$ (stimulated emission)

$B_{12}=\frac{\pi}{\hbar\varepsilon c^3}g_2\left|\epsilon\cdot p_e\right|^2$ (absorption)

$A_{21}=4\pi\nu^3\frac{\pi}{\hbar\varepsilon c^3}g_1\left|\epsilon\cdot p_e\right|^2$ (spontaneous emission)

We see that in the above (12) , (13) , (14) relations, the coefficients depend on the polarization versor of the incident photons. The incident electromagnetic wave is however unpolarized , and therefore the system interacts separate which each of two independent polarization states and so instead of $\left|\epsilon\cdot p_e\right|^2$ we will have $\left|\epsilon_1\cdot p_e\right|^2+\left|\epsilon_2\cdot p_e\right|^2$ where ϵ_i , $i=1,2$ with $\epsilon_i\cdot\epsilon_j=\delta_{ij}$ are the two independent orthogonal polarization versors.

If N_i is the state $|\psi_i\rangle$ population , $N_i=N_i(t)$, $i=1,2$ then from (12) , (13) , (14) we have

$$-\left(\frac{\partial N_2}{\partial t}\right)_{st.emission}=\left(\frac{\partial N_1}{\partial t}\right)_{st.emission}=B_{21}n_{\vec{k}}\nu^3\Delta\Omega N_2$$

$$\left(\frac{\partial N_2}{\partial t}\right)_{absorption}=-\left(\frac{\partial N_1}{\partial t}\right)_{absorption}=B_{12}n_{\vec{k}}\nu^3\Delta\Omega N_1$$

$$-\left(\frac{\partial N_2}{\partial t}\right)_{sp.emission}=\left(\frac{\partial N_1}{\partial t}\right)_{sp.emission}=A_{21}N_2$$

It follows $g_2B_{21}=g_1B_{12}$, $A_{21}=4\pi\nu^3B_{21}$ (15)

$$\left(\frac{\partial N_1}{\partial t}\right)_{st.emission}+\left(\frac{\partial N_1}{\partial t}\right)_{absorption}=B_{21}n_{\vec{k}}\nu^3\Delta\Omega\left(N_2-\frac{g_2}{g_1}N_1\right)\qquad(16)$$

In a system at thermodynamical equilibrium temperature *T* we can assume a distribution of states according to Boltzmann distribution :

$\frac{N_i}{N}=\frac{g_i\exp\left(-E_i/(k_bT)\right)}{Z}$ with $N=\sum_i N_i$, $Z=\sum_i g_i\exp\left(-E_i/(k_bT)\right)$,

k_b -the Boltzmann constant, N_i the state $|\psi_i\rangle$ population, $H_0|\psi_i\rangle=E_i|\psi_i\rangle$,

g_i degeneracy of the E_i eigenvalue states.

(see Chap. Classical statistical ensemble)

At thermodynamical equilibrium we have that the net exchange between any two levels $|\psi_1\rangle$, $|\psi_2\rangle$ will be balanced. Also , the equilibrium distribution of photons will be that of a photonic gas at equilibrium and so we can consider

$n_{\vec{k}}=\frac{1}{\exp\left(h\nu/(k_bT)\right)-1}$ with $\|\vec{k}\|=k=2\pi\nu/c$, $h\nu=E_2-E_1$

The delented balancing between levels represented by $|\psi_1\rangle$ and $|\psi_2\rangle$ states gives

$0=\left(\frac{\partial N_1}{\partial t}\right)_{net}=4\pi B_{21}\nu^3 n_{\vec{k}} N_2-4\pi B_{12}\nu^3 n_{\vec{k}} N_1+A_{21}N_2$ and so

$4\pi\nu^3 B_{21} g_2\exp(-E_2/(k_bT))-4\pi\nu^3 g_1 B_{12}\exp(-E_1/(k_bT))+$

$+A_{21}(\exp(h\nu/(k_bT))-1)\exp(-E_2/(k_bT))=0$ (17)

The Einstein coefficients are fixed probabilities per time units, associated witheach atom and do not depend on the state of the gas of which the atoms are a part. Therefore (17) must hold for any $T>0$.

For $T\to\infty$ from (17) we obtain $B_{21}g_2=B_{12}g_1$ and so (17) leads to

$4\pi\nu^3 B_{21}g_2(1-\exp(h\nu/(k_bT)))=g_2A_{21}(1-\exp(h\nu/(k_bT)))$

and we recovered (15) from the balancing of net exchange between levels , and we can see also that if (15) is valid , the net balancing (17) follows.

The rate equations (12) , (13) , (14) refer only to excitation at the particular optical frequency $\nu_0=\frac{1}{h}(E_2-E_1)$.At frequencies offset from ν_0 the strenght of stimulated (or spontaneous emission) will not vanish, it will be decreased according to the so called line shape describing the broadening affecting atomic or molecular resonance. The broadening of the emitted spectrum at a particular resonance frequency occurs because the difference between the excited state and the lower one final state can have fluctuations. If the fluctuation is due to a phenomenon that is the same for each quantum emitter, there is a homogeneous broadening . If each quantum emitter has a different type of fluctuation, there is a inhomogeneous broadening.

Therefore the emission probability rate for a frequency in the interval (ν , $\nu+d\nu$) will be (for stimulated emission) $\frac{dW_{21}}{dt}=B_{21}\nu^3 n_{\vec{k}}\Delta\Omega g(\nu)d\nu$ where vers$\vec{k}$ is in the solid angle $\Delta\Omega$, $k=\|\vec{k}\|=2\pi\nu/c$ and $g=g(\nu)$ is the spectral line shape function defined as a distribution of frequencies such that $\int_B g(\nu)d\nu$ is interpreted as the probability that a photon with a wave number $k=2\pi\nu/c$, $\nu\in B$ actually has a resonant frequency which causes the emission.

An example of situation where the fluctuation which determines a spectral line shape function is the same for each individual system of a statistical ensemble (homogeneous broadening) are natural or lifetime broadening fluctuations. The uncertainity principle relates the mean lifetime τ of an excited state with the uncertainity of its energy $\Delta E=h\Delta\nu$ as $\tau\Delta E\geq\frac{\hbar}{2}$, $\tau\Delta\nu\geq\frac{1}{4\pi}$ and so any frequency in an interval $(\nu_0,\nu_0+\Delta\nu)$ can determine an emission.

When ν is an effective resonant frequency , causing emission, the atom (or molecule) system absorbs from the photonic electromagnetic oscillator and dissipates during positional fluctuations on the electronic orbit a mean power $\widetilde{P}(\nu)$ which is proportional to the probability that photons with frequency in an

interval $(\nu, \nu+d\nu)$ actually determine an emission.
Hence we have merely a process similar to forced oscillations described by a motion equation of the form
$a_0\ddot{q}=Q_e+Q_f+Q_a=-kq-\alpha\dot{q}+Q_0\cos(\omega t)$ with
$Q_e=-kq$ -elastic force , $Q_f=-\alpha\dot{q}$ -dissipative friction force,
$Q_a=Q_0\cos(\omega t)$ -active oscillating force .

For $\frac{\alpha}{a_0}=2\delta$, $\frac{k}{a_0}=\omega_0^2$, $\frac{Q_0}{a_0}=\beta$ we have

$\ddot{q}+2\delta\dot{q}+\omega_0^2 q=\beta\cos(\omega t)$ (18)

The homogeneous equation $\ddot{q}+2\delta\dot{q}+\omega_0^2 q=0$ has for $\delta<\omega_0$ a general real solution of the form $q_0(t)=\exp(-\delta t)\,b\cos(t\sqrt{\omega_0^2-\delta^2}+\varphi)$ where b, φ are constants.
A particular solution of (18) of the form $q_1(t)=A\sin(\omega t)+B\cos(\omega t)$ leads to the system in A, B

$A(\omega_0^2-\omega^2)-2B\delta\omega=0$
$2A\delta\omega+B(\omega_0^2-\omega^2)=\beta$

with solution $A=\beta\frac{2\delta\omega}{(\omega^2-\omega_0^2)^2+4\delta^2\omega^2}=A_A$, $B=\beta\frac{\omega_0^2-\omega^2}{(\omega^2-\omega_0^2)^2+4\delta^2\omega^2}=A_D$

and so $q_1(t)=A_A\sin(\omega t)+A_D\cos(\omega t)=\bar{A}\cos(\omega t-\phi)$ where

$\bar{A}=\sqrt{A_A^2+A_D^2}=\beta((\omega_0^2-\omega^2)^2+4\delta^2\omega^2)^{-1/2}$, $\phi=\arctan(\frac{A_A}{A_D})=\arctan\left(\frac{2\delta\omega}{\omega_0^2-\omega^2}\right)$.

For $t\to\infty$ we have $q_0(t)\to 0$ and so we can take for the absorbed power
$P_A(t)=Q_a\dot{q}_1(t)=Q_0\cos(\omega t)(\omega A_A\cos(\omega t)-\omega A_D\sin(\omega t))$

The mean absorbed power on a period $\frac{2\pi}{\omega}$ is

$$P_A=\frac{1}{2}Q_0\,\omega A_A=\frac{Q_0^2}{a_0}\frac{\delta\omega^2}{(\omega_0^2-\omega^2)^2+4\delta^2\omega^2}$$

The dissipated power is
$P_D(t)=-Q_f\dot{q}_1(t)=\alpha\dot{q}_1^2=2\delta a_0(\omega A_A\sin(\omega t)-\omega A_D\cos(\omega t))^2$
The mean dissipated power on a period is

$$P_D=a_0\delta\omega^2(A_A^2+A_D^2)=\frac{Q_0^2}{a_0}\frac{\delta\omega^2}{(\omega_0^2-\omega^2)^2+4\delta^2\omega^2}=P_A$$

We have $\widetilde{P}=\widetilde{P}(\omega)=P_D=P_A=\frac{Q_0^2}{a_0}\frac{\delta\omega^2}{(\omega_0^2-\omega^2)^2+4\delta^2\omega^2}$

$\widetilde{P}$ has a maximum at $\omega=\omega_0$ and the full width at half maximum is

$\Delta\omega_{res}=|\omega_1-\omega_2|$ where $\widetilde{P}(\omega_{1,2})=\frac{1}{2}\widetilde{P}(\omega_0)$.

We obtain for $\omega_{1,2}>0$ that $\omega_{1,2}=\sqrt{\omega_0^2+\delta^2}\pm\delta$, $\Delta\omega_{res}=2\delta$.

We consider δ a small value and so significant values of $\widetilde{P}$ are obtained for $|\omega_0-\omega|\in O(\varepsilon)$ with $\varepsilon>0$ a small value and so

$\widetilde{P}=\frac{Q_0^2}{a_0}\frac{\delta}{(\omega_0-\omega)^2+4\delta^2}+O(\varepsilon)$, $\widetilde{P}(\nu)\approx C\frac{\Gamma/2}{(\nu-\nu_0)^2+(\Gamma/2)^2}$ where C is a constant and Γ is the full width at half maximum. $\widetilde{P}(\nu)$ has maximum value at $\nu=\nu_0$. Therefore considering ν_0 sufficiently large we obtain in the case of homogeneous broadening the Lorentz frequency distribution

$g(\nu)\approx\frac{1}{\pi}\frac{\Gamma/2}{(\nu-\nu_0)^2+(\Gamma/2)^2}$.

Inhomogeneous broadening occurs for example due the Doppler effect resulting from the distribution of velocities in a gas at a certain temperature.

If $\vec{v}$ is the velocity of the atom (molecule) in a gas and the angle between $\vec{v}$ and the perturbing electromagnetic wave is θ with $\frac{v}{c}\in O(\varepsilon)$, $v=\|\vec{v}\|$, ε small , the frequency shift is $\Delta\nu=\nu\frac{v}{c}\cos\theta+O(\varepsilon^2)$ (see Chap. Doppler effect . . .)

The dispersion $(\langle(\Delta\nu)^2\rangle)^{1/2}$ over all values of $\vec{v}$ and θ will be σ with

$\sigma^2=\nu_0^2\frac{\langle\vec{v}^2\rangle}{c^2}\langle\cos^2\theta\rangle+O(\varepsilon^2)\approx\nu_0^2\frac{\langle\vec{v}^2\rangle}{2c^2}$

According to Chap. Classical statistical ensemble we will have $\langle\vec{v}^2\rangle=\frac{2}{m}3k_bT$ where T is the absolute temperature of the gas and m is the mass of the gas atom or molecule. Therefore the dispersion is $\sigma=\frac{\nu_0}{c}\left(\frac{3k_bT}{m}\right)^{1/2}$ and the spectral line in the case of inhomogeneous broadening due the Doppler effect in a gas can be a Gaussian distribution with mean value ν_0 and dispersion σ:

$$g(\nu)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{1}{2}\left(\frac{\nu-\nu_0}{\sigma}\right)^2\right)$$

Suppose we have two types of fluctuations *a* and *b* which have spectral line shape functions g_a respective g_b and produce a shift in resonance frequency $(\Delta\nu)_a$ and respective $(\Delta\nu)_b$.

Therefore we have on the probability space (Φ,P) of photons with the probability $P:\wp(\Phi)\to[0,1]$ where $P(\{\varphi\})$ is the probability that the photon φ has a resonant frequency that causes emission, the random variables $(\Delta\nu)_a,(\Delta\nu)_b:\Phi\to\mathbb{R}$ such that $(\Delta\nu)_{a,b}(\varphi)$ is the shift in resonance frequency that is present when the photon φ perturbs the Hamiltonian of an atom.

From the interpretation of $g(\nu)$ follows that

$P\circ(\tilde{\nu}+(\Delta\nu)_{a,b})^{-1}$ where $\tilde{\nu}:\Phi\to\mathbb{R}$ is defined by $\tilde{\nu}(\varphi)$ -frequency of the photon φ, has the density $g_{a,b}$ and we must have $P\circ\tilde{\nu}^{-1}=\varepsilon_{\nu 0}$ because ν_0 is the only resonant frequency when we have no fluctuations.

(where $\varepsilon_{\nu 0}(\{\nu\})=\begin{cases}1 & \text{if } \nu=\nu_0\\ 0 & \text{if } \nu\neq\nu_0\end{cases}$, $\varepsilon_{\nu 0}$ has density function $\delta(\nu-\nu_0)$) .

If $\rho_{a,b}$ are the densities of $(\Delta\nu)_{a,b}$, from the rule for densities of sums of independent random variables we have $g_{a,b}(\nu)=(\delta(\nu-\nu_0)*\rho_{a,b})(\nu)=\rho_{a,b}(\nu-\nu_0)$ (* -the convolution operation)

The total fluctuation $a+b$ produces a shift $(\Delta\nu)_a+(\Delta\nu)_b=(\Delta\nu)_{a+b}$ and assuming the fluctuations are independent we will have

$g_{a+b}(\nu)=\rho_{a+b}(\nu-\nu_0)=(\rho_a*\rho_b)(\nu-\nu_0)=(g_a(\nu+\nu_0)*g_b(\nu+\nu_0))(\nu-\nu_0)=$

$=\int g_a(\nu-\nu_0-\nu'+\nu_0)g_b(\nu'+\nu_0)\,d\nu'=(g_a*g_b)(\nu+\nu_0)$

$g_{a+b}(\nu)=(g_a*g_b)(\nu+\nu_0)$

As proven we have $\left(\frac{\partial N_1}{\partial t}\right)_{st.emission}=B_{21}n_{\vec{k}}\,\nu^3\Delta\Omega\,g(\nu)\,d\nu N_2$ and in the same way $\left(\frac{\partial N_1}{\partial t}\right)_{absorption}=-\frac{g_2}{g_1}B_{21}n_{\vec{k}}\,\nu^3\Delta\Omega\,g(\nu)\,d\nu N_1$.

Therefore from stimulated emission we have a gain in emitted power

$$P_{net}=h\nu\left(\left(\frac{\partial N_1}{\partial t}\right)_{st.emission}+\left(\frac{\partial N_1}{\partial t}\right)_{absorption}\right)=h\nu B_{21}\Delta N\,n_{\vec{k}}\,\nu^3\Delta\Omega\,g(\nu)\,d\nu$$

which is positive only when we have a population inversion $\Delta N=N_2-\frac{g_2}{g_1}N_1>0$.

The stimulated emission cross section σ_{21} is defined as the probability rate of stimulated emission transition divided by the flux number of photons (number of photons crossing an unit area of surface normal to propagation direction in unit time). If the medium is refractive (n -dimensionless refractive index) the flux will be affected by the medium . The flux is equal to $\rho\,v$ where ρ is the density number of photons per unit volume and v is the propagation velocity.

For the considered electromagnetic wave, the number of photons in the volume V for a wave vector $\vec{k}$ in a $d^3\vec{k}$ volume element in $\vec{k}$ -space is

$2n_{\vec{k}}\frac{V}{(2\pi)^3}d^3\vec{k}=2n_{\vec{k}}\frac{V}{(2\pi)^3}k^2\,dk\,\Delta\Omega$ (we have a factor of 2 because we are considering the two independent polarization states).

$k=\frac{2\pi}{\lambda_m}=\frac{2\pi}{v}\nu=\frac{2\pi}{c}n\nu$

(λ_m is the wavelenght of the elctromagnetic wave in the medium) and so

$\rho = 2\, n_{\vec{k}} \frac{1}{c^3} n^3\, \nu^2 d\,\nu \Delta\Omega$ and the flux will be $\Phi = \rho v = \rho \frac{c}{n} = 2\, n_{\vec{k}} \frac{n^2}{\lambda^2} d\,\nu \Delta\Omega$

where $\lambda = \frac{c}{\nu}$ is the wavelenght of the electromagnetic wave in vacuum.

Hence $\sigma_{21} = \frac{\frac{dW_{21}}{dt}}{\Phi} = \frac{B_{21} n_{\vec{k}}\, \nu^3 \Delta\Omega\, g(\nu) d\,\nu}{2\, n_{\vec{k}}\, d\,\nu \Delta\Omega} \frac{\lambda^2}{n^2} = \frac{1}{8\pi} A_{21} \frac{\lambda^2}{n^2} g(\nu)$,

$\sigma_{21}(\nu) = \frac{1}{8\pi} A_{21} \frac{\lambda^2}{n^2} g(\nu)$

Consider now a gain medium where we have a population inversion per unit volume $\Delta \widetilde{N} = \frac{1}{V}\left(N_2 - \frac{g_2}{g_1} N_1\right)$ and an incident coherent beam of photons in the z -axis direction. The number of photons in the beam crossing a normal to z -axis surface Σ of area A in a small time interval Δt is N_σ .

We look at the stimulated emissions that take place in a cylindrical region along the z -axis with basis Σ having volume $V = A\,\Delta z$ (with Δz small) .

The number of photons crossing the surface Σ in the same interval Δt and are perturbing the states of electrons in the gain medium atoms is N_p . As long as the incident beam signal intensity is small enough (that is far from saturation) so that it does not have a significant effect on the magnitude of the population inversion which would increase the gain in emitted power, and therefore since the stimulated emission photons have the same wave vector , phase and polarization as the incident beam photons would overcrease N_p , we can consider $N_p = N_\sigma$ within the time interval we considered for counting N_σ .

The intensity of the incident beam is $I = \frac{N_\sigma}{A \Delta t} h\,\nu$. Since the stimulated emission photons have the same wave vector , phase and polarizations as the incident beam photons we have an increase of N_σ in the time interval Δt due the difference between stimulated emission photons and absorption photons which, ignoring the spontaneous emission, is $(\Delta N_1)_{net} = (\Delta N_1)_{st.emission} + (\Delta N_1)_{absorption}$

$(\Delta N_1)_{st.emission}$ gives the number of stimulated emission photons,

$(\Delta N_1)_{absorption}$ gives the number of absorbed photons.

Therefore $\Delta N_\sigma = (\Delta N_1)_{net} = (\Delta N_1)_{st.emission} + (\Delta N_1)_{absorption}$ (19)

If Γ_{21} is the transition probability rate for stimulated emission, from (12) ,(13), (16) and (19) follows $\Gamma_{21} \Delta \widetilde{N} A \Delta z = \frac{\Delta N_\sigma}{\Delta t}$.

The flux of perturbing photons is $\Phi=\frac{N_p}{A\Delta t}$ which in the case of a small signal is $\Phi=\frac{N_\sigma}{A\Delta t}$. For a small signal that not affects $\Delta\widetilde{N}$, taking $\gamma_0(\nu)=\sigma_{21}(\nu)\Delta\widetilde{N}$ we derive $\frac{\Delta I}{\Delta z}=h\nu\frac{\Delta N_\sigma}{A\Delta t\Delta z}=h\nu\Gamma_{21}\Delta\widetilde{N}=h\nu\frac{\Gamma_{21}}{\Phi}\frac{N_\sigma}{A\Delta t}\Delta\widetilde{N}=\sigma_{21}\Delta\widetilde{N}I$ and so the small signal equation for the optical intensity $\frac{dI}{dz}=\gamma_0(\nu)I(z)$ leading to $I(z)=\exp(\gamma_0(\nu)z)I_{\text{in}}$ where $I_{\text{in}}=I(0)$ is the optical intensity of the input signal.

Consider a crystal lattice of a semiconductor material with unit cells $(\Omega_0+R_{\boldsymbol{n}})_{\boldsymbol{n}}$ (see Chap. Covalent crystal lattice) , $R_{\boldsymbol{n}}=\sum_{i=1}^{3}n_i\vec{a}_i$, $\boldsymbol{n}=(n_i)_{i=\overline{1,3}}$, $\Omega_0=\{(a_ix_i)_{i=\overline{1,3}}|x_i\in[-\frac{1}{2},\frac{1}{2}]\text{ for }i=\overline{1,3}\}$, $\vec{b}_i=\frac{2\pi}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}(\vec{a}_i\times\vec{a}_j)\epsilon_{ijk}$ (with no summation over j,k) .

We consider a volume $V=N\Omega_0$, $n_i=\overline{0,N_i}$ of $N=N_1N_2N_3$ cells.

We consider simplified a rectangular lattice $\vec{k}=(k_i)_{i=\overline{1,3}},k_ia_i=2\pi\frac{m_i}{N_i}$, $m_i\in\mathbb{Z}$

An orthonormalized complete set of wave functions of electrons in the crystal will be of the form $(\widetilde{\psi}_{\vec{k}\alpha})_{\vec{k}\alpha}$ with $\widetilde{\psi}_{\vec{k}\alpha}=\exp(-\frac{i}{\hbar}E_\alpha(\vec{k})t)\,\psi_{\vec{k}\alpha}(x)$

with $(t,x)\in\mathbb{R}^4$ time-space coordinates and

$\psi_{\vec{k}\alpha}(x)=\frac{1}{\sqrt{N\Omega_0}}\exp(i\vec{k}\cdot x)u_{\vec{k}\alpha}(x)$, $u_{\vec{k}\alpha}(x)=\sum_{\boldsymbol{n}}\exp(i\vec{k}(R_{\boldsymbol{n}}-x))u_{0\alpha}(x-R_{\boldsymbol{n}})$

where $u_{0\alpha}=u_{0\alpha}(x)\in\mathbb{R}$ is a solution of $\nabla^2u_{0\alpha}(x)+\frac{2m_0}{\hbar^2}(E_{0\alpha}-V_0(x))u_{0\alpha}(x)=0$

$E_{0\alpha}$ -energy levels of a electron in a single atom cell system.

Since we can roughly consider that $u_{0\alpha}$ vanishes outside of the cell Ω_0 we take the normalization $\int u_{0\alpha}(x-R_{\boldsymbol{n}})u_{0\beta}(x-R_{\boldsymbol{m}})d^3x=\delta_{\boldsymbol{nm}}\delta_{\alpha\beta}\Omega_0$

We have $\psi_{\vec{k}\alpha}(x)=\frac{1}{\sqrt{N\Omega_0}}\sum_{\boldsymbol{n}}\exp(i\vec{k}\cdot R_{\boldsymbol{n}})u_{0\alpha}(x-R_{\boldsymbol{n}})$ and since $\psi_{\vec{k}\alpha}$ are periodic with respect to $\vec{k}$ with period $\left(\frac{2\pi}{a_i}\right)_{i=\overline{1,3}}$ it is sufficient to consider only values $\vec{k}=(k_i)_{i=\overline{1,3}}$ with $k_i\in\left[-\frac{\pi}{a_i},\frac{\pi}{a_i}\right)$ (the first Brillouin zone)

We can verify that we have

$\langle\psi_{\vec{k}\alpha},\psi_{\vec{k}'\beta}\rangle=\sum_{\boldsymbol{n},\boldsymbol{m}}\exp(i\vec{k}'\cdot R_{\boldsymbol{n}}-i\vec{k}R_{\boldsymbol{m}})\frac{1}{N\Omega_0}\int u_{0\beta}(x-R_{\boldsymbol{n}})u_{0\alpha}(x-\boldsymbol{R}_{\boldsymbol{m}})d^3x=\delta_{\vec{k}\vec{k}'}\delta_{\alpha\beta}$

and so we have chosen the correct normalization.
The energy levels in the Linear combination of atomic orbitals tight binding approximation (see Chap. Covalent crystal lattices …) are given by

$$E_\alpha(\vec{k})=E_{0\alpha}-\delta_\alpha-2\gamma_\alpha(\cos(k_1a_1)+\cos(k_2a_2)+\cos(k_3a_3)) \quad (20)$$ where

$$\delta_\alpha=-\frac{1}{\Omega_0}\int u_{0\alpha}(x)(V(x)-V_0(x))u_{0\alpha}d^3x$$

$$\gamma_\alpha=-\frac{1}{\Omega_0}\sum_{i=1}^{3}\int\frac{1}{2}(u_{0\alpha}(x-\vec{a}_i)+u_{0\alpha}(x+\vec{a}_i))(V(x)-V_0(x))u_{0\alpha}(x)d^3x$$

$$V(x)=\sum_{\boldsymbol{n}}V_0(x-R_{\boldsymbol{n}}) \ .$$

Since the $u_{0\alpha}$ roughly vanish outside Ω_0 we can assume that

$$\int u_{0\alpha}(x-R_{\boldsymbol{n}})\nabla u_{0\beta}(x-R_{\boldsymbol{m}})d^3x\approx 0 \quad \text{for } \boldsymbol{n}\neq\boldsymbol{m} \text{ and therefore}$$

$$\int\psi^*_{\vec{k}\alpha}(x)(\hat{p}\,\psi_{\vec{k}'\beta})(x)d^3x=$$

$$=\frac{1}{N\Omega_0}\int\sum_{\boldsymbol{n}}\exp(-i(\vec{k}-\vec{k}')\cdot R_{\boldsymbol{n}})(-u_{0\alpha}(x)i\hbar\nabla u_{0\beta}(x))d^3x=$$

$$=-\delta_{\vec{k}\vec{k}'}\frac{i\hbar}{\Omega_0}\int u_{0\alpha}(x)\nabla u_{0\beta}(x)d^3x=i\delta_{\vec{k}\vec{k}'}\frac{m_0}{\Omega_0}\frac{E_{0\alpha}-E_{0\beta}}{\hbar}\int u_{0\alpha}(x)\,x\,u_{0\beta}(x)d^3x$$

$$\langle\psi_{\vec{k}\alpha}|\hat{p}|\psi_{\vec{k}'\beta}\rangle=i\delta_{\vec{k}\vec{k}'}\frac{m_0}{e}\mu_{\alpha\beta}\frac{E_{0\alpha}-E_{0\beta}}{\hbar} \quad (21)$$

where $\mu_{\alpha\beta}=\frac{1}{\Omega_0}\int u_{0\alpha}(x)e\,x\,u_{0\beta}(x)d^3x$ is the transition dipole moment.

In the general $(\vec{a}_i)_{i=\overline{1,3}}$ case the relation (20) becomes

$$E_\alpha(\vec{k})=E_{0\alpha}-\delta_\alpha-2\gamma_\alpha(\cos(2\pi\tilde{k}_1)+\cos(2\pi\tilde{k}_2)+\cos(2\pi\tilde{k}_3))$$

with $\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i=\sum_{i=1}^{3}\tilde{k}_i\vec{b}_i$, $\vec{k}\cdot\vec{a}_i=2\pi\tilde{k}_i$ and we take $(\tilde{k}_i)_{i=\overline{1,3}}=\vec{\tilde{k}}$, $\tilde{k}=\|\vec{\tilde{k}}\|$,

noticing that the number of $\vec{k}$ -states in a volume $d\tilde{k}_1d\tilde{k}_2d\tilde{k}_3=d^3\vec{\tilde{k}}$

is $Nd^3\vec{\tilde{k}}=N\tilde{k}^2\Delta\tilde{\Omega}$ and the first Brillouin zone corresponds to $(\tilde{k}_i)_{i=\overline{1,3}}\in\left[-\frac{1}{2},\frac{1}{2}\right)^3$

The valence band of electrons in the semiconductor crystal lattice is defined by by states $\psi_{\vec{k}v}$ whose energy levels $E_1(\vec{k})$ for small wave numbers, and $\vec{k}$ in the first Brillouin zone are, according to (20) approximated by

$$E_1(\vec{k})=E_1(0)+\gamma_v4\pi^2\tilde{k}^2 \text{ with } E_1(0)=E_v=E_{0v}-\delta_v-2\gamma_v$$

The conduction band of electrons is defined by states $\psi_{\vec{k}c}$ whose energy levels for the same $\vec{k}$ values are approximated by

$$E_2(\vec{k})=E_2(0)+\gamma_c4\pi^2\tilde{k}^2 \text{ with } E_2(0)=E_c=E_{0c}-\delta_c-2\gamma_c$$

We have $E_c > E_v$ and at $\vec{k}=0$, $E_1(\vec{k})$ has a maximum and $E_2(\vec{k})$ has a minimum. Therefore we must have $\gamma_v < 0$, $\gamma_c > 0$ and $E_g = E_c - E_v$ is the band gap.

Consider a electromagnetic wave with vector potential :

$\vec{A} = \epsilon(A\exp(i(\vec{q}\cdot x - \omega t)) + A^+ \exp(-i(\vec{q}\cdot x - \omega t)))$ with $\omega = q\frac{c}{n}$, n -refraction index of the semiconductor medium, $A \in \mathbb{C}$, ϵ -polarization versor , $\omega \in \mathbb{R}_+$, $\vec{q} \in \mathbb{R}^3$, $q = \|\vec{q}\|$, $\epsilon \cdot \vec{q} = 0$

The Hamiltonian perturbation for the electrons in valence band and conduction band can be estimated as $\widetilde{H} = \frac{e}{2m_0}(p\cdot\vec{A} + \vec{A}\cdot p)$ (m_0 mass of the electron) and focusing on emission (photoluminiscence), the transition probability rate from an electron state $\psi_{\vec{k}'c} = |i\rangle$ of the conduction band to an electron state $\psi_{\vec{k}v}$ in the valence band will be $\Gamma_{if} = \frac{2\pi}{\hbar}|\langle \psi_{\vec{k}'v}|\widetilde{H}|\psi_{\vec{k}c}\rangle|^2 \delta(E_2(\vec{k}) - E_1(\vec{k}) - \hbar\omega)$.

We can evaluate $|\langle \psi_{\vec{k}'v}|\widetilde{H}|\psi_{\vec{k}c}\rangle|^2 = \frac{e^2}{m_0^2}\langle A^+ A\rangle |\langle \psi_{\vec{k}'v}|\epsilon\cdot p|\psi_{\vec{k}c}\rangle|^2 =$

$= \langle A^+ A\rangle \frac{(E_{0c} - E_{0v})^2}{\hbar^2}|\mu_{vc}\cdot\epsilon|^2 \delta_{\vec{k}'\vec{k}}$ where $\mu_{vc} = \frac{1}{\Omega_0}\int u_{0v}(x)\, e\, x\, u_{0c}(x) d^3x$ is the transition dipole moment and we used (21) .

To obtain the total transition probability rate, we must sum over all $\vec{k}, \vec{k}'$ -states and consider the spin degeneracy of the final states . Hence the total transition probability rate is

$\Gamma(\omega) = \frac{4\pi}{\hbar^3}\langle A^+ A\rangle (E_{0c} - E_{0v})^2 |\mu_{vc}\cdot\epsilon|^2 N \int 4\pi\widetilde{k}^2 \delta(\hbar\omega - E_g - 4\pi^2(\gamma_c - \gamma_v)\widetilde{k}^2) d\widetilde{k} =$

$= \frac{1}{\pi}\langle A^+ A\rangle \frac{N}{\hbar^3}\frac{(E_{0c} - E_{0v})^2}{(\gamma_c - \gamma_v)^{3/2}}|\mu_{vc}\cdot\epsilon|^2 \sqrt{\hbar\omega - E_g}$ (22) , $N = \frac{V}{\Omega_0}$

Since $\widetilde{k}$ must be small for making the $\cos(2\pi\widetilde{k}_i) \approx 1 - 2\pi^2\widetilde{k}_i^2$ approximation in relation (20) , the relation (22) is valid only for $\hbar\omega$ close to E_g and $\hbar\omega > E_g$.

Also it follows that the power emitted by photoluminiscence in an unit volume is given by $P_{cv}(\omega) = N_c \Gamma(\omega)\hbar\omega$ where N_c is the volumic concentration of conduction electrons.

If we consider an unpolarized perturbing electromagnetic wave we wil replace in the above relation $|\mu_{vc}\cdot\epsilon|^2$ by $|\mu_{vc}\cdot\epsilon_1|^2 + |\mu_{vc}\cdot\epsilon_2|^2$ with ϵ_1, ϵ_2 two orthogonal polarization direction versors.

Electrical conductivity arises due to the presence of electrons in states that are delocalized (extended through the material) , how are the states near the bottom of the conduction band E_c and near the top of the valence band E_v . In order to transport electrons, a state must be partially filled, containing an electron part of time.

An electron in the conduction band that moves in *j* direction will move with the group velocity $v_g=\frac{\partial \omega}{\partial k_j}(\vec{k})=\frac{1}{\hbar}\frac{\partial E_2}{\partial k_j}(\vec{k})$ (see Chap. Wave propagation) with $\vec{k}$ having only the j component not equal to zero. Therefore $\dot{v}_g=\frac{1}{\hbar}\frac{\partial^2 E_2}{\partial k_j^2}\frac{d k_j}{d t}$.

The momentum of the electron has only the j component which is equal to $\hbar k_j$.

The force acting on the electron is in j direction equal to $F_j=\hbar\frac{d k_j}{d t}$ and we take $F_j=m\dot{v}_g$ with m -the effective mass of the electron in direction j .

Therefore, for motion in direction j the $\psi_{\vec{k}c}$ state electron with $\vec{k}=k_j(\delta_{ij})_{i=\overline{1,3}}$, has an effective mass $m_{je}=\frac{\hbar^2}{\partial^2 E_2/\partial k_j^2}$ (we consider the quasicontinuous variation $k_j=k_j(t)$ for the wave vector of the transported electron).

With $\vec{a}_l=(a_{li})_{i=\overline{1,3}}$ for $l=\overline{1,3}$ we have $\vec{k}=\sum_{i=1}^{3}\tilde{k}_i\vec{b}_i$, $\tilde{k}_l=\frac{1}{2\pi}\vec{k}\cdot\vec{a}_l$, $E_2=E_c+4\pi^2\tilde{k}^2$

$\frac{\partial E_2}{\partial k_j^2}=2\gamma_c\sum_{i=1}a_{ij}^2$, $m_{je}=\frac{\hbar^2}{2\gamma_c\sum_{i=1}^{3}a_{ij}^2}$ and so, since $\gamma_c>0$ conduction electrons have positive effective mass.

If an electron is taken out of the valence band then the trajectory that the electron would normally have taken is now missing its charge. This combination of the full valence band minus the electron can be converted into a picture of a completely empty band containing a positively charged particle that moves in the same way as the electron. This particle is called a hole. In the same way as above we derive an effective mass in direction *j* of a electron near the top of the valence band as $m_{jp}=\frac{\hbar^2}{2\gamma_v\sum_{i=1}^{3}a_{ij}^2}$. The electrons near the top of the the valence band have negative effective mass, since $\gamma_v<0$.

Since force= mass x acceleration , a negative-effective-mass electron near the top of the valence band would move the opposite direction as a positive-effective-mass electron near the bottom of the conduction band, in response to a given electric or magnetic force. Therefore a hole move this way as well. Thus a hole is a positive charge, positive-effective-mass of value – m_{jp} quasiparticle.

Partial filling of the states at the bottom of the conduction band can be understood as adding electrons to that band. Partial filling of the states at the top of the valence band can be understood as taking out electrons of that band or adding holes to that band.

An electron may be excited out of its energy level by a striking photon, generating a electron-hole pair. Electron-hole pairs are constantly generated by thermal energy as well, in the absence of any energy source. Electron-hole pairs are also apt to

recombine. The precise mechanism of generation and recombination are governed by the conservation of energy and conservation of momentum. In a recombination event an electron loses an amount of energy larger than the band gap and thermal energy (in the form of phonons) or radiation (in the form of photons) is emitted.
A quantum state is partially filled only if its energy is near the Fermi level which expresses the thermodynamic quantity of work required from the body maintaining thermodynamical equilibrium to add an electron to the body or equally the work obtained by removing an electron from the body at thermodynamical equilibrium. Therefore V_A - V_B , the observed voltage between two points A ,B in an electric circuit, is exactly related to the corresponding chemical potential (see Chap. Thermodynamics) difference μ_A - μ_B in Fermi levels by the formula

$$V_A - V_B = \frac{\mu_A - \mu_B}{e}$$ (e -electron charge).

It can be seen that electrons will move from a body of high μ (low voltage) to low μ (high voltage) if a simple path is provided. This flow of electrons will cause the lower μ to increase and likewise the higher μ to decrease (due to charging or other repulsive effects). This leads to the fact that an electric circuit in thermodynamical equilibrium (off) state will have a constant Fermi level throughout its connected parts. (Thermodynamical equilibrium requires that the circuit be internally connected and not contain any batteries or other power sources nor any variations in temperature).
At thermodynamical equilibrium the probability that a state of energy ε is occupied by an electron is given by the Fermi-Dirac distribution

$$f(\varepsilon) = \frac{1}{1 + \exp((\varepsilon - \mu)/(k_b T))}$$ (see Chap. Quantum statistical ensemble)

where T -absolute equilibrium temperature , k_b -Boltzmann constant , μ -Fermi level.
In an insulator, the Fermi level lies within a large band gap far away from any states that are able to carry current (partially filled states).
In a metal (material with high conductivity) the Fermi level lies within a delocalized band. A large number of states nearby the Fermi level are thermally active and readily carry current.
In an intrinsic or lightly doped semiconductor the Fermi level is close enough to a band edge that there are a diluted number of thermally excited carriers residing near the band edge (in p-type semiconductors the Fermi level is closer to the valence band and in n-type semiconductors the Fermi level is closer to the conduction band).

Photoluminiscence is typically initiated by photoexcitation (photons excite electrons to a higher energy level) . Following excitation various relaxation processes occur (transition between band states for example in semiconductors) and other photons are re-radiated. The reemitted photons can have a longer wavelenght as the photoexcitation photons (redshift) because intermediate transitions between states at higher level in the conduction band to a lower level which is closer to the bottom of the conduction band E_c or between states at a lower level in the valence band to a level which is closer to the top of of the valence band E_v can occur before a electron-hole recombination with a emission of a photon having a energy close to and above the band gap $E_g = E_c - E_v$ occurs.

A steady value of conduction electrons concentration can be obtained by applying a electric field to the crystal. Thermal activation and electric field liberate atomic electrons (from donor levels) into the conduction band. Many of these electrons are accelerated by the field and collide with luminiscent centers ionizing them(creating holes).Light is emitted in the normal way as soon an electron recombines with a hole . The effect dies away when constant voltage is applied, since the electric field would separate electrons and holes. Therefore an alternating voltage may be used to create a sustained light emission.
Also when an electrode contacts a crystal to provide a flow of electrons or holes or a voltage is applied to a p-n junction causing a current to flow, a steady electrons concentration in the conduction band can be obtained.In both cases the electrons lose energy recombining with holes accompanied by the emission of light . The phenomenon is called electroluminiscence (direct conversion of electric energy into visible light as in LED-s (Light Emission Diodes)).

26. Two component Dirac equation
Non-relativistic limit of Dirac equation
Pauli-Schroedinger equation

Two component Dirac equation
Non-relativistic limit of Dirac equation
Pauli-Schroedinger equation

Taking the Dirac spinor as $\psi=\begin{pmatrix}\widetilde{\psi}_A\\ \widetilde{\psi}_B\end{pmatrix}$ where $\widetilde{\psi}_A, \widetilde{\psi}_B$ are two-component fields, we write the Dirac equation (in the Dirac basis) as a system in the two-component fields:

$$i\frac{\partial}{\partial t}\widetilde{\psi}_A+i\,\vec{\sigma}\cdot\nabla\,\widetilde{\psi}_B=m\,\widetilde{\psi}_A$$

$$-i\,\vec{\sigma}\cdot\nabla\,\widetilde{\psi}_A-i\frac{\partial}{\partial t}\widetilde{\psi}_B=m\,\widetilde{\psi}_B$$

and with $\psi=\exp(-iEt)\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}$, $(\psi_A,\psi_B)=(\psi_A,\psi_B)(\vec{x})$, $\hat{\vec{p}}=-i\nabla$, the above system becomes the Dirac equation eigenvalue problem :

$$E\,\psi_A-\vec{\sigma}\cdot\hat{\vec{p}}\,\psi_B=m\,\psi_A$$

$$\vec{\sigma}\cdot\hat{\vec{p}}\,\psi_A-E\,\psi_B=m\,\psi_B$$

where for simplification by choosing right measuring units we have taken $\hbar=1$ (reduced Planck constant) and $c=1$ (speed of light in vacuum). We can always restore this constants by dimensional analysis.

In the presence of an electromagnetic field (see Chap. Lagrangian of electromagnetism) we must take

$E\to E-eA_0$, $\hat{\vec{p}}\to\hat{\vec{p}}+e\vec{A}$ where $A=(A^\mu)_{\mu=\overline{0,3}}(\vec{x})$ is a stationary electromagnetic potential, $e=-|e|$ is the electron charge and $\vec{A}=(A_k)_{k=\overline{1,3}}$ and we have :

$$(E+eA_0-m)\,\psi_A=\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A})\,\psi_B \qquad (1)$$

$$\psi_B=\frac{1}{E-eA_0+m}\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A})\,\psi_A \qquad (2)$$

Eliminating ψ_B we obtain an equation for ψ_A :

$$\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A})\frac{1}{E-eA_0+m}\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A})\,\psi_A=(E-eA_0-m)\,\psi_A \qquad (3)$$

(We notice that $\hat{\vec{p}}$ is a differential operator and therefore is acting on $A=A(\vec{x})$)

In a non-relativistic situation we have

$$\vec{p}^{\,2}\ll m^2,\ E=E_{NR}+m,\ E_{NR}\ll m,\ \bar{\alpha}=\frac{E_{NR}-eA_0}{2m}\ll 1,\ (\vec{p}+e\vec{A})^2\ll m^2\ ,\ |\psi_B|\ll|\psi_A|$$

Thus $$\frac{1}{E-eA_0+m}=\frac{1}{2m}\left(1-\frac{E_{NR}-eA_0}{2m}+O(\bar{\alpha}^2)\right) \qquad (4)$$

Taking in (4) the $O(\bar{\alpha})$ approximation, relation (3) becomes:

$$E_{NR}\,\psi_A=\left(e\,A_0+\frac{1}{2m}(\vec{\sigma}\cdot(\hat{\vec{p}}+e\,\vec{A}))^2\right)\psi_A \quad .$$

We have $(\vec{\sigma}\cdot(\hat{\vec{p}}+e\,\vec{A}))^2\,\psi_A=((\hat{\vec{p}}+e\,\vec{A})^2+i\,\epsilon_{klm}\,\sigma_k(\hat{p}_l+e\,A_l)(\hat{p_m}+e\,A_m))\,\psi_A$,
$i\,\epsilon_{klm}\,\sigma_k(\hat{p}_l+e\,A_l)(\hat{p_m}+e\,A_m)=e\,\sigma_k\,\epsilon_{klm}(\partial_l(A_m\,\psi_A)+A_l\partial_m\,\psi_A)=-e\,\sigma_k\,B_k\,\psi_A$
where $(B_k)_{k=\overline{1,3}}=\vec{B}=-\nabla\times\vec{A}$ is the magnetic induction field (see Chap. Electromagnetic four-potential).
Therefore in $O(\bar{\alpha})$ approximation we obtain the Schroedinger-Pauli equation for the ψ_A two component spinor in the non-relativistic case:

$$\left(\frac{1}{2m}(\hat{\vec{p}}+e\,\vec{A})^2+e\,A_0-\frac{1}{2m}e\,\vec{\sigma}\cdot\vec{B}\right)\psi_A=E_{NR}\,\psi_A$$

which leads to a non-relativistic Hamiltonian for the two-component spinor field ψ_A interacting with an electromagnetic field of stationary potential $(A_\mu)_\mu=(A_0,\vec{A})$ as:

$$\hat{H}=\frac{1}{2m}(\hat{\vec{p}}+e\,\vec{A})^2+e\,A_0-\frac{1}{2m}\vec{\sigma}\cdot\vec{B} \quad .$$

By gauge invariance we can choose $A_0 = 0$ and for a constant magnetic field we can choose $A_1=\frac{1}{2}B\,x^2$, $A_2=-\frac{1}{2}B\,x^1$, $A_3=0$.
Then $(\hat{\vec{p}}+e\,\vec{A})^2=-\nabla^2+e^2\,\vec{A}^2-2\,ie\,A_k\,\partial_k=-\nabla^2-ie\,B(x^2\partial_1-x^1\partial_2)+O(\vec{A}^2)=$
$=-\nabla^2-e\,\vec{B}\cdot\hat{\vec{L}}+O(\vec{A}^2)$ where $\hat{\vec{L}}=\vec{x}\times\hat{\vec{p}}$ is the orbital angular momentum operator.
Thus $\hat{H}=-\frac{1}{2m}\nabla^2-\frac{1}{2m}e\,\vec{B}\cdot(\hat{\vec{L}}+2\,\vec{S})+e\,A_0$, where $\vec{S}=\frac{1}{2}\hbar\,\vec{\sigma}$ is the spin angular momentum operator.
We derive a magnetic moment for the charged e = - | e |, spin ½ particle given by $\mu=-\mu_B\,g_s\frac{\vec{S}}{\hbar}$ where $\frac{\vec{S}}{\hbar}$ is the spin operator and $\mu_B=\frac{|e|}{2m}\hbar$ is the Bohr magneton.
Hence we have a value g_s = 2 for the so called gyromagnetic ratio of the electron. However we will show in Chap. Anomalous magnetic moment of the electron that quantum fluctuations lead to a value $g_s\approx 2\left(1+\frac{e^2}{8\,\pi^2}\right)\approx 2(1+0.00116)$.

The term $-\frac{1}{2m}e\,\vec{B}\cdot(\vec{L}+2\,\vec{S})$ or $-\frac{1}{2m}e\,\vec{B}\cdot(g_l\,\vec{L}+g_s\,\vec{S})$ (g_l, g_s gyromagnetic ratios for orbital magnetic moment respective spin magnetic moment, $g_l=1, g_s\approx 2$, g_s having an anomalous contribution due to quantum fluctuations) which is the potential energy corresponding to the orbital respective spin magnetic moments of the electron $\mu_{le}=-\mu_B\,g_l\frac{\vec{L}}{\hbar}$, $\mu_{se}=-\mu_B\,g_s\frac{\vec{S}}{\hbar}$ provides the explication of the Zeeman effect on splitting the spectral lines of an element in the presence of a static magnetic field.(see Chap. Perturbation theory for the two-component Dirac equation).

Bohr model

We use an approximation of the atom as a system of electron orbiting according to classical mechanics a circular orbit of radius *r* around a nucleus of charge *-Ze*. (*Z* the atomic number, *e* the electron charge) and the orbit satisfies, to be stable, the standing wave condition for the quantum de Broglie wave associated to the electron. Thus, if λ is the de Broglie wavelenght of the electron wave function we must have $n\lambda=2\pi r \quad , \quad n\in\mathbb{N}^*$.
If *v* is the speed of the electron moving on a circular orbit, according to classical mechanics, in the Coulomb central forces potential $e\,c\,A_0=-\frac{Ze^2}{4\pi r}$ we will have:

$\frac{mv^2}{r}=\frac{Ze^2}{4\pi r^2} \quad , \quad mv^2=\frac{Ze^2}{4\pi r}$ (charge units are so that $\varepsilon=1$ permittivity in vacuum)

and acording to quantum mechanics de Broglie rule we must have :

$mv=p=\frac{h}{\lambda} \quad , \quad mvr=n\hbar$ and so $mv^2=\frac{Ze^2}{2n\lambda} \quad , \quad v=\frac{Ze^2}{2nh} \quad , \quad r=\frac{4\pi n^2\hbar^2}{Ze^2m}$.

The energy levels are $E_n=\frac{mv^2}{2}-\frac{Ze^2}{4\pi r}=-\frac{Ze^2}{8\pi r}=-\frac{(Ze^2)^2m}{32\pi^2n^2\hbar^2}$

Taking $E_{NR}=E_n$ we obtain $\bar{\alpha}=\frac{(Ze^2)^2}{64\pi^2n^2}$ and thus we can assume that the Schroedinger-Pauli Hamiltonian describes the electron in the nucleus Coulomb potential with $O(\alpha^2)$ approximation if we take $\alpha=\frac{e^2}{4\pi}$ the fine structure constant.

We notice also that in the Bohr model we obtain $\frac{p}{m}=v=\frac{Ze^2}{4\pi n}$ (we obviously take $\hbar=1$, $c=1$)

To describe the electron in the Coulomb force potential of the nucleus system with an $O(\alpha^4)$ approximation, we take in (4) the $O(\bar{\alpha}^2)$ approximation and also $e\,A_0=-\frac{Ze^2}{4\pi r}$, $r=\|\vec{x}\|$ considering $\left\|\frac{\vec{p}}{m}\right\|=O(\alpha)$, $\vec{A}=0$ and so (3) becomes

$$\frac{1}{2m}\vec{\sigma}\cdot\hat{\vec{p}}\left(1-\frac{1}{2m}(E_{NR}-e\,A_0)\right)\vec{\sigma}\cdot\hat{\vec{p}}\,\psi_A=(E_{NR}-e\,A_0)\,\psi_A \qquad (5).$$

From (2) we have :

$$\psi_B=\frac{1}{2m}\left(1-\frac{E_{NR}-e\,A_0}{2m}\right)\vec{\sigma}\cdot\hat{\vec{p}}\,\psi_A=\frac{\vec{\sigma}\cdot\hat{\vec{p}}}{2m}\,\psi_A+O(\alpha^3)\,\psi_A \quad ,$$

$$\langle\psi_B|\psi_B\rangle\approx\langle\psi_A|\frac{\hat{\vec{p}}^2}{4m^2}|\psi_A\rangle+O(\alpha^4)\langle\psi_A|\psi_A\rangle$$

We take a normalization condition derived from the unit charge condition:

$$1=\int J^0 d^3\vec{x}=\int \psi^+ \psi d^3\vec{x}=\langle \psi_A|\psi_A\rangle+\langle \psi_B|\psi_B\rangle=\langle \psi_A|\left(1+\frac{\hat{\vec{p}}^2}{4m^2}\right)|\psi_A\rangle+O(\alpha^4)\ .$$

Therefore we have a normalization

$$\psi_A=\left(1-\frac{1}{8}\frac{\hat{\vec{p}}^2}{m^2}\right)\varphi+O(\alpha^4) \quad (\text{ since } \frac{1}{\sqrt{1+\alpha^2}}=1-\frac{1}{2}\alpha^2+O(\alpha^4)\ ).$$

Introducing this in (5) and multiplying both sides of the equation by $\left(1-\frac{\hat{\vec{p}}^2}{8m^2}\right)$ and keeping only terms to order $O(\alpha^4)$ we obtain after some calculus:

$$\left(\frac{\hat{\vec{p}}^2}{2m}-\frac{\hat{\vec{p}}^4}{8m^3}+e\,A_0+\frac{e\,\vec{\sigma}\cdot\hat{\vec{p}}\,A_0\,\vec{\sigma}\cdot\hat{\vec{p}}}{4m^2}\right)\varphi=\left(E_{NR}+\frac{\hat{\vec{p}}^2}{8m^2}e\,A_0+e\,A_0\frac{\hat{\vec{p}}^2}{8m^2}\right)\varphi \text{ with } \hat{\vec{p}}^4=\hat{\vec{p}}^2\hat{\vec{p}}^2.$$

Taking $\vec{E}=-\nabla A_0$ the electric field, we have $\vec{E}=-Ze\frac{\vec{x}}{4\pi r^3}$,

$$\vec{E}\times\hat{\vec{p}}=-\frac{Ze}{4\pi r^3}\hat{\vec{L}}\ ,\ \nabla\cdot\vec{E}=-Ze\,\delta^3(\vec{x})$$

$$\hat{\vec{p}}^2 A_0\,\varphi=(-\nabla^2 A_0+2i\vec{E}\cdot\hat{\vec{p}}+A_0\hat{\vec{p}}^2)\varphi$$

$$\vec{\sigma}\cdot\hat{\vec{p}}\,A_0\,\vec{\sigma}\cdot\hat{\vec{p}}=-\vec{\sigma}\cdot(\vec{E}\times\hat{\vec{p}})+i\vec{E}\cdot\hat{\vec{p}}+A_0\hat{\vec{p}}^2\ .$$

Therefore for $\vec{S}=\frac{1}{2}\vec{\sigma}$ the spin operator we obtain the following equation in the normalized two-component spinor φ :

$$\left(\frac{\hat{\vec{p}}^2}{2m}-\frac{Ze^2}{4\pi r}-\frac{\hat{\vec{p}}^4}{8m^3}+\frac{Ze^2\hat{\vec{L}}\cdot\vec{S}}{8\pi m^2 r^3}+\frac{Ze^2}{8m^2}\delta^3(\vec{x})\right)\varphi=E_{NR}\,\varphi \quad (6)$$

This equation gives a $O(\alpha^4)$ approximation of the Dirac equation eigenvalue problem.

$$\psi_A=\left(1-\frac{\hat{\vec{p}}^2}{8m^2}\right)\varphi\ ,\ \psi_B=\frac{1}{m}\left(1-\frac{E_{NR}-e\,A_0}{2m}\right)\vec{S}\cdot\hat{\vec{p}}\,\psi_A\ ,\ A_0=-\frac{Ze}{4\pi r}\ .$$

The first two terms in the left side of (6) are the kinetic and potential energy for the unperturbed Hydrogen Hamiltonian. The third term is the relativistic correction to the kinetic energy. The fourth term is the correct spin-orbit interaction. The fifth term is the so called Darwin term.

We can consider that in the left side operator applied to solutions of (6) equation , the radius r goes not far below the Bohr radius $a_0=\frac{\hbar^2}{m\alpha}$ and $\delta^3(\vec{x})=\frac{1}{(2\pi)^3}R^3\delta_{\vec{x}\vec{0}}$ where $R = O(m)$ is the range of momentum. Therefore the left side of (6) operator is $m\,O(\alpha)$ and so if we formulate the (6) equation for ψ_A instead of φ , having $\varphi=\left(1+\frac{\hat{\vec{p}}^2}{8m^2}\right)\psi_A+O(\alpha^4)\,\psi_A$ and $E_{NR}=mO(\alpha^2)$ according to the Bohr model, we get a $O(\alpha^3)$ approximation of the Dirac equation eigenvalue problem.

27. Solutions of the Dirac equation for the Hydrogen atom

Solutions of the Dirac equation for the Hydrogen atom

We choose measure units for distance,time and electric charge respective, such that the reduced Planck constant $\hbar=1$, the speed of light in vacuum constant $c=1$ the electric permittivity in vacuum constant $\varepsilon=1$. The mass of the electron is m .
The Dirac equation satisfied by the Dirac spinor field of the electron , $\psi=\psi(t,\vec{x})$ in presence of the Coulomb potential of the atomic nucleus with atomoic number Z , $(A_\mu)_\mu=(A_0,0,,0,0)$, $A_0=-\frac{Ze}{4\pi r}$ with $e=-|e|$ charge of the electron, $r=\|\vec{x}\|$ is $i\gamma^\mu(\partial_\mu+ieA_\mu)\psi-m\psi=0$. This leads to a Hamiltonian operator $H=\gamma^0\gamma^k p_k+eA_0+\gamma^0 m$ with $\vec{p}=(p_k)_{k=\overline{1,3}}=-i\nabla$ the momentum operator

$\vec{S}=\frac{1}{2}\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}$ the spin operator, $\vec{\sigma}$ the Pauli matrices vector.

The Dirac equation written as a Schroedinger equation has the form :

$$i\frac{\partial}{\partial t}\psi=\begin{pmatrix}eA_0+m & \vec{\sigma}\cdot\vec{p}\\ \vec{\sigma}\cdot\vec{p} & eA_0-m\end{pmatrix}\psi .$$

We have solutions of the form $\psi=\exp(-iEt)\begin{pmatrix}\widetilde{\psi}_A\\ \widetilde{\psi}_B\end{pmatrix}$ where $\widetilde{\psi}_A=\widetilde{\psi}_A(\vec{x}),\widetilde{\psi}_B=\widetilde{\psi}_B(\vec{x})$ are two-component fields and so we have the eigenvalue problem

$$\begin{pmatrix}\vec{\sigma}\cdot\vec{p} & 0\\ 0 & \vec{\sigma}\cdot\vec{p}\end{pmatrix}\begin{pmatrix}\widetilde{\psi}_B\\ \widetilde{\psi}_A\end{pmatrix}=\begin{pmatrix}E-A_0-m & 0\\ 0 & E-eA_0+m\end{pmatrix}\begin{pmatrix}\widetilde{\psi}_A\\ \widetilde{\psi}_B\end{pmatrix}$$

with E the Hamiltonian eigenvalue or energy level .

We consider the operators $\vec{L}=\vec{x}\times\vec{p}$, $\vec{J}=\vec{L}+\vec{S}$, $K=\gamma^0 2\vec{S}\cdot\vec{J}-\frac{1}{2}\gamma^0$

and as we know from Chap. Spin representations we have
$[L_i,L_j]=\epsilon_{ijk}L_k$, $[S_i,S_j]=\epsilon_{ijk}S_k$.
On the space H_l of spherical harmonics of degree $l\in\mathbb{N}^*$ that is

$H_l=\left\{Y:S(\vec{0},1)\to\mathbb{C}\right|$ the function $f:\mathbb{R}^3\to\mathbb{C}$, $f(\vec{x})=\|\vec{x}\|^l Y\left(\frac{\vec{x}}{\|\vec{x}\|}\right)$ is a harmonic homogeneous polynomial of degree l in the variables $(x_1,x_2,x_3)\}$, the $(L_i)_{i=\overline{1,3}}$ are the generators of a spin l irreducible representations, having $S(\vec{0},1)=\{\vec{x}\in\mathbb{R}^3|\|\vec{x}\|=1\}$ and an orthonormal basis of eigenvectors for L_3 given by

the functions $Y_l^m=(-1)^m\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}P_l^{|m|}(\cos\theta)\exp(i m\varphi)$

with $m\in\{-l,-l+1,...0,1,...,l\}$, $Y_l^m=Y_l^m(\theta,\varphi)$,

$x_1=r\sin\theta\cos\varphi$, $x_2=r\sin\theta\sin\varphi$, $x_3=r\cos\theta$,

$P_l^{|m|}$ the associated Legendre polynomials $P_l^m(x)=(1-x^2)^{m/2}\frac{d^m}{dx^m}(P_l(x))$ for

$m\in\mathbb{N}$, $P_l(x)=\frac{1}{2^l l!}\frac{d^l}{dx^l}((x^2-1)^l)$ for $x\in\mathbb{R}$, $\vec{L}^2=(\vec{x}\times\vec{p})^2$, $\vec{L}^2Y_l^m=l(l+1)Y_l^m$,

$L_3Y_l^m=mY_l^m$, $L_3=-i\frac{\partial}{\partial\varphi}$ and the scalar product

$$\langle Y,Y'\rangle=\int\limits_{S(\vec{0},1)}Y^*(\Theta)Y'(\Theta)d\sigma(\Theta)$$

We have $[H,L_3]=\gamma^0[\gamma^k p_k,x_1p_2-x_2p_1]$ (since $[A_0,x_1p_2-x_2p_1]=0$ because

$$p_iA_0=-i\frac{x_i}{r}\frac{dA_0}{dA_r}\ ,\ A_0=A_0(r)\ )$$

Since $[x_k,p_l]=i\delta_{kl}$ we obtain $[H,L_3]=i\gamma^0(\gamma^2p_1-\gamma^1p_2)$, $[H,\vec{L}]=-i\gamma^0(\vec{\gamma}\times\vec{p})$.

Also $[H,S_3]=\frac{1}{2}[\gamma^0\gamma^k p_k,i\gamma^1\gamma^2]=-i\gamma^0(\gamma^2p_1-\gamma^1p_2)$, $[H,\vec{S}]=i\gamma^0(\vec{\gamma}\times\vec{p})$.

Therefore $[H,\vec{J}]=0$. Further we have :

$$[H,K]=[H,\gamma^0(2\vec{S}\cdot\vec{J}-\frac{1}{2})]=[H,\gamma^0](2\vec{S}\cdot\vec{J}-\frac{1}{2})+\gamma^0[H,2\vec{S}]\cdot\vec{J}=$$

$$=-2\vec{\gamma}\cdot\vec{p}(2\vec{S}\cdot\vec{J}-\frac{1}{2})+2i(\vec{\gamma}\times\vec{p})\cdot\vec{J}$$

$$(\vec{\gamma}\cdot\vec{p})(2\vec{S}\cdot\vec{p})=\frac{1}{2}\gamma^k p_k i\epsilon_{qlm}\gamma^l\gamma^m J_q=p_qJ_q\gamma^0\gamma^5-i\epsilon_{qkm}\gamma^m p_kJ_q=$$

$$=\vec{p}\cdot\vec{J}\,\gamma^0\gamma^5+i(\vec{\gamma}\times\vec{p})$$

$$[H,K]=-2i\gamma^1\gamma^2\gamma^3\vec{p}\cdot\vec{S}+\vec{\gamma}\cdot\vec{p}=\frac{1}{2}\gamma^1\gamma^2\gamma^3p_k\epsilon_{klm}\gamma^l\gamma^m+\gamma^kp_k=0\ ,\ [H,K]=0.$$

$$[K,\vec{J}]=[\gamma^0 2\vec{S}\cdot\vec{J}-\frac{1}{2}\gamma^0,\vec{J}]=\gamma^0[2\vec{S}\cdot\vec{J},\vec{J}]+[\gamma^0,\vec{J}]2\vec{S}\cdot\vec{J}-\frac{1}{2}[\gamma^0,\vec{J}]=\gamma^0[2\vec{S}\cdot\vec{J},\vec{J}]$$

$[2\vec{S}\cdot\vec{J},\vec{J}]=[2\vec{S}\cdot\vec{L},\vec{J}]=[2\vec{S}\cdot\vec{L},\vec{L}]+[2\vec{S}\cdot\vec{L},\vec{S}]=2iS_k\epsilon_{kjl}L_l+2i\epsilon_{kjl}S_lL_k=0$ and so

$[K,\vec{J}]=0$ (because $[L_i,S_j]=0$, $[L_i,L_j]=i\epsilon_{ijk}L_k$, $[S_i,S_j]=i\epsilon_{ijk}S_k$)

It follows also $[J_i,J_j]=i\epsilon_{ijk}J_k$, $[\vec{J}^2,J_3]=0$.

We have four mutually commuting operators $H,\vec{J}^2,J_3,K$ and we can seek for solutions of the Dirac equation which are sums of functions of the form

$\psi=\begin{pmatrix} f(r)\,\psi_A \\ i\,g(r)\,\psi_B \end{pmatrix}$ where ψ_A, ψ_B are two-component functions on the $S(\vec{0},1)$ sphere with $(\psi_A, \psi_B)=(\psi_A, \psi_B)(\theta,\varphi)$ in spherical coordinates

$$(x_1, x_2, x_3)=r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \quad , \quad r=\|\vec{x}\|$$

and $f, g: \mathbb{R}^* \to \mathbb{R}$, $H\,\psi=E\,\psi$, $\vec{J}^2\,\psi=j(j+1)\,\psi$, $J_3\,\psi=m\,\psi$, $K\,\psi=\kappa\,\psi$ where $j\in\mathbb{R}^*$ since $\vec{J}^2$ is hermitian.

We have $K=\begin{pmatrix} \vec{\sigma}\cdot\vec{L}+\boldsymbol{I} & 0 \\ 0 & -\vec{\sigma}\cdot\vec{L}-\boldsymbol{I} \end{pmatrix}$ (1)

$$K^2=(\gamma^0 2S_k L_k+\gamma^0)^2=L_k L_l(\delta_{kl}+2i\,\epsilon_{klq}S_q)+4\,S_k L_k+\boldsymbol{I}=\vec{L}^2+i2\vec{S}\cdot(\vec{L}\times\vec{L})+4\,S_k L_k+\boldsymbol{I}$$

$$\vec{L}\times\vec{L}=(\epsilon_{klm}\,\epsilon_{lij}\,\epsilon_{mpq}\,x_i\,p_j\,x_p\,p_q)_k=(-i\,\epsilon_{klm}\,\epsilon_{lij}\,\epsilon_{mpq}\,\delta_{jp}\,x_i\,p_q)_k=$$

$$=(i\,\epsilon_{klm}(\delta_{lm}\,\delta_{iq}-\delta_{lq}\,\delta_{im})\,x_i\,p_q)_k=i\,\vec{L}$$

$$K^2=\vec{L}^2+2\vec{S}\cdot\vec{L}+\boldsymbol{I} \qquad (2)$$

$$\vec{J}^2=(\vec{L}+\vec{S})^2=\vec{L}^2+2\vec{S}\cdot\vec{L}+\frac{3}{4}\boldsymbol{I}=K^2-\frac{1}{4}\boldsymbol{I} \qquad (3)$$

Let $\vec{J}^0=\vec{L}+\frac{1}{2}\vec{\sigma}$, $\vec{J}=\begin{pmatrix} \vec{J}^0 & 0 \\ 0 & \vec{J}^0 \end{pmatrix}$.

Since ψ is an eigenstate of K it follows from (3) that ψ_A , ψ_B are eigenstates of $\vec{J}^{02}$ and from (1) it follows that they are also eigenstates of $\vec{\sigma}\cdot\vec{L}$.

From (3) we have $\vec{J}^{02}=\vec{L}^2+\vec{\sigma}\cdot\vec{L}+\frac{3}{4}\boldsymbol{I}$ (4) , $\kappa^2=j(j+1)+\frac{1}{4}=\left(j+\frac{1}{2}\right)^2>0$

$$\vec{J}^{02}\,\psi_A=j(j+1)\,\psi_A \quad , \quad \vec{J}^{02}\,\psi_B=j(j+1)\,\psi_B \quad .$$

From (4) follows now that ψ_A, ψ_B are eigenstates of $\vec{L}^2$.

Also we have $J_3^0\,\psi_A=m\,\psi_A$, $J_3^0\,\psi_B=m\,\psi_B$ (5)

Let $\vec{L}^2\,\psi_A=l_A(l_A+1)\,\psi_A$, $\vec{L}^2\,\psi_B=l_B(l_B+1)\,\psi_B$ (6)

and as we know we must have $l_A, l_B\in\mathbb{N}$.

From (4) we obtain now $\vec{\sigma}\cdot\vec{L}\,\psi_A=(j(j+1)-l_A(l_A+1)-\frac{3}{4})\,\psi_A$,

$$\vec{\sigma}\cdot\vec{L}\,\psi_B=(j(j+1)-l_B(l_B+1)-\frac{3}{4})\,\psi_B \qquad (7)$$

From (1) follows :

$$\kappa-1=j(j+1)-l_A(l_A+1)-\frac{3}{4}=\kappa^2-l_A(l_A+1)-1$$

$$\kappa+1=l_B(l_B+1)-j(j+1)+\frac{3}{4}=l_B(l_B+1)-\kappa^2+1$$

$2\kappa=l_B(l_B+1)-l_A(l_A+1)$ and so $\kappa\in\mathbb{Z}^*$, $|\kappa|=j+\frac{1}{2}\in\mathbb{N}^*$

For $\kappa>0$ we obtain $l_A=\kappa-1=j-\frac{1}{2}$, $l_B=\kappa=j+\frac{1}{2}\in\mathbb{N}^*$

and for $\kappa<0$ we obtain $l_A=-\kappa=j+\frac{1}{2}\in\mathbb{N}^*$, $l_B=-\kappa-1$.

Since as we know the spherical harmonics Y_l^k for $k=\overline{-l,l}$ are the eigenfunctions of L_3 for k eigenvalue with eigenspace dimension equal to 1 and generate the l-order spherical harmonics satisfying $\vec{L}^2Y=l(l+1)Y$ we obtain from (5) that

$\psi_A=\alpha_A Y_{l_A}^{m-\frac{1}{2}}\chi_+ +\beta_A Y_{l_A}^{m+\frac{1}{2}}\chi_-$, $\psi_B=\alpha_B Y_{l_B}^{m-\frac{1}{2}}\chi_+ +\beta_B Y_{l_B}^{m+\frac{1}{2}}\chi_-$ where

$\alpha_A,\beta_A,\alpha_B,\beta_B\in\mathbb{C}$, $m-\frac{1}{2}\in\mathbb{Z}$, $\chi_+=\begin{pmatrix}1\\0\end{pmatrix}$, $\chi_-=\begin{pmatrix}0\\1\end{pmatrix}$

From (7) we obtain :

$$\begin{aligned}&\vec{\sigma}\cdot\vec{L}\,\psi_A=l_A\,\psi_A \ , \ \vec{\sigma}\cdot\vec{L}\,\psi_B=-(l_B+1)\,\psi_B \text{ for } \kappa>0\\ &\vec{\sigma}\cdot\vec{L}\,\psi_A=-(l_A+1)\,\psi_A \ , \ \vec{\sigma}\cdot\vec{L}\,\psi_B=l_B\,\psi_B \text{ for } \kappa<0 \ .\end{aligned} \tag{8}$$

Let $Y=\alpha Y_l^{m-\frac{1}{2}}\chi_+ +\beta Y_l^{m+\frac{1}{2}}\chi_-$ and we have

$\vec{\sigma}\cdot\vec{L}\,Y=\sigma_3 L_3 Y+\frac{1}{2}((\sigma_1+i\,\sigma_2)(L_1-iL_2)+(\sigma_1-i\,\sigma_2)(L_1+iL_2))Y$.

Since $(L_1-iL_2)Y_l^{m+\frac{1}{2}}=c\,Y_l^{m-\frac{1}{2}}$, $(L_1+iL_2)Y_l^{m-\frac{1}{2}}=c'\,Y^{m+\frac{1}{2}}$ with $c,c'\in\mathbb{C}$ (9)

as we can derive from the commutation relations $[L_i,L_j]=i\,\epsilon_{ijk}L_k$ and the fact that the eigenspaces of L_3 are one-dimensional and since also

$(\sigma_1-i\,\sigma_2)\chi_+=2\chi_-$, $(\sigma_1+i\,\sigma_2)\chi_-=2\chi_+$, $(\sigma_1-i\,\sigma_2)\chi_-=(\sigma_1+i\,\sigma_2)\chi_+=0$

we obtain $\vec{\sigma}\cdot\vec{L}\,Y=(\alpha(m-\frac{1}{2})+\beta c)\,Y_l^{m-\frac{1}{2}}+(-\beta(m+\frac{1}{2})+\alpha c')\,Y_l^{m+\frac{1}{2}}$

Because $(L_1+iL_2)(L_1-iL_2)=\vec{L}^2-L_3^2+L_3$ from (8) follows

$c\,c^+=c\,c'=l(l+1)-(m+\frac{1}{2})^2+m+\frac{1}{2}=(l+\frac{1}{2})^2-m^2$ and so $c'=c^*$.

The condition $\vec{\sigma}\cdot\vec{L}\,Y=sY$ leads to

$s\alpha=\alpha(m-\frac{1}{2})+\beta c$, $s\beta=-\beta(m+\frac{1}{2})+\alpha c'$ which has a non-zero solution in (α,β)

if and only if $c\,c'=(s+\frac{1}{2})^2-m^2$ (10)

With s from the (8) conditions for $\vec{\sigma}\cdot\vec{L}\,Y=sY$ with $Y=\psi_A,\ l=l_A;\ Y=\psi_B,\ l=l_B$ the (10) condition is satisfied in both cases $\kappa>0$ respective $\kappa<0$

and we must take $d=\frac{\alpha}{\beta}=\frac{d(m-\frac{1}{2})+c}{-m-\frac{1}{2}+d\,c'}$, $d=(m\pm(l+\frac{1}{2}))/c'$

$$s=-(m+\frac{1}{2})+m\pm(l+\frac{1}{2})=-\frac{1}{2}\pm(l+\frac{1}{2})$$

Therefore we must take

$\frac{\alpha_A}{\beta_A}=(m+l+\frac{1}{2})/c'$, $l=l_A$ and $\frac{\alpha_B}{\beta_B}=(m-l-\frac{1}{2})/c'$, $l=l_B$ for $\kappa>0$,

$\frac{\alpha_A}{\beta_A}=(m-l-\frac{1}{2})$, $l=l_A$ and $\frac{\alpha_B}{\beta_B}=(m+l+\frac{1}{2})/c'$, $l=l_B$ for $\kappa<0$

If $m-\frac{1}{2}=l$ we take $\beta=0$. If $m+\frac{1}{2}=l$ we take $\alpha=0$.

Normalizing ψ_A and ψ_B such that $|\alpha_A|^2+|\beta_A|^2=1$, $|\alpha_B|^2+|\beta_B|^2=1$ we can always change ψ_A and ψ_B each with an arbitrary phase factor $\exp(i\theta_A)$, $\exp(i\theta_B)$ and the conditions $K\psi=\kappa\psi$, $J_3\psi=m\psi$, $J^2\psi=j(j+1)\psi$, $L^2\psi_A=l_A(l_A+1)\psi_A$, $L^2\psi_B=l_B(l_B+1)\psi_B$ and (8) for $\vec{\sigma}\cdot\vec{L}$ and ψ_A , ψ_B are still satisfied.

Let $\kappa>0$. Then $\vec{\sigma}\cdot\vec{L}\,\psi_A=l_A\,\psi_A$, $J_3^0\,\psi_A=m\,\psi_A$, $l_A=\kappa-1=j-\frac{1}{2}$,

$\vec{\sigma}\cdot\vec{L}\,\psi_B=-(l_B+1)\,\psi_B=-(l_A+2)\,\psi_B$, $l_B=\kappa=j+\frac{1}{2}=l_A+1$.

Let $Y=\frac{\vec{\sigma}\cdot\vec{x}}{r}\,\psi_A$. We have

$$[L_j,\frac{x_i}{r}]=\epsilon_{jkl}x_k[p_l,\frac{x_i}{r}]=\epsilon_{jkl}x_k x_i\,i\frac{x_l}{r^3}-i\,\epsilon_{jkl}\frac{x_k}{r}\delta_{il}=i\,\epsilon_{jik}\frac{x_k}{r}$$ and so

$$[J_3^0,\frac{\vec{\sigma}\cdot\vec{x}}{r}]=[L_3,\frac{\vec{\sigma}\cdot\vec{x}}{r}]+[\frac{1}{2}\sigma_3,\frac{\vec{\sigma}\cdot\vec{x}}{r}]=\vec{\sigma}\cdot[L_3,\frac{\vec{x}}{r}]+\frac{1}{2}[\sigma_3,\vec{\sigma}]\cdot\frac{\vec{x}}{r}=$$

$=i\,\sigma_j\,\epsilon_{3jk}\frac{x_k}{r}+i\,\epsilon_{3jk}\sigma_k\frac{x_j}{r}=0$. Since $J_3^0\,\psi_A=m\,\psi_A$ we obtain now $J_3^0 Y=mY$ (11)

We have also

$(\vec{\sigma}\cdot\vec{x})(\vec{\sigma}\cdot\vec{L})=\sigma_k x_k\,\sigma_l\,\epsilon_{lij}x_i p_j=(\delta_{kl}+i\,\epsilon_{klq}\sigma_q)\,\epsilon_{lij}x_k x_i p_j=$

$=i(\delta_{kj}\delta_{qi}-\delta_{ki}\delta_{qj})\,\sigma_q x_k x_i p_j=\vec{\sigma}\cdot\vec{x}\left(r\frac{\partial}{\partial r}\right)-ir^2\vec{\sigma}\cdot\vec{p}$

$$\vec{\sigma}\cdot\vec{p}=\frac{1}{r}\frac{\vec{\sigma}\cdot\vec{x}}{r}\left(-ir\frac{\partial}{\partial r}+i\,\vec{\sigma}\cdot\vec{L}\right)\qquad(11')$$

$[\vec{\sigma}\cdot\vec{L},\frac{\vec{\sigma}\cdot\vec{x}}{r}]=\sigma_k[L_k,\frac{\sigma_j x_j}{r}]+[\sigma_k,\frac{\sigma_j x_j}{r}]L_k=\sigma_k\,\sigma_j[L_k,\frac{x_j}{r}]+[\sigma_k,\sigma_j]\frac{x_j}{r}L_k=$

$=-2\frac{\vec{\sigma}\cdot\vec{x}}{r}+2\left(ir\,\vec{\sigma}\cdot\vec{p}-\frac{\vec{\sigma}\cdot\vec{x}}{r}x_j\partial_j\right)=-2\frac{\vec{\sigma}\cdot\vec{x}}{r}+2\,ir\,\vec{\sigma}\cdot\vec{p}-2\frac{\vec{\sigma}\cdot\vec{x}}{r}r\frac{\partial}{\partial r}=$

$=-2\frac{\vec{\sigma}\cdot\vec{x}}{r}-2\frac{\vec{\sigma}\cdot\vec{x}}{r}\vec{\sigma}\cdot\vec{L}$ and we obtain $\vec{\sigma}\cdot\vec{L}\,Y=-(l_A+2)Y$ (12) .

Because ψ_A is a combination of l_A -order spherical harmonics it follows that $r^{l_A}\psi_A(\theta,\varphi)$ is a homogeneous harmonical polynomial of degree l_A and $r^{l_B}Y$ is a homogeneous polynomial of degree $l_B=l_A+1$ in the variables x_1,x_2,x_3 . Thus if

we show that $\nabla^2(r^{l_B}Y)=0$, we can derive that $\vec{L}^2 Y=l_B(l_B+1)Y$.
We have $\nabla^2(r^{l_B}Y)=\nabla^2(r^{l_A}\vec{\sigma}\cdot\vec{x}\,\psi_A)=r^{l_A}\psi_A(\nabla^2(\vec{\sigma}\cdot\vec{x}))+2\partial_j(\sigma_k x_k)\partial_j(r^{l_A}\psi_A)+$
$+\vec{\sigma}\cdot\vec{x}\,\nabla^2(r^{l_A}\psi_A)=2i\vec{\sigma}\cdot\vec{p}(r^{l_A}\psi_A)=\frac{2}{r}\frac{\vec{\sigma}\cdot\vec{x}}{r}\left(r\frac{\partial}{\partial r}(r^{l_A})\psi_A-r^{l_A}\vec{\sigma}\cdot\vec{L}\,\psi_A\right)=0$.
(because $\vec{\sigma}\cdot\vec{L}$ acts only on the angular part of $r^{l_A}\psi_A$) and so $\vec{L}^2 Y=l_B(l_B+1)Y$ (13).
Considering (11) , (12) and (13) it follows now that *Y* is determined up to a phase factor $\exp(i\theta_B)$ by α_B,β_B with $\frac{\alpha_B}{\beta_B}=\left(m-l_B-\frac{1}{2}\right)/c'$, since we have normalized ψ_A , ψ_B and $\left(\frac{\vec{\sigma}\cdot\vec{x}}{r}\right)^2=\boldsymbol{I}$, as $Y=\exp(i\theta_B)\psi_B$ and so $\psi_B=\exp(-i\theta_B)\frac{\vec{\sigma}\cdot\vec{x}}{r}\psi_A$.
We can always choose the phase factors $\exp(i\theta_A),\exp(i\theta_B)$ such that
$\psi_B=-\frac{\vec{\sigma}\cdot\vec{x}}{r}\psi_A$, $\psi_A=-\frac{\vec{\sigma}\cdot\vec{x}}{r}\psi_B$.
In a similar way we treat the case $\kappa<0$ interchanging the roles of *A* and *B* .
Taking $\widetilde{\psi}_A=f(r)\psi_A$, $\widetilde{\psi}_B=ig(r)\psi_B$, $F=rf(r),G=rg(r)$, $\alpha=\frac{e^2}{4\pi}$
considering (11') , the eigenvalue problem for $\psi=\begin{pmatrix}\widetilde{\psi}_A\\ \widetilde{\psi}_B\end{pmatrix}$ becomes the system :

$$\begin{cases} G'+\frac{\kappa G}{r} &= \left(m-E-\frac{Z\alpha}{r}\right)F \\ F'-\frac{\kappa F}{r} &= \left(m+E+\frac{Z\alpha}{r}\right)G \end{cases}$$

With the guidance of the non-relativistic solution (see Chap. Perturbation theory for the two-component Dirac equation) we may assume that $E^2 < m^2$ and taking $\rho=\sqrt{m^2-E^2}r$, $k_1=m+E$, $k_2=m-E$ the system becomes:

$$\begin{cases} \left(\frac{\partial}{\partial\rho}+\frac{\kappa}{\rho}\right)G &= \left(\sqrt{\frac{k_2}{k_1}}-\frac{Z\alpha}{\rho}\right)F \\ \left(\frac{\partial}{\partial\rho}-\frac{\kappa}{\rho}\right)F &= \left(\sqrt{\frac{k_1}{k_2}}+\frac{Z\alpha}{\rho}\right)G \end{cases}$$

Considering again the non-relativistic solutions we will postulate a solution of the form:
$F=\exp(-\rho)\rho^s\sum_{m=0}^{\infty}a_m\rho^m$, $G=\exp(-\rho)\rho^s\sum_{m=0}^{\infty}b_m\rho^m$ where obviously we do not confuse the index *m* with the mass *m*.
The system above leads to recursion relations :

$$\begin{cases} -b_m+b_{m+1}(s+m+1)+\kappa b_{m+1}-a_m\sqrt{\frac{k_2}{k_1}}+a_{m+1}Z\alpha &= 0 \\ -a_m+a_{m+1}(s+m+1)-\kappa a_{m+1}-b_m\sqrt{\frac{k_1}{k_2}}-b_{m+1}Z\alpha &= 0 \end{cases}$$

We assume that the ρ^s term is the lowest order term in the series for (F,G) and so we have $b_{-1}=a_{-1}=0$, $(a_0,b_0)\neq(0,0)$ in the recursion relation with $m\in\mathbb{Z}$ which can be written as :

$$\begin{pmatrix} s+m+1+\kappa & Z\alpha \\ -Z\alpha & s+m+1-\kappa \end{pmatrix}\begin{pmatrix} b_{m+1} \\ a_{m+1} \end{pmatrix}=\begin{pmatrix} 1 & \sqrt{\frac{k_2}{k_1}} \\ \sqrt{\frac{k_1}{k_2}} & 1 \end{pmatrix}\begin{pmatrix} b_m \\ a_m \end{pmatrix} \qquad (14)$$

Therefore $s^2=\kappa^2-Z^2\alpha^2$ and for the solution to be finite at $\rho=0$ we must take $s=\sqrt{\kappa^2-Z^2\alpha^2}$ and $\frac{s+\kappa}{Z\alpha}=-\frac{a_0}{b_0}$ (κ is a non-zero integer and $Z\alpha$ is small).

The recursion relation (14) implies :

$$\begin{pmatrix} b_{m+1} \\ a_{m+1} \end{pmatrix}=\frac{1}{(m+1)(2s+m+1)}\begin{pmatrix} s+m+1-\kappa & -Z\alpha\sqrt{\frac{k_1}{k_2}} \\ Z\alpha & (s+m+1+\kappa)\sqrt{\frac{k_1}{k_2}} \end{pmatrix}\begin{pmatrix} 1 & \sqrt{\frac{k_2}{k_1}} \\ 1 & \sqrt{\frac{k_2}{k_1}} \end{pmatrix}\begin{pmatrix} b_m \\ a_m \end{pmatrix} \text{ and}$$

$$b_{m+1}+\sqrt{\frac{k_2}{k_1}}a_{m+1}=\frac{1}{(m+1)(m+1+2s)}\left(2(s+m+1)+Z\alpha\left(\sqrt{\frac{k_2}{k_1}}-\sqrt{\frac{k_1}{k_2}}\right)\right)\left(b_m+\sqrt{\frac{k_2}{k_1}}a_m\right)$$

If for a value $m=m_0\in\mathbb{N}$ we have $b_{m0}+\sqrt{\frac{k_2}{k_1}}a_{m0}=0$, because obviously we have $(s+m_0+1)^2-\kappa^2+Z^2\alpha^2>0$ (with $s=\sqrt{\kappa^2-Z^2\alpha^2}$) it follows from (14) that $b_{m0+1}=a_{m0+1}=0$ and by induction $b_m=a_m=0$ for $m\in\mathbb{N}$, $m>m_0$.

Hence, excepting the trivial solution $F=\exp(-\rho)\rho^s a_0$, $G=\exp(-\rho)\rho^s b_0$ with $s=\sqrt{\kappa^2-Z^2\alpha^2}$, $\frac{s+\kappa}{Z\alpha}=-\frac{a_0}{b_0}=\sqrt{\frac{k_1}{k_2}}$ leading to

$$E=E_0=m-\frac{Z^2\alpha^2}{\kappa(\kappa+s)}=\frac{(s+\kappa)^2-Z^2\alpha^2}{(s+\kappa)^2+Z^2\alpha^2}m \ ,$$

we can assume $b_0+\sqrt{\frac{k_2}{k_1}}a_0\neq 0$ and so we will have

$$b_{m+1}+\sqrt{\frac{k_2}{k_1}}a_{m+1}=\left(\prod_{n=0}^{m}\frac{2(s+n+1)+Z\alpha\left(\sqrt{\frac{k_2}{k_1}}-\sqrt{\frac{k_1}{k_2}}\right)}{(n+1)(n+1+2s)}\right)\left(b_0+\sqrt{\frac{k_2}{k_1}}a_0\right)\ .$$

If for $m_0=\left\lfloor Z\alpha\left(\sqrt{\frac{k_1}{k_2}}-\sqrt{\frac{k_2}{k_1}}\right)\right\rfloor+1$ we have that for $k=\overline{0,m_0}$ is satisfied

$2(s+k+1)+Z\alpha\left(\sqrt{\frac{k_2}{k_1}}-\sqrt{\frac{k_1}{k_2}}\right)\neq 0$ then we obtain from the recursion that

$b_{m0}+\sqrt{\frac{k_2}{k_1}}a_{m0}\neq 0$ and

$$\left|\sum_{m=0}^{\infty}b_m\rho^m+\sqrt{\frac{k_2}{k_1}}a_m\rho^m\right|\geq-\left|\sum_{m=0}^{m0}b_m\rho^m+\sqrt{\frac{k_2}{k_1}}a_m\rho^m\right|+$$

$$+\left|b_{m0}+\sqrt{\frac{k_2}{k_1}}a_{m0}\right|\left|\sum_{m=1}^{\infty}\frac{1}{(m_0+1)\ldots(m_0+m)}\rho^{m0+m}\right|\geq-\left|\sum_{m=0}^{m0}b_m\rho^m+\sqrt{\frac{k_2}{k_1}}a_m\rho^m\right|-$$

$$-\left|b_{m0}+\sqrt{\frac{k_2}{k_1}}a_{m0}\right|\left|\sum_{m=0}^{m0}\frac{1}{m!}\rho^m\right|m_0!+\left|b_{m0}+\sqrt{\frac{k_2}{k_1}}a_{m_0}\right|m_0!\exp(\rho)$$

Therefore we obtain $G+\sqrt{\frac{k_2}{k_1}}F>\frac{1}{2}\rho^s\left|b_{m0}+\sqrt{\frac{k_2}{k_1}}a_{m0}\right|m_0!$ for large ρ , $\rho\to\infty$

and so the ψ function would be a not normalizable function.

Hence we must consider that exists $n=n_r\in\mathbb{N}^*$ such that we have

$$2(s+n_r)+Z\alpha\left(\sqrt{\frac{k_2}{k_1}}-\sqrt{\frac{k_1}{k_2}}\right)=0 \qquad (15)$$

The energy levels are therefore quantized as

$E=E_{nr,j}$, $n_r\in\mathbb{N}^*$, $\kappa=\pm\left(j+\frac{1}{2}\right)\in\mathbb{Z}^*$, $j\geq 0$ with E determined from (15)

$$E_{nr,j}=\frac{mc^2}{\sqrt{1+\frac{Z^2\alpha^2}{\left(n_r+\sqrt{\left(j+\frac{1}{2}\right)^2-Z^2\alpha^2}\right)^2}}}$$

We normalize $\widetilde{\psi}_B$ with $b_0=1$ and then $a_0=\frac{s+\kappa}{Z\alpha}$, (a_0,b_0) are determined by

$\kappa=\pm\left(j+\frac{1}{2}\right)$ and for a given n_r we have $E=E_{nr,j}$, f,g determined.

The solutions are $\psi=\begin{pmatrix} f(r)\,\psi_A \\ i\,g(r)\,\psi_B \end{pmatrix}$ with

$$\psi_A=\psi^{mj}_{l_A,j}=\alpha_A Y^{mj-\frac{1}{2}}_{l_A}\chi_+ +\beta_A Y^{mj+\frac{1}{2}}_{l_A}\chi_-$$
$$\psi_B=\psi^{mj}_{l_B,j}=\alpha_B Y^{mj-\frac{1}{2}}_{l_B}\chi_+ +\beta_B Y^{mj+\frac{1}{2}}_{l_B}\chi_-$$

for $\kappa=j+\frac{1}{2}$ we have $\begin{cases} \frac{\alpha_A}{\beta_A}=\left(m_j+l_A+\frac{1}{2}\right)/c' & , l_A=j-\frac{1}{2} \\ \frac{\alpha_B}{\beta_B}=\left(m_j-l_B-\frac{1}{2}\right)/c' & , l_B=j+\frac{1}{2} \end{cases}$

for $\kappa=-j-\frac{1}{2}$ we have $\begin{cases} \frac{\alpha_A}{\beta_A}=\left(m_j-l_A-\frac{1}{2}\right)/c' & , l_A=j+\frac{1}{2} \\ \frac{\alpha_B}{\beta_B}=\left(m_j+l_B+\frac{1}{2}\right)/c' & , l_B=j-\frac{1}{2} \end{cases}$

Also we have $\frac{\vec{\sigma}\cdot\vec{x}}{r}\,\psi^{mj}_{l_A,j}=-\,\psi^{mj}_{l_B,j}$.

For any j , m_j there are two solutions (determined up to a multiplication with a constant) having the same energy level $E_{nr,j}$ (corresponding to $\kappa=\pm\left(j+\frac{1}{2}\right)$) .

The energy level $E_{nr,j}$ has a degeneracy $2\left(2\left(j+\frac{1}{2}\right)+1\right)$, corresponding to the $m=m_j\in\frac{1}{2}+\mathbb{Z}$ satisfying $|m|\le j$ for $\kappa>0$; $|m|\le j+1$ for $\kappa<0$ for $j\in\mathbb{N}^*-\frac{1}{2}$

28. Unperturbed two component Dirac equation for the Hydrogen atom

Perturbation theory for the two component Dirac equation for the Hydrogen atom

Unperturbed two-component Dirac equation
Perturbation theory for the two-component Dirac equation

We can consider a Hamiltonian for the electron in the Coulomb potential field of the atomic nucleus which leads to the (6) equation in $O(\alpha^3)$ approximation of the Dirac equation for the ψ_A component of the electron Dirac spinor field in Chap. Non-relativistic limit of the Dirac equation, considered without the relativistic correction to kinetic energy term , the spin-orbit interaction term and the Darwin term.
The unperturbed Hamiltonian is therefore

$H_0=\frac{\hat{\vec{p}}^2}{2m}+V$ which applies to the ψ_A component of the Dirac spinor with

$V=-\frac{Z\alpha}{r}$, $r=\|\vec{x}\|$ and $\alpha=\frac{e^2}{4\pi}$ the fine structure constant.

The corresponding time independent Schroedinger equation is:

$$\left(\nabla^2+\frac{Z\alpha}{r}+E\right)\psi_A=0 \qquad (1)\ .$$

Following the solutions in Chap. Solutions of the Dirac equation for the Hydrogen atom we search for solutions ψ_A of (1) that are eigenfunctions of the operators

$$\vec{J}^2,\vec{L}^2,\vec{\sigma}\cdot\vec{L} \text{ and } J_3 \text{ where } \vec{J}=\vec{L}+\vec{S}\ ,\ \vec{S}=\frac{1}{2}\vec{\sigma} \text{ such that}$$

$$\vec{J}^2\psi_A=j(j+1)\psi_A\ ,\ j\geq 0\ ;\ \vec{L}^2\psi_A=l(l+1)\psi_A\ ,\ l=j\pm\frac{1}{2}\ ,\ l\in\mathbb{N}$$

$$\vec{\sigma}\cdot\vec{L}\,\psi_A=l\,\psi_A \text{ if } l=j-\frac{1}{2}\ \ (\ \kappa>0\ )\ ;\ \vec{\sigma}\cdot\vec{L}\,\psi_A=-(l+1)\psi_A \text{ if } l=j+\frac{1}{2}\ \ (\ \kappa<0\ )$$

$$J_3\psi_A=m\,\psi_A\ ,\ m\in\frac{1}{2}+\mathbb{Z}\ ,\ |m|\leq j \text{ for } l=j-\frac{1}{2}\ ,\ |m|\leq j+1 \text{ for } l=j+\frac{1}{2}$$

and so we take $\psi_A=\frac{F(r)}{r}Y$, $Y=Y_{lm}=\bar{\alpha}Y_l^{m-\frac{1}{2}}\chi_+ +\bar{\beta}Y_l^{m+\frac{1}{2}}\chi_-$ with

Y_l^k the spherical harmonics and $\chi_+=\begin{pmatrix}1\\0\end{pmatrix}$, $\chi_-=\begin{pmatrix}0\\1\end{pmatrix}$,

$$\frac{\bar{\alpha}}{\bar{\beta}}=\frac{m+j}{c^*} \text{ for } l=j-\frac{1}{2}\ ,\ \frac{\bar{\alpha}}{\bar{\beta}}=\frac{m-j-1}{c^*} \text{ for } l=j+\frac{1}{2},$$

$$\bar{\beta}=0 \text{ if } m+\frac{1}{2}>l\ ,\ \bar{\alpha}=0 \text{ if } m-\frac{1}{2}<-l\ ;\ |\bar{\alpha}|^2+|\bar{\beta}|^2=1,$$

$$(L_1-iL_2)Y_l^{m+\frac{1}{2}}=cY_l^{m-\frac{1}{2}}\ ,\ (L_1+iL_2)Y_l^{m-\frac{1}{2}}=c^*Y_l^{m+\frac{1}{2}}.$$

Since $\nabla^2=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\vec{L}^2$ the (1) equation becomes:

$$F''-\frac{l(l+1)}{r^2}F+\frac{2mZ\alpha}{r}F+2mEF=0 \qquad (2).$$

Taking $F(r)=G(\xi)$ with $\xi=2\sqrt{2m|E|}r$ for $E<0$ the equation (2) becomes the Whittaker function equation $\frac{d^2G}{d\xi^2}+\left(-\frac{1}{4}+\frac{k}{\xi}+\frac{\frac{1}{4}-\mu^2}{\xi^2}\right)G=0$ with parameters $k=\sqrt{\frac{m}{2|E|}}$, $\mu=l+\frac{1}{2}$.

The Whittaker equation has a fundamental system of solutions $M_{k,\mu}$, $W_{k,\mu}$ given by

$$M_{k,\mu}(z)=z^{\frac{1}{2}+\mu}\exp(-\frac{1}{2}z)\left(1+\sum_{p=1}^{\infty}\frac{(\frac{1}{2}+\mu-k)...(\frac{1}{2}+\mu-k+p-1)}{p!(2\mu+1)...(2\mu+p)}z^p\right)$$

$$W_{k,\mu}(z)=\frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-k)}M_{k,\mu}(z)+\frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-k)}M_{k,-\mu}(z)$$

As in Chap. Solutions of the Dirac equation for the Hydrogen atom we conclude that the only acceptable solutions for which the ψ_A is a normalizable function are $G(\xi)=M_{k,\mu}(\xi)$ with $k=l+1+n_r$ where $n_r\in\mathbb{N}$, $M_{k,\mu}(\xi)$ being in this case a polynomial of degree n_r .

(the $M_{k,-\mu}(z)$ makes the ψ_A inacceptable in 0 and for $n_r\notin\mathbb{N}$, as in Chap. Solutions of the Dirac equation for the Hydrogen atom, the $M_{k,\mu}(z)$ increases not less than a $Cz^{\frac{1}{2}+\mu}$ for $z\to\infty$).

Therefore the energy levels are quantized by $n=l+1+n_r$, $n_r\in\mathbb{N}$, $l\in\mathbb{N}$ with $\sqrt{\frac{m}{2|E|}}Z\alpha=n$, $E_n=-\frac{mZ^2\alpha^2}{2n^2}$, $n\in\mathbb{N}^*$ and the solutions for F are (3) :

$$F_{nl}(r)=M_{n,l+\frac{1}{2}}(\frac{2Zm\alpha}{n}r)=M_{n,l+\frac{1}{2}}(\frac{2Z}{na_0}r)=\exp(-\frac{\xi}{2})\xi^{l+1}\frac{(n-l-1)!(2l+1)!}{(n+l)!}L_{n-l-1}^{(2l+1)}(\xi)$$

where $a_0=\frac{1}{m\alpha}$ is the Bohr radius and $\xi=\frac{2Zr}{na_0}$, $L_n^{(\beta)}$ is the generalized Laguerre polynomial for $n\in\mathbb{N}$, $L_n^{(\beta)}(x)=x^{-\beta}e^x\frac{1}{n!}\frac{d^n}{dx^n}(e^{-x}x^{n+\beta})$, $e^x=\exp(x)$, $L_n^{(\beta)}(0)=\frac{\Gamma(n+\beta+1)}{n!\Gamma(\beta+1)}$.

We have $\int_0^\infty x^{\beta+1}e^{-x}(L_n^{(\beta)}(x))^2dx=\int_0^\infty\frac{1}{(n!)^2}\frac{d^n}{dx^n}(e^{-x}x^{n+\beta})x^{-\beta+1}e^x\frac{d^n}{dx^n}(e^{-x}x^{n+\beta})dx=$

$$=\int_0^\infty \frac{1}{(n!)^2}(-1)^n e^{-x}x^{n+\beta}\frac{d^n}{dx^n}\left(x^{-\beta+1}e^x\frac{d^n}{dx^n}(e^{-x}x^{n+\beta})\right)dx=$$

$$=\int_0^\infty \frac{1}{(n!)^2}e^{-x}(x^{n+\beta+1}(n+1)!-x^{n+\beta}n(n+\beta)n!)dx=\frac{\Gamma(n+\beta+1)}{n!}(2n+\beta+1)\ .$$

With F_{nl} given by (3), $R_{nl}=\frac{F_{nl}(r)}{r}$ we will have for $n=k+l+1$, $\beta=2l+1$

$$\int_0^\infty R_{nl}^2(r)r^2dr=\frac{na_0}{2Z}\int_0^\infty e^{-\xi}\xi^{\beta+1}\left(\frac{(n-l-1)!(2l+1)!}{(n+l)!}\right)^2(L_k^{(\beta)}(\xi))^2d\xi$$

$\int_0^\infty R_{nl}^2(r)r^2dr=\frac{n^2a_0}{2Z}\frac{(n-l-1)!}{(n+l)!}((2l+1)!)^2$ and so the normalized solutions are:

$$\psi_{nlm}(\vec{x})=\frac{2}{n^2}\left(\frac{Z}{a_0}\right)^{3/2}\sqrt{\frac{(n-l-1)!}{(n+l)!}}\exp(-\xi/2)\xi^l L_{n-l-1}^{(2l+1)}(\xi)Y_{lm}(\theta,\varphi)$$ where

$$\vec{x}=(r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta)\ ,\ \xi=\frac{2Zr}{na_0}\ ,$$

$$l\in\mathbb{N}\ ,\ n\in l+1+\mathbb{N}\ ,\ m\in\frac{1}{2}+\mathbb{Z}\ ,\ |m|\le l+\frac{1}{2}$$

We notice that we have two sets of ψ_{nlm} solutions: one with Y_{lm} determined for $l=j-s$ and one with Y_{lm} determined for $l=j+s$ having the specifications $s=\frac{1}{2}$, $\vec{J}^2\psi_A=j(j+1)\psi_A$, $j>0$. We denote the two set solutions ψ_{nlmj}, $j=l\pm s$.

Another complete set of E_n eigenstates are the

$\psi_{nlm\pm}$ with $\psi_{nlm\pm}=R_{nl}(r)Y_l^{m\mp\frac{1}{2}}(\theta,\varphi)\chi_\pm$, $m=m_j=m_l+m_s$, $m_s=\pm\frac{1}{2}$

The ψ_{nlmj} are $H_0,\vec{L}^2,\vec{J}^2,\vec{S}\cdot\vec{L},J_z$ eigenstates with eigenvalues

respective $E_n, l(l+1), j(j+1), \frac{1}{2}l$ if $l=j-\frac{1}{2}$,

$-\frac{1}{2}(l+1)$ if $l=j+\frac{1}{2}$ (for $\vec{S}\cdot\vec{L}$) and $m=m_j$.

The $\psi_{nlm\pm}$ are $H_0,\vec{L}^2,\vec{J}^2,L_z,S_z$ eigenstates with eigenvalues

respective $E_n, l(l+1), j(j+1), m_l=m\mp\frac{1}{2}, m_s=\pm\frac{1}{2}$.

We notice also that we have $\psi_{nlm}(0)=0$ for $l>0$ and $|\psi_{n0m}(0)|=\frac{1}{\sqrt{\pi}}\left(\frac{Z}{na_0}\right)^{3/2}$ (4).

Let $\psi=\psi_{nlm}=R_{ln}(r)Y_{lm}(\theta,\varphi)$, $R_{nl}(r)=\frac{u(r)}{r}$

and for $s\in\mathbb{Z}$: $\langle r^s\rangle=\langle\psi|r^s|\psi\rangle=\int_0^\infty u^2(r)r^s dr$.

Considering (2) we obtain

$u''=\left(\frac{l(l+1)}{r^2}-\frac{2}{ar}+\frac{1}{n^2a^2}\right)u$ where $a=\frac{a_0}{Z}$ and so

$$r^s u''=\left(l(l+1)r^{s-2}-\frac{2}{a}r^{s-1}+\frac{1}{n^2a^2}r^s\right)u$$

$$\int_0^\infty u r^s u'' dr=l(l+1)\langle r^{s-2}\rangle-\frac{2}{a}\langle r^{s-1}\rangle+\frac{1}{n^2a^2}\langle r^s\rangle \qquad (5).$$

$\int_0^\infty u r^s u'' dr=-I_1-I_2$ with $I_1=\int_0^\infty u' r^s u' dr$, $I_2=s\int_0^\infty u r^{s-1}u' dr$

$$I_1=-\frac{2}{s+1}\int_0^\infty u' r^{s+1}u'' dr=-\frac{2}{s+1}\int_0^\infty u' r^{s+1}\left(\frac{l(l+1)}{r^2}-\frac{2}{a}\frac{1}{r}+\frac{1}{n^2a^2}\right)u dr$$

For any k we have $\int_0^\infty u' r^k u dr=-\int_0^\infty u r^k u' dr-k\int_0^\infty u r^{k-1}u dr$ and so

$$\int_0^\infty u' r^k u dr=-\frac{k}{2}\langle r^{k-1}\rangle \ , \ I_2=-\frac{s(s-1)}{2}\langle r^{s-2}\rangle \ ,$$

$$\int_0^\infty u' r^{s+1}u'' dr=-\frac{l(l+1)(s-1)}{2}\langle r^{s-2}\rangle+\frac{s}{a}\langle r^{s-1}\rangle-\frac{s+1}{2n^2a^2}\langle r^s\rangle.$$

Thus $(s+1)I_1=l(l+1)(s-1)\langle r^{s-2}\rangle-\frac{2s}{a}\langle r^{s-1}\rangle+\frac{s+1}{n^2a^2}\langle r^s\rangle$

$$(s+1)\int_0^\infty u r^s u'' dr=-l(l+1)(s-1)\langle r^{s-2}\rangle+2\frac{s}{a}\langle r^{s-1}\rangle-\frac{s+1}{n^2a^2}\langle r^s\rangle+\frac{s(s^2-1)}{2}\langle r^{s-2}\rangle \quad (6).$$

Considering (5) and (6) we obtain now the Kramers-Pasternak relation:

$$\frac{s+1}{n^2}\langle r^s\rangle-(2s+1)a\langle r^{s-1}\rangle+\frac{s}{4}((2l+1)^2-s^2)a^2\langle r^{s-2}\rangle=0 \qquad (6')$$

For $s=0$ it follows $\left\langle\frac{1}{r}\right\rangle=\frac{1}{n^2a}$ (7)

and for $s=-1$ it follows $a\langle r^{-2}\rangle=l(l+1)a^2\langle r^{-3}\rangle$ (8) .

Suppose now we have a Hamiltonian depending on a parameter $H = H(\lambda)$ and the normalized states $\psi=|\psi(\lambda)\rangle$ satisfying for $E(\lambda)\in\mathbb{R}$: $H(\lambda)|\psi(\lambda)\rangle=E(\lambda)|\psi(\lambda)\rangle$

Since the states are normalized we have

$E(\lambda)=\langle\psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle$ (9)

$\left(\frac{d}{d\lambda}\langle\psi(\lambda)|\right)|\psi(\lambda)\rangle+\langle\psi(\lambda)|\left(\frac{d}{d\lambda}|\psi(\lambda)\rangle\right)=0$ and from (9) we will obtain the Feynman-Hellmann theorem:

$\frac{dE(\lambda)}{d\lambda}=\langle\psi(\lambda)|\frac{dH(\lambda)}{d\lambda}|\psi(\lambda)\rangle$ (10) .

Taking $\lambda=l$ as a real parameter, with

$H(l)=-\frac{1}{2m}\frac{d^2}{dr^2}+\frac{l(l+1)}{2mr^2}-\frac{1}{2m}\frac{2}{r}\frac{d}{dr}-\frac{Z\alpha}{r}$, $|\psi(l)\rangle\propto R_{nl}(r)$, $n=n_r+l+1$,

$R_{nl}:\mathbb{R}_+\to\mathbb{R}$ belonging to the Hilbert space $L^2_{r^2}([0,\infty),\mathbb{R})$ having scalar product

$\langle u,v\rangle=\int_0^\infty uvr^2dr$,

$E(l)=-\frac{1}{2m}\frac{1}{(n_r+l+1)^2a^2}$ for fixed $n_r\in\mathbb{N}$ we have $\frac{dH(l)}{dl}=\frac{2l+1}{2mr^2}$ and so

plugging into (10) we obtain for $l\in\mathbb{N}$ that $\left\langle\frac{1}{r^2}\right\rangle=\frac{1}{l+\frac{1}{2}}\frac{1}{n^3a^2}$ (11)

and with (8) : $\left\langle\frac{1}{r^3}\right\rangle=\frac{1}{l(l+\frac{1}{2})(l+1)}\frac{1}{n^3a^3}$ (12).

Consider now the unperturbed Hamiltonian which is assumed to have no time dependence, H_0 , having eigenvalues $(E_n^{(0)})_{n\in\mathbb{N}^*}$ and let for a given eigenvalue E^0 , an orthonormal set of eigenfunctions, $(|k^0\rangle)_{k\in D}$ which is complete in the eigenspace of E^0 having $E^0=E_k^{(0)}$, $H_0|k^0\rangle=E^0|k^0\rangle$ for any $k\in D$.

Let λV a Hamiltonian representing a weak physical disturbance (with λ a dimensionless parameter , $\lambda\ll1,\lambda\geq0$) .

The perturbed Hamiltonian is $H=H_0+\lambda V$.

For $V_{kl}=\langle k^0|V|l^0\rangle$, $k,l\in D$ we have that $(V_{kl})_{k,l}$ is a self-adjoint complex matrix and we find $(\alpha_{kl})_{k,l}$ an unitary matrix such that $\sum_{l,k\in D}\alpha^*_{pl}V_{lk}\alpha_{nk}=\delta_{pn}\epsilon_p$ with $\epsilon_p\in\mathbb{R}$ for any $p,n\in D$. Thus with Einstein summation convention for $l,k\in D$ we have $\langle\alpha_{pl}l^0|V|k^0\alpha_{nk}\rangle=\delta_{pn}\epsilon_n$ for any $p,n\in D$.

The perturbed eigenstates $|n\rangle$ depend on λ and satisfy

$(H_0+\lambda V)|n\rangle=E_n|n\rangle$ (13)

$|n\rangle=|n^{(0)}\rangle+\lambda|n^{(1)}\rangle+\lambda^2|n^{(2)}\rangle+...$

$E_n=E_n^{(0)}+\lambda E_n^{(1)}+\lambda^2E_n^{(2)}+...$

where $|n^{(0)}\rangle=\sum_{k\in D}\alpha_{nk}|k^0\rangle$, $|n^{(l)}\rangle=\frac{1}{l!}\left|\frac{dn}{d\lambda}\right\rangle(0)$, $E_n^{(l)}=\frac{1}{l!}\frac{dE_n}{d\lambda}(0)$ for $l\in\mathbb{N}$,

$E_n^{(0)}=E_k^{(0)}=E_0$ for $n\in D$, $k\in D$ with E_0 the eigenvalue corresponding to the $\mathrm{Sp}[(|k^0\rangle)_{k\in D}]$ eigenspace of H_0.

We can define $|n\rangle$ such that $\langle n|n\rangle=1$ and $\langle n|n^{(0)}\rangle\in\mathbb{R}$.

Differentiating (13) with respect to λ and making $\lambda=0$ we obtain $H_0|n^{(1)}\rangle+V|n^{(0)}\rangle=E_n^{(1)}|n^{(0)}\rangle+E_n^{(0)}|n^{(1)}\rangle$ (14) and multiplying this with $\langle n^{(0)}|$ follows $E_n^{(1)}=\langle n^{(0)}|V|n^{(0)}\rangle=\epsilon_n$.

Since $\langle n|n\rangle=1$, by differentiation with respect to λ we derive $\langle n^{(0)}|n^{(1)}\rangle+\langle n^{(1)}|n^{(0)}\rangle=0$ and because $\langle n|n^{(0)}\rangle\in\mathbb{R}$ it follows $\langle n^{(0)}|n^{(1)}\rangle=0$.

Let $(|l^{(0)}\rangle)_{l\notin D}$ the other eigenstates forming with $(|k^0\rangle)_{k\in D}$ a complete orthonormal system of eigenfunctions for H_0 having $H_0|l^{(0)}\rangle=E_l^{(0)}|l^{(0)}\rangle$, $E^0=E_n^{(0)}\neq E_l^{(0)}\in\mathbb{R}$ for any $l\notin D$. Multiplying (14) with $\langle l^{(0)}|$ with $l\notin D$ it follows

$$\langle l^{(0)}|n^{(1)}\rangle=\sum_{k\in D}\frac{\langle l^{(0)}|V|\alpha_{nk}k^0\rangle}{E_n^{(0)}-E_l^{(0)}}\ .$$

Taking $|n\rangle=\sum_{k\in D}\alpha_{nk}|k^0\rangle+\lambda\sum_{l\notin D,k\in D}\frac{\langle l^{(0)}|V|\alpha_{nk}k^0\rangle}{E_n^{(0)}-E_l^{(0)}}|l^{(0)}\rangle+O(\lambda^2)$ (15)

we verify that $\langle m^{(0)}|(H_0+\lambda V-E_n)|n\rangle=O(\lambda^2)$ for any $|m^{(0)}\rangle=\sum_{k\in D}\alpha_{mk}|k^0\rangle$, $m\in D$ and $\langle l^{(0)}|(H_0+\lambda V-E_n)|n\rangle=O(\lambda^2)$ for any $l\notin D$.

Therefore $|n\rangle$ given by (15) is a weak solution to the time-independent Schroedinger equation $(H_0+\lambda V)|n\rangle=E_n|n\rangle$ to $O(\lambda^2)$ approximation on the equation.

The above formulas for eigenstates and eigenvalues corrections $|\lambda n^{(1)}\rangle$ and $\lambda E_n^{(1)}$ to the unperturbed $|n^{(0)}\rangle$ and $E_n^{(0)}$ implies that the perturbation theory can be legitimately used when the perturbation λV satisfies

$$\sum_{l\notin D}\left|\frac{\langle l^{(0)}|\lambda V|n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\right|^2\ll 1\ ,\ \|(\lambda V_{kl})_{k,l\in D}\|\ll|E_n^{(0)}|\text{ for any }n\in D\qquad(*).$$

Suppose we have to compute the corrections to eigenvalues and eigenstates for a unperturbed Hamiltonian H_0 and a total of two small perturbations λV_1 and λV_2 with a perturbed Hamiltonian $H = H_0 + \lambda V_1 + \lambda V_2$.

We can proceed in two ways:

1) First we calculate the corrections produced for the $H_1 = H_0 + \lambda V_1$ Hamiltonian:

$$E_{n1}=E_n^{(0)}+\lambda E_{n1}^{(1)}+O(\lambda^2)$$
$$|n_1\rangle=|n^{(0)}\rangle+\lambda|n_1^{(1)}\rangle+O(\lambda^2)\ .$$

Then we calculate the corections produced for the $H_2 = H_0 + \lambda V_2$ Hamiltonian:

$$E_{n2}=E_n^{(0)}+\lambda E_{n2}^{(1)}+O(\lambda^2)$$
$$|n_2\rangle=|n^{(0)}\rangle+\lambda|n_2^{(1)}\rangle+O(\lambda^2)\ .$$

To obtain the final corrections we add the H_1 and H_2 corrections:

$$E_n=E_n^{(0)}+\lambda E_{n1}^{(1)}+\lambda E_{n2}^{(1)}+O(\lambda^2)$$
$$|n\rangle=|n^{(0)}\rangle+\lambda|n_1^{(1)}\rangle+\lambda|n_2^{(1)}\rangle+O(\lambda^2)\ .$$

Obviously we have $E_{ni}^{(1)}=\langle n^{(0)}|V_i|n^{(0)}\rangle$

$$\left|n_i^{(1)}\right\rangle=\sum_{l\neq n}\frac{\langle l^{(0)}|V_i|l^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\left|l^{(0)}\right\rangle \text{ for } i=1,2 \quad .$$

2) First we calculate the corrections produced for the $H_1 = H_0 + \lambda V_1$ Hamiltonian as in the precedent case.

Then we consider H_1 as an unperturbed Hamiltonian on which we apply the λV_2 perturbation taking the corrections with $E_{\bar{n}}^{(0)}=E_{n1}$, $\left|\bar{n}^{(0)}\right\rangle=\left|n_1\right\rangle$:

$E_{\bar{n}}=E_{n1}+\lambda E_{\bar{n}}^{(1)}+O(\lambda^2)$

$\left|\bar{n}\right\rangle=\left|n_1\right\rangle+\lambda\left|\bar{n}^{(1)}\right\rangle+O(\lambda^2)$

with $\left|\bar{n}^{(1)}\right\rangle=\sum_{\bar{l}\neq\bar{n}}\frac{\langle\bar{l}^{(0)}|V_2|\bar{n}^{(0)}\rangle}{E_{\bar{n}}^{(0)}-E_{\bar{l}}^{(0)}}\left|\bar{l}^{(0)}\right\rangle$, $E_{\bar{n}}^{(1)}=\langle n_1|V_2|n_1\rangle$

$\left|\bar{l}^{(0)}\right\rangle=\left|l_1\right\rangle=\left|l^{(0)}\right\rangle+\lambda\left|l_1^{(1)}\right\rangle+O(\lambda^2)$, $E_{\bar{l}}^{(0)}=E_{l1}=E_l^{(0)}+\lambda E_{l1}^{(1)}+O(\lambda^2)$ where

$H_1\left|l_1\right\rangle=E_{l1}\left|l_1\right\rangle$, $H_1\left|n_1\right\rangle=E_{n1}\left|n_1\right\rangle$.

The final perturbed states and energy eigenvalues are in case 2) the $\left|\bar{n}\right\rangle$ respective $E_{\bar{n}}$.

We can verify that we have :

$\left|\bar{n}^{(0)}\right\rangle=\left|n_1\right\rangle=\left|n^{(0)}\right\rangle+O(\lambda)$, $\left|\bar{l}^{(0)}\right\rangle=\left|l^{(0)}\right\rangle+O(\lambda)$

$E_{\bar{n}}^{(0)}=E_{n1}=E_n^{(0)}+O(\lambda)$, $E_{\bar{l}}^{(0)}=E_{l1}=E_l^{(0)}+O(\lambda)$

$E_{\bar{n}}^{(1)}=E_{n2}^{(1)}+O(\lambda)$, $\left|\bar{n}^{(1)}\right\rangle=\left|n_2^{(1)}\right\rangle+O(\lambda)$

$E_{\bar{n}}=E_n+O(\lambda^2)$, $\left|\bar{n}\right\rangle=\left|n\right\rangle+O(\lambda^2)$.

Therefore, to $O(\lambda^2)$ approximation we obtain approximatively the same result for both ways 1) and 2) in calculation of the corrections for the unperturbed Hamiltonian H_0 perturbed with $\lambda V_1 + \lambda V_2 = \lambda V$. Obviously we will usually proceed the 1) way.

As we proved in Chap. Non-relativistic limit of the Dirac equation, for the ψ_A first two-component part of the Dirac spinor describing the electron in the atomic nucleus Coulomb potential field, we have the $O(\alpha^3)$ approximation for the Dirac equation eigenvalue problem as a time-independent two complex components Schroedinger equation:

$$\left(\frac{\hat{\vec{p}}^2}{2m}-\frac{Z\alpha}{r}-\frac{\hat{\vec{p}}^4}{8m^3}+\frac{Z\alpha}{2m^2r^3}\hat{\vec{L}}\cdot\vec{S}+\frac{\pi}{2}\frac{Z\alpha}{m^2}\delta^3(\vec{x})\right)\psi_A=E_{NR}\,\psi_A \text{ where}$$

$\psi_A:\mathbb{R}^3\to\mathbb{C}^2$, $\psi_A=\psi_A(\vec{x})$, $\alpha=\frac{e^2}{4\pi}$ is the fine structure constant, m is the electron rest mass , Z is the atomic number of the nucleus.

Hence we have the unperturbed Coulomb potential Hamiltonian

$H_0=\frac{\hat{\vec{p}}^2}{2m}-\frac{Z\alpha}{r}$ and three perturbations known as $\lambda V_{\text{kin}}=-\frac{\hat{\vec{p}}^4}{8m^3}$,

$\lambda V_{\text{sp.or}}=\frac{Z\alpha}{2m^2r^3}\hat{\vec{L}}\cdot\vec{S}$, $\lambda V_{\text{Darwin}}=\frac{\pi}{2}\frac{Z\alpha}{m^2}\delta^3(\vec{x})$.

We show that λV_{kin} is indeed the relativistic correction to the kinetic energy, $\lambda V_{\text{sp.or}}$ is the correction from the spin-orbit interaction while $\lambda V_{\text{Darwin}}$ is a correction that comes precisely from the Dirac equation.

The relativistic form of the kinetic energy is

$$T=\sqrt{\vec{p}^2+m^2}-m=\frac{\vec{p}^2}{2m}-\frac{\vec{p}^4}{8m^3}+mO\left(\left(\frac{\vec{p}^2}{m^2}\right)^3\right) \quad .$$

In the Bohr model (see Chap. Two-component Dirac equation) we have $\frac{p}{m}=\frac{Z\alpha}{n}=O(\alpha)$ and so λV_{kin} is a $mO(\alpha^6)$ approximation to the kinetic energy.

To apply perturbation theory for the λV_{kin} perturbation we must verify that the (*) relations are satisfied for $\lambda V = \lambda V_{\text{kin}}$ and $\psi = \psi_{nlm}$ solutions to the unperturbed Hamiltonian eigenvalue problem corresponding to energy level

$E_n^{(0)}=-m\frac{Z^2\alpha^2}{2n^2}=-\frac{1}{2mn^2a^2}$, $n\in\mathbb{N}$, $n\geq l+1$, $a=\frac{a_0}{Z}=\frac{1}{m\alpha Z}$.

The $-\lambda V_{\text{kin}}=\frac{\hat{\vec{p}}^4}{8m^3}$ is positive semi-definite and so for any $|\varphi\rangle,|\eta\rangle$ we have

$$\left|\langle\varphi|\lambda V_{kin}|\eta\rangle\right|^2\leq\langle\varphi|\lambda V_{kin}|\varphi\rangle\langle\eta|\lambda V_{kin}|\eta\rangle \qquad (16)$$

Therefore, considering the sum for the λV_{kin} perturbation

$S_n=\sum_{l\notin D}\left|\frac{\langle l^{(0)}|\lambda V|n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\right|^2$ we have

$$|\langle l^{(0)}|\lambda V|n^{(0)}\rangle|^2\leq\langle l^{(0)}|\lambda V|l^{(0)}\rangle\langle n^{(0)}|\lambda V|n^{(0)}\rangle$$

$$\langle\psi|\lambda V|\psi\rangle=-\frac{1}{2m}\left\langle\frac{\hat{\vec{p}}^2}{2m}\psi\middle|\frac{\hat{\vec{p}}^2}{2m}\psi\right\rangle=-\frac{1}{2m}\langle\psi|\left(E_n^{(0)}+\frac{Z\alpha}{r}\right)^2|\psi\rangle=$$

$$=-\frac{1}{2m}\left(E_n^{(0)2}+Z^2\alpha^2\left\langle\frac{1}{r^2}\right\rangle+2E^{(0)}Z\alpha\left\langle\frac{1}{r}\right\rangle\right)=\frac{m}{8n^4(2l+1)}Z^4\alpha^4(6l+3-8n) \qquad (17) .$$

where we used (7) and (11) .

Thus having (16) and (17) and considering for an energy level $k\notin D$ all ψ_{kqm} with $q=\overline{0,k-1}$, $|m|\leq q+\frac{1}{2}$, $m\in\frac{1}{2}+\mathbb{Z}$, $j=q\pm\frac{1}{2}$ solutions for the unperturbed Hamiltonian eigenvalue problem with eigenvalue $E_k^{(0)}$ we obtain:

$$S_n \le \sum_{k\neq n,\, k\le 2n} \left(Z^4\alpha^4 4\left(\frac{1}{k^2}-\frac{1}{n^2}\right)^{-2} \frac{8n-6n-3}{8n^4(2l+1)} \sum_{q=0}^{k-1} \frac{2(2q+3)(8k-6q-3)}{8k^4(2q+1)} \right) +$$

$$+ \sum_{k=2n+1}^{\infty} \frac{8}{9} Z^4\alpha^4 \frac{8n-6l-3}{2l+1} \frac{4}{8k^4}(8k^2-3k-3k(k-1)).$$

After some increasings and using $\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}$ we obtain

$$S_n \le 2Z^4\alpha^4 \frac{8n-6l-3}{2l+1}\left(\frac{5}{16}n^2+\frac{10}{9}\right)\frac{\pi^2}{6} \le Cn^3Z^4\alpha^4 = O(\alpha^4) \ll 1 \ .$$

considering (17) , $\|(\lambda V_{kl})_{k,l\in D}\|$ for $\lambda V = \lambda V_{\text{kin}}$ can be estimated as the equivalent norm $C_n = \sum_{k\in D} \lambda_{|\epsilon_k|} = \sum_{k\in D} -\langle k^{(0)}|\lambda V_{\text{kin}}|k^{(0)}\rangle = \sum_{q=0}^{n-1} \frac{2(2q+3)(8n-6q-3)}{8n^4(2q+1)} mZ^4\alpha^4$

and so $C_n \le \frac{10}{4n^2} mZ^4\alpha^4 \ll |E_n^{(0)}| = \frac{mZ^2\alpha^2}{2n^2}$.

Therefore the (*) conditions are satisfied for the kinetic energy correction perturbation and we can use perturbation theory for this perturbation.
Thus for $\lambda V = \lambda V_{\text{kin}}$ for the perturbation theory we take

$|k^0\rangle = \psi_{nlmj}$, $|l^0\rangle = \psi_{nl'm'j'}$ and have $V_{kl} = -\langle \psi_{nmlj}|\frac{\hat{\vec{p}}^4}{8m^3}|\psi_{nl'm'j'}\rangle =$

$$= -\frac{1}{2m}\langle \psi_{nlmj}|\left(E_n^{(0)}+\frac{Z\alpha}{r}\right)^2|\psi_{nl'm'j'}\rangle = \delta_{ll'}\delta_{mm'}\delta_{jj'}\frac{6l+3-8n}{8n^4(2l+1)} mZ^4\alpha^4 .$$

(Obviously we do not confuse the *m* index of the solution with the *m* of the electron mass).

Hence the $(V_{kl})_{k,l\in D}$ matrix is already diagonalized by the chosen ψ_{nlmj} with fixed $n\in\mathbb{N}^*$ and l,m,j describing the indexed set D of $E_n^{(0)}$ eigenfunctions and the first order corrections to the energy level $|n^{(0)}\rangle = \psi_{nlmj}$ unperturbed eigenstate are: $\lambda E_n^{(0)} = \frac{6l+3-8n}{8n^4(2l+1)} mZ^4\alpha^4 = -\frac{1}{2m} E_n^{(0)2}\left(\frac{4n}{l+\frac{1}{2}}-3\right)$.

As we learned in Chap. Magnetic moment of the electron, the electron has a magnetic moment $\vec{\mu} = -\mu_B g_S \frac{\vec{S}}{\hbar}$ where $\mu_B = \frac{|e|}{2m}\hbar$ is the Bohr magneton and $g_S \approx 2$ is the gyromagnetic ratio.

The electron is considered moving with velocity $\vec{v}$ in the rest frame of the nucleus, in the Bohr atom model approximation. In the rest frame of the electron, in a non-relativistic approximation we have a magnetic field
$\vec{B} = -\vec{v}\times\vec{E}$ (we take $c=1, \hbar=1$) where (see Chap. Relativistic dynamics)

$\vec{E}=-\nabla A_0=\nabla\frac{Ze}{4\pi r}=-\frac{Ze}{4\pi}\frac{\vec{x}}{r^3}$ is the electric field in the rest frame of the nucleus.

The corresponding energy of the magnetic moment in this magnetic field is (see Chap. Magnetic moment) $\Delta H_L=-\vec{\mu}\cdot\vec{B}$ and ΔH_L is called the spin-orbit Larmor interaction energy.

We have $\vec{B}=-\vec{x}\times\vec{v}\frac{Ze}{4\pi r^3}=-\frac{1}{m}\frac{Ze}{4\pi r^3}\vec{L}$

$$\Delta H_L=-\frac{1}{m}\mu_B g_S\frac{Ze}{4\pi r^3}\vec{L}\cdot\vec{S}=g_S\frac{Z\alpha}{2m^2r^3}\vec{L}\cdot\vec{S}.$$

Consider now the nucleus rest frame *R* and at moment of time *t* in *R* the rest frame of the electron *R'* which moves in *R* with velocity $\vec{v}(t)$. The space-time coordinates of a point in *R* are *X* and in *R'* are *X'* (as column vectors).

Then (see Chap. Lorentz transformations) we have :

$$X'=B(\vec{v})(X-(t,\vec{0})^T) \text{ with}$$

$$B(\vec{v})=\begin{pmatrix}\gamma & (-\gamma v_i)_{i=\overline{1,3}}^T\\ (-\gamma v_i)_{i=\overline{1,3}} & \left(\delta_{ij}+\frac{\gamma-1}{v^2}v_iv_j\right)_{i,j=\overline{1,3}}\end{pmatrix} \text{ where } \gamma=\frac{1}{\sqrt{1-v^2}}.$$

At the moment $t'=t+\Delta t$ we have an instantaneous rest frame *R"* so that when *X"* are the coordinates in *R"*, we have

$X''=B(\vec{v}+\Delta\vec{v})(X-(t,\vec{0})^T)$, $\Delta\vec{v}=\vec{v}(t')-\vec{v}(t)$, $X''=B(\vec{v}+\Delta\vec{v})B(-\vec{v})X'$.

Since $B(\vec{v}+\Delta\vec{v})B(-\vec{v})$ is a Lorentz transformation we have

$B(\vec{v}+\Delta\vec{v})B(-\vec{v})=R(\Delta\theta,\vec{n})B(\Delta\vec{b})$.

Then considering an infinitesimal time interval Δt we obtain $R(\Delta\theta,\vec{n})$ an infinetesimal rotation of angle $\Delta\theta$ around an axis with a versor $\vec{n}$ orientation and $B(\Delta\vec{b})$ an infinitesimal boost given by the infinitesimal velocity $\Delta\vec{b}$.

Then taking the Lorentz group generators $(J_k)_{k=\overline{1,3}},(K_k)_{k=\overline{1,3}}$ with

$(J_k)_{ij}=-\epsilon_{ijk}$, $(J_k)_{0\alpha}=(J_k)_{\alpha 0}=0$, $(K_k)_{0i}=(K_k)_{i0}=\delta_{ik}$, $(K_k)_{00}=(K_k)_{ij}=0$ for $i,j,k=\overline{1,3}$, $\alpha=\overline{0,3}$ we will have

$R(\Delta\theta,\vec{n})=\exp(-\Delta\theta n_k J_k)\approx\boldsymbol{I}-\Delta\vec{\theta}\cdot\vec{J}$, $B(\Delta\vec{b})=\exp(-\Delta\vec{b}\cdot\vec{K})\approx\boldsymbol{I}-\Delta\vec{b}\cdot K$

$$B(\vec{v}+\Delta\vec{v})B(-\vec{v})\approx\boldsymbol{I}-\Delta\vec{\theta}\cdot\vec{J}-\Delta\vec{b}\cdot\vec{K}$$

Therefore $X'=(\boldsymbol{I}+\Delta\vec{\theta}\cdot\vec{J}+\Delta\vec{b}\cdot\vec{K})X''$.

Whitout loss of generality we can suppose that

$\vec{v}=(\beta,0,0)=\vec{\beta}$, $\Delta\vec{v}=(\Delta\beta_x,\Delta\beta_y,0)=\Delta\vec{\beta}$ and so

$$B(-\vec{v})=\begin{pmatrix}\gamma & \gamma\beta & 0 & 0\\ \gamma\beta & \gamma & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$$

We neglect the $O((\Delta\beta)^2)$ and $O(\beta^4)$ terms and after some calculus we obtain

$$|\vec{v}+\Delta\vec{v}|^2\approx\beta^2+2\beta\Delta\beta_x \ , \ \frac{1}{\sqrt{1-(\vec{v}+\Delta\vec{v})^2}}\approx\gamma+\gamma^3\beta\Delta\beta_x$$

$$B(\vec{v}+\Delta\vec{v})\approx\begin{pmatrix} \gamma+\gamma^3\beta\Delta\beta_x & -(\gamma\beta+\gamma^3\Delta\beta_x) & -\gamma\Delta\beta_y & 0 \\ -(\gamma\beta+\gamma^3\Delta\beta_x) & \gamma+\gamma^3\beta\Delta\beta_x & \frac{\gamma-1}{\beta}\Delta\beta_y & 0 \\ -\gamma\Delta\beta_y & \frac{\gamma-1}{\beta}\Delta\beta_y & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\Lambda=B(\vec{\beta}+\Delta\vec{\beta})B(-\vec{\beta})\approx\begin{pmatrix} 1 & -\gamma^2\Delta\beta_x & -\gamma\Delta\beta_y & 0 \\ -\gamma^2\Delta\beta_x & 1 & -\frac{1-\gamma}{\beta}\Delta\beta_y & 0 \\ -\gamma\Delta\beta_y & \frac{1-\gamma}{\beta}\Delta\beta_y & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Let $\Delta\vec{\beta}_{\parallel}=(\Delta\beta_x,0,0)$, $\Delta\vec{\beta}_{\perp}=(0,\Delta\beta_y,0)$ and in general, rotational invariance defines $\Delta\vec{\beta}_{\parallel}=(\vec{v}\cdot\Delta\vec{v})\frac{\vec{v}}{||\vec{v}||}$, $\Delta\vec{\beta}_{\perp}=\vec{v}-(\vec{v}\cdot\Delta\vec{v})\frac{\vec{v}}{||\vec{v}||}$ and we have

$$\Lambda\approx\boldsymbol{I}-\frac{\gamma-1}{\beta^2}(\vec{\beta}\times\Delta\beta)\cdot\vec{J}-\gamma(\gamma\Delta\vec{\beta}_{\parallel}+\Delta\vec{\beta}_{\perp})\cdot\vec{K} \text{ and so}$$

$$\Delta\vec{\theta}\approx\frac{\gamma^2}{\gamma+1}\vec{v}\times\Delta\vec{v} \ , \ \Delta\vec{b}\approx\gamma(\gamma\Delta\vec{v}_{\parallel}+\Delta\vec{v}_{\perp}) \qquad (18).$$

R' is the instantaneous rest frame of the electron at time $\tau = t$ in *R* and *R"* is the instantaneous rest frame of the electron at time $\tau = t + \Delta t$ in *R* .
Consider a particle P at rest in the frame *R"*
on location $\vec{r}''$ and time coordinate variable s'' in R'' so that we have

$$X_P{''}^T=X_P{''}^T(s'')=(s'',\vec{r}'') \ , \ X_P-(t,\vec{0})^T=X_P(\tau)-(t,\vec{0})^T=B(-\vec{v}(\tau))X_P{''}(s'')$$

$$X_{P0}(\tau)=\tau \ , \ s''=s''(\tau) \ , \ s''(t)=0 \ , \ \vec{v}(\tau)=\vec{v}(t)+\Delta\vec{v}(\tau) \ , \ \tau=t+\Delta t$$

$$X_P{'}=X_P{'}(s')=B(\vec{v}(t))B(-\vec{v}(\tau))X_P{''}(s'')=(\boldsymbol{I}+\Delta\vec{\theta}\cdot\vec{J}+\Delta\vec{b}\cdot\vec{K})X_P{''}(s'')=$$

$$=(s''+\Delta\vec{b}\cdot\vec{r}'',s''\Delta\vec{b}+\vec{r}''-\Delta\vec{\theta}\times\vec{r}'')^T=(s',(s'-\Delta\vec{b}\cdot\vec{r}'')\Delta\vec{b}+\vec{r}''-\Delta\vec{\theta}\times\vec{r}'')^T$$

$$s'=s'(\tau)=s''+\Delta\vec{b}\cdot\vec{r}'' \ , \ s'(t)=\Delta\vec{b}(t)\cdot\vec{r}''=0 \ , \ \Delta\vec{b}(t)=\vec{0} \ , \ \Delta\vec{\theta}(t)=\vec{0} \ .$$

The velocity of the particle P in the *R'* frame at time $\tau = t$ is

$$\vec{w}=\lim_{\tau\to t}\left(\frac{X_{Pi}{'}(s'(\tau))-X_{Pi}{'}(s'(t))}{s'(\tau)-s'(t)}\right)_{i=\overline{1,3}}=$$

$$=\lim_{\tau\to t}\frac{(s'(\tau)-\Delta\vec{b}(\tau)\cdot\vec{r}'')\Delta(\vec{b})(\tau)-\Delta\vec{\theta}(\tau)\times\vec{r}''}{s'(\tau)-s'(t)}=-\frac{\Delta\vec{\theta}}{\Delta s'}(t)\times\vec{r}'' \qquad (18').$$

Since *R'* is the instantaneous rest frame for the electron at time $\tau = t$ and *R"* is the instantaneous rest frame for the electron at time $\tau = t + \Delta t$ we have $\frac{\Delta t}{\Delta s'}(s'(t)) = \gamma$ and so $\frac{\Delta \vec{\theta}}{\Delta s'} = \gamma \frac{\Delta \vec{\theta}}{\Delta t}(t)$ and from (18) , (18') follows now that the instantaneous rest frame of the electron experiences an instantaneous rotation of angular velocity $\vec{\omega}_T = -\frac{\Delta \vec{\theta}}{\Delta s'} = -\frac{\gamma^3}{\gamma+1}\vec{v}\times\vec{a}$ where $\vec{a} = \frac{d\vec{v}}{dt}$ is the electron acceleration in *R* , the rest frame of the nucleus fact known as the Thomas precession effect.

We represent the spin ½ electron with spin angular momentum $\vec{S}$ as a rotating ball B of radius R with center in the origin of the R' frame and spinning with a constant angular velocity $\vec{\omega}$ having a uniformly distributed mass with density ρ such that :

$\vec{S} = \int_B \rho \vec{x} \times (\vec{\omega} \times \vec{x}) d^3\vec{x}$. Let $\vec{\omega} = (0, 0, \omega)$ and so we have

$$\vec{S} = \int_B \rho(\vec{x}^2 \vec{\omega} - (\vec{x}\cdot\vec{\omega})\vec{x}) d^3\vec{x} = \int_0^R \rho r^4 4\pi \vec{\omega} dr - \int_B \rho z^2 \omega e_z d^3\vec{x} =$$

$$= 4\pi \frac{R^5}{5}\rho\vec{\omega} - 2\pi\omega e_z \int_0^R \rho \int_0^\pi r^4 \cos^2(\theta)\sin(\theta) d\theta dr = \vec{\omega}\frac{R^5}{5} 2\pi\rho(2 - \frac{2}{3}) = \frac{8}{15}\pi R^5 \rho\vec{\omega} .$$

The spin angular momentum is collinear with the magnetic moment since we have $\vec{\mu} = -\mu_B g_S \vec{S}$ and the magnetic moment must align with the magnetic field which is $\vec{B} = -\vec{x}\times\vec{v}\frac{Ze}{4\pi r^3}$. In the Bohr model the electron orbits a circular orbit with constant angular velocity which is collinear with $\vec{L}$ and so $\vec{B} = \frac{-Ze}{4\pi r^3}\frac{1}{m}\vec{L}$, $\vec{a} = -\frac{\vec{v}^2}{a_0^2}\frac{Z^2}{n^4}\vec{x}$, where $a_0 = \frac{1}{m\alpha}$ is the Bohr radius.

Therefore $\vec{\omega}_T \| \vec{x}\times\vec{v} \| \vec{B} \| \mu \| \vec{S} \| \vec{\omega}$ and we can consider $\vec{\omega} = \lambda\vec{\omega}_T$, $\lambda \in \mathbb{R}$.

The instantaneous rotation with angular velocity ω_T , known as Thomas precession produces as we know three inertial forces acting on the spinning in the electron rest frame *R'* electron ball *B* which has a distribution of velocities in *R'* given by $\vec{v}' = \vec{\omega}\times\vec{x}'$ and we have $\vec{S} = \int_B \rho\vec{x}\times(\vec{\omega}\times\vec{x}) d^3\vec{x} = \frac{8}{15}\pi R^5\rho\vec{\omega}$.

The inertial forces are:

- the Euler force with density $-\rho\frac{d\vec{\omega}_T}{ds'}\times\vec{x}'$
- the centrifugal force with density $-\rho\vec{\omega}_T\times(\vec{\omega}_T\times\vec{x}')$
- the Coriolis force with density $-2\rho(\vec{\omega}_T\times\vec{v}') = -2\rho(\vec{\omega}_T\times(\vec{\omega}\times\vec{x}'))$.

We have $\frac{d\vec{\omega}_T}{ds'}=\frac{dt}{ds'}\frac{d\vec{\omega}_T}{dt}=\frac{-\gamma^4}{\gamma+1}\vec{v}\times\frac{d\vec{a}}{dt}$. Taking $\vec{a}=-\frac{\vec{v}^2}{a_0^2}\frac{Z^2}{n^4}\vec{x}$ we obtain

$\frac{d\vec{a}}{dt}=-\frac{Z^2}{a_0^2 n^4}\vec{v}^2\vec{v}$ and so $\frac{d\vec{\omega}_T}{ds'}=0$ and the Euler force is vanishing.

The energy corresponding to the centrifugal force field is

$E_{cf}=\int_B\left(\int_{\Gamma(\vec{x})}-\rho\left(\vec{\omega}_T\times\left(\vec{\omega}_T\times\vec{x}'\right)\right)\cdot d\vec{x}'\right)d^3\vec{x}$ where $\Gamma(\vec{x})$ is a path in B from the origin $\vec{0}$ to $\vec{x}\in B$ and the origin is the zero energy point for the centrifugal field.

Hence $E_{cf}=\int_B\left(\int_{\Gamma(\vec{x})}\rho\left(\vec{\omega}_T{}^2\vec{x}'-\vec{\omega}_T\left(\vec{\omega}_T\cdot\vec{x}'\right)\right)\cdot d\vec{x}'\right)d^3\vec{x}=\int_B\frac{1}{2}\rho\Big(\left(\omega_{T1}^2+\omega_{T2}\right)x_3^2+$

$+\left(\omega_{T1}^2+\omega_{T3}^2\right)x_2^2+\left(\omega_{T2}^2+\omega_{T3}^2\right)x_1^2\Big)d^3\vec{x}=\int_0^R\rho\,\vec{\omega}_T{}^2 r^4\int_0^\pi\cos^2(\theta)\sin(\theta)\,d\theta\int_0^{2\pi}d\varphi\,dr$

$E_{cf}=\frac{4\pi\rho R^5}{15}\vec{\omega}_T{}^2$ (19) .

Because as we established $\vec{\omega}=\lambda\vec{\omega}_T$, in the same way we obtain for the energy corresponding to the Coriolis force field $E_{cor}=\frac{8\pi\rho R^5}{15}\vec{\omega}\cdot\vec{\omega}_T=\vec{S}\cdot\vec{\omega}_T$ (20)

We have also $\frac{E_{cf}}{E_{cor}}=\frac{\omega_T}{\omega}=\frac{\omega_T}{\|\vec{S}\|}\frac{8\pi\rho}{15}R^5=\frac{4}{5}\omega_T R^2 m$ (21)

(since $\|\vec{S}\|=\frac{1}{2}$ and $m=\frac{4}{3}\pi R^3\rho$)

We have to estimate the electron radius *R* considering the energy necessary to assemble an amount of charge *q* into a given sphere of radius *r*.

The electrostatic potential at a distance r from a charge q is $V(r)=\frac{q}{4\pi r}$.

To bring an additional amount of charge *dq* from infinity necessitates putting energy into the system by an amount $dU=V(r)\,dq$ (22).

If the sphere is assumed to have a constant charge density ρ then

$q=\rho\frac{4}{3}\pi r^3$, $dq=\rho 4\pi r^2 dr$.

Integrating (22) from zero to the final radius *R* yields the expression for the total energy *U*.

$U=\int_0^R\frac{1}{4\pi r}\rho^2\frac{16\pi^2}{3}r^5\,dr=\frac{4}{15}\pi R^5\rho^2=\frac{q^2}{4\pi}\frac{3}{5}\frac{1}{R}$.

q is now interpreted as the electron charge *e* and the energy *U* is set to the relativistic rest mass energy of the electron *m* and so we must have

$m=\frac{e^2}{4\pi}\frac{3}{5}\frac{1}{R}$, $R=\frac{3}{5}\frac{\alpha}{m}$.

As we proved , in a non-relativistic approximation of the electron orbiting the nucleus:

$$\vec{\omega}_T = -\frac{\gamma^3}{\gamma+1}\vec{v}\times\vec{a} = -\frac{1}{2}\vec{v}\times\vec{a} \text{ and from the Bohr model follows}$$

$$\vec{a} = -\frac{\vec{v}^2}{a_0^2}\frac{Z^2}{n^4}\vec{x} \quad , \quad \|\vec{a}\| = \frac{m}{n^4}Z^3\alpha^3 \quad , \quad a_0 = \frac{1}{m\alpha} \ ,$$

$$\|\vec{v}\| = \frac{Z\alpha}{n} \quad , \quad \omega_T = \frac{Z^4\alpha^4}{n^5}m$$

Thus $\frac{E_{cf}}{E_{cor}} = \frac{4}{5}\frac{Z^4\alpha^4 m}{n^5}\frac{9}{25}\frac{\alpha^2}{m^2}m = \frac{36}{125}\frac{Z^4\alpha^6}{n^5} = O(\alpha^6)$ and we can neglect the centrifugal inertial forces potential energy and we have a energy from the Thomas precession given by

$$E_{cor} = \vec{S}\cdot\vec{\omega}_T = -\vec{S}\cdot\frac{1}{2}\vec{v}\times\vec{a} = -\frac{1}{2}\frac{\vec{S}\cdot Z^4\alpha^4 m^2}{n^6}\vec{x}\times\vec{v} = -\frac{1}{2}\frac{Z\alpha}{m^2 r^3}\vec{L}\cdot\vec{S} \quad ,$$

because from the Bohr model we have $r = \frac{n^2}{Zm\alpha}$.

Therefore we have a spin-orbit interaction correction given by

$\Delta H_{SO} = \Delta H_L + E_{cor} = Z\alpha\frac{g_S - 1}{2m^2 r^3}\vec{L}\cdot\vec{S}$ which for $g_S \approx 2$ leads to the

$$\lambda V_{\text{sp.or}} = \frac{Z\alpha}{2m^2 r^3}\vec{L}\cdot\vec{S}$$

The ψ_{nlmj} solutions of the unperturbed eigenvalue problem are also eigenfunctions of the $\vec{S}\cdot\vec{L}$ operator with $\vec{S}\cdot\hat{\vec{L}}\left|\psi_{nlmj}\right\rangle = \frac{1}{2}l\left|\psi_{nlmj}\right\rangle$ if $l = j - \frac{1}{2}$,

$\vec{S}\cdot\hat{\vec{L}}\left|\psi_{nlmj}\right\rangle = -\frac{1}{2}(l+1)\left|\psi_{nlmj}\right\rangle$ if $l = j + \frac{1}{2}$ and so $(V_{kl})_{k,l\in D}$ is already diagonalized for the $\lambda V = \lambda V_{\text{sp.or}}$ perturbation since it follows from the structure of the ψ_{nlmj} solutions that $\langle \psi_{nlmj}|\frac{1}{r^3}|\psi_{nl'm'j'}\rangle \propto \delta_{ll'}\delta_{mm'}\delta_{jj'}$.

Therefore, with the perturbation $\lambda V = \lambda V_{\text{sp.or}}$, $\left|k^{(0)}\right\rangle = \psi_{nlmj}$, $\left|l^{(0)}\right\rangle = \psi_{n'l'm'j'}$

we have $|\langle k^{(0)}|\lambda V|l^{(0)}\rangle|^2 \le \delta_{ll'}\delta_{mm'}\delta_{jj'}s_l^2\frac{Z^2\alpha^2}{4m^4}(g_S-1)^2\langle k^{(0)}|\frac{1}{r^3}|k^{(0)}\rangle\langle l^{(0)}|\frac{1}{r^3}|l^{(0)}\rangle =$

$$= \left(\frac{s_l}{l(l+\frac{1}{2})(l+1)}\right)^2\frac{Z^2\alpha^2}{4m^4}(g_S-1)^2\frac{\delta_{ll'}\delta_{mm'}\delta_{jj'}}{n^3 n'^3 a^6}$$

where $s_l = \frac{1}{2}l$ if $l = j - \frac{1}{2}$, $s_l = -\frac{1}{2}(l+1)$ if $l = j + \frac{1}{2}$.

It follows now , after some increasings and calculus that

$$\|(\lambda V_{kl})_{k,l\in D}\|\frac{1}{\left|E_n^{(0)}\right|}\leq\left(2+\sum_{l=1}^{n-1}\frac{2l+3}{l^2}\right)\frac{2n^2}{Z^2\alpha^2 m}m\frac{Z^4\alpha^4}{n^3}\leq\frac{6+\pi^2+4\log n}{n}Z^2\alpha^2\ll 1\ ,$$

$$S_n=\sum_{l\notin D}\left|\frac{\langle l^{(0)}|\lambda V|n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\right|^2\leq\sum_{k\neq n}\frac{4}{m^2Z^4\alpha^4}\left(\frac{1}{n^2}-\frac{1}{k^2}\right)^{-2}\frac{Z^8\alpha^8m^2}{n^3k^3}\left(2+\sum_{l=1}^{k-1}(2l+3)\frac{1}{(l(l+1))^2}\right)\leq$$

$$\leq Z^4\alpha^4\sum_{k\neq n}\left(\frac{1}{n^2}-\frac{1}{k^2}\right)^{-2}\left(1+\pi^2+\frac{1}{k}\right)\frac{1}{n^3k^3}\leq Z^4\alpha^4\sum_{k=2n}^{\infty}\frac{16}{9}\left(1+\pi^2+\frac{1}{k}\right)\frac{n}{k^3}+$$

$$+Z^4\alpha^4\left(\frac{1}{n^2}-\frac{1}{(n+1)^2}\right)^{-2}\sum_{k=1}^{\infty}\left(1+\pi^2+\frac{1}{k}\right)\frac{n}{k^3}\leq Z^4\alpha^4\frac{n(n+4)^2}{4}\sum_{k=1}^{\infty}\left(1+\pi^2+\frac{1}{k}\right)\frac{1}{k^3}=$$

$$=\frac{n(n+4)^2}{4}((1+\pi^2)\zeta(3)+\zeta(4))Z^4\alpha^4=O(\alpha^4)\ll 1\ .$$

Thus the (*) conditions are satisfied for the spin-orbit interaction perturbation and we can use perturbation theory for this perturbation.

For $\psi_{nlmj}=|n^{(0)}\rangle$ unperturbed eigenstate we have the energy level corrections of first order are given by $\lambda E_n^{(1)}=\langle n^{(0)}|\lambda V_{\text{sp.or}}|n^{(0)}\rangle=\frac{Z\alpha}{2m^2}(g_S-1)s_l\left\langle\frac{1}{r^3}\right\rangle$

where $s_l=\frac{1}{2}l$ if $l=j-\frac{1}{2}$ and $s_l=-\frac{1}{2}(l+1)$ if $l=j+\frac{1}{2}$.

$\lambda E_n^{(1)}=\frac{1}{2m}E_n^{(0)2}(g_S-1)\frac{4n}{(2l+1)(l+1)}$ for $l=j-\frac{1}{2}$

$\lambda E_n^{(1)}=-\frac{1}{2m}E^{(0)2}(g_S-1)\frac{4n}{l(2l+1)}$ for $l=j+\frac{1}{2}$.

For the $\lambda V=\lambda V_{\text{Darwin}}=\frac{\pi}{2}\frac{Z\alpha}{m^2}\delta^3(\vec{x})$ perturbation we have

$\langle\psi_{nlm}|\lambda V|\psi_{n'l'm'}\rangle=\psi^+_{nlm}(\vec{0})\,\psi_{n'l'm'}(\vec{0})\frac{\pi}{2}\frac{Z\alpha}{m^2}$ and so this perturbation affects only states $|n^{(0)}\rangle=\psi_{n0m}$ with $l=0$.

Since the Darwin term affects only the l = 0 states , the D set for the Darwin term perturbation and unperturbed energy level $E_n^{(0)}$ can be taken as $\left\{\sqrt{\frac{Z}{2\pi a_0 n}}R_{n0}\chi_+,\sqrt{\frac{Z}{2\pi a_0 n}}R_{n0}\chi_-\right\}$ and so $(\lambda V_{kl})_{k,l\in D}$ is already diagonalized and

$$S_n=\sum_{l\notin D}\left|\frac{\langle l^{(0)}|\lambda V|n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\right|^2=\sum_{k\neq n}\left(\frac{1}{n^2}-\frac{1}{k^2}\right)^{-2}\frac{4}{Z^4\alpha^4m^2}\frac{\pi^2}{4}\frac{Z^2\alpha^2}{m^4}\frac{1}{\pi^2}\frac{Z^6\alpha^6m^6}{n^3k^3}\leq$$

$$\leq Z^4\alpha^4\frac{n(n+4)^2}{4}\zeta(3)=O(\alpha^4)\ll 1$$

The energy level corrections at first order for the Darwin term perturbation for the unperturbed $E_n^{(0)}$ eigenvalues and $l = 0$ states are

$$\lambda E_n^{(1)} = \langle n^{(0)} | \lambda V | n^{(0)} \rangle = \frac{\pi}{2} \frac{Z\alpha}{m^2} \frac{1}{\pi} \frac{Z^3 \alpha^3 m^3}{n^3} = \frac{1}{2} \frac{Z^4 \alpha^4 m}{n^3} = \frac{Z^2 \alpha^2}{n} \left| E_n^{(0)} \right| = \frac{1}{2m} 4n E_n^{(0)2} \ .$$

Therefore we see that perturbation theory can be applied for the Darwin term and we have the above correction to energy levels.

The total energy level correction for the combined relativistic kinetic energy, spin-orbit interaction and Darwin term perturbations, according to the above considerations is

$$\Delta E_n = -\frac{E_n^{(0)2}}{2m} \left(\frac{4n}{l + \frac{1}{2}} - 3 - (g_S - 1) \frac{4n}{2\left(l + \frac{1}{2}\right)(l+1)} - 4n \delta_{l0} \right) \text{ for } l = j - \frac{1}{2} \text{ and}$$

$$\Delta E_n = -\frac{E_n^{(0)2}}{2m} \left(\frac{4n}{l + \frac{1}{2}} - 3 + (g_S - 1) \frac{4n}{2l\left(l + \frac{1}{2}\right)} \right) \text{ for } l = j + \frac{1}{2}.$$

From the Dirac equation solution (see Chap. Solutions to the Dirac equation for the Hydrogen atom) we have a $O(\alpha^6)$ approximation of the energy levels given by

(for $n = n_r + j + \frac{1}{2}$)

$$E_n \approx \frac{m}{\sqrt{1 + \frac{Z^2 \alpha^2}{\left(n - \frac{1}{2} Z^2 \alpha^2 \left(j + \frac{1}{2} \right)^{-1} \right)^2}}} \approx m \left(1 - \frac{Z^2 \alpha^2}{2n^2} - \frac{1}{2} \frac{Z^4 \alpha^4}{n^3} \left(j + \frac{1}{2} \right)^{-1} + \frac{3}{8} \frac{Z^4 \alpha^4}{n^4} \right) =$$

$$= m + E_n^{(0)} - \frac{1}{2m} E_n^{(0)2} \left(\frac{4n}{j + \frac{1}{2}} - 3 \right) \ .$$

For $l = j - \frac{1}{2}$ we have $\frac{4n}{j + \frac{1}{2}} = \frac{4n}{l + \frac{1}{2}} - \frac{4n}{2\left(l + \frac{1}{2}\right)(l+1)}$

and for $l = j + \frac{1}{2}$ we have $\frac{4n}{j + \frac{1}{2}} = \frac{4n}{l + \frac{1}{2}} + \frac{4n}{2l\left(l + \frac{1}{2}\right)}$.

With $g_S = 2$ we conclude that to $O(\alpha^6)$ approximation, the perturbation energy level coincides with the Dirac equation solution energy level , except the case $l = 0$ for which the computed spin-orbit correction by perturbation theory is always undetermined due the $\frac{l}{l\left(l + \frac{1}{2}\right)(l+1)} = \frac{0}{0}$ indetermination which occurs (since $l \in \mathbb{N}$)

because $\left\langle \frac{1}{r^3} \right\rangle = C \frac{1}{l\left(l+\frac{1}{2}\right)(l+1)} = \infty$ for $l=0$.

Since $\vec{S}\cdot\hat{\vec{L}}\left|\psi_{n0m_j}\right\rangle = 0$, in the case $l=0$ we must take the spin-orbit correction to the energy level to be zero and so, since for $l=0$ we have $j=\frac{1}{2}$, $\frac{4n}{j+\frac{1}{2}} = \frac{4n}{l+\frac{1}{2}} - 4n$

the pertubation theory energy level is equal, in $O(\alpha^6)$ approximation, to the Dirac equation solutions energy level even in the $l=0$ case.

In Chap. Non-relativistic limit of the Dirac equation we derived a magnetic moment of the electron $\vec{\mu} = -\mu_B(g_L\vec{L} + g_S\vec{S})$ with $g_L = 1$, $g_S \approx 2$ and $\mu_B = \frac{|e|}{2m}$ the Bohr magneton, g_L orbital angular momentum gyromagnetic ratio, g_S spin angular momentum gyromagnetic ratio. Thus in the presence of a constant magnetic field $\vec{B}$ we have a perturbation of the electron in the Coulomb potential field of the atomic nucleus Hamiltonian H given by $\lambda V_M = -\vec{\mu}\cdot\vec{B}$.

If the field $\vec{B}$ is weak, the spin-orbit interaction dominates over the effect of the external magnetic field (through the Larmor interaction energy) and we must include in H at least the spin-orbit interaction perturbation $\lambda V_{\text{sp.or}}$. The diagonalization of $(V_{kl})_{k,l\in D}$ for the $\lambda V_{\text{sp.or}} + \lambda V_M$ perturbation will occur (since $|\lambda V_M| \ll |\lambda V_{\text{sp.or}}|$) then with a good approximation for the same states $(\sum_{k\in D} \alpha_{nk}\left|k^0\right\rangle)_{n\in D} = (\left|n^{(0)}\right\rangle)_{n\in D}$ for which occurs for the $\lambda V_{\text{sp.or}}$ perturbation , that means for the $(\psi_{nlmj})_{n,l,m,j} = (\left|k^{(0)}\right\rangle)_{k\in D}$ with $l = \overline{0, n-1}$, $m \in \frac{1}{2} + \mathbb{Z}$, $|m| \le l + \frac{1}{2}$, $j = l \pm \frac{1}{2}$ for each energy level $E_n^{(0)}$, $n \in \mathbb{N}^*$. Moreover, the spin angular momentum generating a magnetic moment $-\mu_B g_S \vec{S}$ will be parallel with the magnetic field in the electron rest frame which being approximatively aligned with the orbital angular momentum as we derived for the Larmor interaction energy (since the external magnetic field is weak and the magnetic moment tends to align with the acting on it magnetic field) leads to the conclusion that we can consider that the expectation values of the $\vec{S}$ and $\vec{L}$ operators are parallel and since $\vec{J} = \vec{S} + \vec{L}$ we have

$$\langle g_L\vec{L} + g_S\vec{S} \rangle = \left\langle g_L \frac{\vec{J}\cdot\vec{L}}{\vec{J}^2}\vec{J} + g_S \frac{\vec{S}\cdot\vec{J}}{\vec{J}^2}\vec{J} \right\rangle \qquad (23) .$$

The first energy level correction introduced by λV_M + $\lambda V_{\text{sp.or}}$ is $\langle k^{(0)}|\lambda V_M + \lambda V_{\text{sp.or}}|k^{(0)}\rangle$ and therefore the correction corresponding to λV_M is $\lambda E_n^{(1)} = \langle k^{(0)}|\lambda V_M|k^{(0)}\rangle$ with $\left|k^{(0)}\right\rangle = \left|\psi_{nlmj}\right\rangle$.

The $|\psi_{nlmj}\rangle$ are $H,\vec{J}^2,\vec{L}^2,J_z,\vec{S}\cdot\vec{L}$ eigenstates and therefore also $\frac{\vec{J}\cdot\vec{L}}{\vec{J}^2}$ and $\frac{\vec{J}\cdot\vec{S}}{\vec{J}^2}$ eigenstates and we have, considering without loss of generality that $\vec{B}=(0,0,B)$, the energy level correction introduced by λV_M, considering (23) is

$$\lambda E_n^{(1)}=\mu_B B m_j\langle\psi_{nlmj}|g_L\frac{\vec{J}\cdot\vec{L}}{\vec{J}^2}+g_S\frac{\vec{J}\cdot\vec{S}}{\vec{J}^2}|\psi_{nlmj}\rangle \text{ and since } \vec{J}=\vec{S}+\vec{L},$$

$\vec{J}\cdot\vec{L}=\frac{1}{2}(\vec{J}^2+\vec{L}^2-\vec{S}^2)$, $\vec{J}\cdot\vec{S}=\frac{1}{2}(\vec{J}^2-\vec{L}^2+\vec{S}^2)$, $\vec{S}^2=\frac{3}{4}\boldsymbol{I}$ we obtain, taking $g_L=1$ that

$$\lambda E_n^{(1)}=\mu_B B m_j\frac{1}{2j(j+1)}(j(j+1)+l(l+1)-\frac{3}{4}+g_S(j(j+1)-l(l+1)+\frac{3}{4}))$$

$$\lambda E_n^{(1)}=\mu_B B m_j(1\pm\frac{g_S-1}{2l+1}) \text{ with } + \text{ for } j=l+\frac{1}{2} \text{ and } - \text{ for } j=l-\frac{1}{2}.$$

The relativistic kinetic energy correction splits an unperturbed energy level $E_n^{(0)}$ in n sublevels $(E_{nl})_{l=\overline{0,n-1}}$. The spin-orbit interaction adds more splitting of each E_{nl} in two sublevels for $j=l\pm\frac{1}{2}, E_{nlj}$. A weak constant uniform magnetic field splits each E_{nlj} in $2l+2$ levels for each $m_j\in\frac{1}{2}+\mathbb{Z}$ with $|m_j|\le l+\frac{1}{2}$. This splitting of atomic energy levels in the presence of a weak magnetic field is known as the Zeeman effect.

If the field $\vec{B}$ is sufficiently strong to disrupt the spin-orbit coupling, the $(|n^{(0)}\rangle)_{n\in D}$ diagonalizing $(V_{kl})_{k,l\in D}$ for the $\lambda V_M+\lambda V_{\text{sp.or}}$ perturbation system of unperturbed eigenstates for a $E_n^{(0)}=E^0$ unperturbed energy eigenvalue will be in a good approximation the system that diagonalizes the $(V_{kl})_{k,l\in D}=(\langle k^0|V_M|l^0\rangle)_{k,l\in D}$ matrix for the λV_M perturbation, which considering $\vec{B}=(0,0,B)$ is $(\psi_{nlm\pm})_{l=\overline{0,n-1},\left|m\mp\frac{1}{2}\right|\le l}$. (with $m\in\frac{1}{2}+\mathbb{Z}$)

Thus the energy level correction introduced by λV_M perturbation for a sufficiently strong magnetic field is

$\lambda E_n^{(1)}=\mu_B B\langle\psi_{nlm\pm}|g_L L_z+g_S S_z|\psi_{nlm\pm}\rangle=\mu_B B(m_l+g_S m_s)$ where we take $g_L=1$.

The splitting of atomic energy levels in the presence of a strong magnetic field is known as the Paschen-Back effect.

Taking $\vec{B}=(0,0,B)$ in the Zeeman effect case, for $l\notin D, |n^{(0)}\rangle=|\psi_{nlmj}\rangle$ we have $|l^{(0)}\rangle=|\psi_{n'l'm'j'}\rangle$, $n'\neq n$,

$$\langle l^{(0)}|\lambda V_M|n^{(0)}\rangle=\langle l^{(0)}|\mu_B B(g_L L_z+g_S S_z)|n^{(0)}\rangle=\langle l^{(0)}|\mu_B B g_L J_z|n^{(0)}\rangle+$$

$$+(g_S-g_L)\mu_B B\langle l^{(0)}|S_z|n^{(0)}\rangle=(g_S-g_L)\mu_B B\langle l^{(0)}|S_z|n^{(0)}\rangle,$$

$$S_z\left|\psi_{nlmj}\right\rangle=\frac{1}{2}R_{nl}(r)\left(\alpha_j Y_l^{m-\frac{1}{2}}(\theta,\varphi)\chi_+-\beta_j Y_l^{m+\frac{1}{2}}(\theta,\varphi)\chi_-\right)$$

$$\left|\psi_{n'l'm'j'}\right\rangle=R_{n'l'}(r)\left(\alpha_{j'} Y_{l'}^{m'-\frac{1}{2}}(\theta,\varphi)\chi_+ +\beta_{j'} Y_{l'}^{m'+\frac{1}{2}}(\theta,\varphi)\chi_-\right) .$$

Hence if $\langle l^{(0)}|S_z|n^{(0)}\rangle\neq 0$ we must have $l=l'$, $m=m'$, $\alpha_j\alpha_{j'}^*\neq\beta_j\beta_{j'}^*$, $n=n'$.
Since $n'\neq n$ we conclude that in the Zeeman effect case the first order corrections to the energy eigenstates, namely $\lambda\left|n^{(1)}\right\rangle$ must vanish.
Also in the Paschen-Back effect case, since the unperturbed eigenstates $\left|\psi_{nlm\pm}\right\rangle=\left|n^{(0)}\right\rangle$ are obviously $\lambda V_M=\mu_B B(g_L L_z+g_S S_z)$ (for $\vec{B}=(0,0,B)$) eigenstates, the $\lambda\left|n^{(1)}\right\rangle$ first order corrections to the energy eigenstates vanish.

Consider the electron in the Coulomb potential field of the atomic nucleus and in presence of a constant magnetic field $\vec{B}=(0,0,B)$ and of a perturbing electromagnetic wave field having a four-potential $A=A(t,\vec{x})=(A_\mu)_{\mu=\overline{0,3}}=(0,\vec{A})$ with $\vec{A}=\left(\frac{1}{2\omega V}\right)^{1/2}\left(a_k\exp(i\vec{k}\vec{x})\exp(-i\omega t)+a_k^+\exp(-i\vec{k}\vec{x})\exp(i\omega t)\right)\vec{\epsilon}$
(see Chap. Quantization of a electromagnetic field) where
V is the volume of the box where the system is confined ,
$\omega=\|\vec{k}\|$ (we consider $\varepsilon=1$,electric permittivity of vacuum , $c=1$, speed of light in vacuum, $\hbar=1$, reduced Planck constant, by suitable choosing of measure units for length, time and electric charge),
$\vec{\epsilon}$ is the polarization versor, having $\vec{k}\cdot\vec{\epsilon}=0$.
Then the Schroedinger-Pauli Hamiltonian for the ψ_A two-component spinor field is (see Chap. Two-component Dirac equation)

$$H=\frac{1}{2m}(\vec{p}+e\vec{A}+e\vec{A}')^2-\frac{Z\alpha}{r}-\frac{1}{2m}e2\vec{S}\cdot(\vec{B}-\nabla\times\vec{A}) \text{ where}$$

$$\vec{A}'=(\frac{1}{2}Bx^2,-\frac{1}{2}Bx^1,0) .$$

Ignoring the (small) $O\left((\|\vec{A}\|+\|\vec{A}'\|)^2\right)$ terms we obtain

$$H=H_0-\frac{1}{2m}e\vec{B}\cdot(\vec{L}+g_S\vec{S})+F\exp(-i\omega t)+F^+\exp(i\omega t)=H_B+H' \text{ where}$$

$$H'=F\exp(-i\omega t)+F^+\exp(i\omega t)$$

$$F=\frac{e}{m}\left(\frac{1}{2\omega V}\right)^{1/2}a_k\exp(i\vec{k}\vec{x})(\vec{\epsilon}\cdot\vec{p}+i(\vec{k}\times\vec{\epsilon})\cdot\vec{S})$$

H_B is the Hamiltonian of the electron in the Coulomb potential field of the atomic nucleus in presence of the constant magnetic field $\vec{B}=(0,0,B)$ and may include spin-orbit interaction and relativistic kinetic energy corrections.
Given $\left|f\right\rangle$ and $\left|i\right\rangle$ H_B eigenstates with energy levels E_f respective E_i , the transition probability rate from state $\left|i\right\rangle$ to state $\left|f\right\rangle$ by absorption of a $\hbar\omega$ energy photon in presence of the perturbing electromagnetic wave field is

$\frac{dw_{fi}}{dt}=2\pi|\langle f|F|i\rangle|^2\,\delta(E_f-E_i-\omega)$

and the transition probability rate from state $|i\rangle$ to state $|f\rangle$ by emission of a $\hbar\omega$ energy photon in presence of the perturbing electromagnetic wave field is

$\frac{dw_{fi}}{dt}=2\pi|\langle f|F^+|i\rangle|^2\,\delta(E_i-E_f-\omega)$ (we have taken as mentioned $\hbar=1$) .

(see Chap. Fermi's golden rule)

For resonant absorption fo example we will have a transition probability rate estimated as

$\frac{dw_{fi}}{dt}=2\pi\frac{e^2}{m^2}\frac{1}{2\omega V}|\langle f|\vec{\epsilon}\cdot\vec{p}+i(\vec{k}\times\vec{\epsilon})\cdot\vec{S}|i\rangle|^2\langle a_k^+ a_k\rangle\,\delta(E_f-E_i-\omega)$ where $\langle a_k^+ a_k\rangle=n_k$ stands for the number of photons in the perturbing electromagnetic field (for spontaneous emission we take n_k = 1).

Since, as we noticed above, the first order corrections to the eigenfunctions introduced by the constant uniform magnetic field vanish we can take in first order approximation $|f\rangle$ and $|i\rangle$ as $|\psi_{n'l'm'j'}\rangle$ respective $|\psi_{nlmj}\rangle$ in the case of a weak $\vec{B}$ field and as $|\psi_{n'l'm'\varepsilon'}\rangle$ respective $|\psi_{nlm\varepsilon}\rangle$ with $\varepsilon,\varepsilon'\in\{\pm\}$ in the case of a strong $\vec{B}$ field.

For the transition probability rate not to be equal to zero, if a photon is supposed to be emitted or absorbed we must have $E_f\neq E_i$ and so in the weak field regime we must have $(n,l,m,j)\neq(n',l',m',j')$. If $(n,l)\neq(n',l')$ then $\langle f|\vec{S}|i\rangle=0$.

If we consider the perturbing electromagnetic wave vector $\vec{k}$ parallel to $\vec{B}$ (the stimulated emission photons have the same wave vectors as the incident beam, and so in stimulated emission and also in absorption the wave vector can be determined , while in spontaneous emission the perturbing electromagnetic wave field is an electromagnetic random fluctuation) $(\vec{k}\times\vec{\epsilon})\cdot\vec{S}$ involves only S_1 and S_2 operators.

In this case (wave vector parallel to magnetic field and weak magnetic field)we have:

$$|f\rangle=R_{n'l'}(r)(\alpha' Y_{l'}^{m'-\frac{1}{2}}(\theta,\varphi)\chi_+ +\beta' Y_{l'}^{m'+\frac{1}{2}}(\theta,\varphi)\chi_-)$$

$S_q|i\rangle=R_{nl}(r)(\alpha_q Y_l^{m-\frac{1}{2}}(\theta,\varphi)\chi_- +\beta_q Y_l^{m+\frac{1}{2}}(\theta,\varphi)\chi_+)$ for $q=1,2$

and so a transition will be allowed by the $(\vec{k}\times\vec{\epsilon})\cdot\vec{S}$ term only if $n=n'$, $l=l'$ and $\Delta m_j=m'-m=\pm1$.

In the strong field regime, $E_f\neq E_i$ implies $(n',l',m_l',m_s')\neq(n,l,m_l,m_s)$ and we have $\langle f|\vec{S}|i\rangle=0$ if $(n',l',m_l')\neq(n,l,m_l)$.

Also in the strong field regime, if $\vec{k}$ is parallel to $\vec{B}$ a transition will be allowed by the $(\vec{k}\times\vec{\epsilon})\cdot\vec{S}$ only if $(n',l',m_l')=(n,l,m_l)$ and $\Delta m_s=m_s'-m_s=\pm1$.

Sincefor the associated Legendre polynomials we have $P_l^m(-\cos\theta)=(-1)^{l+m}P_l^m(\cos\theta)$ changing integration variables $\vec{x}\to-\vec{x}$,equivalent $(\theta,\varphi)\to(\theta+\pi,\varphi)$ we derive $\langle f|\vec{\epsilon}\cdot\vec{p}|i\rangle=0$ if $\Delta(l+m_j)=l'+m_j'-l-m_j\equiv0(\mathrm{mod}\,2)$

in the weak field regime and $\Delta(l+m_l)=l'+m_l'-l-m_l\equiv 0(\mathrm{mod}\,2)$ in the strong field regime.

If $\vec{k}$ is parallel to $\vec{B}$ since $\vec{k}\cdot\vec{\epsilon}=0$ it follows that $\vec{\epsilon}\cdot\vec{p}$ involves only $\widehat{p_1}=-i\partial_1$ and $\widehat{p_2}=-i\partial_2$ operators and therefore, changing integration variables on $\langle f|\vec{\epsilon}\cdot\vec{p}|i\rangle$ as $(x^1,x^2,x^3)\rightarrow(-x^1,-x^2,x^3)$, equivalent $(\theta,\varphi)\rightarrow(\theta,\varphi+\pi)$ we can derive $\langle f|\vec{\epsilon}\cdot\vec{p}|i\rangle=0$ if $\Delta m_j=m_j'-m_j\equiv 0(\mathrm{mod}\,2)$ in the weak field regime and $\Delta m_l=m_l'-m_l\equiv 0(\mathrm{mod}\,2)$ in the strong field regime.

Hence transitions are forbidden if

1) in the weak field regime
   a) for perturbing wave vector parallel to the magnetic field
   $(\Delta(l+m_j)\equiv 0$ or $\Delta m_j\equiv 0\ (\mathrm{mod}\ 2))$ and $(((\Delta n\neq 0)$ or $(\Delta l\neq 0))$ or $\Delta m_j\neq\pm 1)$
   b) for an arbitrary perturbing wave vector direction
   $(\Delta(l+m_j)\equiv 0\ (\mathrm{mod}\ 2))$ and $(\Delta n\neq 0$ or $\Delta l\neq 0)$;
2) in the strong field regime
   a) for perturbing wave vector parallel to the magnetic field
   $(\Delta(l+m_l)\equiv 0$ or $\Delta m_l\equiv 0\ (\mathrm{mod}\ 2)$ or $\Delta m_s\neq 0)$ and $(\Delta n\neq 0$ or $\Delta l\neq 0$ or or $\Delta m_l\neq 0$ or $\Delta m_s=0)$
   b) for an arbitrary perturbing wave vector direction
   $(\Delta(l+m_l)\equiv 0\ (\mathrm{mod}\ 2)$ or $\Delta m_s\neq 0)$ and $(\Delta n\neq 0$ or $\Delta l\neq 0$ or $\Delta m_l\neq 0)$.

The above selection rules for allowed transitions determine the form of absorption spectra of atomic energy levels and the stimulated emission resonant frequencies of a medium.

If some transitions are classified as forbidden this does not mean that these transitions cannot occur, only that they merely occur at a lower rate. In such a case the transition is termed electric dipole forbidden and the transitions between such levels must be approximated by higher order transitions appearing from the higher momentum operator powers, $\frac{(\vec{p}+e\vec{A})^4}{8m^3}$ for example in considering relativistic kinetic energy correction to the Hamiltonian.

Virtual photons created through vacuum energy fluctuations can interact with the electron as it moves around the Hydrogen nucleus leading to an anomalous difference in energy between two orbitals in a Hydrogen like atom. The phenomenon is called Lamb shift.

The fluctuating electromagnetic field has a four-vector potential given by

$$A=(0,\vec{A})=(A_\mu)_{\mu=\overline{0,3}},$$

$$\vec{A}(t,\vec{x})=\int\left(\frac{1}{(2\pi)^3 2\omega_k}\right)^{1/2}\sum_{a=1}^{2}(a_k\exp(-i\omega_k t+i\vec{k}\vec{x})+a_k^+\exp(i\omega_k t-i\vec{k}\vec{x}))\vec{\epsilon}_k^a d^3\vec{k}$$

where $\omega_k=\|\vec{k}\|$, $\vec{\epsilon}_k^a$ are polarization vectors, $\vec{k}\cdot\vec{\epsilon}_k^a=0$, $\vec{\epsilon}_k^a\cdot\vec{\epsilon}_k^b=\delta_{ab}$, $a,b=1,2$ $\vec{k}\in\mathbb{R}^3$, $[a_k,a_{k'}^+]=\delta^3(\vec{k}-\vec{k}')$.

The fluctuating electromagnetic field perturbs the electric potential due to atomic nucleus $V(\vec{x})=-\frac{Z\alpha}{r}$ causing fluctuations in the position of the electron, which explains the energy shift. The difference of potential energy is given by

$$\Delta V=V(\vec{x}+\delta\vec{x})-V(\vec{x})=\delta\vec{x}\cdot\nabla V(\vec{x})+\frac{1}{2}(\delta\vec{x}\cdot\nabla)^2V(\vec{x})+...$$

where $\delta\vec{x}$ is the position fluctuation operator.

If $|0\rangle$ is the ground state in the photon field states Hilbert space S , since the fluctuations are supposed to be isotropic we have

$$\langle 0|Q\,\delta\vec{x}|0\rangle=\langle 0|\delta\vec{x}|0\rangle \qquad (24)$$

$$\langle 0|((Q\,\delta\vec{x})\cdot\nabla)^2|0\rangle=\langle 0|(\delta\vec{x}\cdot\nabla)^2|0\rangle \qquad (25)$$

for any orthogonal matrix operator $Q=(Q_{kl})_{k,l=\overline{1,3}}$ acting on S with $Q_{kl}Q_{kn}=\delta_{ln}\boldsymbol{I}_S$ for $l,n=\overline{1,3}$

Taking in (24) Q any constant orthogonal matrix it follows $\langle 0|\delta\vec{x}|0\rangle=0$ (26) .

Taking in (25) Q such that $Q_{ki}\delta x_i=\sqrt{(\delta\vec{x})^2}\,\delta_{kq}$ we obtain for any $q=\overline{1,3}$ that

$$\langle 0|(\delta\vec{x}\cdot\nabla)^2|0\rangle=\langle 0|\delta_{kq}\delta_{lq}(\delta\vec{x})^2\nabla_k\nabla_l|0\rangle=\langle 0|(\delta\vec{x})^2\nabla_q^2|0\rangle \qquad (27).$$

From (27) follows now that $\langle 0|(\delta\vec{x}\cdot\nabla)^2|0\rangle=\frac{1}{3}\langle 0|(\delta\vec{x})^2\nabla^2|0\rangle$ and so,

using (26) , (27) we have $\langle\Delta V\rangle=\frac{1}{6}\langle 0|(\delta\vec{x})^2|0\rangle\langle\psi|\nabla^2\left(-\frac{Z\alpha}{r}\right)|\psi\rangle$,

$$\langle\Delta V\rangle=\frac{2}{3}\pi\langle 0|(\delta\vec{x})^2|0\rangle Z\alpha|\psi(0)|^2 \text{ (since } \nabla^2\frac{1}{r}=-4\pi\delta^3(\vec{x})\text{)} \qquad (26')$$

for any electron atomic orbital state ψ.

The electron displacement field induced by a single mode of fluctuating electromagnetic field of wave vector $\vec{k}$ and pulsation $\omega=\|\vec{k}\|$ satisfies the classical equation of motion

$$m\frac{d^2}{dt^2}(\delta\vec{x})=e\vec{E}=e\frac{\partial\vec{A}}{\partial t}=$$

$$=e\int-\frac{i}{(2\pi)^{3/2}}\left(\frac{k}{2}\right)^{1/2}\sum_{a=1}^{2}(a_k\exp(-ikt+i\vec{k}\vec{x})-a_k^+\exp(ikt-i\vec{k}\vec{x}))\vec{\epsilon}_k^a d^3\vec{k}$$

and so

$$\delta\vec{x}=\frac{i}{(2\pi)^{3/2}}\frac{e}{m}\int\frac{1}{k^2}\left(\frac{k}{2}\right)^{1/2}\sum_{a=1}^{2}(\exp(-ikt+i\vec{k}\vec{x})a_k-\exp(ikt-i\vec{k}\vec{x})a_k^+)\vec{\epsilon}_k^a d^3\vec{k}+C \ .$$

Because $\langle 0|\delta\vec{x}|0\rangle=0$ and $a_k|0\rangle=0$ it follows $C=0$ and further due to creation and anihilation operators commutation relation we derive

$$\langle 0|(\delta\vec{x})^2|0\rangle=\frac{1}{(2\pi)^3}\frac{e^2}{m^2}\int\frac{2}{k^4}\frac{k}{2}d^3\vec{k}=\frac{e^2}{2\pi^2}\frac{1}{m^2}\int_0^\infty\frac{1}{k}dk \ . \ (28)$$

This result diverges when no limits about the integral. The electron is unable to respond to the fluctuating field if the fluctuations are smaller than the natural orbital frequency which in the Bohr model corresponds to a pulsation

$\omega_n = \frac{v}{r} = \frac{Z\alpha/n}{n^2/(Zm\alpha)} = \frac{Z^2\alpha^2 m}{n^3}$.

Uncertainity in position of the electron defines a range domain that is a ball with radius $\frac{\hbar}{2mc}$ (the half reduced Compton wavelenght - see Chap. Relativistic dynamics) since the uncertainity in position must be greater than half of the reduced Compton wavelenght. Because we must consider fluctuating photons that actually interact with the electron as a well defined particle , the considered fluctuating photons must have a wavelenght greater than the reduced Compton wavelenght of the electron.

Hence in (28) we must integrate with $\frac{Z^2\alpha^2 m}{n^3} < k < 2\pi m$.

Therefore $\langle 0|(\delta\vec{x})^2|0\rangle = \frac{2}{\pi}\frac{\alpha}{m^2}\log\left(\frac{2\pi n^3}{Z^2\alpha^2}\right)$ and considering (4) , (26') we have that the energy level shift due to electromagnetic vacuum energy fluctuations is

$\langle \Delta V\rangle = \frac{4}{3\pi} m \frac{Z^3\alpha^4}{n^3}\log\left(\frac{2\pi n^3}{Z^2\alpha^2}\right)\delta_{l0}$.

We see that the Lamb shift affects only states $\psi_{n\,l\,m}$ with $l = 0$.

The Darwin term can also be interpreted as a result of the apparent fluctuations of the position of the electron produced by the interference between the energy states corresponding to the electron respective positron of the virtual electron-positron pairs created by quantum fluctuations as solutions to the Dirac relativistic wave equation. Thus the Darwin term changes the potential energy of the electron as a smearing out of the electrostatic interaction between the electron and the nucleus due to these rapid quantum oscillations or zitterbewegung of the electron.

To show how zitterbewegung arises we consider the Dirac equation for electrons in free space:

$H\,\psi(t,\vec{x}) = i\partial_0\,\psi(t,\vec{x})$ with $H = m\gamma^0 + \gamma^0\gamma^k\hat{p}_k$, $\hat{p}_k = -i\partial_k$, $\vec{x} = (x_j)_{j=\overline{1,3}}$ and with summation over k index in the H expression.

As we know (see Chap. Quantum statistical ensemble) for any observable that not depends explicitly on time , A , we have :

$\frac{d\langle A\rangle_t}{dt} = i\langle [H,A]\rangle_t$ and this leads for the averaged position x_k and the averaged velocity $\alpha_k = \frac{dx_k}{dt}$ of the electron to approximative equations

$\alpha_k(t) = i[H,\hat{x}_k] = \gamma^0\gamma^k$, $\frac{d\alpha_k}{dt} = \frac{d^2x_k}{dt^2} = i[H,\alpha_k] = 2i\gamma^k m + 2\sigma^{kl}p_l = 2i(p_k - \gamma^0\gamma^k H)$

$\alpha_k = \exp(iHt)\,\alpha_k(0)\exp(-iHt)$, $\alpha_k(0) = \gamma^0\gamma^k$ where we used the

commutation relations $[\hat{p}_k,\hat{x}_l]=-i\,\delta_{kl}$, $\sigma^{kl}=\frac{i}{2}[\gamma^k,\gamma^l]$.

Because p_k and H are both time-independent the above equation can be integrated twice to find the explicit time-dependence of the position for the electron.

Thus $\alpha_k(t)=(\alpha_k(0)-p_k H^{-1})\exp(-2iHt)+p_k H^{-1}$

$x_k(t)=x_k(0)+p_k H^{-1}t+\frac{1}{2}iH^{-1}(\alpha_k(0)-p_k H^{-1})(\exp(-2iHt)-1)$.

The resulting expression consists of a initial position, a motion proportional to time and a oscillation term with an amplitude approximate by $\frac{\sqrt{3}}{2}\frac{1}{m}$ where $\frac{1}{m}=\frac{\hbar}{mc}$ is the reduced Compton wavelenght (we obviously used $H\approx m$, $p\ll m$ and derived $\langle\vec{\xi}^2\rangle=\langle\left(\frac{1}{2}iH^{-1}(\gamma^0\gamma^k-p_kH^{-1})\right)\left(\frac{1}{2}iH^{-1}(\gamma^0\gamma^k-p_kH^{-1})^+\right)\rangle\approx\frac{3}{4}\frac{1}{m^2}$). (29)

Quantum fluctuations allow the creation of virtual electron-positron pairs with a lifetime estimated by the uncertainity principle $\Delta t\approx\frac{\hbar}{\Delta E}\approx\frac{\hbar}{mc^2}=\frac{1}{m}$. The distance the particles can move during this time is $\xi\approx c\,\Delta t=\frac{\hbar}{mc}=\frac{1}{m}$ the reduced Compton wavelenght. The electrons of the atom interact with those pairs and this yields a fluctuating electron position $\vec{x}+\vec{\xi}$ and the effect on the potential V can be estimated as $V(\vec{x}+\vec{\xi})=V(\vec{x})+\vec{\xi}\cdot\nabla V(\vec{x})+\frac{1}{2}(\vec{\xi}\cdot\nabla)^2V(\vec{x})+...$

Averaging over the fluctuations we get (as for the fluctuations that cause the Lamb shift exposed above) :

$\langle\vec{\xi}\rangle=0$, $\langle\xi_i\,\xi_j\rangle=\frac{1}{3}\langle\vec{\xi}^2\rangle\,\delta_{ij}$, $V(\vec{x}+\vec{\xi})\approx V(\vec{x})+\frac{1}{6}\langle\vec{\xi}^2\rangle\nabla^2V(\vec{x})$.

(The $(\xi_i)_{i=\overline{1,3}}$ can be wieved as three independent random variables having the same probability distribution and a zero average value.)

Considering (29) this leads to a perturbation of the potential due to electron-positron fluctuations given by

$\delta V\approx\frac{1}{8m^2}\nabla^2V$ and with $V=-\frac{Z\alpha}{r}$ we have $\nabla^2V=4\pi Z\alpha\,\delta^3(\vec{x})$

$\delta V\approx\frac{\pi}{2}\frac{Z\alpha}{m^2}\delta^3(\vec{x})$ which is precisely the Darwin term .

29. Energy momentum tensor operator and Angular momentum tensor operator in quantum field theory

Energy-momentum tensor operator
Angular momentum tensor operator

Consider a quantum field system described by a Lagrangian density
$\mathscr{L}\left(\left(\Phi_a, \partial\Phi_a\right)_a\right)$ with $\Phi_a = \Phi_a(x)$, $x = (t, \vec{x}) = (x^\mu)_{\mu=\overline{0,3}}$,
$(\eta^{\mu\nu})_{\mu,\nu}$ the Minkowski metric tensor in four-dimensional Minkowski space with signature (+ , - , - , -) (speed of light is considered $c = 1$) .
We have infinitesimal translations and Lorentz rotations so that the coordinates and fields transform as
$x^\mu \to x'^\mu = x^\mu + \eta^{\mu\nu}\theta_\nu + O(\theta^2)$
$\Phi_a(x) \to \Phi'_a(x') = \Phi_a(x)$
for translations of infinetisimal parameters $(\theta_\nu)_\nu \in \mathbb{R}^4$;
$x^\mu \to x'^\mu = x^\mu + \varepsilon^{\mu\nu} x_\nu + O(\varepsilon^2)$
$\Phi_a(x) \to \Phi'_a(x') = \Phi_a(x) + \sum_{\mu<\nu} I^b_{a\mu\nu}\Phi_b(x)\varepsilon^{\mu\nu} + O(\varepsilon^2)$
for rotation real infinitesimal rotation parmeters $\varepsilon^{\mu\nu} = -\varepsilon^{\nu\mu}$, $\mu, \nu = \overline{0,3}$
with rotation independent constants $I^b_{a\mu\nu} = -I^b_{a\nu\mu}$.
Considering the field arguments of the Lagrangian density function as field operator functions we define the canonical momenta operators :
$\pi^{a\mu} = \pi^{a\mu}(x) = \frac{\partial \mathscr{L}}{\partial(\partial_\mu \Phi_a(x))}$ and define the energy-momentum density tensorial operator $T^{\mu\nu} = T^{\mu\nu}(x) = \pi^{a\mu}(x)(\partial^\nu \Phi_a(x)) - \eta^{\mu\nu}\mathscr{L}(x)$
$(T^{\mu\nu})_\mu$ is the Noether current (see Chap. Noether theorem) corresponding to invariance under ν translations and if the action $S = \int \mathscr{L}\, d^4x$ is invariant under ν translations we have $\partial_\mu T^{\mu\nu} = 0$ and so the four-momentum operator $P_\nu(x^0) = \int\limits_{x^0=const} T_{0\nu}(x)\, d^3\vec{x}$ is a conserved quantity: $\frac{dP_\nu}{dx^0} = 0$
The total angular momentum density operator is defined as the Noether current corresponding to invariance under $\mu\nu$ rotations and is given by
$M^\lambda_{\mu\nu}(x) = L^\lambda_{\mu\nu}(x) + S^\lambda_{\mu\nu}(x)$ where
$L^\lambda_{\mu\nu}(x) = x_\mu T^\lambda_{\ \nu}(x) - x_\nu T^\lambda_{\ \mu}(x)$ orbital angular momentum density operator,
$S^\lambda_{\mu\nu}(x) = \pi^{a\lambda}(x)(\Phi_b(x)) I^b_{a\mu\nu}$ spin angular momentum density operator.
Under rotations invariance we have $\partial_\lambda M^\lambda_{\mu\nu}(x) = 0$ and defining angular momentum operators: $L_{\mu\nu}(x^0) = \int\limits_{x^0=const} L^0_{\mu\nu}(x)\, d^3\vec{x}$ -orbital angular momentum operator and $S_{\mu\nu}(x^0) = \int\limits_{x^0=const} S^0_{\mu\nu}(x)\, d^3\vec{x}$ -spin angular momentum operator, $M_{\mu\nu}(x^0) = L_{\mu\nu}(x^0) + S_{\mu\nu}(x^0)$ we have $\frac{dM_{\mu\nu}}{dx^0} = 0$.

The total angular momentum operator is a conserved quantity.
The orbital respective spin angular momentum operators are in general not conserved quantities under rotations invariance.
We have

$$\partial_\lambda L^{\lambda}_{\mu\nu} = T_{\mu\nu} - T_{\nu\mu} \qquad (1)$$

$$\partial_\lambda S^{\lambda}_{\mu\nu} + \partial_\lambda L^{\lambda}_{\mu\nu} = 0 \qquad (2)$$

Let $t_{\mu\nu}(x) = \int_0^{x^0} (T_{\mu\nu}(x) - T_{\nu\mu}(x))\, dx^0 = -t_{\nu\mu}(x)$ (3)

$${}^0S_{\mu\nu}(x^0) = \int_{x^0=const} (S^0_{\mu\nu}(x) + t_{\mu\nu}(x))\, d^3\vec{x}$$

$${}^0L_{\mu\nu}(x^0) = \int_{x^0=const} (L^0_{\mu\nu}(x) - t_{\mu\nu}(x))\, d^3\vec{x}$$

From (1) , (2) , (3) we derive :

$$\frac{d^0 L_{\mu\nu}}{dx^0}(x^0) = \int_{x^0=const} d^3\vec{x}\,(\partial_0 L^0_{\mu\nu}(x) - \partial_0 t_{\mu\nu}(x)) = -\int_{x^0=const} \partial_i L^i_{\mu\nu}(x)\, d^3\vec{x} \qquad (4)$$

$$\frac{d^0 S_{\mu\nu}}{dx^0} = \int_{x^0=const} d^3\vec{x}\,(\partial_0 S^0_{\mu\nu}(x) + \partial_0 t_{\mu\nu}(x)) = \int_{x^0=const} d^3\vec{x}\,\big(-\partial_i S^i_{\mu\nu}(x) - \partial_\lambda L^{\lambda}_{\mu\nu}(x) + T_{\mu\nu}(x) - T_{\nu\mu}(x)\big) = -\int_{x^0=const} \partial_i S^i_{\mu\nu}(x)\, d^3\vec{x} \qquad (5)$$

(greek indices for indexing from 0 to 3 , latin indices for indexing from 1 to 3)
If we suppose that the field operators tend to zero sufficiently fast at spatial infinity we conclude from (4) and (5) (by flux-divergence theorem) that

$$\frac{d^0 L_{\mu\nu}}{dx^0} = 0 \quad , \quad \frac{d^0 S_{\mu\nu}}{dx^0} = 0$$

${}^0L_{\mu\nu}$ and ${}^0S_{\mu\nu}$ are conserved quantities under rotation invariance and in particular $S_{\mu\nu}$ and $L_{\mu\nu}$ are conserved quantities if $t_{\mu\nu} = 0$ or more if T is a symmetric tensor .

30. Covalent crystal lattices of metals

Covalent crystal lattices of metals

In a covalent crystal, the positive kernels of metal atoms are kept in the stable positions of a latticial grid $\Gamma=\{n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3 | n_i=\overline{0,N_i}\ ,\ i=\overline{1,3}\}$ (with $\vec{a}_1,\vec{a}_2,\vec{a}_3\in\mathbb{R}^3$, $N_1,N_2,N_3\in\mathbb{N}$) by the common field of interaction between the kernels and the electronic shells of the crystal composing atoms.

Wave functions of the electrons in the crystal satisfy a time independent Schroedinger equation $\left(-\frac{\hbar^2}{2m_0}\nabla^2+V(x)\right)\psi(x)=E\,\psi(x)$ (1) with $x=(x_1,x_2,x_3)\in\mathbb{R}^3$

where $V = V(x)$ contains all interactions of the electron with the other electrons and the kernel nodes of the lattice.

Let $\boldsymbol{R_n}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$ for $\boldsymbol{n}=(n_1,n_2,n_3)\in\mathbb{Z}^3$

The equation (1) must be invariant under $\boldsymbol{R_n}$ translations and so $V(x+\boldsymbol{R_n})=V(x)$ and the wavve functions ψ satisfy cyclic boundary conditions

$\psi(x+N_i\vec{a}_i)=\psi(x)$ for $i=\overline{1,3}$ (no summation over i index) (2)

Consider the translation operator $\hat{T}_{\boldsymbol{n}}$ defined by $\hat{T}_{\boldsymbol{n}}\,\psi(x)=\psi(x+\boldsymbol{R_n})$.

Because $\int|\psi(x+\boldsymbol{R_n})|^2 d^3x=\int|\psi(x)|d^3x$ it follows that the eigenvalues of $\hat{T}_{\boldsymbol{n}}$, $\langle\hat{T}_{\boldsymbol{n}}\rangle$ satisfy $|\langle\hat{T}_{\boldsymbol{n}}\rangle|=1$ and therefore we have $\vec{k}\in\mathbb{R}^3$ such that $\langle\hat{T}_{\boldsymbol{n}}\rangle=\exp(i\vec{k}\cdot\boldsymbol{R_n})$ for any $\boldsymbol{n}\in\mathbb{Z}^3$. Now the Born-Karman cyclic conditions (2) lead to $\vec{k}\in\mathbb{R}^3$ with $\vec{k}\cdot\vec{a}_i=\frac{2\pi m_i}{N_i}$, $m_i\in\mathbb{Z}$ for $i=\overline{1,3}$ and so

$\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i$ where $\vec{b}_i=\frac{2\pi}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}(\vec{a}_j\times\vec{a}_k)\epsilon_{ijk}$ (no summation over j,k indices)

Since $V(x)=V(x+\boldsymbol{R_n})$, $\hat{T}_{\boldsymbol{n}}$ commutes with $\hat{H}=-\frac{\hbar^2}{2m_0}\nabla^2+V(x)$ and so any system of functions $(\psi_{\vec{k}})_{\vec{k}}$, $\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i$ with $\psi_{\vec{k}}(x)=\exp(i\vec{k}\cdot x)u_{\vec{k}}(x)$ where $u_{\vec{k}}$ satisfies $u_{\vec{k}}(x+\boldsymbol{R_n})=u_{\vec{k}}(x)$ for any $x\in\mathbb{R}^3$, $\boldsymbol{n}\in\mathbb{Z}^3$ and

$$\nabla^2 u_{\vec{k}}(x)+2i\vec{k}\cdot\nabla u_{\vec{k}}(x)+\frac{2m_0}{\hbar^2}\left(E(\vec{k})-\frac{\hbar^2}{2m_0}\vec{k}^2-V(x)\right)u_{\vec{k}}(x)=0 \qquad (3)$$

for the energy level $E(\vec{k})$ eigenvalue is a system of eigenfunctions for $\hat{H}$ and $\hat{T}_{\boldsymbol{n}}$ for any $\boldsymbol{n}\in\mathbb{Z}^3$.

Obviously we have $E(\vec{k})=\frac{\langle\psi_{\vec{k}}|\hat{H}|\psi_{\vec{k}}\rangle}{\langle\psi_{\vec{k}}|\psi_{\vec{k}}\rangle}$ for the energy levels, depending on the wave vector $\vec{k}$ which an electron can have in the crystal.

For the solutions of (3) we can take a liniar combination of atomic orbitals approximations, taking $V(x)=\sum_{\boldsymbol{n}} V_0(x-\boldsymbol{R_n})$, $\psi_{\vec{k}}(x)=\sum_{\boldsymbol{n}} \exp(i\vec{k}\cdot\boldsymbol{R_n})u_0(x-\boldsymbol{R_n})$ where u_0 satisfies the single atom Schroedinger equation

$$\nabla^2 u_0(x)+\frac{2m_0}{\hbar^2}(E_0-V_0(x))u_0(x)=0 \qquad (4)$$

We will have $u_{\vec{k}}(x)=\sum_{\boldsymbol{n}} \exp(i\vec{k}\cdot(\boldsymbol{R_n}-x))u_0(x-\boldsymbol{R_n})$

We can take $u_0(x)\in\mathbb{R}$ since $V_0(x)\in\mathbb{R}$ and because V_0 is considered to have its support in $\{\alpha_1\vec{a}_1+\alpha_2\vec{a}_2+\alpha_3\vec{a}_3 | \alpha_i\in(-\frac{1}{2},\frac{1}{2}) , i=\overline{1,3}\}$ we can normalize such that $\int u_0(x-\boldsymbol{R_n})u_0(x-\boldsymbol{R_m})d^3x=\delta_{\boldsymbol{nm}}$.

For a structure with $N = N_1 \mathrm{N}_2 N_3$ lattice nodes we have:

$\int \psi_{\vec{k}}^* \psi_{\vec{k}} d^3x=\sum_{\boldsymbol{m}}\sum_{\boldsymbol{n}} \exp(i\vec{k}\cdot(\boldsymbol{R_n}-\boldsymbol{R_m}))\delta_{\boldsymbol{nm}}=N$ and so the normalized form of $\psi_{\vec{k}}$ is

$\psi_{\vec{k}}=N^{-1/2}\sum_{\boldsymbol{n}} \exp(i\vec{k}\cdot\boldsymbol{R_n})u_0(x-\boldsymbol{R_n})$.

Considering (4) we obtain :

$$\hat{H}\,\psi_{\vec{k}}(x)=N^{-1/2}\sum_{\boldsymbol{n}} \exp(i\vec{k}\cdot\boldsymbol{R_n})\hat{H}\,u_0(x-\boldsymbol{R_n})=$$

$=E_0\,\psi_{\vec{k}}(x)+N^{-1/2}\sum_{\boldsymbol{n}} \exp(i\vec{k}\cdot\boldsymbol{R_n})(V(x)-V_0(x-\boldsymbol{R_n}))u_0(x-\boldsymbol{R_n})$ and therefore

$$E(\vec{k})=E_0+$$

$$+N^{-1}\sum_{\boldsymbol{m}}\sum_{\boldsymbol{n}}(\int u_0(x-\boldsymbol{R_m})(V(x)-V_0(x-\boldsymbol{R_n}))u_0(x-\boldsymbol{R_n})d^3x)\exp(i\vec{k}\cdot(\boldsymbol{R_n}-\boldsymbol{R_m})) \quad (5)$$

We consider a hight binding approximation in which we take in the sum from (5) only the terms with $\boldsymbol{m}-\boldsymbol{n}=(\pm\delta_{il})_{l=\overline{1,3}}$ for $i\in\{1,2,3\}$ or with $\boldsymbol{m}=\boldsymbol{n}$.

Since obviously we must have $E(\vec{k})=E(\vec{k})^*\in\mathbb{R}$, we will have in the hight binding approximation that $E(\vec{k})=E_0-\alpha-2\gamma(\cos(\vec{k}\cdot\vec{a}_1)+\cos(\vec{k}\cdot\vec{a}_2)+\cos(\vec{k}\cdot\vec{a}_3))$ where E_0 is a single atom electron energy level and

$\alpha=-\int u_0(x)(V(x)-V_0(x))u_0(x)d^3x$,

$\gamma=-\sum_{i=1}^{3}\int \frac{1}{2}(u_0(x-\vec{a}_i)+u_0(x+\vec{a}_i))(V(x)-V_0(x))u_0(x)d^3x$.

For a rectangular lattice with $\vec{a}_i\cdot\vec{a}_j=\delta_{ij}a_ia_j$ for $i,j=\overline{1,3}$ the energy levels relation from above becomes

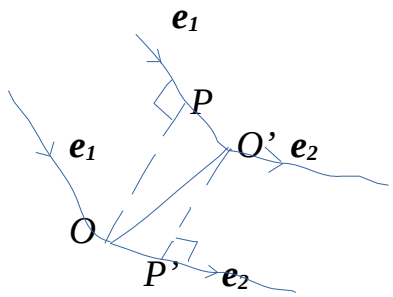
$$E(\vec{k})=E_0-\alpha-2\gamma(\cos(k_1a_1)+\cos(k_2a_2)+\cos(k_3a_3)) \qquad (6)$$

where $\vec{k}=(k_i)_i$, $\vec{a}_i=a_i(\delta_{il})_{l=\overline{1,3}}$, $k_ia_i=2\pi\tilde{k}_i$, $\tilde{k}_i=\frac{m_i}{N_i}$, $m_i\in\mathbb{Z}$

From (6) follows that if $k_i=\frac{n_i\pi}{a_i}$, $n_1\equiv n_2\equiv n_3 \pmod 2$ $i=\overline{1,3}$ in the energy spectrum $(E(\vec{k}))_{\vec{k},\alpha,\gamma,E_0}$ appear jumps over forbidden zones.

For example, for given E_0, α, γ there are two forbidden zones of $E(\vec{k})$ with upper respective lower end at a distance 12 γ from each other ,
12 γ being the lenght of an allowed zone corresponding to the first Brillouin zone of $\vec{k}$ defined by $k_i \in [-\frac{\pi}{a_i}, \frac{\pi}{a_i}]$ for $i=\overline{1,3}$ and the given E_0, α, γ.

The existence of forbidden zones can be confirmed by electromagnetic X-radiation diffraction on crystals.
In a simple rectangular crystal lattice, the coherent diffusion processes on the orbitals of *O* and *O'* nodal atoms experienced by a beam of X-rays coming in the direction of versor $\boldsymbol{e_1}$ cause a diffraction pattern in the direction of versor $\boldsymbol{e_2}$ due the interference of diffracted X-rays coming from *O* respective *O'* in direction $\boldsymbol{e_2}$.



According to figure the optical path difference is $d=\|OP'\|-\|O'P\|=\overrightarrow{OO'}\cdot(\boldsymbol{e_2}-\boldsymbol{e_1})$
Thus for $\overrightarrow{OO'}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$ the phase difference between the two diffracted rays is $\varphi=\frac{2\pi}{\lambda}(n_1\vec{a}_1\cdot\boldsymbol{e}+n_2\vec{a}_2\cdot\boldsymbol{e}+n_2\vec{a}_3\cdot e)$ where $\boldsymbol{e}=\boldsymbol{e_2}-\boldsymbol{e_1}$
Taking 2θ as the angle between $\boldsymbol{e_1}$ and $\boldsymbol{e_2}$ we will have $\boldsymbol{e}=2\sin\theta\sum_{i=1}^{3}\alpha_i \operatorname{vers}\vec{a}_i$
with $\sum_{i=1}^{3}\alpha_i^2=1$ and interference maxima can be obtained for
$2a_i\alpha_i\sin\theta=h_i\lambda$ with $h_i\in\mathbb{Z}$ for $i=\overline{1,3}$
Hence interference maxima will appear at angles θ satisfying

$$2\sin\theta=\lambda n\sqrt{\frac{h_1^2}{a_1^2}+\frac{h_2^2}{a_2^2}+\frac{h_3^2}{a_3^2}} \text{ where } n,h_1,h_2,h_3\in\mathbb{N} \qquad (7)$$

However , interference patterns determined by (7) relations will fail to appear if $\Delta E=\frac{hc}{\lambda}$ (h -Planck constant) is equal to the difference between two allowed energy levels of the $(E(\vec{k}))_{\vec{k},E_0,\alpha,\gamma}$ spectrum, since in that case the wave can be absorbed in a $E(\vec{k})$ level to $E(\vec{k}')$ level transition process.

Kroning-Penney model

To consider an one-dimensional model for a crystal lattice we assume that the metal atomic kernels create a periodic potential field of forces such that the time independent Schroedinger equations for the electrons in the crystal , are those of a succession of potential gaps and barriers :

$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}E\psi=0$ for $x\in[n(a+b),(n+1)a+nb]$

$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-V_0)\psi=0$ for $x\in[(n+1)a+nb,(n+1)(a+b)]$

with $V_0>E$ where E is the energy level and $n\in\mathbb{Z}$;

V_0,a,b are positive constants, $a+b=d$ is the constant of the one-dimensional lattice.

Solutions of the time independent Schroedinger equations are

$\psi=\psi_n(x)=A_n\sin(k_1x_n)+B_n\cos(k_1x_n)$ for $x_n\in[0,a]$

$\psi=\overline{\psi_n}(x)=\overline{A_n}\sinh(k_2(x_n-d))+\overline{B_n}\cosh(k_2(x_n-d))$ for $x_n\in[a,a+b]$

where $x_n=x-nd$, $k_1^2=\frac{2m_0E}{\hbar^2}$, $k_2^2=\frac{2m_0}{\hbar^2}(V_0-E)$.

the function ψ must be continuous differentiable at

$x_n=a$ and $x_n=a+b$ for any $n\in\mathbb{Z}$

For $x_n=d$ ($x=(n+1)d$) we will have $\overline{B_n}=B_{n+1}$, $\overline{A_n}=\frac{k_1}{k_2}A_{n+1}$;

for $x_n=a$ ($x_n-d=-b$) we will have

$A_n\sin(k_1a)+B_n\cos(k_1a)=-\overline{A_n}\sinh(k_2b)+\overline{B_n}\cosh(k_2b)$,

$A_n\cos(k_1a)-B_n\sin(k_1a)=\frac{k_2}{k_1}(\overline{A_n}\cosh(k_2b)-\overline{B_n}\sinh(k_2b))$

We will assume that the parameter

$P=\frac{k_2^2ab}{2}$ (a measure for the area of a potential barrier) is constant for $V_0\to\infty$, $b\to0$ and therefore we can approximate $\sinh(k_2b)\approx k_2b$, $\cosh(k_2b)\approx1$, $a\approx d$ and we have:

$A_n\sin(k_1d)+B_n\cos(k_1d)+B_n\cos(k_1d)=B_{n+1}$

$A_n\cos(k_1d)-B_n\sin(k_1d)=A_{n+1}-\frac{2P}{k_1d}B_{n+1}$.

$\begin{pmatrix}B_{n+1}\\A_{n+1}\end{pmatrix}=M\begin{pmatrix}B_n\\A_n\end{pmatrix}$ where $M=\begin{pmatrix}\cos(k_1d) & \sin(k_1d)\\ \frac{2P}{k_1d}\cos(k_1d)-\sin(k_1d) & \frac{2P}{k_1d}\sin(k_1d)+\cos(k_1d)\end{pmatrix}$

We have $\det M=1$, $M\in M_{2\times 2}(\mathbb{R})$ and therefore we find $X\in M_{2\times 2}(\mathbb{C})$,
$\Lambda=\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}$ or $(\Lambda=\begin{pmatrix}\lambda & 1\\ 0 & \lambda\end{pmatrix}$ with $\lambda=\pm 1$, $\frac{P}{k_1 d}\sin(k_1 d)+\cos(k_1 d)=\pm 1)$
such that $M=X^{-1}\Lambda X$, $\begin{pmatrix}B_{n+1}\\ A_{n+1}\end{pmatrix}=X^{-1}\Lambda^n X\begin{pmatrix}B_0\\ A_0\end{pmatrix}$
Since ψ must be bounded it follows that $X\begin{pmatrix}B_{n+1}\\ A_{n+1}\end{pmatrix}=\Lambda^n X\begin{pmatrix}B_0\\ A_0\end{pmatrix}$ must be
bounded for $n\in\mathbb{Z}$ and so $|\lambda_1|=|\lambda_2|=1$ which can occur only if
$\frac{P}{k_1 d}\sin(k_1 d)+\cos(k_1 d)=\cos(k d)\in[-1,1]$, (7)
$\lambda_{1,2}=\cos(k d)\pm i\sin(k d)$, $E=E(k)=\frac{\hbar^2}{2m_0}k_1^2$.
For $P=0$ we have $k=k_1$ and the electrons behave like free electrons
(no potntial barriers) . For $P=\infty$ we must have $\sin(k_1 d)=0$ and the energy is
quantized by $k_1=\frac{n\pi}{d}$, $n\in\mathbb{N}$.
For $0<P<\infty$ we observe that are allowed only energy levels that satisfy
$\frac{P}{k_1 d}\sin(k_1 d)+\cos(k_1 d)\in[-1,1]$. The forbidden energy zones appear for
$k=\frac{\pm n\pi}{d}$, $n\in\mathbb{N}$ at boundary.
From (7) we derive that we have $\alpha,\beta,\gamma,\delta$ constants depending on P,k_1,d
such that $\psi=\psi_n(x)=\exp(ik n d)(\alpha\sin(k_1 x_n)+\beta\cos(k_1 x_n))+$
$+\exp(-ik n d)(\gamma\sin(k_1 x_n)+\delta\cos(k_1 x_n))$ for $x=x_n+nd$, $x_n\in[0,a]$, $n\in\mathbb{N}$.
For a chain of *N* potential barriers we require Born-Karman cyclic condition
$\psi(x+L)=\psi(x)$ where $L=N d$ and therefore we must have $k=\frac{2\pi m}{N d}$, $m\in\mathbb{Z}$.
The maximum lenght of an interval for k with $E(k)$ in the same allowed energy
zone is $\frac{2\pi}{d}$ ($k\in[-\frac{\pi}{d},\frac{\pi}{d}]$ -the first Brillouin zone)
Because $k=\frac{2\pi m}{N d}$, $m\in\mathbb{Z}$ in a N potential barriers chain we have N energy
modes in each allowed energy zone.

31. Phonons in three-dimensional crystals

Phonons in three-dimensional crystals

Consider a cubic three-dimensional crystal lattice $\Gamma=([0,2M-1]a\cap\mathbb{Z}a)^3$ for $a>0, M\in\mathbb{N}$. The atoms in the nodes of the lattice have mass m.
We suppose that the atoms can oscillate around the equilibrium positions at the nodes having displacements $\boldsymbol{r}_{\boldsymbol{n}}=(r_{\boldsymbol{n}\alpha})_{\alpha=\overline{1,3}}$, $\boldsymbol{r}_{\boldsymbol{n}}=\boldsymbol{r}_{\boldsymbol{n}}(t)$ with respect to node $\boldsymbol{n}\in\Gamma$, (t-time coordinate). The kinetic energy is $K=\frac{m}{2}\sum_{\boldsymbol{n}}\dot{\boldsymbol{r}}_{\boldsymbol{n}}^{\,2}$ and in a harmonic approximation, the potential energy of the crystal is $U=\frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{m}\in\Gamma}V_{\alpha\beta}(\boldsymbol{n}-\boldsymbol{m})r_{\boldsymbol{n}\alpha}r_{\boldsymbol{m}\beta}$ with summation over α,β indices, $V_{\alpha\beta}$ depending only on the differences $\boldsymbol{n}-\boldsymbol{m}$, considering the invariance of the crystal system under $a(\delta_{\alpha\beta})_{\beta=\overline{1,3}}$ translations for $\alpha=\overline{1,3}$. We have also $V_{\alpha\beta}(\boldsymbol{n}-\boldsymbol{m})=V_{\beta\alpha}(\boldsymbol{m}-\boldsymbol{n})$.
The resultant force of all other atoms acting on an atom in the crystal at node $\boldsymbol{m}$ is $(F_{\boldsymbol{m}\beta})_{\beta}=-\left(\frac{\partial U}{\partial r_{\boldsymbol{m}\beta}}\right)_{\beta}=(-\sum_{\boldsymbol{n}}V_{\alpha\beta}(\boldsymbol{n}-\boldsymbol{m})r_{\boldsymbol{n}\alpha})_{\beta}$.
If the crystal moves as a whole we have $\boldsymbol{r}_{\boldsymbol{n}}=\vec{v}\,dt$ for any $\boldsymbol{n}\in\Gamma$ and $F_{\boldsymbol{m}\beta}=0$ for any $\boldsymbol{m}\in\Gamma$, $\beta=\overline{1,3}$ and since $\vec{v}\in\mathbb{R}^3$ can take arbitrary values we derive $\sum_{\boldsymbol{n}}V_{\alpha\beta}(\boldsymbol{n}-\boldsymbol{m})=0$ for any $\alpha,\beta,\boldsymbol{m}$ (1).
Introducing cyclic boundary conditions for the extended crystal lattice we must have $\boldsymbol{r}_{\boldsymbol{n}+\boldsymbol{a}(\boldsymbol{i})L}=\boldsymbol{r}_{\boldsymbol{n}}$ where $L=2M$, $\boldsymbol{a}(\boldsymbol{i})=a(\delta_{ij})_{j=\overline{1,3}}$ for any $\boldsymbol{n}$.
We can take $r_{\boldsymbol{n}\alpha}=\frac{1}{\sqrt{mN}}\sum_{\vec{k}}e_{\alpha}(\vec{k})A_{\vec{k}}\exp(i\vec{k}\cdot\boldsymbol{n})$ where $N=(2M)^3$ and the over $\vec{k}$ is taken for $\vec{k}=(k_i)_{i=\overline{1,3}}\in R$, $R=(\frac{2\pi}{aL}[-M,M)\cap\frac{2\pi}{aL}\mathbb{Z})^3$ with $A_{\vec{k}}=A_{\vec{k}}(t)\in\mathbb{C}$, $e_{\alpha}(\vec{k})=e_{\alpha}(-\vec{k})\in\mathbb{R}$, $A_{\vec{k}}=A_{-\vec{k}}^{*}$, $\alpha=\overline{1,3}$.
We can easy prove that :
$\frac{1}{N}\sum_{\boldsymbol{n}}\exp(i(\vec{k}-\vec{k}')\cdot\boldsymbol{n})=\delta_{\vec{k}\vec{k}'}$, $\frac{1}{N}\sum_{\vec{k}}\exp(i(\boldsymbol{n}-\boldsymbol{n}')\cdot\vec{k})=\delta_{\boldsymbol{n}\boldsymbol{n}'}$,
$e_{\alpha}(\vec{k})A_{\vec{k}}=\sqrt{\frac{m}{N}}\sum_{\boldsymbol{n}}r_{\boldsymbol{n}\alpha}\exp(-i\vec{k}\cdot\boldsymbol{n})$
Let $A_{\vec{k}}=A_{\vec{k}1}+iA_{\vec{k}2}$ and we have therefore generalized coordinates given by
$q=((A_{\vec{k}1},A_{\vec{k}2})e_{\alpha}(\vec{k}))_{\vec{k}\in R,\alpha=\overline{1,3}}$ and $K=\frac{1}{2}\sum_{\vec{k}}e_{\alpha}(\vec{k})e_{\alpha}(k)\dot{A}_{\vec{k}}\dot{A}_{-\vec{k}}$ (2),
$U=\frac{1}{2}\sum_{\vec{k}}D_{\alpha\beta}(\vec{k})e_{\alpha}(\vec{k})e_{\beta}(\vec{k})A_{\vec{k}}A_{-\vec{k}}$ (3)
where $D_{\alpha\beta}(\vec{k})=D_{\beta\alpha}(\vec{k})^{*}=D_{\alpha\beta}(-\vec{k})^{*}=D_{\alpha\beta}(-\vec{k})=\frac{1}{m}\sum_{\boldsymbol{n}}V_{\alpha\beta}(\boldsymbol{n})\exp(i\vec{k}\cdot\boldsymbol{n})$

The Lagrangian is $L=K-U$ and having $A_{\vec{k}}A_{-\vec{k}}=A_{\vec{k}1}^2+A_{\vec{k}2}^2$

$$\frac{\partial}{\partial(\dot{A}_{\vec{k}}e_\alpha(\vec{k}))}=\frac{1}{2}\frac{\partial}{\partial(\dot{A}_{\vec{k}1}e_\alpha(\vec{k}))}-\frac{1}{2}i\frac{\partial}{\partial(\dot{A}_{\vec{k}2}e_\alpha(\vec{k}))}$$

$$\frac{\partial}{\partial(A_{\vec{k}}e_\alpha(\vec{k}))}=\frac{1}{2}\frac{\partial}{\partial(A_{\vec{k}1}e_\alpha(\vec{k}))}-\frac{1}{2}i\frac{\partial}{\partial(A_{\vec{k}2}e_\alpha(\vec{k}))},$$

the Euler-Lagrange equations $\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}}\right)-\frac{\partial L}{\partial q}=0$ lead to

$$e_\alpha(\vec{k})\ddot{A}_{\vec{k}i}+D_{\alpha\beta}(\vec{k})e_\beta(\vec{k})A_{\vec{k}i}=0 \text{ for } i=1,2 \qquad (4)$$

We assume that $\Re D(\vec{k})$ commutes with $\Im D(\vec{k})$ for any $\vec{k}$ which happens if $V(\boldsymbol{n})$ commutes with $V(\boldsymbol{n}')$ for any $\boldsymbol{n},\boldsymbol{n}'$.

We have harmonical oscillation in direction $(e_\alpha(\vec{k}))_\alpha$ terms and we take $\dot{A}_{\vec{k}}=-i\omega(\vec{k})A_{\vec{k}}$, $\ddot{A}_{\vec{k}}=-\omega^2(\vec{k})A_{\vec{k}}$ and so from (4) we have

$$\omega^2(\vec{k})e_\alpha(\vec{k})-D^{(c)}_{\alpha\beta}(\vec{k})e_\beta(\vec{k})=0 \text{ for } c=1,2\ ,\ (D^{(1)},D^{(2)})=(\Re D,\Im D) \qquad (5)$$

Since $D_{\alpha\beta}(\vec{k})=D_{\beta\alpha}(\vec{k})^*=D_{\alpha\beta}(-\vec{k})^*$ and $[D^{(1)},iD^{(2)}]=0$ we conclude that D is hermitian and we can can take a real orthonormate system $(\boldsymbol{e}^s(\vec{k}))_{s=\overline{1,3}}$, and three real eigenvalues of $D(\vec{k})$: $\omega_s^2(\vec{k})$, $s=\overline{1,3}$.

We assume that the potential energy (3) is positive definite and so we have three branches of oscillations in orthogonal directions $\boldsymbol{e}^s$, s = 1,2,3

$D(\vec{k})\boldsymbol{e}^s(\vec{k})=\omega_s^2(\vec{k})\boldsymbol{e}^s(\vec{k})$ for $\vec{k}\in\mathbb{R}^3$, $\omega_s(\vec{k})>0$.

Because of (1) we will have $D_{\alpha\beta}(\vec{k})\to 0$ for $\vec{k}\to\vec{0}$ and so $\omega_s(\vec{k})\to 0$ for $k\to 0$, (with $\|\vec{k}\|=k$) .

The summation of the three branches lead to a total displacement

$$r_{\boldsymbol{n}\alpha}=\frac{1}{\sqrt{mN}}\sum_{\boldsymbol{n},s}e^s_\alpha(\vec{k})A_{s\vec{k}}(t)\exp(i\vec{k}\cdot\boldsymbol{n}) \text{ with } \ddot{A}_{s\vec{k}}=-\omega_s^2(\vec{k})A_{s\vec{k}} \ ,$$

$$K=\frac{1}{2}\sum_{\vec{k},s}\dot{A}_{s\vec{k}}\dot{A}_{s-\vec{k}} \ , \quad U=\frac{1}{2}\sum_{\vec{k},s}\omega_s^2(\vec{k})A_{s\vec{k}}A_{s-\vec{k}} \qquad (6)$$

and generalized coordinates $(A_{s\vec{k}1},A_{s\vec{k}2})_{\vec{k}\in R,\,s=\overline{1.3}}$, $A_{s\vec{k}}=A_{s\vec{k}1}+iA_{s\vec{k}2}$.

We have $P_{s\vec{k}}=\frac{\partial(K-U)}{\partial\dot{A}_s\vec{k}}=\dot{A}_{s-\vec{k}}$

$$\sum_s e^s_\alpha(\vec{k})A_{s\vec{k}}=\sqrt{\frac{m}{N}}\sum_{\boldsymbol{n}}r_{\boldsymbol{n}\alpha}\exp(-i\vec{k}\boldsymbol{n}) \qquad (7)$$

From $\boldsymbol{e}^s\cdot\boldsymbol{e}^{s'}=\delta_{ss'}$ it follows $\sum_s e^s_\alpha(\vec{k})e^s_{\alpha'}(\vec{k})=\delta_{\alpha\alpha'}$ and so from (7) we obtain

$$A_{s\vec{k}}=\sqrt{\frac{m}{N}}\sum_{\boldsymbol{n}}e^s_\alpha(\vec{k})r_{\boldsymbol{n}\alpha}\exp(-i\vec{k}\cdot\boldsymbol{n}) \quad (\text{ with summation over } \alpha=\overline{1,3}\ ) \qquad (7')\ .$$

Taking $p_{\boldsymbol{n}\alpha}=m\dot{\boldsymbol{r}}_{\boldsymbol{n}\alpha}$ we derive

$$P_{s\vec{k}}=\frac{1}{\sqrt{mN}}\sum_{\boldsymbol{n}} e^{s}_{\alpha}(\vec{k})\,p_{\boldsymbol{n}\alpha}\exp(i\vec{k}\cdot\boldsymbol{n})\ .$$

Considering the corresponding quantum operators $\hat{r}_{\boldsymbol{n}\alpha},\hat{p}_{\boldsymbol{n}\alpha},\hat{A}_{s\vec{k}},\hat{P}_{s\vec{k}}$ we will have the commutation relations $[\hat{r}_{\boldsymbol{n}\alpha},\hat{p}_{\boldsymbol{n}'\beta}]=i\hbar\,\delta_{\alpha\beta}\delta_{\boldsymbol{n}\boldsymbol{n}'}$ and so

$$[\hat{A}_{s\vec{k}},\hat{P}_{s'\vec{k}'}]=\sum_{\boldsymbol{n},\boldsymbol{n}'}\frac{1}{N}e^{s}_{\alpha}(\vec{k})e^{s'}_{\beta}(\vec{k}')i\hbar\,\delta_{\alpha\beta}\delta_{\boldsymbol{n}\boldsymbol{n}'}\exp(i(\vec{k}'\cdot\boldsymbol{n}'-\vec{k}\,\boldsymbol{n}))=i\hbar\,\delta_{ss'}\delta_{\vec{k}\vec{k}'}\quad(8)\ .$$

The Hamiltonian is $H = K + U$ and so the Hamiltonian operator is

$$\hat{H}=\frac{1}{2}\sum_{\vec{k},s}(\hat{P}_{s\vec{k}}\hat{P}_{s-\vec{k}}+\omega_s^2(\vec{k})\hat{A}_{s\vec{k}}\hat{A}_{s-\vec{k}})\qquad(9)$$

We define creation and anihilation operators $b^{+}_{s\vec{k}}$ and respective $b_{s\vec{k}}$ by relations

$$\hat{A}_{s\vec{k}}=\sqrt{\frac{\hbar}{2\,\omega_s(\vec{k})}}(b_{s\vec{k}}+b^{+}_{s-\vec{k}})\quad,\quad\hat{P}_{s\vec{k}}=i\sqrt{\frac{\hbar\,\omega_s(\vec{k})}{2}}(b^{+}_{s\vec{k}}-b_{s-\vec{k}})\qquad(10)$$

Relation (8) is satisfied if

$$[b_{s\vec{k}},b^{+}_{s'\vec{k}'}]=i\hbar\,\delta_{ss'}\delta_{\vec{k}\vec{k}'}\quad,\quad[b_{s\vec{k}},b_{s'\vec{k}'}]=0\quad\text{for }\vec{k},\vec{k}'\in R\ ;\ s,s'\in\{1,2,3\}\quad(11)\ .$$

With the commutation relations (11) , from (9) and (10) follows now

$$\hat{H}=\sum_{\vec{k},s}\hbar\,\omega_s(\vec{k})(b^{+}_{s\vec{k}}b_{s\vec{k}}+\frac{1}{2})=\sum_{\vec{k},s}\hbar\,\omega_s(\vec{k})(\hat{b}^{+}_{s\vec{k}}\hat{b}_{s\vec{k}}+\frac{1}{2})$$

and from (6) follows $\hat{r}_{\boldsymbol{n}}=\sqrt{\frac{\hbar}{2mN}}\sum_{\vec{k},s}\frac{\boldsymbol{e}^{s}(\vec{k})}{\sqrt{\omega_s(\vec{k})}}(b_{s\vec{k}}\exp(i\vec{k}\cdot\boldsymbol{n})+b^{+}_{s\vec{k}}\exp(-i\vec{k}\cdot\boldsymbol{n}))$

$b_{s\vec{k}}=b_{s\vec{k}}(t)=\hat{b}_{s\vec{k}}\exp(-i\,\omega_s(\vec{k})t)$ with $\hat{b}_{s\vec{k}}$ -anihilation operator , $\hat{b}^{+}_{s\vec{k}}$ -creation operator of a phonon of wave vector $\vec{k}$ and polarization s acting on a Hilbert space of oscillations of the crystall lattice which has a ground state (corresponding to no oscillation) denoted $|0\rangle$ and single phonon states $\hat{b}^{+}_{s\vec{k}}|0\rangle$ having also $\hat{b}_{s\vec{k}}|0\rangle=0$, $[\hat{b}_{s\vec{k}},\hat{b}^{+}_{s'\vec{k}'}]=i\hbar\,\delta_{ss'}\delta_{\vec{k}\vec{k}'}$, $[\hat{b}_{s\vec{k}},\hat{b}_{s'\vec{k}'}]=0$ for any $s\in\{1,2,3\}$, $\vec{k}\in\mathbb{R}^3$.

In the same way as for the electromagnetic field quantization we can consider the crystal lattice oscillations as a system of a number of phonons having different wave vectors and polarizations defined by a state $\prod_{\vec{k},s}\hat{b}^{+}_{s\vec{k}}|0\rangle$. Thus , with the commutation relations (11) we derive a number of particles operator $\hat{N}_{s\vec{k}}=\hat{b}^{+}_{s\vec{k}}\hat{b}_{s\vec{k}}$ in the same way as for the quantized electromagnetic field , as the particles number of phonons oscillating in direction $\boldsymbol{e}^{s}(\vec{k})$ and propagating with wave vector $\vec{k}$ and pulsation $\omega_s(\vec{k})$.

Since $\boldsymbol{r_n}$ transforms like a vector under a spatial coordinates rotation the phonons can be considerated spin 1 particles having three polarization directions s = 1,2,3 with a field operator function defined (in a continuum limit for the $\boldsymbol{n}$ domain of latticial

nodes) by the displacements field $\vec{u}(t,\boldsymbol{n})=\boldsymbol{r}_{\boldsymbol{n}}(t)$ as $\vec{\varphi}(t,x)=\sqrt{\frac{mN}{V}}\boldsymbol{r}_{\boldsymbol{n}}(t)=$

$$=\frac{\sqrt{\hbar V}}{(2\pi)^3}\int\sum_s\frac{1}{\sqrt{2\omega_s(\vec{k})}}\boldsymbol{e}^s(\vec{k})\left(\hat{b}_{s\vec{k}}\exp(-i\omega_s(\vec{k})t+i\vec{k}\cdot x)+\right.$$
$$\left.+\hat{b}^{+}_{s\vec{k}}\exp(i\omega_s(\vec{k})t-i\vec{k}\cdot x)\right)d^3\vec{k}$$

where $\boldsymbol{n}$ is identified in the continuum limit with the spatial x variable and V is the volume of the crystal, N is the number of nodes.

Consider the example when the covalent metallic crystal medium is assimilable to a liniar elastic homogeneous material and so we have the liniar elastic potential energy given by $U=\frac{1}{2}\sum_{\boldsymbol{n}}a^3C_{ijkl}u^{(\boldsymbol{n})}_{i,j}u^{(\boldsymbol{n})}_{k,l}$ where $u^{(\boldsymbol{n})}_{i,j}=\frac{\boldsymbol{r}_{\boldsymbol{n}+\boldsymbol{a}(j)\,i}-\boldsymbol{r}_{\boldsymbol{n}\,i}}{a}$ and $C_{ijkl}=C_{ijlk}=C_{klij}$ with $i,j,k,l=\overline{1,3}$ (and summation over i,j,k,l in the expression for U).

It follows that :

$$U=\frac{1}{2}a\left(\sum_{\boldsymbol{n}}\sum_{j\neq l}C_{ijkl}\boldsymbol{r}_{\boldsymbol{n}+\boldsymbol{a}(j)\,i}\boldsymbol{r}_{\boldsymbol{n}+\boldsymbol{a}(l)\,k}+\sum_{\boldsymbol{n}}\left(C_{ijkl}\delta_{jl}+\sum_{p,q}C_{ijkl}\delta_{jp}\delta_{lq}\right)\boldsymbol{r}_{\boldsymbol{n}\,i}\boldsymbol{r}_{\boldsymbol{n}\,k}-\right.$$
$$\left.-2\sum_{\boldsymbol{n}}\sum_{q}C_{ijkl}\delta_{jq}\boldsymbol{r}_{\boldsymbol{n}\,i}\boldsymbol{r}_{\boldsymbol{n}+\boldsymbol{a}(l)\,k}\right)$$
$$V_{\alpha\beta}(0)=a\left(C_{\alpha\gamma\beta\varepsilon}\delta_{\gamma\varepsilon}+\sum_{p,q}C_{\alpha\gamma\beta\varepsilon}\delta_{\gamma p}\delta_{\varepsilon q}\right)$$
$$V_{\alpha\beta}(-\boldsymbol{a}(\varepsilon))=-a\sum_{q}C_{\alpha\gamma\beta\varepsilon}\delta_{\gamma q}$$
$$V_{\alpha\beta}(\boldsymbol{a}(\gamma))=-a\sum_{q}C_{\alpha\gamma\beta\varepsilon}\delta_{\varepsilon q}$$
$$V_{\alpha\beta}(\boldsymbol{a}(\gamma)-\boldsymbol{a}(\varepsilon))=aC_{\alpha\gamma\beta\varepsilon}\ \text{ if }\ \gamma\neq\varepsilon$$

If the material is liniar elastic isotrope we have
$C_{\alpha\gamma\beta\varepsilon}=\lambda\delta_{\alpha\gamma}\delta_{\beta\varepsilon}+\mu(\delta_{\alpha\beta}\delta_{\gamma\varepsilon}+\delta_{\alpha\varepsilon}\delta_{\gamma\beta})$ with $\lambda,\mu\in\mathbb{R}$ the Lame coefficients.
Hence if the crystal medium is assimilable to a liniar elastic isotrope homogeneous material we obtain :

$$D_{\alpha\beta}(\vec{k})=\frac{1}{m}\sum_{\boldsymbol{n}}V_{\alpha\beta}(\boldsymbol{n})\exp(i\vec{k}\cdot\boldsymbol{n})=\frac{a}{m}\left(\lambda+\mu+6\mu\delta_{\alpha\beta}-\lambda\left(\exp(-ik_\beta a)+\exp(ik_\alpha a)-\right.\right.$$
$$\left.-\exp(i(k_\alpha-k_\beta)a)\right)-\mu(\exp(-ik_\alpha a)+\exp(ik_\beta a)-\exp(i(k_\beta-k_\alpha)a))+$$
$$\left.-\sum_{\varepsilon}\mu\delta_{\alpha\beta}(\exp(-ik_\varepsilon a)+\exp(ik_\varepsilon a))\right)$$

We observe that for $\vec{k}=\vec{0}$ we have $D_{\alpha\beta}(\vec{k})=0$.

Further for $k^2a^2\ll 1$ we can approximate

$$D_{\alpha\beta}(\vec{k})=\frac{a}{m}((\lambda+\mu)k_\alpha k_\beta a^2+\mu\delta_{\alpha\beta}k^2a^2+O(k^3a^3))$$

Having $\frac{m}{a^3}=\rho$ -the density of the material we conclude that for small wave numbers ($k^2a^2\ll 1$) we obtain $D_{\alpha\beta}(\vec{k})=\frac{\lambda+\mu}{\rho}k_\alpha k_\beta+\frac{\mu}{\rho}\delta_{\alpha\beta}\vec{k}^2$ $D_{\alpha\beta}(\vec{k})k_\beta=\frac{\lambda+2\mu}{\rho}k^2k_\alpha$ and if $k_\beta u_\beta=0$ we have $D_{\alpha\beta}(\vec{k})u_\beta=\frac{\mu}{\rho}k^2u_\alpha$. Therefore in the liniar elastic isotrope case , for small wave numbers *k* we have three oscillation modes: a longitudinal mode with $\omega_\parallel(\vec{k})=\sqrt{\frac{\lambda+2\mu}{\rho}}\|\vec{k}\|$ and two transversal modes $\omega_\perp(\vec{k})=\sqrt{\frac{\mu}{\rho}}\|\vec{k}\|$. The corresponding phase velocities are $\frac{\omega_\parallel}{k}=\sqrt{\frac{\lambda+2\mu}{\rho}}$ and respective $\frac{\omega_\perp}{k}=\sqrt{\frac{\mu}{\rho}}$ the longitudinal respective transversal elastic waves propagation velocities.

32. Photonic gas. Black-body radiation Phononic gas. Specific heat of crystals

Photonic gas. Black-body radiation
Phononic gas. Specific heat of crystals

As we noticed in Chap. Classical statistical ensemble and Chap. Quantum statistical ensemble, in the case of a system consisting of identical particles having an energy levels spectrum $(\varepsilon_s)_s$ we have the occupation numbers at thermodynamical equilibrium given by

$N_s = g_s \exp\left(\frac{\mu - \varepsilon_s}{k_b T}\right)$ for classical statistical ensemble (1)

$N_s = \frac{g_s}{\exp((\varepsilon_s - \mu)/(k_b T)) - 1}$ for bosonic quantum statistical ensemble (2)

$N_s = \frac{g_s}{\exp((\varepsilon_s - \mu)/(k_b T)) + 1}$ for fermionic quantum statistical ensemble (3)

where μ -chemical potential of particles , T equilibrium temperature , k_b -Boltzmann costant .

However , we can approximate in some cases the energy levels spectrum with a continuous spectrum and since , as we mentioned in Chap. Canonical quantization of a scalar field, the minimum accessible volume in phase space for a particle is $(2\pi\hbar)^f$ (with f -number of freedom degrees for a particle), in the case of a continuous spectrum approximation we must replace the g_s degeneracy coefficients with infinitesimal values $\frac{g}{a}\left(\prod_{i=1}^{f} dq_i\, dp_i\right)$ where $a = (2\pi\hbar)^f$ and g can be for example the spin multiplicity (or polarization multiplicity for photons or phonons) of the considered particles and $(q_i\ ,\ p_i)_{i=\overline{1,f}}$ are the phase space coordinates for a single particle subsystem.

The radiation emitted by a black-body (a cavity which reflects no incident radiation of its external walls) which is equal to the thermal radiation emitted from the body to stay in thermal equilibrium at absolute temperature T with the absorbed incident radiation can be considered as a photonic gas, a system of photons with a continuous spectrum of energy levels and chemical potential $\mu = 0$ (since the number of photons is indefinite) and so we have a infinitesimal occupation number of the $(\varepsilon\ ,\ \varepsilon + d\,\varepsilon)$ energy levels interval given by

$dN = \frac{2}{a}\frac{1}{\exp(\varepsilon/(k_b T)) - 1} 4\pi V p^2 dp$ because $g = 2$ for the two polarization states a photon can have and V is the volume of the cavity, $p = \frac{\varepsilon}{c}$, $\prod_{i=1}^{3} dq_i\, dp_i = 4\pi V p^2 dp$ $f = 3$, $a = (2\pi\hbar)^3$, c speed of light .

Therefore the total thermal energy radiation amount is

$$U=V\int\rho(\varepsilon,T)\,d\varepsilon$$

with $\rho(\varepsilon,T)=\frac{8\pi}{c^3(2\pi\hbar)^3}\frac{\varepsilon^3}{\exp(\varepsilon/(k_bT))-1}$ -spectral density.

If we use classical considerations we will have (according to energy equipartition from Chap. Classical statistical ensemble) an average energy for a wave state

$$k_bT=\frac{\int_0^\infty \varepsilon\exp(-\varepsilon/(k_bT))\,d\varepsilon}{\int_0^\infty \exp(-\varepsilon/(k_bT))\,d\varepsilon}$$ and a infinitesimal number of states

$dN=g\frac{V}{(2\pi)^3}d^3\vec{k}=8\pi\frac{V}{c^3}\nu^2 d\nu$ with ν -photon frequencies and so it follows

a spectral density like the Rayleigh-Jeans law $\bar{\rho}(\nu,T)=\frac{8\pi}{c^3}\nu^2 k_bT$ giving

$U=V\int_0^\infty\bar{\rho}(\nu,T)\,d\nu$ and we will have an ultraviolet catastrophe : spectral density of energy goes to infinity as the frequency increases.

However experimental data lead to the adopting of quantization of photon energies and the quantum approach for the photonic gas :

$\varepsilon=\hbar\omega$, $dN=\frac{2}{a}\frac{1}{\exp(\varepsilon/(k_bT))-1}\frac{1}{c^3}\varepsilon^2 d\varepsilon$, $\rho(\varepsilon,T)=\frac{8\pi}{c^3(2\pi\hbar)^3}\frac{\varepsilon^3}{\exp(\varepsilon/(k_bT))-1}=$

$=\frac{1}{\pi^2c^3}\frac{\omega^3}{\exp(\hbar\omega/(k_bT))-1}$ spectral density of energy (Planck law) .

We have $\int_0^\infty\frac{\varepsilon^3}{\exp(\varepsilon/(k_bT))-1}d\varepsilon=(k_bT)^4\int_0^\infty\frac{x^3}{\exp(x)-1}dx$

$\int_0^\infty\frac{x^3dx}{\exp(x)-1}=\int_0^\infty\sum_{k=0}^\infty x^3\exp(-x)\exp(-kx)dx=(\sum_{k=1}^\infty\frac{1}{k^4})\int_0^\infty u^3\exp(-u)du=\sum_{k=1}^\infty\frac{6}{k^4}.$

The system of functions $\left(\frac{1}{\sqrt{2\pi}},\left(\frac{1}{\sqrt{\pi}}\cos(kx),\frac{1}{\sqrt{\pi}}\sin(kx)\right)_{k\in\mathbb{N}^*}\right)$ is orthonormal complete in $L^2((0,2\pi))$ and so in $L^2((0,2\pi))$ we have

$x=\frac{1}{2\pi}\int_0^{2\pi}u\,du+\frac{1}{\pi}\sum_{k=1}^\infty\left(\cos(kx)\frac{1}{k^2}\int_0^{2k\pi}u\cos u\,du+\sin(kx)\frac{1}{k^2}\int_0^{2k\pi}u\sin u\,du\right)=$

$=\pi-\sum_{k=1}^\infty\frac{2}{k}\sin(kx)$

$$x^2=\frac{1}{2\pi}\int_0^{2\pi}u^2\,du+\frac{1}{\pi}\sum_{k=1}\left(\cos(kx)\frac{1}{k^3}\int_0^{2k\pi}u^2\cos u\,du+\sin(kx)\frac{1}{k^3}\int_0^{2k\pi}u^2\sin u\,du\right)=$$

$$=\frac{4}{3}\pi^2+\sum_{k=1}^{\infty}\left(\frac{4}{k^2}\cos(kx)-\frac{4\pi}{k}\sin(kx)\right)=\frac{4}{3}\pi^2+2(x-\pi)\pi+\sum_{k=1}^{\infty}\frac{4}{k^2}\cos(kx)$$

$$x^2-2\pi x+\frac{2}{3}\pi^2=4\sqrt{\pi}\sum_{k=1}^{\infty}\frac{1}{k^2}\frac{1}{\sqrt{\pi}}\cos(kx)\quad\text{and so}$$

$$\sum_{k=1}^{\infty}\frac{1}{k^4}=\frac{1}{16\pi}\int_0^{2\pi}\left(x^2-2\pi x+\frac{2}{3}\pi^2\right)^2dx=\frac{\pi^4}{90}$$

Thus the radiated total energy density is

$$u(T)=\frac{U}{V}=\frac{8\pi^5}{15c^3(2\pi\hbar)^3}k_b^4T^4=\sigma T^4\ ,\ \sigma=\frac{8\pi^5k_b^4}{15c^3(2\pi\hbar)^3}\ \text{(the Stefan-Boltzmann law)}$$

Let $L_{\theta,\varphi}$ the thermal equilibrium amount of radiation energy radiated in direction (θ,φ) in an unit time interval through a unit area surface element normal to the direction from a surface element dS situated at the origin of the spherical coordinates reference system (r,θ,φ) , $\theta\in(0,\pi)$, $\varphi\in(0,2\pi)$ on the boundary of the radiating body ($\theta=0$ direction being the outwards normal direction to dS) and in a unit solid angle for (θ,φ) directions. Then the radiated infinitesimal power from surface element dS in direction (θ,φ) in the solid angle $d\Omega$ is $P_{d\Omega}=\int_{(d\Omega)}L_{\theta,\varphi}dS\cos\theta d\Omega$ with $d\Omega=\sin\theta d\theta d\varphi$.

Considering the radiating body as a Lambert source we suppose that $L_{\theta,\varphi}=L$ not depends on θ , φ .

The total radiated power from surface element dS is therefore given by :

$$P=dS\left(\int_0^{2\pi}\int_0^{\pi/2}L\cos\theta\sin\theta\,d\theta\,d\varphi\right)=\pi L\,dS\ .$$

The radiated photons have speed c and the radiated energy density in an energy level interval $(\varepsilon,\varepsilon+d\varepsilon)$ is $\rho(\varepsilon,T)d\varepsilon$ and so from the interpretation of $L_{\theta,\varphi}$ follows

$LdS=\frac{1}{4\pi}\int_0^{\infty}c\,\rho(\varepsilon,T)d\varepsilon dS$ (since the radiated photons emerge from dS in any direction of a solid angle 4π with velocity c) .

Thus $P=\pi LdS=\frac{c}{4}\left(\int_0^{\infty}\rho(\varepsilon,T)d\varepsilon\right)dS$ and the total radiated power per unit area of body boundary surface is $\frac{P}{dS}=\frac{\pi^2}{60c^2\hbar^3}k_b^4T^4$

We observe also that for

$\varepsilon=\hbar\omega\ll k_bT$ we obtain $\rho(\varepsilon,T)d\varepsilon=\frac{8\pi}{c^3(2\pi\hbar)^3}\frac{\hbar^3\omega^3k_bT}{\hbar\omega}\hbar\,d\omega=\frac{1}{\pi^2c^3}\omega^2k_bT\,d\omega$

(the Rayleigh-Jeans law) .

In a crystal lattice with N nodes heat is generated by independent propagating oscillations of the atoms in the nodes which can be expressed in the form of a gas of phonons behaving like a system of bosons which has a Hamiltonian operator $\hat{H}=\sum_{\vec{k},s}\hbar\,\omega_s(\vec{k})(\hat{b}^{+}_{\vec{k},s}\hat{b}_{\vec{k},s}+\frac{1}{2})$ with $\hat{b}^{+}_{\vec{k},s},\hat{b}_{\vec{k},s}$ -creation respective anihilation operators acting on the Hilbert space of oscillation states of the crystal lattice nodes.

$\hat{N}_{\vec{k},s}=\hat{b}^{+}_{\vec{k},s}\hat{b}_{\vec{k},s}$ is the particles number operator of phononic oscillations in direction $\boldsymbol{e}^{s}(\vec{k})$ propagating with wave vector $\vec{k}$ and pulsation $\omega_s(\vec{k})$.

At thermal equilibrium with temperature T the particles number is $N_{\vec{k},s}=\frac{g_s}{\exp(\hbar\,\omega_s(\vec{k})/k_bT)-1}$ and we have two oscillation modes in normal to propagation direction $\vec{k}$ which have a phase velocity c_T (transversal elastic waves) and one oscillation mode in parallel to propagation direction $\vec{k}$ which have a phase velocity c_P (longitudinal elastic waves), considering only long wavelenght acoustic phonons: $s=\overline{1,3}$, $\omega_1(\vec{k})=\omega_2(\vec{k})=c_T\|\vec{k}\|$, $\omega_3(\vec{k})=c_P\|\vec{k}\|$, $\vec{k}\cdot\boldsymbol{e}^{j}(\vec{k})=0$ for $j=1,2$, $\vec{k}\|\boldsymbol{e}^{3}(\vec{k})$.

For a cubic lattice of edgelenght L we have $\vec{k}\in(\frac{2\pi}{L}\mathbb{Z})^3$.

(see Chap. Phonons in three-dimensional crystals)

Taking the continuous spectrum approximation we have the total energy of the phonons in the crystal given by

$$U=\sum_{\vec{k},s}g_s\left(\frac{\hbar\,\omega_s(\vec{k})}{\exp(\hbar\,\omega_s(\vec{k})/k_bT)-1}+\frac{\hbar\,\omega_s(\vec{k})}{2}\right)=$$

$$=\frac{3V}{(2\pi\hbar)^3}\int_0^{\omega_{max}}4\pi\left(\frac{\hbar\,\omega}{\exp(\hbar\,\omega/k_bT)-1}+\frac{\hbar\,\omega}{2}\right)p^2\,dp$$ where $p=\frac{\hbar\,\omega}{u}$ with $\frac{3}{u^3}=\frac{2}{c_T^3}+\frac{1}{c_P^3}$ and ω_{max} can be determined as the maximal pulsation from the condition that the total number of oscillators is $3N$, that is $3N=\frac{3V}{(2\pi\hbar)}\int_0^{\omega_{max}}4\pi\frac{\hbar^3}{u^3}\omega^2\,d\,\omega$ leading to $\omega_{max}=u\left(\frac{6N\pi^2}{V}\right)^{1/3}$. We define the Debye temperature θ by $k_b\,\theta=\hbar\,\omega_{max}$ and it follows $U=\frac{3k_b^4T^4V}{\hbar^3u^3 2\pi^2}\int_0^{\theta/T}\frac{x^3\,dx}{\exp(x)-1}+\frac{9}{8}N\,k_b\,\theta$

For $\frac{\theta}{T}\ll 1$ we can approximate $\frac{x^3}{\exp(x)-1}\approx x^2$ and so

$U\approx\frac{9}{8}N\,k_b\,\theta+3\,N\,k_bT\approx 3\,N\,k_bT$.

For $\frac{\theta}{T}\gg 1$ we have $\int_0^{\theta/T}\frac{x^3\,dx}{\exp(x)-1}\approx\int_0^{\infty}\frac{x^3\,dx}{\exp(x)-1}=\frac{\pi^4}{15}$ and so

$U\approx\frac{\pi^2 k_b^4 T^4 V}{10\hbar^3 u^3}+\frac{9}{8}N k_b\theta$

The specific heat is $C_V=\left(\frac{\partial U}{\partial T}\right)_V$ and therefore

$C_V=3Nk_b$ for $\frac{\theta}{T}\ll 1$ and $C_V=\frac{2\pi^2 k_b^4 T^3 V}{5\hbar^3 u^3}$ for $\frac{\theta}{T}\gg 1$ and in the general case

we have $U=3Nk_bT\,D(\frac{\theta}{T})+\frac{9}{8}Nk_b\theta$

$C_V=3Nk_b\left(D(\frac{\theta}{T})-\frac{\theta}{T}D'(\frac{\theta}{T})\right)$ where

$D(\frac{\theta}{T})=\frac{3}{(\theta/T)^3}\int_0^{\theta/T}\frac{x^3\,dx}{\exp(x)-1}$.

33. Quantum electrodynamics scattering

Quantum electrodynamics scattering

Electron-proton scattering

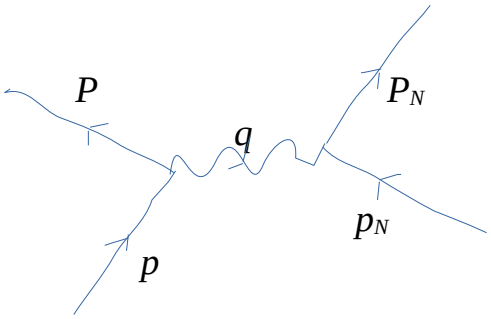


fig.1

Let p , p_N respective the incoming electron and nucleon four-momenta and P , P_N the corresponding outgoing four-momenta.
Applying the Feynman rules (see Chap. Feynman amplitudes amd lattice gauge theory) for the fig. 1 diagram we obtain the Feynman amplitude

$$A_F(P,P_N)=(2\pi)^4(-ie)(ie)\frac{i}{(P-p)^2+i\varepsilon}(-\eta_{\mu\nu})(\bar{u}(P)\gamma^\mu u(p))(\bar{u}(P_N)\gamma^\nu u(p_N))$$

$$\delta^4(P+P_N-p-p_N)=(2\pi)^4 M(P,P_N)\,\delta^4(P+P_N-p-p_N)\ .$$

To obtain the cross section we have to square $|M(P,P_N)|$.
(We have suppressed the particles spin indexes and consider averaging over the incoming particles spin polarizations and summation over the outgoing particles spin polarizations (the incoming particles are unpolarized and the outgoing spin polarizations are not measured)) .
Thus averaging and summing $|M(P,P_N)|^2$ and considering that

$$\sum_s u_\alpha(p,s)\overline{u_\beta}(p,s)=\left(\frac{\not{p}+m}{2m}\right)_{\alpha\beta}$$ we have:

$$|M(P,P_N)|^2=\frac{e^2}{4((P-p)^2)^2}\,\mathrm{tr}\left(\frac{(\not{P}+m)\gamma^\mu(\not{p}+m)\gamma^\lambda}{(2m)^2}\right)\mathrm{tr}\left(\frac{(\not{P}_N+M)\gamma_\mu(\not{p}_N+M)\gamma_\lambda}{(2M)^2}\right)$$

where $\not{p}=\gamma^\mu p_\mu$ and m respective M are the electron and proton mass.
Since the trace of an odd number product of gamma matrices vanishes and
$\mathrm{tr}(\gamma^\mu\gamma^\nu)=4\eta^{\mu\nu}$ with $(\eta^{\mu\nu})_{\mu,\nu}$ the Minkowski metric coefficients , (1)
$\mathrm{tr}(\gamma^\mu\gamma^\nu\gamma^\lambda\gamma^\sigma)=4(\eta^{\mu\nu}\eta^{\lambda\sigma}-\eta^{\mu\lambda}\eta^{\nu\sigma}+\eta^{\mu\sigma}\eta^{\nu\lambda})$ we obtain
$\frac{1}{2}\mathrm{tr}((\not{P}+m)\gamma^\mu(\not{p}+m)\gamma^\lambda)=2(P^\mu p^\lambda-\eta^{\mu\lambda}(P\,p)+P^\lambda p^\mu+m^2\eta^{\mu\lambda})$ and with
$P+P_N=p+p_N$ after some calculus we derive:

$$|M(P,P_N)|^2=\frac{e^4}{4m^2M^2}\frac{2(P\,p_N)(P_N\,p)+2(P\,P_N)(p\,p_N)+(P-p)^2(M^2+m^2)}{((P-p)^2)^2}\ .$$

Then according to calculations we made in Chap. Canonical quantization of a scalar field , the differential cross section for the scattering in the center of mass frame is:

$$d\sigma=\frac{1}{|\vec{v}_1-\vec{v}_2|}\frac{1}{(2\pi)^2}\frac{m^2M^2}{p_N^0\,p^0\,E^2}((E^2-(m+M)^2)(E^2-(M-m)^2))^{1/2}|M(P,P_N)|^2d\Omega$$

where $\vec{p}=m\frac{\vec{v}_1}{\sqrt{1-\vec{v}_1^2}}=-\vec{p}_N=-M\frac{\vec{v}_2}{\sqrt{1-\vec{v}_2^2}}$, $p_0=\sqrt{\vec{p}^2+m^2}$, $p_{N0}=\sqrt{\vec{p}_N^2+M^2}$

$$\vec{P}=-\vec{P}_N=\frac{1}{2E}((E^2-(m+M)^2)(E^2-(M-m)^2))^{1/2}(\cos\theta,\sin\theta\cos\varphi,\sin\theta\sin\varphi)$$

$$P^0=\sqrt{\vec{P}^2+m^2}\ ,\ P_N^0=\sqrt{\vec{P}^2+M^2}\ ,\ E=p^0+p_N^0$$

$(\theta,\varphi)\in(0,\pi)\times(0,2\pi)$ are the solid angle $d\Omega$ variables.

Electron-electron scattering

In a scattering process of two electrons incoming four-momenta p_1 , p_2 and P_1 , P_2 outgoing four-momenta we have to consider that we cannot distinguish between the two outgoing electrons. The electron carrying momentum P_1 could have "come from" the incoming electron carrying momentum p_1 or the incoming electron carrying momentum p_2 . Now there are two Feynman diagrams we have to consider:

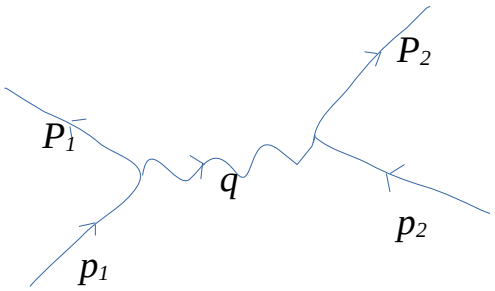


fig.2

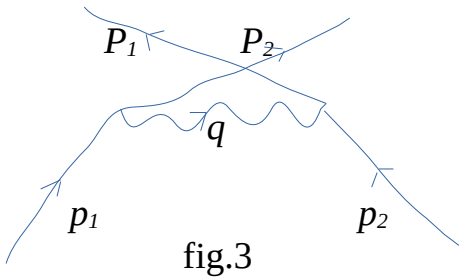


fig.3

The Feynman amplitude for the fig.2 diagram is

$$A_F(P_1,P_2)=(2\pi)^4\frac{(-i)(ie)^2}{(P_1-p_1)^2}(\bar{u}(P_1)\gamma^\mu u(p_1))(\bar{u}(P_2)\gamma_\mu u(p_2))\,\delta^4(P_1+P_2-p_1-p_2)=$$

$$=(2\pi)^4M(P_1,P_2)\delta^4(P_1+P_2-p_1-p_2)$$

In computing $M(P_1,P_2)$, as we did for the electron-proton scattering , we average over the incoming spin polarizations and sum over the outgoing spin polarizations . Also, we study the electron-electron scattering in the reltivistic limit in which the electron mass m may be neglected compared to the momenta so we can nevertheless set m to 0 wherever possible.

By Fermi statistics the amplitude for the fig.3 diagram where the P_1 , P_2 electrons are interchanged is then $-A_F(P_2, P_1)$.

Thus the Feynman amplitude for the scattering process to order $O(e^2)$ is

$A_F(P_1,P_2)-A_F(P_2,P_1)=(2\pi)^4 M\,\delta^4(P_1+P_2-p_1-p_2)$ with

$M=M(P_1,P_2)-M(P_2,P_1)$.

Squaring the $|M|$ to compute cross sections we obtain

$|M|^2=|M(P_1,P_2)|^2+|M(P_2,P_1)|^2-2\Re(M^*(P_1,P_2)M(P_2,P_1))$.

Using the computations from electron-proton scattering, neglecting m when compared to the momenta , we will have :

$$|M(P_1,P_2)|^2+|M(P_2,P_1)|^2=\frac{e^4}{2m^4}\left(\frac{(P_1p_2)(P_2p_1)+(P_1P_2)(p_1p_2)}{((P_1-p_1)^2)^2}+\right.$$
$$\left.+\frac{(P_2p_2)(P_1p_1)+(P_1P_2)(p_1p_2)}{((P_2-p_1)^2)^2}\right)$$

$$2\Re(M^*(P_1,P_2)M(P_2,P_1))=\frac{e^4}{64m^4}\frac{1}{(P_1-p_1)^2(P_2-p_1)^2}\left(\mathrm{tr}(\not p_1\gamma^\mu\not P_1\gamma^\nu\not p_2\gamma_\mu\not P_2\gamma_\nu)+\right.$$
$$\left.+\mathrm{tr}(\not P_1\gamma^\mu\not p_1\gamma^\nu\not P_2\gamma_\mu\not p_2\gamma_\nu)\right)$$.

Using the (1) identities and the identities

$\gamma^\mu\not p\gamma_\mu=-2\not p$, $\gamma^\mu\not p\not q\gamma_\mu=4\not p\not q$, $\gamma^\mu\not p\not q\not r\gamma_\mu=-2\not r\not q\not p$ (2) after calculus we derive:

$\mathrm{tr}(\not p_1\gamma^\mu\not P_1\gamma^\nu\not p_2\gamma_\mu\not P_2\gamma_\nu)=-32(p_1p_2)(P_1P_2)$.

Therefore we obtain :

$$|M|^2=\frac{e^4}{2m^4}\left(\frac{(P_1p_2)(P_2p_1)+(P_1P_2)(p_1p_2)}{((P_1-p_1)^2)^2}+\frac{(P_2p_2)(P_1p_1)+(P_1P_2)(p_1p_2)}{((P_2-p_1)^2)^2}+\right.$$
$$\left.+\frac{2(p_1p_2)(P_1P_2)}{(P_1-p_1)^2(P_2-p_1)^2}\right)$$

In the relativistic limit, in the center of mass frame we have:

$p_1=E(1,0,0,1)$, $p_2=E(1,0,0,-1)$, $E\vec v_1=\vec p_1$, $E\vec v_2=\vec p_2$,

$P_1=E(1,\sin\theta,0,\cos\theta)$, $P_2=E(1,-\sin\theta,0,-\cos\theta)$

According to calculations we made in Chap. Canonical quantization of a scalar field and Chap. Feynman amplitudes and lattice gauge theory we obtain a differential cross section given by

$$d\sigma=\frac{1}{2}\frac{16m^4}{(2\pi)^2}\frac{1}{4E^2}\frac{1}{8(2E)^2}(2E)^2|M|^2d\Omega=\frac{m^4}{(2\pi)^2E^2}2|M|^2d\Omega$$.

After some calculus we find out that :

$2|M|^2=\frac{e^4}{4m^4}f(\theta)$ with $f(\theta)=32\left(\frac{1}{\cos^4(\theta/2)}+\frac{1}{\sin^4(\theta/2)}+1\right)$ and so

$\frac{d\sigma}{d\Omega}=\frac{\alpha^2}{E^2}f(\theta)$ (*) where $\alpha=\frac{e^2}{4\pi}$ is the fine structure constant,

The (*) relation can be used for experimental determination of the fine structure constant.

Photon-electron scattering (Compton scattering)

for the scattering of a photon carrying four-momentum *k* on an electron carrying four-momentum *p* with *k'* outgoing photon four-momentum and *p'* outgoing elctron four-momentum we have to consider to order e^2 two Feynman diagrams shown in fig.4 , fig.5 , since the electron can either absorb the *k* photon first or emit the *k'* photon first. (The electron comes along, absorbs and then emits a photon or emits and the absorbs a photon and continues its way.)

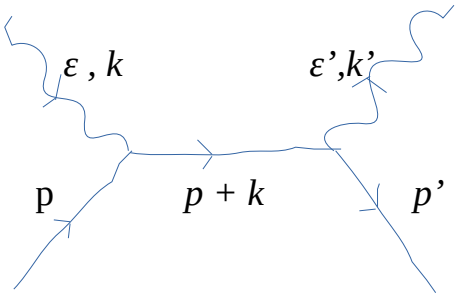


fig.4

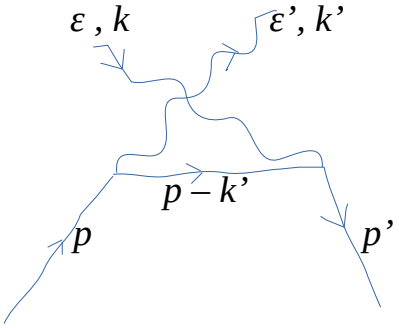


fig.5

ε and ε' are the polarization four-vectors of the *k* respective *k'* photon. We choose the transverse gauge in which in one frame with vers $\vec{k}=(1,0,0)$ we have $\varepsilon\in\{(0,0,1,0),(0,0,0,1)\}$ and the same is valid for ε' and k' . (see Chap. Quantization of an electromagnetic field and Chap. Feynman amplitudes and lattice gauge theory).

In a rest frame of the incoming electron we have $p = (m, 0 , 0, 0)$ and $\varepsilon p = 0$ and so in any frame we will have $\varepsilon k=\varepsilon p=\varepsilon' p=0=\varepsilon' k'=0$, $\varepsilon^2=\varepsilon'^2=-1$ (3)

The Feynman amplitude corresponding to the fig.4 diagram is

$$A(\varepsilon',k',\varepsilon,k)=(2\pi)^4(ie)^2\bar{u}(p')\not{\varepsilon}'\frac{i}{\not{p}+\not{k}-m}\not{\varepsilon}u(p)\delta^4(p+k-p'-k')=$$

$$=(2\pi)^4 M(\varepsilon,k',\varepsilon,k)\delta^4(p+k-p'-k') .$$

The Feynman amplitude corresponding to the fig.5 diagram is

$$A(\varepsilon,-k,\varepsilon',-k')=(2\pi)^4 M(\varepsilon,-k,\varepsilon',-k')\delta^4(p+k-p'-k') .$$

The total Feynman amplitude is

$$A=A(\varepsilon',k',\varepsilon,k)+A(\varepsilon,-k,\varepsilon',-k')=(2\pi)^4 M\,\delta^4(p+k-p'-k') .$$

We have $\not{p}u(p)=mu(p)$ and since $\varepsilon p=\varepsilon k=0$ we obtain

$$(\not{p}+\not{k}+m)\not{\varepsilon}u(p)=\not{\varepsilon}(-\not{p}-\not{k}+m)u(p)=-\not{\varepsilon}\not{k}u(p)$$

The electrons and the photons are obviously on mass shell having $p^2 = m^2$, $k^2 = 0$ and so we will have

$$M(\varepsilon',k',\varepsilon,k)=ie^2\bar{u}(p')\frac{\not\varepsilon'\not\varepsilon\not k}{2pk}u(p) \quad ,$$

$$M(\varepsilon,-k,\varepsilon',-k')=ie^2\bar{u}(p')\frac{\not\varepsilon\not\varepsilon'\not k'}{2pk'}u(p) \quad .$$

The squared total absolute Feynman amplitude , after we average over incoming spin polarizations and sum over outgoing spin polarizations of the electrons will be given by

$$|M|^2=\frac{1}{(8m^2)}\left(\frac{e^4\,\mathrm{tr}((\not p'+m)\not\varepsilon'\not\varepsilon\not k(\not p+m)\not k\not\varepsilon\not\varepsilon')}{(2pk)^2}+\frac{e^4\,\mathrm{tr}((\not p'+m)\not\varepsilon\not\varepsilon'\not k'(\not p+m)\not k'\not\varepsilon'\not\varepsilon)}{(2pk')}+\right.$$

$$\left.+\frac{e^4}{(2pk)(2pk')}(\mathrm{tr}((\not p'+m)\not\varepsilon'\not\varepsilon\not k(\not p+m)\not k'\not\varepsilon'\not\varepsilon)+\mathrm{tr}((\not p'+m)\not\varepsilon\not\varepsilon'\not k'(\not p+m)\not k\not\varepsilon\not\varepsilon'))\right) .$$

In evaluating the first trace above we keep in mind that the trace of an odd number product of gamma matrices vanishes , so the m term vanishes and also the m^2 term vanishes since it contains $k^2 = 0$. Considering relations (1) and (3) and the identity $\not a\not b+\not b\not a=2ab$ we can compute the remaining term and obtain

$\mathrm{tr}(\not p'\not\varepsilon'\not\varepsilon\not k\not p\not k\not\varepsilon\not\varepsilon')=8k\,p(2(k\varepsilon')^2+pk')$.

Let $T=\mathrm{tr}((\not p'+m)\not\varepsilon'\not\varepsilon\not k(\not p+m)\not k'\not\varepsilon'\not\varepsilon)$.

We take as allowed $p'=p+k-p$ and obtain $T=P+Q_1+Q_2$ where

$P=\mathrm{tr}(\not p\not\varepsilon'\not\varepsilon\not k\not p\not k'\not\varepsilon'\not\varepsilon)+m^2\,\mathrm{tr}(\not\varepsilon'\not\varepsilon\not k\not k'\not\varepsilon'\not\varepsilon)$

$Q_1=\mathrm{tr}(\not k\not\varepsilon'\not\varepsilon\not k\not p\not k'\not\varepsilon'\not\varepsilon)$

$Q_2=-\mathrm{tr}(\not k'\not\varepsilon'\not\varepsilon\not k\not p\not k'\not\varepsilon'\not\varepsilon)$.

For the first term in P we let $\not p$ pass the $\not\varepsilon$' and $\not\varepsilon$(since $p\,\varepsilon' = p\,\varepsilon = 0$) to find out the combination $\not p\not k\not p = 2\,k\,p - m^2\not k$.

The m^2 term gives a contribution that cancels the second term in P leaving us with

$P=8(pk)(pk')(2(\varepsilon'\varepsilon)^2-1)$,

$Q_1=-8(k\varepsilon')^2(pk')$,

$Q_2=8(k'\varepsilon)^2(pk)$.

Putting it all together we obtain

$$|M|^2=\frac{e^4}{4m^2}\left(\frac{pk'}{pk}+\frac{pk}{pk'}+4(\varepsilon'\varepsilon)^2-2\right) .$$

Writing $pk'=m\omega'$, $pk=m\omega$ where ω,ω' are the pulsations of the photons in the incoming electron rest frame we have

$$|M|^2=\frac{e^4}{4m^2}\left(\frac{\omega}{\omega'}+\frac{\omega'}{\omega}+4(\varepsilon'\varepsilon)^2-2\right) .$$

According to Chap. Feynman amplitudes and lattice gauge theory and Chap. Canonical quantization of a scalar field the differential cross section in the incoming electron rest frame is given by :

$d\sigma=\frac{m}{(2\pi)^2}\frac{1}{2\omega}\frac{d^3\vec{k}'}{2\omega'}\frac{d^3\vec{p}'}{E_{p'}}|M|^2\delta^4(p'+k'-p-k)$ with $E_{p'}=\sqrt{\vec{p}'^2+m^2}$,
$\omega'=\|\vec{k}'\|$, $p=(m,0,0,0)$.
As in Chap. Canonical quantization of a scalar field we can write
$f(E_{p'},\vec{p}')\frac{d^3\vec{p}'}{E_{p'}}=2\theta(p'^0)\delta(p'^2-m^2)f(p')d^4p'$ with θ the Heaviside function.
We have $p'^2-m^2=(p+k-k')^2-m^2=2p(k-k')-2kk'=$
$=2m(\omega-\omega')-2\omega\omega'(1-\cos\theta)$ where θ is the scattering angle of the photon.
Thus $\omega'=\frac{\omega}{1+\frac{2\omega}{m}\sin^2\frac{\theta}{2}}$ giving the frequency shift of the Compton effect.

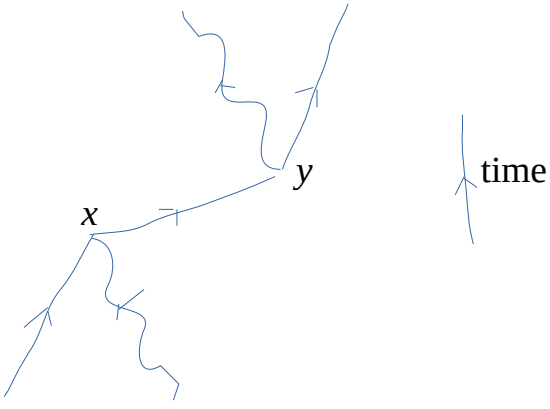
Using the evident relation $\int f(\omega')\delta(a\omega'-b)d\omega'=\frac{1}{a}f(\frac{b}{a})$ it follows:

$$d\sigma=\frac{1}{2\omega}\frac{m}{(2\pi)^2}\frac{\omega'^2}{\omega'}\frac{2}{2m+4\omega\sin^2\frac{\theta}{2}}|M|^2d\Omega$$

$\frac{d\sigma}{d\Omega}=\frac{\alpha^2}{4m^2}\left(\frac{\omega'}{\omega}\right)^2\left(\frac{\omega'}{\omega}+\frac{\omega}{\omega'}+4(\varepsilon'\varepsilon)^2-2\right)$ the Klein-Nishina formula with

$\omega'=\frac{\omega}{1+\frac{2\omega}{m}\sin^2\frac{\theta}{2}}$, $\alpha=\frac{e^2}{4\pi}$, $d\Omega=\sin\theta d\theta d\varphi$, $(\theta,\varphi)\in(0,\pi)\times(0,2\pi)$,
θ the photon scattering angle.

Compton scattering provides a physical argument that special relativity and quantum mechanics mandate antimatter. Consider the fig. 4 scattering diagram as



The electron is hit by the photon at the point *x* in space-time, propagates to the point *y* in space-time and emits a photon. We assumed implicitely that $y^0 - x^0 > 0$.

But according to special relativity another observer moving by (along the 1-direction say) would register the time difference
$y'^0-x'^0=(y^0-x^0)\cosh\varphi-(y^1-x^1)\sinh\varphi$ which could be negative for large enough boost parameter φ , provided that $y^1-x^1>y^0-x^0$ that is if the separation between the two space-time points *x* and *y* were spacelike . Then this observer would see the field disturbance propagating from *y* to *x* . Since we see negative charge propagating from *x* to *y* the other observer must see positive electric charge propagating from *y* to *x*. Without special relativity we simple write down the Schroedinger equation for the electron. Special relativity allows different observers to see different time ordering and hence opposite charges flowing toward the future .

Scattering of two spinless charged particles

A spinless charged particle field has according to Chap. Canonical quantization of a scalar field a Lagrangian density
$\mathscr{L}(\varphi,\partial\varphi)=(\partial\varphi)^+(\partial\varphi)-m^2\varphi^+\varphi$ with $\varphi=\varphi(t,\vec{x})\in\mathbb{C}$ the complex scalar field and m the rest mass of the particle.
In presence of a electromagnetic field, the interaction Lagrangian density will be (replacing ∂_μ with $\partial_\mu+iqA_\mu(x)=D_\mu$ (4) with q the charge of the particle and $(A_\mu)_\mu$ the quantum electrodynamics four-potential of the electromagnetic field or the gauge field and ignoring the $O(q^2A^2)$ terms (see Chap. Lagrangian of electromagnetic field)):

$$\mathscr{L}(\varphi,\partial\varphi,A,\partial A)=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+(\partial\varphi)^+(\partial\varphi)-m^2\varphi^+\varphi-qJ^\mu A_\mu \qquad (5)$$

where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ and $J^\mu=i(\varphi^+(\partial^\mu\varphi)-(\partial^\mu\varphi)^+\varphi)$ is the conserved current.
According to the Hamiltonian of a charged particle in a eletromagnetic field we would have a Schroedinger equation
$i\partial_0\psi=\frac{1}{2m}(\vec{p}+q\vec{A})^2+qA_0$ which leads to the (4) option, since
$\hat{\vec{p}}=-i\nabla$, $iD_0\psi=\frac{1}{2m}(-iD_k)(-iD_k)\psi$.

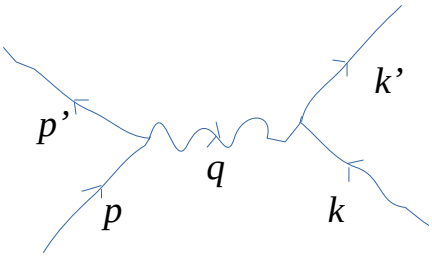
We can see that in applying the Feynman rules for the interaction vertices considering the (5) Lagrangian density, the coupling corresponding to a quantum electrodynamics $-qJ^\mu(x)A_\mu(x)$ interaction term is $iq(k+K)^\mu$ where k and K are the four-momenta of the incoming particle / outgoing antiparticle respective outgoing particle / incoming antiparticle.
For a quantum electrodynamics scattering of spinless particles with charges q_1 respective q_2 and incoming four-momenta *p* respective *k* , outgoing four-momenta *p'* respective *k'* the Feynman diagram in q_1q_2 order is the fig.6 diagram and according to Feynman rules we will have a Feynman amplitude

$$A=(2\pi)^4 M\,\delta^4(p+k-p'-k') \text{ with}$$

$$M=(iq_1)(iq_2)(-i)(p+p')^{\mu}\left(\eta_{\mu\nu}-(1-\xi)\frac{(p-p')_{\mu}(p-p')_{\nu}}{(p-p')^2}\right)\frac{1}{(p-p')^2}(k+k')^{\nu}\ .$$

Since the particles are considered on mass shell we have $(p + p')\,(p - p') = m_1^2 - m_1^2 = 0$ (with m_1 , m_2 the rest masses of the particles) and so we can drop the R_ξ -gauge dependent term from the photon propagator obtaining :

$$M=iq_1q_2\frac{(p+p')(k+k')}{(p-p')^2}\ .$$



$q = p - p'$

fig.6

In the center of mass frame we have

$$\vec{p}+\vec{k}=\vec{p}'+\vec{k}'=\vec{0}\ ,\ \|\vec{p}\|=\|\vec{p}'\|=r=\frac{1}{2E}((E^2-(m_1+m_2)^2)(E^2-(m_1-m_2)^2))^{1/2}\ ,$$

$$p_0=p'_0=\sqrt{r^2+m_1^2}\ ,\ k_0=k'_0=\sqrt{r^2+m_2^2}\ ,\ E=p_0+k_0$$

and the differential cross section of the scattering process is, according to Chap. Canonical quantization of a scalar field :

$$d\sigma=\frac{1}{|v_1-v_2|}\frac{1}{4p_0k_0}\frac{1}{(2\pi)^2}\frac{1}{8E^2}((E^2-(m_1+m_2)^2)(E^2-(m_1-m_2)^2))^{1/2}|M|^2\,d\Omega$$

where $d\Omega=\sin\theta d\theta d\varphi$ is the $(\theta,\varphi)\in(0,\pi)\times(0,2\pi)$ variables differential solid scattering angle, with θ the angle between the $\vec{p}'$ and $\vec{p}$ directions .

In the non-relativistic approximation we have

$$r\ll m_{1,2}\ ,\ p_0=p'_0\approx m_1+\frac{r^2}{2m_1}\ ,\ k_0=k'_0\approx m_2+\frac{r^2}{2m_2}\ ,\ v_1=\frac{r}{m_1}\ ,\ v_2=-\frac{r}{m_2}$$

$$(p-p')^2\approx 2m_1^2-2\left(m_1+\frac{r^2}{2m_1}\right)^2+2r^2\cos\theta\approx -4r^2\sin^2\frac{\theta}{2}\ ,$$

$(p+p')(k+k')=(p+p')(2k+p-p')=2k(p+p')\approx 4m_1m_2$ and so in the

non-relativistic case we obtain :

$$\frac{d\sigma}{d\Omega}=\frac{1}{r}\frac{m_1 m_2}{m_1+m_2}\frac{1}{4m_1 m_2}\frac{1}{(2\pi)^2}\frac{1}{8(m_1+m_2)^2}2r(m_1+m_2)\frac{16m_1^2 m_2^2}{16r^4\sin^4\frac{\theta}{2}}(q_1 q_2)^2 ,$$

$$\frac{d\sigma}{d\Omega}=\left(\frac{\alpha}{r^2}\frac{m_1 m_2}{2(m_1+m_2)}\right)^2\frac{1}{\sin^4\frac{\theta}{2}} \text{ with } \alpha=\frac{q_1 q_2}{4\pi} \text{ and for } m_1 \ll m_2 , r=m_1 v$$

and for $m_1 \ll m_2$, $r=m_1 v$ we recognize the Rutherford formula for Coulomb scattering : $\frac{d\sigma}{d\Omega}=\left(\frac{\alpha}{2m_1 v^2}\right)^2\frac{1}{\sin^4\frac{\theta}{2}}$

(see I. Inţa , S. Dumitru Complenente de fizică , Editura tehnică , Bucureşti)

In the relativistic approximation of $m_{1,2} \ll r$ we will have:

$$p_0=p'_0=k_0=k'_0\approx r , E=2r , v_1=-v_2\approx 1 ,$$

$$(p-p')^2\approx -4r^2\sin^2\frac{\theta}{2} ,$$

$$(p+p')(k+k')=2k(p+p')\approx 4r^2\cos^2\frac{\theta}{2} ,$$

$$\frac{d\sigma}{d\Omega}=\frac{1}{2}\frac{1}{4r^2}\frac{1}{(2\pi)^2}\frac{1}{32r^2}4r^2\frac{16r^4\left(1+\cos^2\frac{\theta}{2}\right)^2}{16r^4\sin^4\frac{\theta}{2}}(q_1 q_2)^2 ,$$

$$\frac{d\sigma}{d\Omega}=\left(\frac{\alpha}{4E}\right)^2\left(\frac{2}{\sin^2\frac{\theta}{2}}-1\right)^2 .$$

At small scattering angles the differential cross section in the relativistic approximation is near to the Rutherford Coulomb scattering formula differential cross section.

Scattering of electromagnetic waves on electrically neutral spinless particle

In Rayleigh scattering (see Chap. Electric dipole … Dipole radiation) light scatters on air molecules which can be considered spinless neutral particles.

In an effective field theory we can describe the air molecules by a scalar field Φ with a lagrangian density

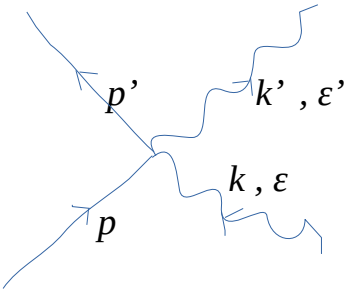
$$\mathscr{L}=\frac{1}{2}\left((\partial\Phi)^2-m^2\Phi^2\right) .$$

Since Φ is neutral the lowest dimension gauge invariant interaction term that can be added to $\mathscr{L}$ is $\frac{1}{2M^2}\Phi^2 F_{\mu\nu}F^{\mu\nu}$ with M some mass scale.

The two powers of derivative in $F_{\mu\nu}F^{\mu\nu}$ (with $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, $(A_\mu)_\mu$ the electromagnetic four-potential field) lead to the proportionality $\boldsymbol{M}\propto\omega^2$ for the scattering of photons on Φ particles amplitude. Thus the scattering cross section varies like $\sigma(\omega)\propto\omega^4$ where ω is the pulsation of the electromagnetic wave.

As in Chap. Electric dipole … Dipole radiation , we have the proportionality with the fourth power of frequency : red light scatters less than blue light on air molecules and hence the sky is blue.

Indeed we have a Feynman diagram



The coupling corresponding to the considered interaction term is

$\frac{i}{M^2}(\eta^{\mu\delta}(kk')-k'^{\mu}k^{\delta})$

and the Feynman amplitude according to feynman rules is

$A=(2\pi)^4\frac{i}{M^2}((\varepsilon\varepsilon')(kk')-(\varepsilon k')(\varepsilon' k))$ where ε respective ε' are the incoming and outgoing photon polarization four-vectors.

We write $A=(2\pi)^4\boldsymbol{M}\,\delta^4(p+k-p'-k')$ and considering for the photon a hypothetical mass μ we have for the photons three polarization vectors $\varepsilon(k,s)$ for incoming photon respective $\varepsilon'(k',s)$ for outgoing photon with $s=\overline{1,3}$, $\varepsilon k=\varepsilon' k'=0$,

$\sum_{s=1}^{3}\varepsilon_\lambda(k,s)\,\varepsilon_\nu(k,s)=(-\eta_{\lambda\nu}+\frac{k_\lambda k_\nu}{\mu^2})$, $\sum_{s=1}^{3}\varepsilon'_\lambda(k',s)\,\varepsilon'_\nu(k',s)=(-\eta_{\lambda\nu}+\frac{k'_\lambda k'_\nu}{\mu^2})$

(see Chap. Feynman amplitudes and lattice gaug theory).

Taking $\mu\to 0$ averaging over incoming photon polarizations and summing over outgoing photon polarizations aftersome calculus the terms with μ^2 at the denominator cancel out and we get

$|\boldsymbol{M}|^2=\frac{(kk')^2}{M^4}=4\frac{(\omega\omega')^2}{M^4}\sin^4(\theta/2)$ where $(k_\lambda)_\lambda=(\omega,\vec{k})$, $(k'_\lambda)_\lambda=(\omega',\vec{k}')$, $\|\vec{k}\|=\omega$, $\|\vec{k}'\|=\omega'$ and θ is the angle between $\vec{k}$ and $\vec{k}'$.

Computing as for photon-electron scattering in the spinless particle rest frame we obtain $\omega'=\frac{\omega}{1+2\frac{\omega}{m}\sin^2(\frac{\theta}{2})}$ and a differential cross section given by

$$d\sigma=\frac{1}{(2\pi)^2}\frac{1}{2m}\frac{1}{2\omega}\frac{1}{2\omega'}\frac{4(\omega\omega')^2}{M^4}\sin^4(\frac{\theta}{2})d^3\vec{k}'\,\delta^4(p+k-p'-k')\frac{d^3\vec{p}'}{2\omega_{p'}}=$$

$$=\frac{1}{(2\pi)^2}\frac{1}{2m}\frac{\omega\omega'^3}{M^4}\sin^4(\frac{\theta}{2})\,\delta(\omega'(2m+4\omega\sin^2(\frac{\theta}{2}))-2m\omega)\,d\omega'\,d\Omega \qquad \text{and so}$$

$$\frac{d\sigma}{d\Omega}=\frac{1}{(4\pi)^2}\frac{1}{m^2}\frac{\omega^4}{M^4}\left(\frac{\sin(\theta/2)}{1+2\frac{\omega}{m}\sin(\theta/2)}\right)^4=\frac{1}{(4\pi)^2}\frac{1}{m^2}\frac{1}{M^4}\omega'^4\sin^4(\theta/2)\,.$$

(see Chap. Quantization of a scalar field … cross section and Feynman amplitudes and lattice gauge theory).

The proportionality with the fourth power of frequency is therefore confirmed. (in the visible spectrum we have $\omega\ll m$, $\omega\approx\omega'$).

34. Anomalous magnetic moment of the electron

Anomalous magnetic moment of the electron

In Chap. Two component Dirac equation we derived for the electron in presence of a electromagnetic four-potential $(A_\mu)_\mu=(A_0,\vec{A})(t,\vec{x})$, $x=(x^\alpha)_\alpha=(t,\vec{x})$, $A_0=A_3=0$, $A_1=\frac{1}{2}Bx^2$, $A_2=-\frac{1}{2}Bx^1$, $\vec{B}=-\nabla\times\vec{A}=(0,0,B)$ -the magnetic induction field, a Hamiltonian operator $\hat{H}=-\frac{1}{2m}\nabla^2-\frac{e}{2m}\vec{B}\cdot(g_L\hat{\vec{L}}+g_S\vec{S})$ where $\vec{L}=\vec{x}\times\vec{p}$, $\vec{S}=\frac{1}{2}\hbar\vec{\sigma}$, $\hat{\vec{p}}$ -the momentum operator, $\vec{\sigma}=(\sigma_i)_{i=\overline{1,3}}$ -the Pauli matrices, the gyromagnetic ratios $g_S=2$, $g_L=1$, the electron charge is $e=-|e|$ and m is the rest mass of the electron.

Considering the quantum field theory for the electron with Lagrangian density

$$\mathscr{L}(\psi,\partial\psi)=\overline{\psi}(i\gamma^\mu\partial_\mu-m)\psi-eJ^\mu A_\mu \qquad (1)$$

with $\psi=(\psi_\mu(t,\vec{x}))_\mu$ a Dirac spinor field, $J^\mu=\overline{\psi}\gamma^\mu\psi$ (see Chap. Dirac Lagrangian) we expect that g_L,g_S need corrections if we take in consideration quantum fluctuations of the electron field.

With $\hat{\psi}=\hat{\psi}(t,\vec{x})$ the quantum field operator function acting on a quantum field states Hilbert space having the vacuum state $|0\rangle$ we have the Hamiltonian operator

$$\hat{H}=\int d^3\vec{x}\left(\frac{\partial\mathscr{L}}{\partial(\partial_0\psi)}\partial_0\psi-\mathscr{L}\right)=\int d^3\vec{x}(\hat{\overline{\psi}}(m-i\gamma^k\partial_k)\hat{\psi}+e\hat{J}^\mu A_\mu) \qquad (2)$$

which can be considered as a field expectation value operator

$\hat{H}=\int d^3\vec{x}\,\hat{\psi}^+(m\gamma^0-i\gamma^0\gamma^k\partial_k+e\gamma^0\gamma^\mu A_\mu)\hat{\psi}$,

where as usual we denote with greek letters indexes from 0 to 3 and with latin letters indexes from 1 to 3 , $\gamma^0=\begin{pmatrix}\boldsymbol{I} & 0\\ 0 & \boldsymbol{I}\end{pmatrix}$, $\gamma^k=\begin{pmatrix}0 & \sigma_k\\ -\sigma_k & 0\end{pmatrix}$ are the gamma matrices and

$m\gamma^0-i\gamma^0\gamma^k\partial_k+e\gamma^0\gamma^\mu A_\mu$ is an operator acting on the Hilbert space of the $\psi=(\psi_\mu(.,\vec{x}))_\mu$ functions with scalar product $\langle\psi,\varphi\rangle=\int\psi^+\varphi d^3\vec{x}$.

The matrix element of $\hat{H}$ under a non-relativistic momentum transfer corresponding to $q=p'-p$, $q=(q_\nu)_\nu$ from a four-momentum p and spin polarization s field state $|p,s\rangle$ to a four-momentum p' and spin polarization s' field state $|p',s'\rangle$ where we obviously take $p^2=p'^2=m^2$ since the the electron states are on mass shell is:

$$\langle p',s'|\hat{H}|p,s\rangle=\int\langle p',s'|\hat{\psi}^+\sqrt{\boldsymbol{I}(m^2-\nabla^2)}\,\hat{\psi}|p,s\rangle d^3\vec{x}+$$

$$+e\int\langle p',s'|\hat{J}^\mu A_\mu|p,s\rangle d^3\vec{x}\approx\int\langle p',s'|\hat{\psi}^+\left(m\gamma^0-\frac{\nabla^2}{2m}\right)\hat{\psi}|p,s\rangle+$$

$$+e\int\langle p',s'|\hat{J}^\mu A_\mu|p,s\rangle d^3\vec{x} \ .$$

(we can take $m\gamma^0 - i\gamma^0\gamma^k\partial_k = \sqrt{\boldsymbol{I}(m^2-\nabla^2)} \approx m\gamma^0 - \frac{\nabla^2}{2m}$ because $m\gamma^0 - i\gamma^0\gamma^k\partial_k$ is hermitian and we can consider the analytical $\sqrt{\ }$ function of the operator $(m\gamma^0 - i\gamma^0\gamma^k\partial_k)^2 = \boldsymbol{I}(m^2-\nabla^2)$ as its finite dimensional approximation for the non-relativistic case $\vec{p}^2 \ll m^2$).

As we exposed in Chap. Dirac equation. Quantization of a Dirac field, we have:

$$\hat{\psi}_\alpha(t,\vec{x}) = \int \frac{d^3\vec{p}}{\sqrt{(2\pi)^3 E_p/m}} \sum_s \left(b(p,s) u_\alpha(p,s) \exp(-ipx) + \right.$$

$$\left. + d^+(p,s) v_\alpha(p,s) \exp(ipx) \right) \quad \text{with } E_p = \sqrt{\vec{p}^2 + m^2} \ , \ |p,s\rangle = b^+(p,s)|0\rangle \sqrt{\frac{(2\pi)^3}{V}} \quad (2')$$

$b^+(p,s), d^+(p,s), b(p,s), d(p,s)$ creation respective anihilation operators satisfying the usual anticommutation relations .

Taking $U = U(a,\Lambda)$ the unitary representation of the Poincare group $\{\mathbb{R}^4 \ni x \to \Lambda x + a \in \mathbb{R}^4 | \Lambda \in SO^+(3,1), a \in \mathbb{R}^4\}$ acting on the field states such that $U\hat{\psi}_\alpha(x)U^+ = \hat{\psi}_\alpha(\Lambda x + a)$, $U|0\rangle = |0\rangle$, as we derived in Chap. Spin statistics theorem we must have $U(a,\boldsymbol{I}) = \exp(i\hat{p}a)$ where $\hat{p}$ is the four-momentum operator acting on the field states, having $\hat{p}|p,s\rangle = p|p,s\rangle$.

Thus we will have:

$$\langle p',s'|\hat{J}^\mu(x)|p,s\rangle = \langle p',s'|U(x,\boldsymbol{I})\hat{J}^\mu(0)U^+(x,\boldsymbol{I})|p,s\rangle =$$

$$= \langle p',s'|\hat{J}^\mu(0)|p,s\rangle \exp(i(p'-p)x) \qquad (3) .$$

We consider the momentum transfer process in time interval (0,*T*) and field support volume V with a $|p,s\rangle$ incoming electron and a $|p',s'\rangle$ outgoing electron (on mass shell) , involving a virtual photon of four momentum $q = p' - p$ of an electromagnetic field whose four-potential $(A_\mu)_\mu$ appears in the (1) Lagrangian density expression as a space-time dependent coupling $-ie\gamma^\mu A_\mu(x)$.

The amplitude of all together possible Feynman diagrams for the process is then (see Chap. Feynman amplitudes and lattice gauge theory) :

$$\tilde{A} = V^{-1}(E_{p'}/m)^{1/2}(E_p/m)^{1/2}\bar{u}_\alpha(p',s')u_\beta(p,s)\exp(ip'_0 T)(-ie)\int d^4x\, d^3\vec{z}\, d^3\vec{y}$$

$$\exp(-i\vec{p}'\vec{z})\exp(i\vec{p}\vec{y})\langle 0|\hat{\psi}_\alpha(T,\vec{z})\hat{J}^\mu(x)A_\mu(x)\hat{\bar{\psi}}_\beta(0,\vec{y})|0\rangle =$$

$$= \int -ie\langle p',s'|\hat{J}^\mu(x)A_\mu(x)|p,s\rangle d^4x =$$

$$= -2\pi i e\,\delta(E_{p'} - E_p)\langle p',s'|\hat{J}^\mu(0)|p,s\rangle \int A_\mu(\vec{x})\exp(-i(\vec{p}'-\vec{p})\vec{x})d^3\vec{x} \qquad (4).$$

(For the last equality we considered as initial that the four-potential not depends on time.)

Notice that in the (4) evaluations, the field operator $\hat{\psi}$ is considered in the (1) Lagrangian density theory and no more satisfies (2') as in the non-selfinteracting free theory.

To calculate $\int \langle p',s'|\hat{J}^{\mu}(0)|p,s\rangle A_{\mu}(\vec{x})\exp(-i(\vec{p}'-\vec{p})\vec{x})d^3\vec{x}$ to order $O(\alpha)$ with $\alpha=\frac{e^2}{4\pi}$ we have to evaluate the process amplitude $\widetilde{A}$ in the (1) Lagrangian density field theory considering the amplitudes corresponding to the Feynman diagrams in fig. (a) , fig. (b) , fig. (c) , fig. (d) , fig. (e).

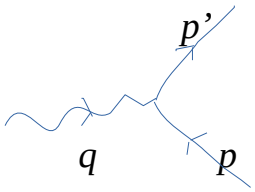


fig. (a)

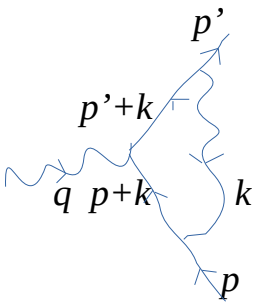


fig. (b)

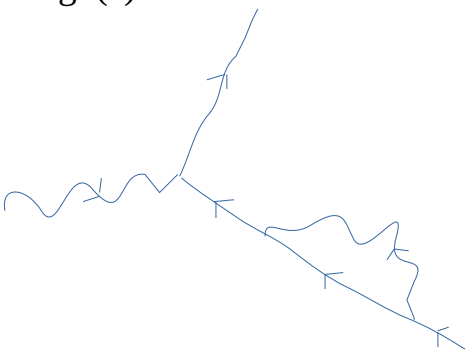


fig. (c)

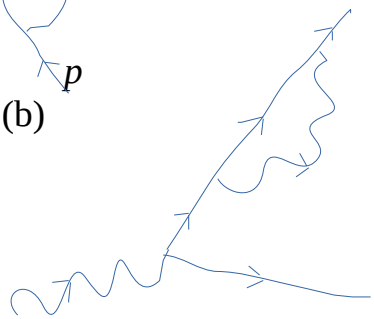


fig. (d)

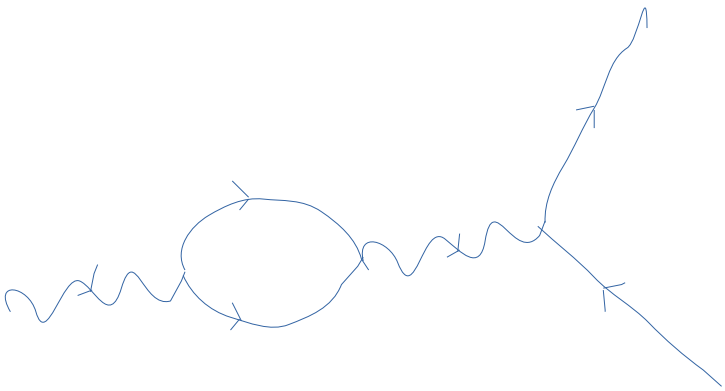


fig. (e)

From current conservation $\partial_{\mu}J^{\mu}=0$ and (3) follows
$q_{\nu}\langle p',s'|J^{\nu}(0)|p,s\rangle=0$ (5) for $q=p'-p$.
$(\langle p',s'|J^{\nu}(0)|p,s\rangle)_{\nu}$ being a Lorentz vector satisfying (5) , we will see that at first order in $\alpha=\frac{e^2}{4\pi}$ we have (5') :

$$\langle p',s'|\hat{J}^{\mu}(0)|p,s\rangle=\bar{u}(p',s')(\gamma^{\mu}F_1(q^2)+i\frac{\sigma^{\mu\nu}}{2m}q_{\nu}F_2(q^2))u(p,s)V^{-1}\left(\frac{E_p}{m}\right)^{-\frac{1}{2}}\left(\frac{E_{p'}}{m}\right)^{-\frac{1}{2}}$$

where F_1, F_2 are scalar functions and $\sigma^{\mu\nu}=\frac{i}{2}[\gamma^{\mu},\gamma^{\nu}]$.

According to Chap. Feynman amplitudes and lattice gauge theory the amplitude for any of the considered Feynman diagrams is given by:
$\widetilde{A}=V^{-1}(E_p/m)^{-1/2}(E_{p'}/m)^{-1/2}A_F$ where A_F is the Feynman amplitude computed following the Feynman rules and has usually the form
$A_F=(2\pi)^4\boldsymbol{M}\,\delta^4(p'-p-q)$. However, since the photon appears as a space dependent coupling of the Dirac field to itself in the interaction vertex term $-e\,\overline{\psi}\gamma^{\mu}\psi A_{\mu}$ we must replace the $(2\pi)^4\delta^4(p'-p-q)$ four-momentum balance factor for the photon with a incident external line interaction factor $\exp(i(p'-p)x)$ taking also for this vertex the coupling $-ie\,\gamma^{\mu}A_{\mu}(x)$ integrating over x.
Except for fig. (b) , all the considered Feynman amplitudes are clearly proportional to $\bar{u}(p',s')\gamma^{\mu}u(p,s)$ and thus contribute to $F_1(q^2)$.
The fig. (b) , fig. (c) , fig. (d) , fig. (e) diagrams amplitudes are of order *O* (e^3) . Since the fig. (a) diagram amplitude is of order *O* (e) , the $F_1(q^2)$ factor is of order $O(e^0)$ and is defined to order *O* (e^2) by the Feynman diagram fig. (a) .
The amplitude for the fig. (a) diagram is according to Feynman rules:

$$\widetilde{A}_1=V^{-1}\left(\frac{E_p}{m}\right)^{-\frac{1}{2}}\left(\frac{E_{p'}}{m}\right)^{-\frac{1}{2}}2\pi\delta(E_{p'}-E_p)(-ie)\int\exp(-i(\vec{p}'-\vec{p})\vec{x})A_{\mu}(\vec{x})\ \bar{u}(p',s')\gamma^{\mu}u(p,s)d^3\vec{x}\ . \quad (6)$$

Comparing now (4) with (5') we must take
$F_1(q^2)=1$ such that $e\,F_1(q^2)$ is the experimentally observed electric charge.
(Except for the fig. (b) diagram all considered diagrams can be reduced to the only diagram fig . (a) by electron mass renormalization and electron charge renormalization acording to Chap. ... Quantum electrodynamics and Chap. ...Electric charge renormalization . Thus with the renormalization of the photon and electron propagators the fig. (a) , fig. (c) , fig. (d) , fig. (e) diagrams become equivalent to a single fig. (a) diagram with mass and charge renormalized.)
According to Feynman rules, the fig. (b) diagram amplitude is

$$\widetilde{A}_2=2\pi\delta(E_{p'}-E_p)(-ie)V^{-1}\left(\frac{E_p}{m}\right)^{-\frac{1}{2}}\left(\frac{E_{p'}}{m}\right)^{-\frac{1}{2}}\int\exp(-i(\vec{p}'-\vec{p})\vec{x})A_{\mu}(\vec{x})\ \bar{u}(p',s')\Gamma^{\mu}u(p,s)d^3\vec{x}\ . \quad (6')$$

where $\Gamma^{\mu}=\int\frac{d^4k}{(2\pi)^4}\frac{(-ie^2)}{k^2+i\varepsilon}\gamma^{\nu}\frac{1}{\not{p}'+\not{k}-m}\gamma^{\mu}\frac{1}{\not{p}+\not{k}-m}\gamma_{\nu}$.
(with $\not{p}=\gamma^{\mu}p_{\mu}$)

We can see that if we will have any kind of momentum transfer with the given electromagnetic field, we must have $E_p = E_{p'}$ and considering (4) , (6) , (6') , (5')

(since we can take in $O(\alpha^2)$ approximation, with mass and charge renormalized to their experimental measured values, $\widetilde{A}=\widetilde{A}_1+\widetilde{A}_2$) , we will have:

$$\langle p',s'|\hat{J}^{\mu}(0)|p,s\rangle=V^{-1}\left(\frac{E_p}{m}\right)^{-\frac{1}{2}}\left(\frac{E_{p'}}{m}\right)^{-\frac{1}{2}}\bar{u}(p',s')(\gamma^{\mu}+\Gamma^{\mu})u(p,s)= \quad (6'')$$
$$=V^{-1}\left(\frac{E_p}{m}\right)^{-\frac{1}{2}}\left(\frac{E_{p'}}{m}\right)^{-\frac{1}{2}}\bar{u}(p',s')(\gamma^{\mu}+\frac{i\sigma^{\mu\nu}}{2m}q_{\nu}F_2(q^2))u(p,s).$$

Using the identities $\bar{u}(p')\not{p}'=m\bar{u}(p')$, $\not{p}u(p)=mu(p)$
and $\bar{u}(p')(\not{p}'\gamma^{\mu}+\gamma^{\mu}\not{p})u(p)=\bar{u}(p')((p'+p)^{\mu}+i\sigma^{\mu\nu}q_{\nu})u(p)$
we derive the Gordon decomposition :

$$\bar{u}(p')\gamma^{\mu}u(p)=\bar{u}(p')\left(\frac{(p'+p)^{\mu}}{2m}+\frac{i\sigma^{\mu\nu}}{2m}q_{\nu}\right)u(p) \qquad (7)$$

Therefore taking $R^{\mu}=\frac{(p'+p)^{\mu}}{2m}F_1(q^2)+\frac{i\sigma^{\mu\nu}}{2m}q_{\nu}(F_1(q^2)+F_2(q^2))$,
with $\hat{\psi}$ from the free Dirac theory we have to order $O(\alpha^2)$ approximation that

$$\langle p',s'|\hat{J}^{\mu}(0)|p,s\rangle=\bar{u}(p',s')R^{\mu}u(p,s)V^{-1}\left(\frac{E_p}{m}\right)^{-\frac{1}{2}}\left(\frac{E_{p'}}{m}\right)^{-\frac{1}{2}}=$$
$$=\langle p',s'|\hat{\bar{\psi}}(0)R^{\mu}\hat{\psi}(0)|p,s\rangle \ .$$

Because $\int\langle p',s'|\hat{\bar{\psi}}(0)q^{\mu}\hat{\psi}(0)|p,s\rangle\exp(iqx)A_{\mu}(x)d^4x=$
$=i\int\langle p',s'|\hat{\bar{\psi}}(0)\hat{\psi}(0)|p,s\rangle\exp(iqx)\partial^{\mu}A_{\mu}(x)d^4x=0$ (since $\partial^{\mu}A_{\mu}=0$)
we derive $\int\langle p',s'|\hat{\bar{\psi}}(0)\frac{(p'+p)^{\mu}}{2m}F_1(q^2)\hat{\psi}(0)|p,s\rangle\exp(iqx)A_{\mu}(x)d^4x=$

$$=\int\langle p',s'|\hat{\bar{\psi}}(x)\frac{2p^{\mu}}{2m}\hat{\psi}(x)|p,s\rangle A_{\mu}(x)d^4x=$$
$$=\frac{1}{2m}\int\langle p',s'|\hat{\bar{\psi}}(x)2iA_{\mu}\partial^{\mu}\hat{\psi}(x)|p,s\rangle d^4x \ .$$

For the considered electromagnetic field we have

$$2iA_{\mu}\partial^{\mu}=-Bi(x^2\partial_1-x^1\partial_2)=-\vec{B}\cdot\hat{\vec{L}} \ .$$

We have also :

$$\int\langle p',s'|\hat{\bar{\psi}}(0)\frac{i\sigma^{\mu\nu}}{2m}q_{\nu}\hat{\psi}(0)|p,s\rangle\exp(iqx)A_{\mu}(x)d^4x=$$
$$=-\int\langle p',s'|\hat{\bar{\psi}}(0)\frac{\sigma^{\mu\nu}}{2m}\hat{\psi}(0)|p,s\rangle\exp(iqx)A_{\mu,\nu}(x)d^4x=$$
$$=-\int\langle p',s'|\hat{\bar{\psi}}(x)\frac{\sigma^{12}B}{2m}\hat{\psi}(x)|p,s\rangle d^4x \ .$$

Hence acting on the larger, dominant component of $\psi=\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}$ which is ψ_A in the Dirac basis (see Chap. Two component Dirac equation) we have for the field expectation value operator $\hat{H}$ the relation

$$\langle p',s'|\hat{H}|p,s\rangle=\int\left\langle p',s'\left|\hat{\psi_A}^{+}(x)\left(m-\frac{\nabla^2}{2m}-\frac{e}{2m}\vec{B}\cdot\hat{\vec{L}}\,F_1(q^2)-\right.\right.\right.$$

$$\left.\left.\left.-\frac{e}{2m}2\vec{B}\cdot\vec{S}\,(F_1(q^2)+F_2(q^2))\right)\hat{\psi_A}(x)\right|p,s\right\rangle d^3\vec{x}\ .$$

Thus we have a correction for the spin angular momentum gyromagnetic ratio by a factor of $1+F_2(q^2)$: $g_S=2(1+F_2(q^2))$ or since we consider small momentum deviations, with $E_p=E_{p'}$ we will take the approximation $g_S\approx 2(1+F_2(0))$ and we must therefore estimate for obtaining the correction of the gyromagnetic ratio, the coefficient F_2 (q^2) when we take $q^2 = 0$.

Considering the Gordon decomposition (7) , from (6") we derive:

$$\bar{u}(p',s')(\gamma^\mu+\Gamma^\mu)u(p,s)=\bar{u}(p',s')(\gamma^\mu(1+F_2(q^2))-\frac{1}{2m}(p'+p)^\mu F_2(q^2))u(p,s) \quad (8)$$

We have

$$\Gamma^\mu=\int\frac{d^4k}{(2\pi)^4}\frac{(-ie^2)}{k^2+i\varepsilon}\frac{\gamma^\nu(\not{p}'+\not{k}+m)\gamma^\mu(\not{p}+\not{k}+m)\gamma_\nu}{((p'+k)^2-m^2+i\varepsilon)((p+k)^2-m^2+i\varepsilon)}=\int\frac{d^4k}{(2\pi)^4}(-ie^2)\frac{N^\mu}{D}\ .$$

Using the identity $\frac{1}{xyz}=2\int_\Delta d\alpha\,d\beta\frac{1}{(z+\alpha(x-z)+\beta(y-z))^3}$ where $\Delta=\{(\alpha,\beta)\in\mathbb{R}^2|0\le\beta\le 1-\alpha \text{ and } \alpha\ge 0\}$ it follows

$\frac{1}{D}=2\int_\Delta d\alpha\,d\beta\frac{1}{(l^2-(\alpha+\beta)^2m^2+i\varepsilon)^3}=2\int_\Delta d\alpha\,d\beta\frac{1}{\overline{D}}$ where we used

$p^2=p'^2=m^2$, $(p'-p)^2=q^2=0$ and take $l=k+\alpha p'+\beta p$.

We defined $N^\mu=\gamma^\nu(\not{l}+\not{P}'+m)\gamma^\mu(\not{l}+\not{P}+m)\gamma_\nu$ (9)

with $P'=(1-\alpha)p'-\beta p$, $P=(1-\beta)p-\alpha p'$ and so we have

$$\Gamma^\mu=2\int_\Delta d\alpha\,d\beta\int\frac{(-ie^2)}{(2\pi)^4}\frac{N^\mu}{(l^2-(\alpha+\beta)^2m^2+i\varepsilon)^3}d^4l\ .$$

Considering (8) we notice that to extract F_2 (0) , we can throw away any term proportional to γ^μ we encounter while processing the (9) expression.

The terms of N^μ are :

-the m^2 term $\propto\gamma^\mu$ and we throw it away;

-the term linear in l which integrates to 0 by symmetry;

-the term quadratic in l given by $\gamma^\nu\not{l}\gamma^\mu\not{l}\gamma_\nu=\gamma^\nu\gamma^\sigma\gamma^\mu\gamma^\tau\gamma_\nu l_\sigma l_\tau$ (10)

Taking $M_{\sigma\tau}=\int\frac{l_\sigma l_\tau}{(l^2-(\alpha+\beta)^2m^2+i\varepsilon)^3}d^4l$ and for $\Lambda\in SO^+(3,1)$ changing the integration variable $l_\sigma\to\Lambda_{\sigma\delta}l_\delta$ we obtain $\Lambda M\Lambda^T=M$ and so if $\eta=(\eta_{\sigma\tau})_{\sigma,\tau}$ is the Minkowski metric coefficients matrix then $\Lambda M\,\eta\Lambda^{-1}=M\,\eta$ and since Λ is arbitrary in $SO^+(3,1)$ it follows $M=\lambda\eta$ with $\lambda\in\mathbb{C}$ and we can replace $l_\sigma l_\tau$ from (10) by $\frac{1}{4}\eta_{\sigma\tau}l^2$ leading to a term proportional to γ^μ .

Hence we can thow away the term quadratic in l ;
-a term independent of l given by
$\gamma^\nu \not{p}' \gamma^\mu \not{p} \gamma_\nu = -2((1-\beta)\not{p} - \alpha \not{p}')\gamma^\mu((1-\alpha)\not{p}' - \beta \not{p})$.
Because $\bar{u}(p')\not{p}' = m\bar{u}(p')$ and $\not{p}u(p) = mu(p)$ we can replace the term by
$-2((1-\beta)\not{p}' - \alpha m)\gamma^\mu((1-\alpha)\not{p} - \beta m)$
This expression has m^2 , m and m^0 terms.
The m^2 term can obviously be thrown away.
Since $\overline{D}$ is symmetric in (α , β) the m term can be symmetrized in (α , β) and gives
$2m(p'+p)^\mu(\alpha(1-\alpha)+\beta(1-\beta))$ considering also that
$\bar{u}(p')(\not{p}\gamma^\mu + \gamma^\mu \not{p}')u(p) = \bar{u}(p')(2p^\mu + 2p'^\mu)u(p) - 2m\bar{u}(p')\gamma^\mu u(p)$.
After some calculus we can verify that
$\bar{u}(p')\not{p}\gamma^\mu \not{p}' u(p) = 2m\bar{u}(p')(p'+p)^\mu u(p) - 3m^2\bar{u}(p')\gamma^\mu u(p)$
and so the m^0 term gives $-4m(1-\alpha)(1-\beta)(p'+p)^\mu$;
-another term independent of l given by
$m(\gamma^\nu \not{P}' \gamma^\mu \gamma_\nu + \gamma^\nu \gamma^\mu \not{P} \gamma_\nu) = 4m((1-2\alpha)p'^\mu + (1-2\beta)p^\mu)$
Since $\overline{D}$ is symmetric in (α , β) this term can be symmetrized and gives
$4m(1-\alpha-\beta)(p'+p)^\mu$.
Putting it all together we obtain

$$-\frac{1}{2m}(p'+p)^\mu F_2(0) =$$

$$= 2\int_\Delta d\alpha d\beta \int \frac{(-ie^2)}{(2\pi)^4} 2m(\alpha+\beta-(\alpha+\beta)^2)(p'+p)^\mu \int \frac{d^4 l}{(l^2-(\alpha+\beta)^2 m^2 + i\varepsilon)^3} .$$

Let $I(\mu) = \int \frac{d^4 l}{(l^2-\mu^2+i\varepsilon)^3} = \int \left(\int \frac{dl_0}{(l_0^2 - \vec{l}^{\,2} - \mu^2 + i\varepsilon)^3} \right) d^3\vec{l}$.

The poles of $F(l_0) = \frac{1}{(l_0^2 - \vec{l}^{\,2} - \mu^2 + i\varepsilon)^3}$ are $z_\pm = \pm(\sqrt{\vec{l}^{\,2} + \mu^2} - i\varepsilon)$ with $\varepsilon > 0$, $\varepsilon \to 0$

Thus $\int F(l_0)dl_0 = 2\pi i \,\mathrm{Rez}(F, z_-) = \int_{-i\infty}^{i\infty} F(z)dz = i\int_{-\infty}^{\infty} F(iz)dz = -i\int \frac{dl_0}{(l_0^2 + \vec{l}^{\,2} + \mu^2)^3}$.

Therefore

$$I(\mu) = -i\int \frac{d^4 k}{(\|k\|_4^2 + \mu^2)^3} = \frac{-2i\pi^2}{\Gamma(2)} \int_0^\infty \frac{k^3}{(k^2+\mu^2)^3} dk = -i\pi^2 \int_0^\infty \frac{k^2}{(k^2+\mu^2)} dk^2 = i\frac{\pi^2}{2\mu^2}$$

$$F_2(0) = -2\int_\Delta d\alpha d\beta \frac{(-ie^2)}{(2\pi)^4} 4m^2(\alpha+\beta-(\alpha+\beta)^2)\frac{(-i\pi^2)}{2(\alpha+\beta)^2 m^2} = \frac{e^2}{8\pi^2} ,$$

$F_2(0) = \frac{\alpha}{2\pi} \approx 0.00118$ and we have the corrected by quantum fluctuations gyromagnetic ratio $g_S = 2.00236$ giving the anomalous magnetic moment of the electron $\vec{\mu}_S = -\frac{g_S \mu_B}{\hbar}\vec{S}$, $\mu_B = \frac{|e|}{2m}\hbar$ being the Bohr magneton while the regular magnetic moment corresponds to $g_S = 2$.

35. Magnetic monopole

Magnetic monopole

For an electromgnetic field with four-potential $(A_\mu)_\mu$ we can define the differential form $A=A_\mu dx^\mu$ and so $F=dA=\frac{1}{2}F_{\mu\nu}dx^\mu dx^\nu=$

$=E_i dx^0 dx^i-B_1 dx^2 dx^3-B_2 dx^3 dx^1-B_3 dx^1 dx^2$.

Taking $(A_\mu)_\mu=(0,\vec{A})$, a magnetic monopole at $\vec{x}=\vec{0}$ with $\vec{x}=(x^i)_{i=\overline{1,3}}$ means that through any spherical surface S with center at $\vec{0}$ we have

$\int_S \vec{B}\cdot\boldsymbol{n}\,dS=g$ (1) with $\boldsymbol{n}$ -the outer normal to S and dS the surface area element on S (The total flux surrounding $\vec{0}$ through the surface S is equal to g which is the magnetic charge of the monopole).

Obviously (1) is equivalent to $\int_S F=-g$ if $\vec{A}=\vec{A}(\vec{x})$ and we must have

$\vec{B}=\frac{g}{4\pi r^2}\frac{\vec{r}}{r}$, $F=-\frac{g}{4\pi}d(\cos\theta)d\varphi$

where $\vec{x}=\vec{r}=(r\cos\theta, r\sin\theta\cos\varphi, r\sin\theta\sin\varphi)$

Hence we can take $A=-\frac{g}{4\pi}\cos\theta d\varphi$ (2) and by gauge invariance we can take any $A+\frac{1}{e}d\Lambda$ where $\Lambda=\Lambda(x)$ gives the gauge transformation

$A_\mu \to A_\mu+\frac{1}{e}\partial_\mu\Lambda$ or $A\to A+\frac{1}{ie}\exp(-i\Lambda(x))d\exp(i\Lambda(x))$

However , φ is not defined at $\theta = 0$ and $\theta = \pi$ which makes A globally indefinite.

We can define A local at $\theta=0$ by $A_N=-\frac{g}{4\pi}(\cos\theta-1)d\varphi$ having $A_N=0$ at $\theta=0$.

In the same way we define A local at $\theta=\pi$ as $A_S=-\frac{g}{4\pi}(\cos\theta+1)d\varphi$.

A_N and A_S must describe the same electromagnetic field and so they must be related by a gauge transformation $A_N=A_S+\frac{1}{ie}\exp(-i\Lambda(x))d\exp(i\Lambda(x))$.

Thus $\frac{1}{ie}\exp(-i\Lambda(x))d\exp(i\Lambda(x))=2\frac{g}{4\pi}d\varphi$ which leads to

$\exp(i\Lambda)=\exp(i(2e\frac{g}{4\pi})\varphi)$. Since $\varphi=0$ and $\varphi=2\pi$ describe the same point, in order for $\exp(i\Lambda)$ to make sense we must have $\exp(i(2e\frac{g}{4\pi})2\pi)=1$ and so we must have $g=\frac{2\pi}{e}n$ with $n\in\mathbb{Z}$.

Therefore the magnetic charge on a magnetic monopole is quantized in units of $\frac{2\pi}{e}$ (e unit electric charge).

If magnetic charges exist , we make the Maxwell equations invariant under a transformation $\vec{E}+i\vec{B}\rightarrow \exp(i\theta)(\vec{E}+i\vec{B})$ by defining the corresponding transformations of electric charge density ρ_e , magnetic charge density ρ_m , electric current density $\vec{j}_e$ and magnetic current density $\vec{j}_m$. The Maxwell equations are

$$\nabla\cdot\vec{E}=\rho_e$$

$$\nabla\cdot\vec{B}=\rho_m$$

$$\nabla\times\vec{B}=\vec{j}_e+\frac{\partial\vec{E}}{\partial t}$$

$$\nabla\times\vec{E}=-\vec{j}_m-\frac{\partial\vec{B}}{\partial t}\ .$$

We will have therefore an electromagnetic duality by transformations $\vec{E}\rightarrow\vec{B}$, $\vec{B}\rightarrow-\vec{E}$, $\rho_e\rightarrow\rho_m$, $\vec{j}_e\rightarrow\vec{j}_m$, $\rho_m\rightarrow-\rho_e$, $\vec{j}_m\rightarrow-\vec{j}_e$.

According to the Meissner effect a single monopole cannot live inside a superconductor since the superconductor material expels any magnetic field. Considering a magnetic antimonopole at distance *R* from the magnetic monopole inside a superconductor, the magnetic flux coming out of the monopole can go into the antimonopole forming a tube connecting the monopole and the antimonopole and obliging the superconductor to give up being a superconductor in the region of the flux tube (Since outside of the tube of radius *r* the magnetic flux is expelled we have that the flux inside the tube is 2 *g* (with *g* the magnetic charge of the monopole, - *g* the magnetic charge of the antimonopole) and so in the flux tube we will have roughly have a constant magnetic field $B=\frac{2g}{\pi r^2}$ parallel to the monopole to antimonopole line). Thus cosidering φ the field or order parameter of the superconductor (the field associated with the condensing Cooper pair bosons (see Chap. Superconductivity)) it is no longer energetically favorable for the field φ to be constant everywhere , instead it vanishes in the region of the flux tube. The energy cost of this arrangement is then given by an energy density $\mathscr{F}=\frac{1}{2}\vec{B}^2$ with $\vec{B}$ the magnetic field in the flux tube and therefore grows with the volume *V* of the flux tube which is proportional to *R*. Hence it costs more and more energy to pull a monopole and a antimonopole apart, and inside a superconductor we will have a confinement of monopoles. Invoking electromagnetic duality, inside a magnetic superconductor, electric charges would be permanently confined.

Also imaging a color magnetic superconductor, we will have permanent confinement of quarks. It seems to be like the ground state of the quantum chromodynamics Lagrangian density system (see Chap. Feynman diagrams and lattice gauge theory

and Chap. Quantum chromodynamics. S U(5) unification) is a color magnetic superconductor since as proved, the energy of a quark-antiquark system also grows with the separation distance , at lower energies, leading to confinement of quarks.

36. Phonon-electron interaction. Superconductivity Meissner effect. Conductivity. Drude model

Phonon-electron interaction. Superconductivity Meissner effect . Conductivity. Drude model

Consider a covalent crystal lattice where positive kernels of metal atoms are kept in stable positions of a lattice grid $\Gamma=\{n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3|n_i=\overline{1,N_i}\ ,\ i=\overline{1,3}\}$ with $\vec{a}_i\in\mathbb{R}^3, N_i\in\mathbb{N}\ ,\ N=N_1N_2N_3\ ,\ i=\overline{1,3}$, by the common field of interaction between the kernels and their electronic shells. Then according to Chap. Covalent crystal lattices of metals, using the linear combination of atomic orbitals with tight binding approximation , the wave functions of the electrons in the crystal are given $\tilde{\psi}_{\vec{k}}(t,x)=\exp(-iE(\vec{k})t)\,\psi_{\vec{k}}(x)$ with $t\in\mathbb{R}, x\in\mathbb{R}^3$ and satisfy the time independent Schroedinger equation $\left(-\frac{1}{2m}\nabla^2+V(x)\right)\psi_{\vec{k}}(x)=E(\vec{k})\,\psi_{\vec{k}}(x)$ (1)

where $V(x)=\sum_{\boldsymbol{n}}V_0(x-\boldsymbol{R_n})$ (we take $\hbar=1$ reduced Planck constant , $c=1$ speed of light in vacuum constant)

$\psi_{\vec{k}}(x)=\sum_{\boldsymbol{n}}\exp(i\vec{k}\cdot\boldsymbol{R_n})u_0(x-\boldsymbol{R_n})$, $\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i=\sum_{i=1}^{3}\tilde{k}_i\vec{b}_i$, $m_i\in\mathbb{Z}$, $i=\overline{1,3}$

$\vec{b}_i=\frac{2\pi}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}(\vec{a}_j\times\vec{a}_k)\,\epsilon_{ijk}$ (no summation over j,k) , $\vec{k}\cdot\vec{a}_i=\frac{2\pi m_i}{N_i}$,

$\psi_{\vec{k}}(x)=\exp(i\vec{k}\cdot x)u_{\vec{k}}(x)$, $u_{\vec{k}}(x+\boldsymbol{R_n})=u_{\vec{k}}(x)$ -the Bloch functions ,

$\boldsymbol{R_n}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$, $\boldsymbol{n}=(n_1,n_2,n_3)\in\mathbb{Z}^3$,

$u_{\vec{k}}(x)=\sum_{\boldsymbol{n}}\exp(i\vec{k}\cdot(\boldsymbol{R_n}-x))u_0(x-\boldsymbol{R_n})$, $u_0=u_0(x)\in\mathbb{R}$ satisfies the single atom time independent Schroedinger equation $\nabla^2u_0(x)+2m(E_0-V_0(x))u_0(x)=0$ and the normalization $\int u_0(x-\boldsymbol{R_n})u_0(x-\boldsymbol{R_m})d^3x=\delta_{\boldsymbol{nm}}$ for $\boldsymbol{n},\boldsymbol{m}\in\mathbb{Z}^3$

We have $E(\vec{k})\approx E_0-\alpha-2\gamma(\cos(2\pi\tilde{k}_1)+\cos(2\pi\tilde{k}_2)+\cos(2\pi\tilde{k}_3))$ (where for a rectangular lattice grid with $\vec{a}_i\cdot\vec{a}_j=a_ia_j\,\delta_{ij}$ we have $k_ia_i=2\pi\tilde{k}_i$, $\vec{k}=(k_i)_i$) for small wave numbers $\tilde{k}_i$, where

$\alpha=-\int u_0(x)(V(x)-V_0(x))u_0(x)d^3x$

$\gamma=-\sum_{i=1}^{3}\int\frac{u_0(x-\vec{a}_i)+u_0(x+\vec{a}_i)}{2}(V(x)-V_0(x))u_0(x)d^3x$

For large N_i we can consider $\vec{k}$ as a continuous variable and so E_0,α,γ determine a continuous zone of the spectrum values $(E(\vec{k}))_{\vec{k}}$.

$E(\vec{k})$ has at $\vec{k}=0$ an extreme value and for small $\|\vec{k}\|$ we have

$E(\vec{k})\approx E(0)+\frac{1}{2}\frac{\partial^2E}{\partial k_\mu\partial k_\nu}(0)k_\mu k_\nu=E(0)+\frac{1}{2m^*_{\nu\mu}}k_\mu k_\nu=E(0)+\epsilon(\vec{k})$.

In the case of a rectangular lattice grid we obtain:

$m^*_{\mu\nu}=0$ if $\mu\neq\nu$ and $m^*_{\nu\nu}=m^*_\nu=\frac{1}{2\gamma a_\nu^2}$ for $\nu=\overline{1,3}$.

Hence if in the crystal we have an additional external field which changes slowly in time defining a Hamiltonian operator

$\widehat{H}_1=-\frac{1}{2m}\nabla^2+V(x)+U(x)$ the study of long wave excitations ($\|\vec{k}\|$ small)

of the electrons can be reduced to the study of the effective Hamiltonian

$\widehat{H}_{eff}=-\frac{1}{2m^*_\nu}\frac{\partial^2}{\partial x_\nu^2}+U(x)+E(0)$

Thus m^*_ν has the role of an effective mass of the electron in direction ν (see also Chap. Fermi's golden rule).

In a cubic lattice crystal $m^*_\nu=m^*$ for any ν , $m^*_\nu=\frac{1}{2\gamma a^2}$, $a=a_\nu$, $\nu=\overline{1,3}$,

(isotropic effective mass) .

As mentioned, if N_1,N_2,N_3 are large we can consider $\vec{k}$ a continuous variable and $(\epsilon(\vec{k}))_{\vec{k}}$ a quasicontinuous spectrum. Thus $d^3\vec{k}=\frac{(2\pi)^3}{\Omega_0}d^3\tilde{\vec{k}}$, $\Omega_0=\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)$ is the cell volume and a volume $d^3\tilde{\vec{k}}$ in $\tilde{k}$-space contains $N d^3\tilde{\vec{k}}$ $\tilde{k}$-states.

The corresponding volume $d^3\vec{k}$ in k-space contains therefore $\frac{N\Omega_0}{(2\pi)^3}d^3\vec{k}=\frac{V}{(2\pi)^3}d^3\vec{k}$ k-states . Considering spin degeneracy $g=2$, the number of states having energy $\epsilon(\vec{k})\in(\epsilon,\epsilon+d\epsilon)$ is $dN_e=\frac{gV}{(2\pi)^3}\int\limits_{E(\vec{k})\in(\epsilon,\epsilon+d\epsilon)}d^3\vec{k}$

We have $\int\limits_{\epsilon(\vec{k})\in(\epsilon,\epsilon+d\epsilon)}d^3\vec{k}=\int\limits_\epsilon^{\epsilon+d\epsilon}\int\frac{dS}{\|\nabla_{\vec{k}}E(\vec{k})\|}d\epsilon$ where dS is the surface $\{\vec{k}|\epsilon(\vec{k})=\epsilon\}$ element . For a isotropic effective mass we have for small $\|\vec{k}\|$ that $\|\nabla_{\vec{k}}E(\vec{k})\|=\frac{\|\vec{k}\|}{|m^*|}$, $\int dS=4\pi k^2$ with $k=\|\vec{k}\|$ and so $\frac{dN_e}{d\epsilon}=\frac{gV}{(2\pi)^3}|m^*|4\pi\|\vec{k}\|$.

The electrons in the conduction band have positive effective mass .

($E(\vec{k})$ has a minimum in the conduction band and so $\gamma>0$, $m^*>0$ (see Chap. Fermi's golden rule)). Measuring the energy levels from the bottom of the corresponding continuous spectrum zone we will have a energetic density of electrons in the conduction band given by $\rho(\epsilon)=\frac{dN_e}{d\epsilon}=\frac{gV}{4\pi^2}(2m^*)^{3/2}\sqrt{\epsilon}$

According to Chap. Quantum statistical ensemble, since electrons obey to Fermi statistics, the probability that a state $|\varepsilon_s\rangle$ of energy $\epsilon(k)=\varepsilon_s$ is occupied by an electron in the conduction band at thermodynamical equilibrium temperature T is:

$p(\epsilon(k))=\frac{\exp((\mu-\epsilon(k))/(k_bT))}{1+\exp((\mu-\epsilon(k))/(k_bT))}$ and the averaged occupation number of the state $|\varepsilon_s\rangle$ is $f(\epsilon(k))=\frac{1}{1+\exp((\epsilon(k)-\mu)/k_bT)}$ where k_b is the Boltzmann constant and μ is the Fermi energy level or chemical potential,(the amount of energy which the particle must carry when entering or leaving the system while the entropy and other extensive parameters remain constant) measured from the E (0) of the corresponding energy levels continuous spectrum zone.

For $T\to 0$ any state with lower energy than the Fermi level is occupied and the states with energy above the Fermi level $\mu=\epsilon_F$ are free of electrons.

Then the total number of electrons in the conduction band is

$$N_e=\int_0^\infty f(\epsilon)\rho(\epsilon)d\epsilon=\frac{gV}{\pi^2\sqrt{2}}(m^*k_bT)^{3/2}F(\frac{\mu}{k_bT})$$

where $F(\frac{\mu}{k_bT})=\int_0^\infty \frac{\sqrt{x}}{1+\exp(x-\frac{\mu}{k_bT})}dx$

For total degeneracy $(T\to 0)$ we have $f(\epsilon)=0$ if $\epsilon>\mu$ and so we take

$$F(\frac{\mu}{k_bT})=\int_0^{\frac{\mu}{k_bT}}\sqrt{x}\,dx=\frac{2}{3}\left(\frac{\epsilon_F}{k_bT}\right)^{3/2}$$

Therefore $N_e=\frac{g\sqrt{2}}{3\pi^2}V(m^*\epsilon_F)^{3/2}$, $\epsilon_F=\frac{1}{2m^*}\left(\frac{6\pi^2N}{gV}\right)^{2/3}$ (2) .

(We can assume $N_e = N$ if we suppose one free (conduction) electron per atom in the crystal lattice)

In the continuous approximation for the $\vec{k}$ variable , in the simplified case of cubic crystal lattice medium assimilable with an isotropic liniar elastic material, we will have a phonon field operator function

$$\vec{\varphi}(t,x)=\frac{1}{\sqrt{(2\pi)^3}}\int\sum_s\frac{\boldsymbol{e}^s(\vec{\boldsymbol{k}})}{\sqrt{2\omega_s(k)}}\left(\hat{b}_{s\vec{k}}\exp(-i\omega_s(k)t+i\vec{k}\cdot x)+\right.$$
$$\left.+\hat{b}^+_{s\vec{k}}\exp(i\omega_s(k)t-i\vec{k}\cdot x)\right)d^3x$$

where $[\hat{b}_{s\vec{k}},\hat{b}^+_{s'\vec{k}'}]=\delta^3(\vec{k}-\vec{k}')\delta_{ss'}$, $[\hat{b}_{s\vec{k}},\hat{b}_{s'\vec{k}'}]=0$, $\hat{b}_{s\vec{k}}|0\rangle=0$, $s=\overline{1,3}$,

$$\omega_1(k)=\sqrt{\frac{\lambda+2\mu}{\rho}}k \quad , \quad \omega_2(k)=\omega_3(k)=\sqrt{\frac{\mu}{\rho}}k \quad , \quad k=\|\vec{k}\| \ ,$$

ρ -density of the isotropic liniar elastic material

λ,μ -Lame coefficients of the isotropic liniar elastic material

$\sqrt{\frac{\lambda+2\mu}{\rho}}=c_P$ and $\sqrt{\frac{\mu}{\rho}}=c_T$ are obviously the longitudinal and respective transversal elastic waves propagation velocities.

$\boldsymbol{e}^1(\vec{k})\times\vec{k}=0$, $\boldsymbol{e}^2(\vec{k})\cdot\vec{k}=\boldsymbol{e}^3(\vec{k})\cdot\vec{k}=0$, $\boldsymbol{e}^i(\vec{k})\cdot\boldsymbol{e}^j(\vec{k})=\delta_{ij}$, $\boldsymbol{e}^i(\vec{k})\in\mathbb{R}^3$, $i,j=\overline{1,3}$.

The Hamiltonian operator corresponding to the phonon field is

$\widehat{H}=\sum_{\vec{k},s}\omega_s(k)(\widehat{\widetilde{b}}^{+}_{s\vec{k}}\widehat{\widetilde{b}}_{s\vec{k}}+\frac{1}{2})$ where $\widehat{\widetilde{b}}_{s\vec{k}}=\sqrt{\frac{(2\pi)^3}{V}}\hat{b}_{s\vec{k}}$ and we have also

$\vec{\varphi}(t,x)=\frac{1}{\sqrt{V}}\sum_{s,\vec{k}}\frac{\boldsymbol{e}^{s}(\vec{k})}{\sqrt{2\omega_s(k)}}(\widehat{\widetilde{b}}_{s\vec{k}}\exp(-i(\omega_s(k)t-\vec{k}\cdot x))+\widehat{\widetilde{b}}^{+}_{s\vec{k}}\exp(i(\omega_s(k)t-\vec{k}\cdot x)))$,

$[\widehat{\widetilde{b}}_{s\vec{k}},\widehat{\widetilde{b}}^{+}_{s'\vec{k}'}]=\delta_{\vec{k}\vec{k}'}\delta_{ss'}$, $\vec{k}$ taking the discrete values $\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i$, $m_i\in\mathbb{Z}$

in the first Brillouin zone $k_i\in[-\frac{\pi}{a},\frac{\pi}{a}]$, $i=\overline{1,3}$.

$\sqrt{\frac{V}{m_0 N}}\vec{\varphi}(t,\boldsymbol{R_n})=\frac{1}{\sqrt{\rho}}\vec{\varphi}(t,\boldsymbol{R_n})=\boldsymbol{r_n}(t)$ where V is the volume of the crystal, m_0 is the mass of a nodal atom kernel , represents the oscillations in time of the node at $x=\boldsymbol{R_n}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$ which in the continuous approximation can be assimilated to the dispalcements field values $\vec{u}(t,x)=\boldsymbol{r_n}(t)$ of the isotropic liniar elastic body.

(see Chap. Phonons in three-dimensional crystals)

After some calculus e derive that a Hamiltonian operator for the phonon field defined by $\widehat{H}=\int\left(\frac{1}{2}(\partial_t\vec{\varphi})^2+\frac{1}{2}(c_P^2(\nabla\cdot\vec{\varphi})^2+c_T^2(\nabla\times\vec{\varphi})^2)\right)d^3x$ leads to

$\widehat{H}=\int\sum_s\omega_s(k)\hat{b}^{+}_{s\vec{k}}\hat{b}_{s\vec{k}}d^3\vec{k}+\delta^3(\vec{0})\int\frac{1}{2}\omega_s(\vec{k})d^3\vec{k}=\sum_{\vec{k},s}\omega_s(k)(\widehat{\widetilde{b}}^{+}_{s\vec{k}}\widehat{\widetilde{b}}_{s\vec{k}}+\frac{1}{2})$

(reminding that $\delta^3(\vec{k}'-\vec{k})=\frac{V}{(2\pi)^3}\delta_{\vec{k}\vec{k}'}$) .

The Lagrangian density of the phonon field, leading to this Hamiltonian operator is defined by $\mathscr{L}(\vec{\varphi},\partial\vec{\varphi})=\frac{1}{2}(\partial_t\vec{\varphi})^2-\frac{1}{2}(c_P^2(\nabla\cdot\vec{\varphi})^2+c_T^2(\nabla\times\vec{\varphi})^2)$ (3)

because we can verify that $\widehat{H}=\int\left(\frac{\partial\widehat{\mathscr{L}}}{\partial(\partial_t\vec{\varphi})}\cdot(\partial_t\vec{\varphi})-\widehat{\mathscr{L}}\right)d^3x$.

We have $\int\mathscr{L}(\vec{\varphi},\partial\vec{\varphi})dt\,d^3x=\int-\frac{1}{2}\varphi_i A_{ij}\varphi_j dt\,d^3x$ with

$A_{ij}=(\delta_{ij}\partial_t^2-c_P^2\partial_i\partial_j-\delta_{ij}c_T^2\partial_k\partial_k+c_T^2\partial_i\partial_j)=\delta_{ij}(\partial_t^2-c_T^2\partial_k\partial_k)-(c_P^2-c_T^2)\partial_i\partial_j$.

The propagator of the phonon field $D_{ij}=D_{ij}(t,x)$ satisfies

$A_{ij}D_{jk}(t,x)=\delta^4((t,x))\delta_{ik}$, $i,j,k=\overline{1,3}$ and obviously summation convention .

For the Fourier transformation of D_{ij} : $D_{ij}(\omega,\vec{k})=\int\exp(-i\omega t+i\vec{k}\cdot x)dt\,d^3x$

we have $(-\delta_{ij}(\omega^2-c_T^2\vec{k}^2)+(c_P^2-c_T^2)k_ik_j)D_{jl}(\omega,\vec{k})=\delta_{il}$ leading to

$D_{jl}(\omega,\vec{k})=\delta_{jl}A+Bk_jk_l$ with

$-\delta_{il}A(\omega^2-c_T^2\vec{k}^2)+k_ik_l(-(\omega^2-c_T^2\vec{k}^2)B+(c_P^2-c_T^2)A+(c_P^2-c_T^2)\vec{k}^2B)=\delta_{il}$,

$A=-\frac{1}{\omega^2-c_T^2\vec{k}^2}$, $B=-\frac{c_P^2-c_T^2}{(\omega^2-c_P^2\vec{k}^2)(\omega^2-c_T^2\vec{k}^2)}$

$$D_{jl}(\omega,\vec{k})=-\frac{1}{\omega^2-c_T^2\vec{k}^2+i\varepsilon}\left(\delta_{jl}+\frac{c_P^2-c_T^2}{\omega^2-c_P^2\vec{k}^2+i\varepsilon}k_jk_l\right)$$

$$D_{jl}(t,x)=\frac{1}{(2\pi)^4}\int\exp(i\omega t-i\vec{k}\cdot x)D_{jl}(\omega,\vec{k})\,d\omega\,d^3\vec{k}$$

Notice that the (3) Lagrangian density breaks the Lorentz invariance. The reference frame in which the crystal lattice is at rest is the preferential frame in which the Lagrangian density (3) describes a phonon system.

The Lagrangian density (3) is invariant under a O(3) transformation of both coordinates and vectorial phonon field that is a rotation of the entire crystal.

In an (infinitesimal) elastic deformation of the crystal the local density of atoms changes. If the density around a point increases, the positive charge density of atomic kernels in the crystal increases at that point, and there appears a potential pit to which the electrons are attracted in the process of the body regaining its initial form after elastic deformation. Thus the energy of the electrons in the deformed crystal region with increased mass density is higher than the energy of the electrons in the undeformed crystal. Increased local density corresponds to negative relative variation of the volume element. The infinitesimal relative variation of the volume element is $\nabla\cdot\vec{u}$ where $\vec{u}=\vec{u}(x)$ is the infinitesimal local displacements field.

Hence, under a small elastic deformation of an isotropic covalent crystal we assume an additional deformation potential $W_d(x)=-\sigma\nabla\cdot\vec{u}(x)$ with $\sigma>0$ in the (1) time independent Schroedinger equation for electrons:

$$\left(-\frac{\nabla^2}{2m}+V(x)+W_d(x)\right)\psi(x)=E(k,\vec{u}(x))\,\psi(x)\ ,\ E(k,\vec{u}(x))=E(k)-\sigma\ \nabla\cdot\vec{u}(x)$$

with σ weak depending on k .

For energy levels $E(k)$ close to the Fermi energy ϵ_F at equilibrium temperatures $T\to 0$ we have $E(k)=\frac{1}{2m^*}\left(\frac{6\pi^2N}{gV}\right)^{2/3}=\epsilon_F$ (according to (2)) and the variation of energy under a local deformation will be $-\sigma\frac{\delta V}{V}=-\sigma\nabla\cdot\vec{u}(x)=\delta\epsilon_F=-\frac{2}{3}\epsilon_F\frac{\delta V}{V}$

and so at $T\to 0$ we have $\sigma=\frac{2}{3}\epsilon_F=\frac{1}{3m^*}\left(\frac{6\pi^2N}{gV}\right)^{2/3}$ (3')

Considering the Hamiltonian field operator for the electron, $\widehat{\widehat{H}}$ as a field expectation value operator, if $\widehat{H_0}$ is the Hamiltonian for the free electron, then

we have for the electrons in the crystal in presence of a phonon excitation (elestic deformation) that :

$$\hat{\hat{H}}=\int(\hat{\psi}^{+}\hat{H}_0\hat{\psi}+\hat{\psi}^{+}V(x)\hat{\psi}+\hat{\psi}^{+}W_d(x)\hat{\psi})d^3x$$

where $\hat{\psi}=\hat{\psi}(t,x)$ is the electron field operator function.

Taking ψ as the Dirac spinor for the electron we have $\hat{H}_0=m\gamma^0-i\gamma^0\gamma^k\partial_k$ with $(\gamma^\alpha)_\alpha$ the gamma matrices, latin letters for indexing from 1 to 3 , greek letters for indexing from 0 to 3 and summation convention. Therefore $\hat{\hat{H}}=\int(\hat{\bar{\psi}}(m-i\gamma^k\partial_k)\hat{\psi}+\hat{\bar{\gamma}}^0V(x)\hat{\psi}-\bar{\sigma}\hat{\bar{\psi}}\gamma^0(\nabla\cdot\hat{\vec{\varphi}})\hat{\psi})d^3x$ where $\vec{\varphi}=\vec{\varphi}(t,x)=\sqrt{\rho}\,\vec{u}(t,x)$ is the phonon field corresponding to the small displacements field and $\bar{\sigma}=\frac{\sigma}{\sqrt{\rho}}$.

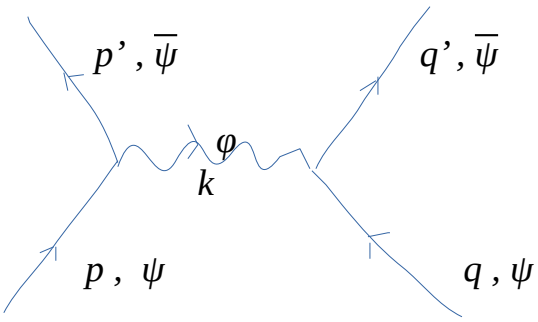
The interaction between electrons and phonons in the crystal lattice can then be expressed by the total Lagrangian density:

$$\mathcal{L}(\psi,\partial\psi,\vec{\varphi},\partial\vec{\varphi})=\bar{\psi}(i\gamma^\alpha\partial_\alpha-m)\psi+\frac{1}{2}(\partial_0\vec{\varphi})^2-\frac{1}{2}c_P^2(\nabla\cdot\vec{\varphi})^2-\frac{1}{2}c_T^2(\nabla\times\vec{\varphi})^2-$$

$$-\bar{\psi}\gamma^0\psi V(x)+\bar{\sigma}\bar{\psi}\gamma^0\psi(\nabla\cdot\vec{\varphi}) \qquad (4)\ .$$

The coupling according to Feynman rules corresponding to the electron-phonon interaction term is $-\bar{\sigma}\,k_j$ with k_j the incoming phonon momentum component.
As we can see, the (4) Lagrangian density breaks Lorentz invariance, the frame where the crystal lattice is at rest being the preferential frame.

The Hamiltonian operator $\hat{H}=\sum_{s,\vec{k}}(\hat{\hat{b}}^{+}_{s\vec{k}}\hat{\hat{b}}_{s\vec{k}}+\frac{1}{2})\omega_s(k)$ for the phonon system is obtained supposing harmonical oscillations of the crystal nodes, only quadratic terms in the energy of deformation (see Chap. Phonons in three-dimensional crystals), the so called harmonic approximation. Otherwise we will have additional phonon self-interaction terms in the Lagrangian density and we have to consider phonon-phonon interactions (we would have non-linear terms in the Euler-Lagrange elastic wave equation).
As we can see from the last term in the (4) Lagrangian density, electrons can interact each with other by exchanging a phonon like in the below Feynman diagram:



$k = p - p' = q' - q$

The Feynman amplitude of this interaction is
$A=(2\pi)^4 M \delta^4(p+q-p'-q')$ with p, q, p', q' incoming respective outgoing four-momenta of the participating electrons,

$$M=\overline{\sigma}^2(\bar{u}(p')\gamma^0 u(p))(\bar{u}(q')\gamma^0 u(q))(-k_j)(-i)\left(\frac{\delta_{jl}}{\omega^2-c_T^2\vec{k}^2+i\varepsilon}+\right.$$

$$\left.+\frac{(c_P^2-c_T^2)k_j k_l}{(\omega^2-c_P^2\vec{k}^2+i\varepsilon)(\omega^2-c_T^2\vec{k}^2+i\varepsilon)}\right)k_j=i\overline{\sigma}^2(\bar{u}(p')\gamma^0 u(p))(\bar{u}(q')\gamma^0 u(q))\frac{\vec{k}^2}{\omega^2-c_P^2\vec{k}^2}$$

with $k=p-p'=q'-q$
(see Chap. Dirac spinor , Quantum electrodynamics, Feynman amplitudes and lattice gauge theory)
We can see that as expected the transversal elastic oscillation with propagation velocity c_T is not involved in the final amplitude expression.
Considering the phononic interaction of two electronic lumps
$J_1^0(t,x)=\delta^3(x-x_0)$ and $J_2^0(t,x)=\delta^3(x-y_0)$ we have an electronic density $J^0(t,x)=\overline{\psi}(t,x)\gamma^0\psi(t,x)=J_1^0(t,x)+J_2^0(t,x)$ acting as a phononic field source in the phonon field Lagrangian density

$$\mathscr{L}(\vec{\varphi},\partial\vec{\varphi})=\frac{1}{2}(\partial_t\vec{\varphi})^2-\frac{1}{2}(c_P^2(\nabla\cdot\vec{\varphi})^2+c_T^2(\nabla\times\vec{\varphi})^2)+\overline{\sigma}J^0\nabla\cdot\vec{\varphi}$$

The action is

$$\int\mathscr{L}(\vec{\varphi},\partial\vec{\varphi})dt\,d^3x=\int\left(\frac{1}{2}(\partial_t\vec{\varphi})^2-\frac{1}{2}(c_P^2(\nabla\cdot\vec{\varphi})^2+c_T^2(\nabla\times\vec{\varphi})^2)-\overline{\sigma}(\partial_i J^0)\varphi_i\right)dt\,d^3x$$

The energy due the presence of the two sources acting on each other through the phonon field is $E = E(x_0 - y_0)$ and if T is the interaction time, satisfies

$$\exp(-iET)=\langle 0|\exp(-i\hat{H}T)|0\rangle=Z(J)=\int D\vec{\varphi}\exp\left(i\int\mathscr{L}(\vec{\varphi},\partial\vec{\varphi})dt\,d^3x\right)=$$

$$=Z(J=0)\exp\left(-\frac{i}{2}\int-\overline{\sigma}\,\partial_j J^0(\bar{x})D_{jl}(\bar{x}-\bar{y})(-\overline{\sigma}\,\partial_l J^0(\bar{y}))d^4\bar{x}\,d^4\bar{y}\right)\quad\text{with}$$

$\bar{x},\bar{y}\in\mathbb{R}^4$, $\bar{x}=(x^0,(x_j)_j)=(x^0,x)$, $\bar{y}=(y^0,(y_j)_j)=(y^0,y)$

Let $W=\int \partial_j J^0(\overline{x}) D_{jl}(\overline{x}-\overline{y}) \partial_l J^0(\overline{y}) d^4\overline{x} d^4\overline{y}$ and we obtain

$$W=-\int J^0(\overline{x}) D_{jl,jl}(\overline{x}-\overline{y}) J^0(\overline{y}) d^4\overline{x} d^4\overline{y}=\int J^0(\overline{x}) J^0(\overline{y}) \int \frac{1}{(2\pi)^4} \exp(i\omega(x^0-y^0))$$

$$\exp(-i\vec{k}\cdot(x-y)) \frac{\vec{k}^2}{\omega^2-c_P^2\vec{k}^2+i\varepsilon} d\omega d^3\vec{k}\, dx^0\, dy^0 d^3x d^3y=$$

$$=\left(\int \frac{1}{(2\pi)^3} dy^0\right)\left(U_0+2\int \exp(-i\vec{k}\cdot(x_0-y_0)) \frac{\vec{k}^2}{-c_P^2\vec{k}^2+i\varepsilon} d^3\vec{k}\right)$$

where U_0 not depends on x_0, y_0 .

Therefore $W=T\frac{U_0}{(2\pi)^3}-T\frac{2}{c_P^2}\int \frac{\exp(-i\vec{k}\cdot(x_0-y_0))}{(2\pi)^3} d^3\vec{k}$ (5)

As we noticed from Chap. Phonons in three dimensional crystals, the three oscillation modes $\omega_1(k)=c_P\|\vec{k}\|$ (longitudinal elastic waves) and $\omega_{2,3}(k)=c_T\|\vec{k}\|$ (transversal elastic waves) corresponding to the acoustic phonons described by the (4) Lagrangian density are valid only for small wave numbers with $\vec{k}^2a^2\ll 1$. Also in a cubic crystal with side lenght L , volume $V=L^3$, $\vec{k}$ takes values $\left(\frac{2\pi}{L}m_i\right)_{i=\overline{1,3}}$ with $m_i\in\mathbb{Z}$. Therefore the integral in (5) must be understood as

$\prod_{i=1}^{3}\left(\sum_{l=-q}^{q}\exp(-i\frac{2\pi}{L}l(x_0^i-y_0^i))\frac{1}{L}\right)=U$ and after some calculus we obtain

$U=\frac{1}{L^3}\prod_{i=1}^{3}\frac{\sin((2q+1)\kappa r_i)}{\sin(\kappa r_i)}$ where $\kappa=\frac{\pi}{L}$, $r_i=x_0^i-y_0^i$, $q\in\mathbb{N}$, $K=2\kappa q$ is defining the range of $\vec{k}$ such that $|k_i|\le K$, $Ka\ll 1$

taking $\vec{r}=(r_i)_i$, $r=\|\vec{r}\|$ we derive

$$U=\frac{1}{L^3}((2q+1)^3-\frac{2}{3}(2q+1)^3q(q+1)(\kappa r)^2+O((Kr)^4))$$

We must have $-iET=-\frac{i}{2}\overline{\sigma}^2W$ and so , with (5), to adding a independent of r constant, we can take for the energy the expression

$$E=E(\vec{r})=\frac{2}{3}\frac{\overline{\sigma}^2}{L^3c_P^2}((2q+1)^3q(q+1)(\kappa r)^2+O((Kr)^4))$$

The interaction force through phonon exchanging, acting on the x_0 electron is wiil be given by $\vec{F}(\vec{r})=-\nabla_{\vec{r}}E(\vec{r})$ and we conclude that if the distance between electrons is of the same magnitude as the lattice constant a , since $Ka\ll 1$ the interaction force is an attractive force $\vec{F}\approx\frac{4}{3}\frac{\overline{\sigma}^2}{L^3c_P^2}(2q+1)^3q(q+1)\kappa^2\vec{r}$.

Thus at growing distance between electrons it costs more and more energy to separate them, because above a specific value of the separation distance the phononic interaction force exceeds the electrostatic photonic interaction repulsive force which it’s shrinking with the inverse square distance.

Hence at low temperatures, electrons are confined in so called Cooper pairs with opposite spin angular momenta (according to Pauli exclusion principle) , which behave like spin 0 bosons.

At low temperatures $(T\to 0)$ the averaged occupation number for states $|\varepsilon_s\rangle$ with energy level ε_s, in the Bose-Einstein statistics satisfied by bosons at equilibrium temperature T is $\langle n_s\rangle=\frac{1}{\exp((\varepsilon_s-\mu)/(k_b T))-1}$ where μ is the chemical potential of the bosons , and tends to 0 for $T\to 0$, $\varepsilon_s>\mu$ and we must have $\varepsilon_s\geq\mu$.

This indicates that at low temperatures (below the Bose-Einstein condensation temperature) all bosons are in the same state which according to considerations in Chap. Quantum statistical ensemble must be the lowest energy state, the fundamental state (the fundamental lowest energy level is supposed to have no degeneracy). Thus the occupation of the fundamental state becomes macroscopic and the bosons form a Bose-Einstein condensate.

In the Bose-Einstein condensate of Cooper pair bosonic particles at low temperatures, all bosons behave in the same way, being in the same state and so under application of an electric field for example, they all move in the same direction, with zero entropy (at low temperatures , as we noticed in Chap. Quantum statistical ensemble , the entropy of the quantum statistical ensemble tends to zero) and superconductivity arises (zero rezistivity of the material).

Consider the field φ associated with the condensing Cooper pair bosons. According to above considerations we have to suppose that φ becomes non-zero below a temperature T_c . The field φ carries two units of electric charge and is therefore complex and so for interaction with an electromagnetic field we have a Lagrangian density $\mathscr{L}(\varphi,\partial\varphi,A,\partial A)=-\frac{1}{4}F^{\mu\nu}F_{\mu\nu}+(D^{\mu}\varphi)^{+}(D_{\mu}\varphi)-a\,\varphi^{+}\,\varphi-\frac{b}{2}(\varphi^{+}\varphi)^2$

where $D_{\mu}=\partial_{\mu}+2ieA_{\mu}$, $A_{\mu}=A_{\mu}(t,x)$, $\varphi=\varphi(t,x)$, $F_{\mu\nu}=\partial_{\mu}A_{\nu}-\partial_{\nu}A_{\mu}$

At equilibrium we have $\varphi=\varphi(x)$ and we admit an external magnetic field $\vec{B}=-\nabla\times\vec{A}$ with $A=(A_{\mu})_{\mu}=(0,\vec{A})$, $A=A(x)$.

At $T\to 0$ the entropy is zero and so the system free energy density is the same as the energy density $\mathscr{F}=\frac{\partial\mathscr{L}}{\partial(\partial_0 A)}(\partial_0 A)+\frac{\partial\mathscr{L}}{\partial(\partial_0\varphi^{+})}(\partial_0\varphi^{+})+\frac{\partial\mathscr{L}}{\partial(\partial_0\varphi)}(\partial_0\varphi)-\mathscr{L}=$

$=\frac{1}{4}F_{ij}F_{ij}+(D_i\varphi)^{+}(D_i\varphi)+a|\varphi|^2+\frac{b}{2}|\varphi|^4$

We suppose that for temperatures $T\approx T_c$ we have $a=a_1(T-T_c)$, $a_1>0$ while b remains positive so that the free energy is minimized by $\varphi=0$ above T_c and by $|\varphi|=\sqrt{-\frac{a}{b}}=v$ below T_c. As we learned in Chap. Effective potential, v is the vacuum expectation value of the field operator $\hat{\varphi}$.

Below T_c at equilibrium the free energy is therefore

$$\mathscr{F}=\frac{1}{4}F_{ij}F_{ij}+(2ev)^2\vec{A}^2-\frac{a^2}{2b}=\frac{1}{2}\vec{B}^2+(2ev)^2\vec{A}^2-\frac{a^2}{2b}$$

The material goes superconducting below T_c and so for constant magnetic field, since $\|\vec{A}\|$ grows as the distance, the total energy grows faster than the volume V (because of the $(2ev)^2\vec{A}^2$ term in the energy density) after the material goes superconducting and φ has a non-zero expectation value. Thus in a superconducting material we have to pay an unacceptable amount of extra energy to maintain the constant magnetic field and so it is more favorable to expel the magnetic field. This is the Meissner effect: magnetic fields are expelled from superconducting materials. The magnetic field leaks into the superconductor a bit over a length scale l determined by the competition between the energy in the magnetic field $F_{ij}^2\sim(\partial A)^2\sim\vec{A}^2/l^2$ and the Meissner term $(2ev)^2\vec{A}^2$. Thus we have the London penetration lenght of the magnetic field into the superconductor $l_L\sim(1/(ev))=\frac{1}{l}\sqrt{\frac{b}{-a}}$.

For a metalic conductor at regular equilibrium temperature T, the Fermi energy level $\mu=\epsilon_F$ is inside the conduction band spectrum and from the relation $N_e=\frac{gV}{\pi^2\sqrt{2}}(m^*k_bT)^{3/2}F(\frac{\mu}{k_bT})$ we established above we can extract $\mu=M(N,T,V)$ and for the energy levels ϵ close to the Fermi level $\mu=\epsilon_F$ we have $f(\epsilon)\approx\frac{1}{2}$ and therefore those energy levels are half occupied being in fact energy levels of conduction electrons. For conduction electrons having an energy close to Fermi level in the quasicontinuous conduction band spectrum we have $\epsilon=E(\vec{k})\approx\mu$ and in the same way as for $T\to 0$ we have $\delta\mu=-\sigma\frac{\delta V}{V}$.

The average energy of conduction electrons is

$$\varepsilon=\frac{1}{N_e}\int_0^\infty f(\epsilon)\rho(\epsilon)\epsilon d\epsilon=k_bT\frac{\int_0^\infty\frac{x^{3/2}dx}{1+\exp(x-\frac{\mu}{k_bT})}}{\int_0^\infty\frac{x^{1/2}dx}{1+\exp(x-\frac{\mu}{k_bT})}}$$ and we have $\varepsilon=\varepsilon(N,T,V)$ (6)

But now we have $\mu = M(N,T,V)$ and so $\frac{\partial M}{\partial V}\delta V = -\sigma\frac{\delta V}{V}$,

$\sigma = -V\frac{\partial M}{\partial V}(N,T,V)$, $\sigma = k_b T\frac{F(\frac{\mu}{k_b T})}{F'(\frac{\mu}{k_b T})}$ with

$F(\frac{\mu}{k_b T}) = \int_0^\infty \frac{\sqrt{x}}{1+\exp(x-\frac{\mu}{k_b T})}dx$, $F'(\frac{\mu}{k_b T}) = \int_0^\infty \frac{\exp(x-\frac{\mu}{k_b T})\sqrt{x}}{(1+\exp(x-\frac{\mu}{k_b T}))^2}dx$.

Thus we have a dependence $\sigma = \sigma(N,T,\mu) = \tilde{\sigma}(N,T,V)$, $\bar{\sigma} = \frac{\sigma}{\sqrt{\rho}}$ (6') .

The phonon-electron coupling constant $\bar{\sigma}$ dependence on thermodynamical parameters T , V and on crystal lattice constants (ρ is here the crystal mass density).
The electric charge transport, as we have seen in Chap. Electromagnetic four-potential … can be described by a charge current density field or charge flux $\vec{J}(t,x) = \rho(t,x)\vec{v}(t,x)$ where ρ is the electric charge density and $\vec{v}$ is the velocities field of the continuous distributed charges.
However in a metalic electric conductor the transported charge is quantized as conduction electrons individual charges e . Those conduction electrons have different velocities, due the random thermal velocity. The average velocity of the conduction electrons, when no electric field field is present , $\langle\vec{v}\rangle = \vec{0}$ since thermal velocities are completely random. When an external electric field is applied, free electrons gain velocity in the direction opposite to the electric field between succesive collisions thus acquiring a velocity component in that direction in addition to its random thermal velocity. As a result, there is a definite small drift velocity of electrons which is superimposed on he random motion of free electrons. Hence the actual charge flux is $\vec{J} = \rho\langle\vec{v}\rangle$ where $\langle\vec{v}\rangle = \vec{u}$ is the average velocity of free electrons in the presence the (constant) electric field and also the drift velocity.
The effects of collisions between different conduction electrons being also completely random compensate themselves and have no effect on the average velocity. Instead , free electrons are accelerated by the constant electric field and lose energy in inelastic collisions with the atomic kernels, nodes of the crystal lattice or equivalent, lose energy by emitting phonons, which are oscillations of the lattice nodes. Thus, equivalent to the effect of this decay of free electrons into lower energy electrons and phonons we introduce a mean friction force $\vec{F}_f = -f\langle\vec{v}\rangle$ (with f a constant positive coefficient) so that in presence of a constant electric field $\vec{E}$ we have an averaged motion equation $m^*\frac{d}{dt}\langle\vec{v}\rangle = e\vec{E} - f\langle\vec{v}\rangle$ where because we have to consider also interactions with the local crystal lattice field we take m^* the effective mass of conduction electrons.
The equation has the solution

$$\vec{u}=\left(\vec{u}_0-\frac{e\vec{E}}{f}\right)\exp\left(-\frac{f}{m^*}t\right)+\frac{eE}{f}\ . \qquad (7)$$

For $t\to\infty$ we obtain $\vec{u}=\frac{e\vec{E}}{f}=\frac{e}{m^*}\tau\vec{E}$ and so we will have a electric current density $\vec{J}=\sigma_c\vec{E}$ with $\sigma_c=\frac{N_e}{V}\frac{e^2}{m^*}\tau$ -the conductivity of the metal, (8)

noticing that $\tau=\frac{m^*}{f}$ is according to (7) the mean time of electrons travelling a distance under the action of electric field and the introduced mean friction force in the reference frame *R* that moves with the constant limit drift velocity $\vec{u}=\frac{e}{m^*}\tau\vec{E}$ with respect to the crystal lattice.

$\vec{J}$ determined by (8) is obviuosly the mean charge flux and if the conductor is a wire with normal to the electric field section area *S* then a charge *J S* passes thruogh the normal section in an unit of time . Thus the current intensity is *I = J S* .

The amount of work done by the field transporting a a positive charge unit along the wire is *U = E l* , where *l* is the length of the wire . Hence the difference in potential between the ends of the wire, known as voltage is

$U=\frac{J}{\sigma_c}l=\frac{l}{\sigma_c S}I$ and so the electric resistance of the wire will be $R=\frac{l}{\sigma_c S}$ having $U=RI$ the well known Ohm's law .

Therefore relation (8) for the charge flux expreesses Ohm’s law in terms of conductivity.

We have seen that the free electrons in the conductor are accelerated under the action of the constant electric field and slowed down under the action of the introduced averaged friction force which equivalates the lose of energy by emission of phonons in inelastic collisions with the nodes of the crystal lattice. Hence electrons are decaying into lower energy electrons and phonons and for this process we have a decay rate *Γ* which leads to a mean lifetime of such electrons equal to $\tilde{\tau}=\frac{1}{\Gamma}$.

From the interpretation of τ we have that τ is the mean time between collisions with crystal nodes and can also considered the mean lifetime of accelerated in the moving reference frame *R* electrons until they lose energy emitting a phonon . Because all accelerated electrons become electrons that suffer a decay we conclude that we must have $\tau=\tilde{\tau}$.

To compute Γ we consider the electron-phonon interaction Lagrangian density (4) (in which we have taken time and distance units such that $\hbar$ = 1 , *c* = 1) .

According to Feynman rules (see Chap. Feynman amplitudes and lattice gauge theory) the order $O(\bar{\sigma})$ Feynman amplitude of a electron decay with phonon emission is $A=(2\pi)^4\boldsymbol{M}\,\delta^4(k-k_1-k_2)$ where k is the incoming electron four-momentum, k_1 is the outgoing electron four-momentum,

$k_2=(\omega,\vec{k}_2)$ is the emitted phonon pulsation and wave vector and $\boldsymbol{M}=\bar{\sigma}\,\bar{u}(k_1,s_1)\gamma^0 u(k,s)\vec{k}_2\cdot\boldsymbol{e}^{s_2}(\vec{k}_2)$ where s_1,s ae the electrons spin polarization indices and s_2 is the phonon polarization index, $\boldsymbol{e}^{s_2}(\vec{k}_2)$ is the phonon polarization versor. It follows that we have to consider only longitudinal polarization direction and so $\omega=c_p\|\vec{k}_2\|$. Since the incoming electrons can have equally both polarizations and outgoing electrons polarizations are not measured, summing over s_1, averaging over s we obtain

$$|\boldsymbol{M}|^2=\frac{1}{2}\bar{\sigma}^2\,\mathrm{tr}\left(\frac{\not{k}_1+m}{2m}\gamma^0\frac{\not{k}+m}{2m}\gamma^0\right)\vec{k}_2^{\,2}$$

with $\not{k}=\gamma^\alpha k_\alpha$, m -the electron mass, $k^2-m^2=k_1^2-m^2=0$.

We have

$$\mathrm{tr}\left(\frac{\not{k}_1+m}{2m}\gamma^0\frac{\not{k}+m}{2m}\gamma^0\right)=1+\frac{k_1^0k^0+\vec{k}_1\cdot\vec{k}}{m^2}\ .$$

According to Chap. Decay rate and cross section and Chap. Feynman amplitudes and lattice gauge theory we have a differential decay rate

$$d\,\Gamma=\frac{m}{E_k}\frac{m\,d^3\vec{k}_1}{(2\pi)^3E_{k1}}\frac{d^3\vec{k}_2}{(2\pi)^3 2\omega}(2\pi)^4|\boldsymbol{M}|^2\delta^4(k-k_1-k_2)\ \text{ with } E_k=k^0=\sqrt{\vec{k}^2+m^2}\ ,$$

$E_{k1}=k_1^0=\sqrt{\vec{k}_1^{\,2}+m^2}$, $k_2^0=\omega=c_P\|\vec{k}_2\|$.

As we know from Chap. Canonical quantization of a scalar field we have

$$f(E_{k1},\vec{k}_1)\frac{d^3\vec{k}_1}{2E_{k_1}}=\theta(k_1^0)\,\delta(k_1^2-m^2)f(k_1)d^4k_1 \text{ with } \theta \text{ -the Heaviside function , so:}$$

$$\Gamma=\frac{m^2\bar{\sigma}^2}{(2\pi)^2}\int\frac{1}{2}\frac{\vec{k}_2^{\,2}}{k^0}\left(1+\frac{k^{02}-k^0c_P\|\vec{k}_2\|+\vec{k}^2-\vec{k}\cdot\vec{k}_2}{m^2}\right)\frac{\delta((c_P^2-1)\vec{k}_2^{\,2}-2k^0c_P\|\vec{k}_2\|+2\vec{k}\cdot\vec{k}_2)}{2c_P\|\vec{k}_2\|}$$

$$\theta(k^0-c_P\|\vec{k}_2\|)d^3\vec{k}_2=\frac{m^2\bar{\sigma}^2}{8\pi c_P}\int_0^{2(\|\vec{k}\|-k^0c_P)/(1-c_P^2)}\frac{r^2(2k^{02}-2k^0c_Pr-(r^2/2)(1-c_P^2))}{2m^2\|\vec{k}\|k^0}dr$$

This relation holds only for $w=\frac{\|\vec{k}\|}{k^0}>c_P$ otherwise following $\Gamma=0$.

The value *w* is the speed of the incoming in the decay process electron and can be taken as the thermal absolute mean velocity $\sqrt{\langle\vec{v}^2\rangle}$ which considering the conduction electrons at equilibrium temperature T, we have

$\varepsilon=\frac{m^*w^2}{2}$ and so we can take $w=\sqrt{2\varepsilon/m^*}$ with ε determined by relation (6). (9)

Obviously the $T\to 0$ expressions are aproximatively valid if we consider $T\ll T_0=\frac{\epsilon_F}{k_b}$ with ϵ_F from the (3') relation . T_0 is called Fermi temperature (degeneracy temperature) and computations show that solid metals at temperatures below the melting point can be considered in the $T\ll T_0$ case.

In this case the (6') relation reduces approximatively to (3') and the (6) relation becomes approximatively $\varepsilon = k_b T \frac{\int_0^{\mu/(k_b T)} x^{3/2} dx}{\int_0^{\mu/(k_b T)} x^{1/2} dx} = \frac{3}{5}\epsilon_F$ with ε_F from (3').

Thus for $w > c_P$ restoring $\hbar$ and c constants we obtain

$$\frac{f}{m^*} = \frac{1}{\tau} = \Gamma = \frac{c}{\hbar} \frac{\bar{\sigma}^2 k^{03}}{30\pi c_P w} \frac{(w - c_P)^3}{(c^2 - c_P^2)^4} (10c^2 - c_P^2 - 6w^2 - 3c_P w) \text{ with } k^0 = \frac{mc^3}{\sqrt{c^2 - w^2}}. \quad (10)$$

Relations (10) , (9) , (6) , (6') (8) determine the conductivity of the metal as a function of N , V , m^*, T, ρ. (we notice the proportionality to the density ρ).

For more accurate approximations, if $T \ll T_0$ we can expand after powers of $\frac{k_b T}{\mu}$.

Thus taking for $n > 0$ the function $K_n(\frac{\mu}{k_b T}) = \left(\frac{k_b T}{\mu}\right)^{n+1} \int_0^{\infty} \frac{x^n dx}{1 + \exp(x - \frac{\mu}{k_b T})}$

we have $F(\frac{\mu}{k_b T}) = \left(\frac{\mu}{k_b T}\right)^{n+1} K_{1/2}(\frac{\mu}{k_b T})$, $\varepsilon = \mu \frac{K_{3/2}(\frac{\mu}{k_b T})}{K_{1/2}(\frac{\mu}{k_b T})}$

and for $T \to 0$ we have $K_n(\frac{\mu}{k_b T}) = \sum_{k=0}^{\infty} \int_0^{\frac{\mu}{k_b T}} (-1)^k \frac{k_b T}{\mu} \left(1 - \frac{k_b T}{\mu} x\right)^n \exp(-kx) dx \approx$

$$\approx \frac{1}{n+1} + \sum_{k=1}^{\infty} n(-1)^{k+1} \left(\frac{k_b T}{\mu}\right)^2 \int_0^{\infty} \frac{1}{k^2} x \exp(-x) dx$$

We have $\sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{k^2} = \zeta(2) - \frac{1}{4}\zeta(2) - \frac{1}{4}\zeta(2) = \frac{1}{2}\zeta(2) = \frac{\pi^2}{12}$

with $\zeta(2) = \sum_{k=1} \frac{1}{k^2}$ the Riemann zeta function.

It follows that $K_n\left(\frac{\mu}{k_b T}\right)\approx\frac{1}{n+1}\left(1+\frac{\pi^2 n(n+1)}{12}\left(\frac{k_b T}{\mu}\right)^2\right)$

$N\approx\frac{2}{3}\frac{g V m^{*3/2}}{\pi^2\sqrt{2}}\mu^{3/2}\left(1+\frac{\pi^2}{16}\left(\frac{k_b T}{\mu}\right)^2\right)$

and taking $\mu_0=\lim_{T\to 0}\mu$, the value of ϵ_F given by (3') we can derive

$\mu\approx\mu_0\left(1-\frac{\pi^2}{24}\left(\frac{k_b T}{\mu_0}\right)^2\right)$, $\varepsilon\approx\frac{3}{5}\mu\left(1+\frac{\pi^2}{4}\left(k_b\frac{T}{\mu}\right)^2\right)\approx\frac{3}{5}\mu_0\left(1+\frac{5\pi^2}{24}\left(\frac{k_b T}{\mu_0}\right)^2\right)$.

$\sigma\approx\frac{2}{3}\mu\left(1-\frac{\pi^2}{12}\left(\frac{k_b T}{\mu}\right)^2\right)\approx\frac{2}{3}\mu_0\left(1-\frac{\pi^2}{8}\left(\frac{k_b T}{\mu_0}\right)^2\right)$.

Solids can conduct heat through the motion of electrons, atoms, ions. To estimate the thermal conductivity of metals, we calculate the contribution of conduction electrons, since metals have a large density of free electrons which have a thermal motion with the average speed *w* as we already established acoording to (9) and (6). Heat in a metalic body crystal lattice is generated by the independent oscillations of atoms in the nodes which can be expressed as a gas of phonons (see Chap. Phononic gas) . The transmission of heat occurs as a net flux of thermal energy (see Chap. Thermodynamics) $\vec{q}=-\kappa\nabla T$ (where κ is the thermal conductivity coefficient and $T=T(x)\in\mathbb{R}_+^*$ with $x\in D\subset\mathbb{R}^3$ is the temperatures field on the domain D of the metal considered as a union of subdomains around each *x* which can be supposed in thermodynamical equilibrium at temperature *T* (*x*)) through collisions of free electrons with the atomic nodes of the crystal lattice in which the electron absorbs or emits a phonon. The mean time between collisions is, as we established, the mean lifetime $\tau=\frac{1}{\Gamma}$ with Γ the above computed electron decay rate.

The net flux at location x in direction $i, \boldsymbol{e_i}=(\delta_{ij})_{j=\overline{1,3}}$ is the difference between what passes from left to right and from right to left.

Therefore taking $u=\frac{1}{\sqrt{3}}$ the mean speed in direction i (since thermal motion is completely random) we have $q_i=\frac{1}{2}n_e u\left(\tilde{\varepsilon}\left(T\left(x-u\,\tau\boldsymbol{e_i}\right)\right)-\tilde{\varepsilon}\left(T\left(x+u\,\tau\boldsymbol{e_i}\right)\right)\right)$ (11)

where $n_e=\frac{N_e}{V}$ is the concentration of conduction electrons and

$n\tilde{\varepsilon}(T)=\frac{U(T)}{V}$ with $n=\frac{N}{V}$ is the energy density of longitudinal phonons (since as we proved only longitudinal phonons interact with electrons).

Also , as we noticed, for a monovalent metalic material we can take $N = N_e$, $n = n_e$.

According to Chap. Phononic gas we have

$U=\frac{k_b^4 T^4 V}{2\hbar^3 c_P^3 \pi^2}\int_0^{\theta/T}\frac{x^3 d\,x}{\exp(x)-1}+\frac{3}{8}N k_b \theta$ with θ -Debye temperature, $k_b\theta=\hbar\,\omega_{max}$

$N=\frac{V}{6\pi^2 c_P^3}\omega_{max}^3$, $\omega_{max}=c_P\sqrt[3]{\frac{6N\pi^2}{V}}$

For $\frac{\theta}{T}\ll 1$ we have $U\approx\frac{3}{8}N k_b\theta+N k_b T\approx N k_b T$

and for $\frac{\theta}{T}\gg 1$ we have $U\approx\frac{\pi^2 k_b^4 T^4 V}{30 c_P^3\hbar^3}+\frac{3}{8}N k_b\theta$

In (11) the factor ½ accounts for the fact that electrons are likely to be moving in either direction. Only half contribute to the flux at a node location *x* .

Therefore $q_i=nu^2\tau\frac{d\varepsilon}{dT}\left(-\frac{\partial T}{\partial x_i}\right)$, $\vec{q}=-\frac{1}{3}w^2\tau\frac{1}{V}\left(\frac{\partial U}{\partial T}\right)_V(\nabla T)$ and so, since

$\frac{\tau}{V}=\frac{m^*}{Ne^2}\sigma_c$ we derive $\frac{\kappa}{\sigma_c}=\frac{1}{3}\frac{m^* w^2}{Ne^2}C_V=\frac{2}{3}\frac{\varepsilon}{Ne^2}C_V$

with $C_V=\left(\frac{\partial U}{\partial T}\right)_V$ -the specific heat of the metal (for longitudinal phonons only)

$C_V=N k_b$ for $\frac{\theta}{T}\ll 1$, $C_V=\frac{2}{15}\pi^2\frac{k_b^4 T^3}{c_P^3\hbar^3}$ for $\frac{\theta}{T}\gg 1$.

Obviously the the total specific heat of the metal is related to the considered above specific heat by a factor of $c_P^3\left(\frac{2}{c_T^3}+\frac{1}{c_P^3}\right)$ (see Chap. Phononic gas).

37. Hall effect. Quantum Hall effect. Fractional Hall effect Topological insulators

Hall effect. Quantum Hall effect
Fractional Hall effect. Topological insulators

Consider a flat rectangular conductor plate of length L in direction x , width w in direction y , and thickness b in direction z .

A constant magnetic field $(0,0,B_z)=\vec{B}$ is applied in direction z and a Hall voltage V_H is applied on the lenght sides from right to left in direction y in the positive oriented frame (O,x,y,z).

V_H is the work done by the system in transporting an unit of charge through the plate in y direction. Thus we have an electric field $\vec{E}=(0,E_y,0)$, $E_y=-\frac{V_H}{w}$.

The Lorentz force acting on conduction electrons which can move freely in the the $(O\,x\,y)$ plane is $\vec{F}=e\vec{E}+e(\vec{v}\times\vec{B})$ where $\vec{v}$ is the velocity of electrons and e is the electron charge.

Solving the $m\dot{\vec{v}}=\vec{F}$ equation of motion with $\vec{v}$ restricted to the $(O\,x\,y)$ plane we find out that

$$m\ddot{v}_x=e\dot{v}_y B_z=\frac{e}{m}(e\,E_y-e\,v_x B_z)B_z$$

$$m\ddot{v}_y=-e\dot{v}_x B_z=-\frac{e^2}{m}v_y B_z^2$$

$$\frac{d^2}{dt^2}(e\,E_y-e\,v_x B_z)=-\left(\frac{e\,B_z}{m}\right)^2(e\,E_y-e\,v_x B_z)$$

and so with $\omega=\frac{e\,B_z}{m}$ we have $v_y=C\sin(\omega t)$, $v_x=-C\cos(\omega t)+\frac{E_y}{B_z}$

Therefore a drift velocity appears in direction x :

$$w_x=\frac{E_y}{B_z}=-\frac{V_H}{w\,B_z}$$

If n is the volumic concentration of conduction electrons in the plate we obtain a current intensity in direction x in the plate given by :

$$I_x=n\,e\,w_x\,w\,b=-\frac{n\,e\,b\,V_H}{B_z}$$ and a Hall resistance $R_H=\frac{V_H}{I_x}=-\frac{B_z}{n\,e\,b}$.

Also the occuring current density in direction x is $j_x=n\,e\,w_x=\frac{n\,e}{B_z}E_y$ and so we have a Hall transversal conductivity $\sigma_{x\,y}=\frac{n\,e}{B_z}$ with $j_x=\sigma_{x\,y}E_y$

In the classical Hall effect a current I flows through a flat conductor plate on which a perpendicular to its surface external magnetic field is applied. The flowing charge carriers in the presence of the external magnetic field are sideway drifting under the action of the Lorentz force and so on the edges of the plate, perpendicular to the

current, a Hall voltage V_H appears so that we have a relation $R_H = V_H / I$ as we established above.

At sufficiently low temperatures and sufficiently strong magnetic fields, the inverse Hall resistance $1/R_H$ takes quantized values due to effects appearing in the quantum Hall system of electrons moving in a plane in presence of an external magnetic field.

If the field $\vec{B}=(0,0,B)$ is sufficiently strong, its effect dominates over the spin-orbit coupling and so all electrons in the quantum Hall system will have spin up (since the magnetic moment of the electrons aligns itself with the magnetic field) and so the can be treated as spinless charged particles.

Considering the gauge with $A=(A_\mu)_\mu=(0,\vec{A})=(0,0,-Bx,0)$ and m the effective mass of the conduction electrons in the plate (defined by $\frac{1}{m}=\frac{\partial^2 E}{\partial k^2}$, $E=E(k)$ -the energy levels corresponding to one single atom unperturbed solution from the crystal lattice) (see Chap. Phonon-electron interaction) , dropping the the z dependence (since the electrons move in the $(O\,x\,y)$ plane) we find out that in the presence of the magnetic field $\vec{B}=-\nabla\times\vec{A}$ the wave functions of the electrons $\psi=\psi(t,\vec{x})=\exp(-iEt)\,\psi(\vec{x})$ with $\vec{x}=(x,y)$ satisfy the time independent Schroedinger equation $\left(\frac{1}{2m}p_x^2+\frac{1}{2m}(p_y-eBx)^2\right)\psi=E\,\psi$ (1) with $p=(p_x,p_y)=-i(\partial_x,\partial_y)$ (considering as usual $c=1$, $\hbar=1$)

Searching for solutions $\psi=\xi(x)\exp(ik_y y)$ we obtain

$$-\frac{1}{2m}\xi''(x)+\frac{1}{2m}(-eBx+k_y)^2\,\xi(x)=E\,\xi(x) \qquad (2)$$

Taking $\zeta=x-\frac{k_y}{eB}$, $u(\zeta)=\xi(x)$ we will have

$$u''(\zeta)+2m\left(E-\frac{(eB)^2}{2m}\zeta^2\right)u(\zeta)=0$$

As in Chap. Quantum harmonic oscillator we obtain for $u = u(\zeta)$ the solutions

$u_n(\zeta)=u_0\exp(-\frac{1}{2}\chi^2)\,H_n(\chi)$ where $\chi=\frac{\zeta}{\zeta_0}$, $\zeta_0^2=\frac{1}{m\omega}$, $\omega=\frac{eB}{m}$ and H_n are the Hermite polynomials

$$H_n(\chi)=(-1)^n\exp(\chi^2)\frac{d^n}{d\chi^n}\exp(-\chi^2)=\sum_{k=0}^{\lfloor n/2\rfloor} n!\,\frac{(-1)^k}{k!(n-2k)!}(2\chi)^{n-2k}$$

which are a complete system in $L^2_{\exp(-\chi^2)}(\mathbb{R})$ having

$$\int_{-\infty}^{\infty} H_n(\chi)\,H_m(\chi)\exp(-\chi^2)\,d\chi=\sqrt{\pi}\,2^n n!\,\delta_{nm}$$

$E=E_n=(n+\frac{1}{2})\omega$, $n\in\mathbb{N}$ quantizes the Landau levels of energy.

(we suppose here $e\,B > 0$)

If L_x is the dimension of the plate in direction x and L_y is the dimension of the plate in direction y , since we assume Born-Karman cyclic boundary conditions

$\psi(x, y + L_y) = \psi(x, y)$ we will have $k_y = \frac{2\pi}{L_y}\kappa$ with $\kappa \in \mathbb{Z}$.
The motion equation corresponding to the Hamiltonian (1) is
$m\ddot{x} = \dot{p}_x = -\frac{2}{2m}(-k_y + eBx)$ and for having periodic motion of the harmonic oscillation, $-k_y + eBx$ must have a vanishing point for x in the $[a, a+L_x]$ domain of the x coordinates of the plate points (the rest point of the oscillator must be in $[a, a+L_x]$) and so $k_y \in [eBa, eBa+eBL_x]$.
Therefore $\kappa \in \left[\frac{eBaL_y}{2\pi}, \frac{eBaL_y}{2\pi} + \frac{eBL_xL_y}{2\pi}\right]$ and any Landau level has a degeneracy of $\frac{|eBS|}{2\pi}$ where $S = L_xL_y$ is the area of the conductor plate.
(we have $L_x = L$, $L_y = w$, $S = Lw$)
The magnetic elementar charge is $\frac{2\pi}{e}$ (see Chap. Magnetic monopole) and so $\frac{|eBS|}{2\pi} = N_\phi$ is also the number of flux quanta passing through the conductor plate.
We define a filling factor $\nu = \frac{N_e}{N_\phi}$ where N_e is the number of conduction electrons in the plate. When the Fermi level is between the ν -th and the ν +1 -th Landau level, the first ν Landau levels are totally filled and the levels above the ν -th Landau level are empty (at low absolute temperature) (see Chap. Phonon-electron interaction) .
So the filling factor is given by ν -th level of the Fermi level as a Landau level.
The current density in direction x is then
$j_x = new_x = \frac{eN_e}{Sb}\frac{E_y}{B} = \frac{e^2}{2\pi b}\frac{N_e}{N_\phi}E_y = \nu\frac{e^2}{2\pi}E_y$ and so (restoring the Planck constant) we obtain $\sigma_{xy} = \nu\frac{e^2}{bh}$, $I_x = j_x wb = -\sigma_{xy}V_H b$, $\frac{1}{R_H} = -\nu\frac{e^2}{h}$
We notice that for $\nu = N_e / N_\varphi$ equal to an integer the Hall fluid of electrons is incompressible. Any attempt to compress it lessens the degeneracy of the Landau levels (the effective area S decreases and so the degeneracy $eBS / 2\pi$ decreases) and forces some of the electrons to the next level , costing lots of energy.
An electric field E_y imposed on the Hall fluid in the y direction produces a current density $j_x = \sigma_{xy}E_y$ in x direction with $\sigma_{xy} = \nu\frac{e^2}{bh}$ (here j_x is the three-dimensional current density. However, the plate has a small thickness and we can consider the two-dimensional current density $J_x = j_x b$ and so $J_x = \tilde{\sigma}_{xy}E_y$ with quantized $\tilde{\sigma}_{xy} = \nu\frac{e^2}{h}$.

By experiments we discover that the Hall fluid is also incompressible for a fractional filling factor $\nu = N_e / N_\varphi$ (more precisely for ν^{-1} being an integer odd number). This is because of the interaction between electrons moving in the presence of the magnetic field. Saying the first Landau level is one third filled for example $\nu = 1/3$ with non-interacting spinless electrons does not define an unique many-body state: there is an enormous degeneracy since each of the electrons can go into any of the $\frac{eBS}{2\pi}$ states available, subject only to Pauli exclusion. But as soon as we consider repulsive interaction between the electrons a presumably unique ground state is picked out within the wast space of degenerate states for certain values of ν .
Suppose that ν^{-1} flux quanta are somehow bound to each electron ($N_\varphi / N_e = \nu^{-1}$) . So we arise to a theory of fractional quasiparticles ($\nu = 1/\kappa$ and an electron state can be considered as a tensorial product of κ qua siparticles states) in which the worldlines of quasiparticles braid around each other in (2+1) space-time (we are still in the case of the plane conductor plate).

Consider two undistinguishable quasiparticles at positions x_1^i, x_2^i at some initial time and end up at positions x_1^f, x_2^f a time T later. In the path integral representation $\langle x_1^f, x_2^f | \exp(-i\hat{H}T) | x_1^i, x_2^i \rangle$ we have to sum over all paths.

In space-time the worldlines of the two particles braid around each other (we are implicitly assuming that the particles cannot go through each other , which is the case if there is a hard core repulsion between them). The path can be divided into topologically distinct classes, characterized by an integer *n* equal to the number of timesthe worldlines of the two particles braid around each other. Since the classes cannot be deformed into each other, the corresponding amplitudes cannot interfere quantum mechanically and with the amplitudes in each class we are allowed to associate an additional phase factor $\exp(i\alpha_n)$ beyond the usual factor coming from the action . The dependence of α_n on *n* is determined by how the quantum amplitudes are to be combined.

Suppose one particle goes around the other through an angle $\Delta\varphi_1$, a history to which we assign an additional phase factor $\exp(if(\Delta\varphi_1))$ with f some as yet unknown function. Suppose this history is followed by another history in which our particle goes around the other by an additional angle $\Delta\varphi_2$. The phase factor $\exp(if(\Delta\varphi_1+\Delta\varphi_2))$ we assign to the combined history has to satisfy the composition law $\exp(if(\Delta\varphi_1+\Delta\varphi_2))=\exp(if(\Delta\varphi_1))\exp(if(\Delta\varphi_2))$. Therefore, since it is supposed to be continuous, *f* must be a linear function of its argument. Weconclude that in (2+1) dimensional space-time we can associate with the quantum amplitude in which one particle goes around the other anticlockwise through an angle $\Delta\varphi$ a phase factor $\exp(i(\theta/\pi)\Delta\varphi)$ with θ an arbitrary real parameter. Note that when one one particle goes around the other clockwise through an angle $\Delta\varphi$, the quantum amplitude acquires a phase factor $\exp(-i(\theta/\pi)\Delta\varphi)$.

When we interchange two such anyons, we have to be careful to specify whether we do it “anticlockwise” or “clockwise ” producing factors exp(*i* θ) and exp(- *i* θ)

respectively. This indicates imediately that parity P (and considering CPT theorem , time reversal T) are violated.

The Lagrangian density describing non-interacting spinless electrons in presence of a electromagnetic field having four-potential $A=(A_\mu)_\mu$ is

$\tilde{\mathscr{L}}_0=\psi^+ i(\partial_0+ie A_0)\psi+\frac{1}{2m}\sum_{j=1}^{3}\psi^+(\partial_j+ie A_j)^2\psi$ with m -effective mass of the electrons $\psi=\psi(t,x)$ complex scalar electron field .

Indeed, rewriting the $\psi^+(\partial_j+ie A_j)^2\psi$ term as the path integral formalism equivalent (by integration by parts) term $-((\partial_j-ie A_j)\psi^+)(\partial_j+ie A_j)\psi$ the motion equations $d_\mu\left(\frac{\partial\tilde{\mathscr{L}}_0}{\partial(\partial_\mu\psi^+)}\right)-\frac{\partial\tilde{\mathscr{L}}_0}{\partial\psi^+}=0$ lead to Schroedinger equation

$i\partial_0\psi=\left(\frac{1}{2m}\sum_{j=1}^{3}(\hat{p}_j+eA_j)^2+A_0\right)\psi$ with $\hat{p}_j=-i\partial_j$ which means that we obtain precisely the Hamiltonian operator of a charged spinless particle in electromagnetic field (we notice that above we have taken the potential as $A=A(x)$ with the gauge $\partial_j A_j=0$) .

Restricting to a (2+1) dimensional space-time we obtain for the invariance of the Lagrangian density under $\psi\to\exp(i\theta)\psi$ with θ as a real infinitesimal parameter (see Chap. Lagrangian field theory. Noether theorem) a conserved current given by $(J^\mu)_{\mu=\overline{0,2}}=(\psi^+\psi,\frac{i}{2m}((\partial_j\psi^+)\psi-\psi^+\partial_j\psi)_{j=1,2})$ and so, ignoring the $O(A^2)$ terms we can write the Lagrangian density as

$\tilde{\mathscr{L}}_0=\psi^+ i\partial_0\psi-\frac{1}{2m}\partial_j\psi^+\partial_j\psi-J^\mu A_\mu=\mathscr{L}_0-J^\mu A_\mu$

The current being conserved we have $\partial_\mu J^\mu=0$ and so we can define a vector potential $(a_\mu)_{\mu=\overline{0,2}}$ such that $J^\mu=-\frac{1}{2\pi}\epsilon^{\mu\nu\lambda}\partial_\nu a_\lambda$ with $\epsilon_{\mu\nu\lambda}=\epsilon^{\mu\nu\lambda}$ the signature of the permutation $\begin{pmatrix}\mu & \nu & \lambda\\ 0 & 1 & 2\end{pmatrix}$. (we consider $B>0$)

When we transform $a_\mu\to a_\mu+\partial_\mu\Lambda$ with $\Lambda=\Lambda(t,\vec{x})$ the current $(J^\mu)_\mu$ remains unchanged and so we can consider $(a_\mu)_\mu$ as a gauge potential.

A gauge invariant theory of the interacting electrons as systems of quasiparticles in a electromagnetic field, interesting only physics at long distances and large time, that is small wave numbers and low frequencies so that second order derivatives in space-time variables can be ignored, will be described by a Lagrangian density

$\mathscr{L}=\frac{\kappa}{4\pi}a_\mu\epsilon^{\mu\nu\lambda}\partial_\nu a_\lambda+\mathscr{L}_q+a_\mu j^\mu-eJ^\mu A_\mu$ (3)

where $\mathscr{L}_q$ is the Lagrangian density for the free quasiparticles field, that is considered as the particles field coupling to the gauge potential $(a_\mu)_\mu$ and has the conserved current $(j^\mu)_\mu$.

As free particles the quasiparticles are fermions and
$\mathscr{L}_q$ can be a Dirac Lagrangian density in (2+1) dimensional space-time or a Lagrangian density for free spinless charged particles.
(it has significance that the quasiparticles obey to Fermi statistics as free from the gauge potential $(a_\mu)_\mu$ particles and that an electron can be considered equivalent to a defined number κ of quasiparticles: $\kappa q = e$ where q is the charge of a quasiparticle) .
In the same way as for the Fadeev-Popov method in Chap.Quantum electrodynamics, we can fix the gauge for $(a_\mu)_\mu$ taking an effective Lagrangian density
$\mathscr{L}_{eff} = \mathscr{L} - \frac{1}{2\xi}(\partial^\mu a_\mu)^2$ and for the gauge $\xi = 0$ corresponding to $\partial^\mu a_\mu = 0$ we find a propagator for the $(a_\mu)_\mu$ field given by

$$D_{\lambda\varepsilon}(k) = (-\frac{2\pi}{\kappa} i\,\epsilon_{\lambda\varepsilon\rho}k^\rho - \xi\eta_{\lambda\varepsilon})\frac{1}{k^2 + i\varepsilon} = -\frac{2\pi}{\kappa} i\,\epsilon_{\lambda\varepsilon\rho}k^\rho$$

$$D_{\lambda\varepsilon}(x-y) = \frac{1}{(2\pi)^3}\int D_{\lambda\varepsilon}(k)\exp(i\,k(x-y))\,d^3k$$

Defining $\tilde{j}^\mu = j^\mu + \frac{e}{2\pi}\epsilon^{\mu\lambda\nu}\partial_\lambda A_\nu$ after integration by parts in the $J^\mu A_\mu$ term and integrating out the gauge field $(a_\mu)_\mu$ in the path integral formalism for the (3) Lagrangian density (see Chap. Path integral formalism) we obtain an equivalent action for the quasiparticles field given by

$$S = \frac{\pi}{\kappa}\int \tilde{j}^\lambda(x)\left(\int \frac{1}{(2\pi)^3}\frac{i\,\epsilon_{\lambda\varepsilon\rho}k^\rho}{k^2}\exp(i\,k(x-y))\,d^3k\right)\tilde{j}^\varepsilon(y)\,d^3x\,d^3y + \int \mathscr{L}_q\,d^3x \quad (4)$$

Expanding the first integrand from (4) we have a $j\,j$ term , a $A\,j$ term and a $A\,A$ term.
The $j\,j$ term is equal to $\frac{\pi}{\kappa}\int j^\mu(x)\frac{\epsilon_{\mu\nu\lambda}\partial_\nu}{\partial^2}j^\lambda(x)\,d^3x$ (4')
With the gauge $\partial^\mu A_\mu = 0$ the $A\,j$ term turns out to be $\int -\frac{e}{\kappa}j^\mu(x)A_\mu(x)\,d^3x$ (4")
and the $A\,A$ term becomes $\frac{e^2}{4\pi\kappa}\int -A_\mu(x)\,\epsilon^{\mu\nu\lambda}\partial_\nu A_\lambda(x)\,d^3x$ (4''')
From (4') we conclude that quasiparticles interact with each other via $\frac{\pi}{\kappa}j^\mu\frac{\epsilon_{\mu\nu\lambda}\partial_\nu}{\partial^2}j^\lambda$, from (4") we derive that quasiparticles must have electric charge $\frac{e}{\kappa} = q$ and taking $\mathscr{L}_{em}(A,\partial A) = -\frac{e^2}{4\pi\kappa}A_\mu\epsilon^{\mu\nu\lambda}\partial_\nu A_\lambda$, considering that $\int \mathscr{L}_{em}d^3x = \int\left(\frac{\partial\mathscr{L}_{em}}{\partial A_\mu} - d_\nu\left(\frac{\partial\mathscr{L}_{em}}{\partial(\partial_\nu A_\mu)}\right)\right)A_\mu + O((A,\partial A)^2)\,d^3x$ we can consider that the electromagnetic term (4''') defines an electromagnetic current $(J^\mu_{em})_\mu$ with

$$e\,J^\mu_{em} = -\left(\frac{\partial\mathscr{L}_{em}}{\partial A_\mu} - d_\nu\left(\frac{\partial\mathscr{L}_{em}}{\partial(\partial_\nu A_\mu)}\right)\right) = \frac{e^2}{2\pi\kappa}\epsilon^{\mu\nu\lambda}\partial_\nu A_\lambda\ .$$

Since $A = (A_0(x), A_1(x), A_2(x))$ in the (2+1) dimensional approach we will have for $\mu = 0$ that the density of electrons is

$\frac{N_e}{S}=J^0_{em}=-\frac{eB}{2\pi\kappa}$ and since the number of flux quanta (for $B>0$) is $N_\phi=-\frac{eBS}{2\pi}$ we obtain a filling factor $\nu=\frac{N_e}{N_\phi}=\frac{1}{\kappa}$ where $B=\partial_2 A_1-\partial_1 A_2$.

For $\mu=2$ we obtain $eJ^1_{em}=\nu\frac{e^2}{h}E_2$ where $E_2=\partial_0 A_1-\partial_1 A_0$ is the electric field in y direction: When an electric field E_y is applied in y direction an electric current appears in x direction having density $J^x=\nu\frac{e^2}{h}E_y$.

This is the fractional Hall effect since as we will prove , the filling factor $\nu = 1/\kappa$ is fractional (an inverse odd number).

From the Lagrangian density (3) we derive Euler-Lagrange equations of motion for the field $(a_\mu)_\mu$: $\frac{\kappa}{2\pi}\epsilon^{\mu\nu\lambda}\partial_\nu a_\lambda=-j^\mu$ (5)

The Lagrangian density for the quasiparticles being $\mathscr{L}_q+j^\mu a_\mu$ from the Aharonov-Bohm effect results that when one quasiparticle moves around another on the $\Gamma=\partial D$, Γ surrounding the quasiparticle in D,the wave function acquires a phase $\Delta\varphi=\int_\Gamma \vec{a}\,d\vec{x}=\int_D(\partial_1 a_2-\partial_2 a_1)d^2\vec{x}=-\frac{2\pi}{\kappa}\int j^0 d^2\vec{x}$.

The surrounded particle is in D and so, since j^0 is the probability density of the quasiparticles, we have $\int_D j^0 d^2\vec{x}=1$.

Thus when a quasiparticle moves around another (in the ($O\,x\,y$) plane) with an angle π anticlockwise the wave function of the particle acquires a phase $-\pi/\kappa$ and so the quasiparticles are anyons with a fractional statistics angle π/κ .

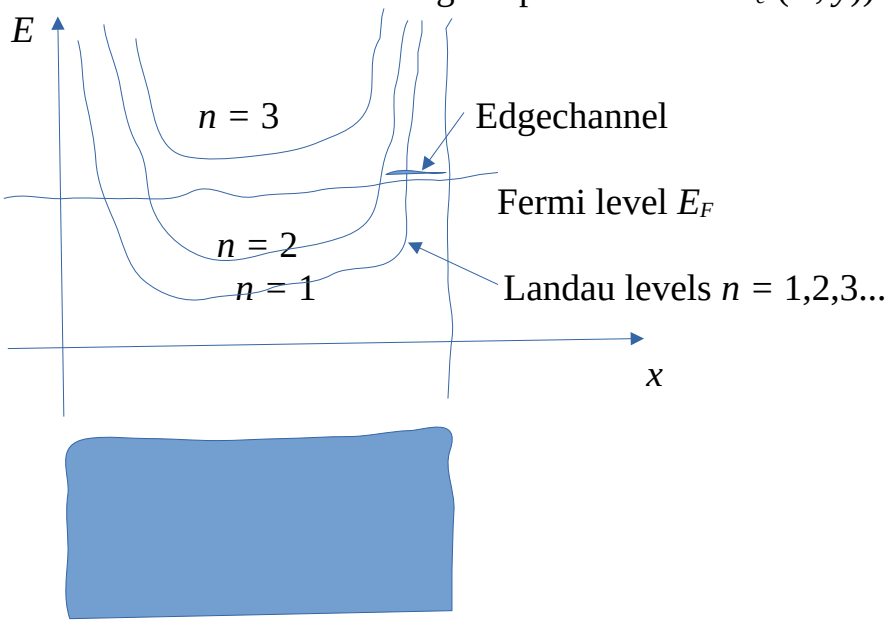
As we mentioned, a conduction electron in the plane conductor plate is equivalent to a product of κ quasiparticles. Thus when we interchange two electrons we interchange κ times two quasiparticles and according to Fermi statistics of quasiparticles, the combined wave function of the two electrons will be multiplied after interchanging with $(-1)^\kappa$. Since electrons are also fermions it follows that $\nu^{-1}=\kappa$ must be an odd integer number.

The interaction of conduction electrons in the conductor plate is now due the interaction of arbitrary quasiparticles which will have the tendency to bond each other into another electrons. Since κ quasiparticles form an electron, bond systems of κ quasiparticles from diferent electrons are forming. Interchanging two such bond systems means moving one bond system around the another with π angle and at the same time rotating each bond system around its center with a π angle.

So we move κ quasiparticles around κ quasiparticles with a π angle which brings a total phase factor $\exp(i\kappa^2\frac{\pi}{\kappa})=\exp(i\kappa\pi)$ and we rotate the coordinates in each bond system of κ quasparticles with π angle which since the quasiparticles are fermions and therefore behave like half integer spin particles brings a phase factor to

the tensorial product wave function of $\exp(i2\kappa\frac{\pi}{2})=\exp(i\kappa\pi)$. So the total phase factor is $\exp(i\kappa\pi)\exp(i\kappa\pi)=1$ and we conclude that the bond systems of κ quasiparticles behave like bosons, obeying to Einstein-Bose statistics.

Considering for a semiconductor or insulator flat plate as a simple example an edge potential $V_e=V_e(\vec{x})$, $\vec{x}=(x,y)\in\mathbb{R}^2$ which has significant values only in the close neighbourhood of the boundary of the plate domain, the time independent Schroedinger equation solutions in presence of an external magnetic field (0 , 0 , B), $(\frac{1}{2m}p_x^2+\frac{1}{2m}(p_y-eBx)+V_e(\vec{x}))\psi=E\psi$ with m -the effective mass of the electrons, $\frac{1}{m}=\frac{\partial^2 E}{\partial k^2}$, $E=E(k)$ the energy levels of electrons corresponding to a single atom unperturbed solution in the crystal lattice, will determine a dependence on (x , y) of the Landau levels at the edges of the sample such that the Landau levels E_n are increasing at the edges (see fig.) (we can understand that in the way that for extracting an electron from the material at the edges we need to do some additional work which translates as overcoming the potential wall V_e (x , y)) .



Since for semiconductors and insulators The Fermi level lays between the valence band and the conduction band, as we can see from figure in the interior of the sample there are no conduction levels below the Fermi level and electrons cannot move freely in the interior of the sample. The average occupation number of a E_n level at equilibrium temperature T is $\langle n\rangle=\frac{1}{1+\exp((E_n-E_F)/(k_bT))}$ and so at the Fermi level, the Landau levels are half occupied and therefore electrons can have transitions between different energy levels when they are at the intersection between the Landau

levels and the Fermi level where the Landau levels are elevated. Therefore in the so arising edgechannels electrons are free to move, not being bounded on a specific location bounding valence band energy level. So conduction is possible in the edgeregions of the sample, in the presence of a magnetic field that induces the Landau levels.

The material is no more an insulator in the topological invariant regions that are determined by the intersections of the Fermi level and the profiles of the Landau levels, which are commonly at the edges of the material.

38. Casimir effect

Casimir effect

Consider two parallel plane plates in vacuum separated by a distance D and the electromagnetic field between the plates with $(\vec{E},\vec{B})=(\vec{E},\vec{B})(t,x)\in\mathbb{R}^6, \vec{E}=(E_i)_{i=\overline{1,3}}$, $\vec{B}=(B_i)_{i=\overline{1,3}}, x=(x^i)_{i=\overline{1,3}}$, $(t,x)\in\mathbb{R}^4$ electric intensity and respective magnetic induction fields between plates. As often before we will consider (by suitable choosing of time , length, electric charge measuring unities) that the speed of light in vacuum constant c = 1, the reduced Planck constant $\hbar$ = 1 , the electric permittivity of vacuum constant ε_0 = 1 .

The electromagnetic field undergoes quantum fluctuations and would contribute with its two polarization degrees of freedom to the energy density of vacuum, the amount $\varepsilon=\int \hbar\,\omega_{\vec{k}}\frac{d^3\vec{k}}{(2\pi)^3}$ energy of vacuum between the plates per unit volume, where because of the established distance between plates, only certain discrete values of the momentum $\vec{k}$ are allowed. (see Chap. Quantization of an electromagnetic field) .

While ε is not observable, the shift $\Delta\varepsilon$ by disturbing the vacuum should be observable since we can control how we disturb the vacuum. The variation of $\Delta\varepsilon$ with the distance D would lead to a force acting between the plates known as the Casimir force.

To calculate this force we vary D , but then we would have to worry about how the energy density outside the plates varies. To avoid this we introduce three plates. We hold the two outer plates fixed and move only the inner plate. The outer plates are at distance L_1 from each to other and the inner plate is at distance D from the left outer plate. If $f(D)$ is the vacuum energy between plates at distance D from each other, the total vacuum energy between plates is $E(D) = f(D) + f(L_1 - D)$ and the Casimir force acting on the inner plate is $-\frac{\partial E}{\partial D}=f'(L_1-D)-f'(D).$

To evaluate $f(D)$ we consider as usual the electromagnetic field between plates confined in a box $B=\{x\in\mathbb{R}^3 | x^1,x^2\in(0,L)\ ,\ x^3\in(0,D)\}$. Also we consider that B has a conducting boundary such that (see Chap. Electric dipole ...) $\vec{E}$ satisfies the boundary conditions $E_i(t,x^1,x^{2,0})=E_i(t,x^1,x^2,D)=0$ for $i=1,2$;

$E_i(t,0,x^2,x^3)=E_i(t,L,x^2,x^3)=0$ for $i=2,3$;

$E_i(t,x^1,0,x^3)=E_i(t,x^1,L,x^3)=0$ for $i=1,3$.

The Maxwell equations are :

$\nabla\times\vec{E}=-\frac{\partial\vec{B}}{\partial t}$ (1) ; $\nabla\cdot\vec{B}=0$ (2) ; $\nabla\cdot\vec{E}=0$ (3) ; $\nabla\times\vec{B}=\frac{\partial\vec{E}}{\partial t}$ (4) ;

leading to $\frac{\partial^2\vec{E}}{\partial t^2}-\nabla^2\vec{E}=0$ (5) ; $\frac{\partial^2\vec{B}}{\partial t^2}-\nabla^2\vec{B}=0$ (6) .

For $t, x^1, x^2 \in \mathbb{R}$ let $F(z) = E_1(t, x^1, x^2, z + \frac{1}{2}D)$. From the boundary conditions we have $F(-\frac{D}{2}) = F(\frac{D}{2}) = 0$

and for $g(z) = \frac{1}{2}(F(z) + F(-z))$, $h(z) = \frac{1}{2}(F(z) - F(-z))$ we have

$g(-\frac{D}{2}) = g(\frac{D}{2}) = h(-\frac{D}{2}) = h(\frac{D}{2}) = 0$.

We can Fourier expand :

$$h = \sum_{m=0}^{\infty} a_m \cos\left(\frac{2\pi m}{D} z\right) + \sum_{m=0}^{\infty} b_m \sin\left(\frac{2\pi m}{D} z\right) \quad \text{with}$$

$$b_m = \frac{2}{D} \int_{-D/2}^{D/2} h(z) \sin\left(\frac{2\pi m}{D} z\right) dz \quad , \quad a_m = \frac{2}{D} \int h(z) \cos\left(\frac{2\pi m}{D} z\right) dz$$

and since h is odd we obtain $h = \sum_{m=0}^{\infty} b_m \sin\left(\frac{2\pi m}{D} z\right)$.

We extend g to $\tilde{g} : [-D, D] \to \mathbb{R}$ by

$\tilde{g}(-\frac{D}{2} - z) = -g(-\frac{D}{2} + z)$, $\tilde{g}(\frac{D}{2} + z) = -g(\frac{D}{2} - z)$ for $z \in [0, \frac{D}{2}]$ and notice that $\tilde{g}$ is a even function on $[-D, D]$.

Fourier expanding :

$$\tilde{g} = \sum_{m=0}^{\infty} c_m \cos\left(\frac{\pi m}{D} z\right) + \sum_{m=0}^{\infty} d_m \sin\left(\frac{\pi m}{D} z\right) \quad \text{with}$$

$c_m = \frac{1}{D} \int_{-D}^{D} \tilde{g}(z) \cos\left(\frac{\pi m}{D} z\right) dz$, $d_m = \frac{1}{D} \int_{-D}^{D} \tilde{g}(z) \sin\left(\frac{\pi m}{D} z\right) dz$ since $\tilde{g}$ is even we obtain $d_m = 0$ and also we have

$$c_{2m} = \frac{1}{D} \int_{-D}^{D} \tilde{g}(z) \cos\left(\frac{2\pi m}{D} z\right) dz = \frac{2}{D} \int_{0}^{D/2} g(z) \cos\left(\frac{2\pi m}{D} z\right) dz +$$

$$+ \frac{2}{D} \int_{0}^{D/2} \tilde{g}(z + \frac{D}{2}) \cos\left(\frac{2\pi m}{D} + m\pi\right) dz = \frac{2}{D} \int_{0}^{D/2} g(z) \cos\left(\frac{2\pi m}{D} z\right) z -$$

$$- \frac{2}{D} \int_{0}^{D/2} g(\frac{D}{2} - z) \cos\left(\frac{2\pi m}{D} z + m\pi\right) dz = 0 .$$

Therefore we will have

$$g = \sum_{m=0}^{\infty} c_{2m+1} \cos\left(\frac{(2m+1)\pi}{D} z\right) ,$$

$$F = g + h = \sum_{m=0}^{\infty} c_{2m+1} \cos\left(\frac{(2m+1)\pi}{D} z\right) + b_m \sin\left(\frac{2\pi m}{D} z\right) .$$

$$E_1(t,x^1,x^2,z)=F(z-\frac{D}{2})=\sum_{m=0}^{\infty}(-1)^m\left(c_{2m+1}\sin\left(\frac{(2m+1)\pi}{D}z\right)+b_m\sin\left(\frac{2m\pi}{D}z\right)\right)$$

$$E_1(t,x^1,x^2,x^3)=\sum_{m=0}^{\infty}A_m(t,x^1,x^2)\sin\left(\frac{m\pi x^3}{D}\right)$$ which multiplied with $\sin\left(\frac{m\pi x^3}{D}\right)$ and integrated over x^3 on $(0,D)$ leads to

$$A_m(t,x^1,x^2)=\frac{2}{D}\int_0^D E_1(t,x^1,x^2,x^3)\sin\left(\frac{m\pi x^3}{D}\right)dx^3$$

and so $A_m(t,x^1,0)=A_m(t,x^1,L)$.

In the same way as above we obtain

$$A_m(t,x^1,x^2)=\sum_{n=0}^{\infty}A_{mn}(t,x^1)\sin\left(\frac{n\pi x^2}{L}\right)$$ and so

$$E_1(t,x^1,x^2,x^3)=\sum_{n2,n3=0}^{\infty}A_{n2n3}(t,x^1)\sin\left(\frac{n_2\pi x^2}{L}\right)\sin\left(\frac{n_3\pi x^3}{D}\right)$$ and we have analog relations for E_2 and E_3 .

Considering the above results we will seek for solutions for the Maxwell system of equations on *B* with the given boundary conditions that have the form

$$E_1=C_1(t)A_1(x^1)\sin\left(\frac{n_2\pi x^2}{L}\right)\sin\left(\frac{n_3\pi x^3}{D}\right)$$

$$E_2=C_2(t)A_2(x^2)\sin\left(\frac{n_1\pi x^1}{L}\right)\sin\left(\frac{n_3\pi x^3}{D}\right)$$

$$E_3=C_3(t)A_3(x^3)\sin\left(\frac{n_1\pi x^1}{L}\right)\sin\left(\frac{n_2\pi x^2}{L}\right)$$

Indexing $(t,x)=(x^\alpha)_{\alpha=\overline{0,3}}$ with the notation $G_{,\alpha}=\frac{\partial G}{\partial x^\alpha}$, from the Maxwell equations we obtain $E_{1,00}=B_{3,02}-B_{2,03}=E_{1,022}+E_{1,033}-E_{2,012}-E_{3,013}$,

$$C_1''(t)A_1(x^1)\sin\left(\frac{n_2\pi x^2}{L}\right)\sin\left(\frac{n_3\pi x^3}{D}\right)=$$

$$=-\left(\frac{n_2^2\pi^2}{L^2}+\frac{n_3^2\pi^2}{D^2}\right)C_1(t)A_1(x^1)\sin\left(\frac{n_2\pi x^2}{L}\right)\sin\left(\frac{n_3\pi x^3}{D}\right)-$$

$$-C_1'(t)A_2'(x^2)\frac{n_1\pi}{L}\cos\left(\frac{n_1\pi x^1}{L}\right)\sin\left(\frac{n_3\pi x^3}{D}\right)-$$

$$-C_3'(t)A_3'(x^3)\frac{n_1\pi}{L}\cos\left(\frac{n_1\pi x^1}{L}\right)\sin\left(\frac{n_2\pi x^2}{L}\right)$$

This relation is of the form

$$\left(C_1''(t)+\left(\frac{n_2^2\pi^2}{L^2}+\frac{n_3^2\pi^2}{D^2}\right)C_1(t)\right)A_1(x^1)H(x^2,x^3)=\cos\left(\frac{n_1\pi x^1}{L}\right)G(t,x^2,x^3)$$

and therefore we must take $A_1(x^1)=C\cos\left(\frac{n_1\pi x^1}{L}\right)$ with C a constant.

Having the freedom of choosing $C_i(t)$ we can take $C=1$.
In the same way we derive similar relations for A_2, A_3 and so we have

$$A_1(x^1)=\cos\left(\frac{n_1\pi x^1}{L}\right)\quad,\quad A_2(x^2)=\cos\left(\frac{n_2\pi x^2}{L}\right)\quad,\quad A_3(x^3)=\cos\left(\frac{n_3\pi x^3}{D}\right)$$

and from (5) we obtain now $C_i''(t)=-\omega_{\vec{k}}^2 C_i(t)$

with $\omega_{\vec{k}}=\|\vec{k}\|$, $\vec{k}=\left(\frac{n_1\pi}{L},\frac{n_2\pi}{L},\frac{n_3\pi}{D}\right)$

Hence the solutions for $\vec{E}$ are of the form $\vec{E}=\sum_{n1,n2,n3\in\mathbb{N}}\vec{E}^{(\vec{k})}+\vec{\widetilde{E}}^{(\vec{k})}$ (7) where

$$E_1^{(\vec{k})}=A_1^{(\vec{k})}\cos(k_1x^1)\sin(k_2x^2)\sin(k_3x^3)\cos(\omega_{\vec{k}}t)$$
$$E_2^{(\vec{k})}=A_2^{(\vec{k})}\sin(k_1x^1)\cos(k_2x^2)\sin(k_3x^3)\cos(\omega_{\vec{k}}t)$$
$$E_3^{(\vec{k})}=A_3^{(\vec{k})}\sin(k_1x^1)\sin(k_2x^2)\cos(k_3x^3)\cos(\omega_{\vec{k}}t)$$
$$\widetilde{E}_1^{(\vec{k})}=\widetilde{A}_1^{(\vec{k})}\cos(k_1x^1)\sin(k_2x^2)\sin(k_3x^3)\sin(\omega_{\vec{k}}t)$$
$$\widetilde{E}_2^{(\vec{k})}=\widetilde{A}_2^{(\vec{k})}\sin(k_1x^1)\cos(k_2x^2)\sin(k_3x^3)\sin(\omega_{\vec{k}}t)$$
$$\widetilde{E}_3^{(\vec{k})}=\widetilde{A}_3^{(\vec{k})}\sin(k_1x^1)\sin(k_2x^2)\cos(k_3x^3)\sin(\omega_{\vec{k}}t)\ .$$

with $\vec{k}\cdot\vec{A}^{(\vec{k})}=0$, $\vec{k}\cdot\vec{\widetilde{A}}^{(\vec{k})}=0$ (because $\nabla\cdot\vec{E}=0$) $\vec{k}=(k_i)_i=\left(\frac{n_1\pi}{L},\frac{n_2\pi}{L},\frac{n_3\pi}{D}\right)$

$\vec{A}^{(\vec{k})}=(A_i^{(\vec{k})})_i$, $\vec{\widetilde{A}}^{(\vec{k})}=(\widetilde{A}_i^{(\vec{k})})_i$.

We notice that if $n_i=0$ then $\vec{E}^{(\vec{k})}$ and $\vec{\widetilde{E}}^{(\vec{k})}$ has only the i-direction component not vanishing and if $n_i\neq 0$ we can decompose $\vec{A}^{(\vec{k})}$ and $\vec{\widetilde{A}}^{(\vec{k})}$ in two normal to $\vec{k}$ components that are independent.
Thus (7) becomes $\vec{E}=\sum_{\vec{k}}\sum_{p\in W_{\vec{k}}}(\vec{E}_{\vec{k}}^{p}\exp(-i(\omega_{\vec{k}}t-\vec{k}\cdot x))+\vec{E}_{\vec{k}}^{p*}\exp(i(\omega_{\vec{k}}t-\vec{k}\cdot x)))$

with $\vec{k}=\left(\frac{n_1\pi}{L},\frac{n_2\pi}{L},\frac{n_3\pi}{D}\right)$, $n_1,n_2,n_3\in\mathbb{Z}$, $\omega_{\vec{k}}=\|\vec{k}\|$, $\vec{k}\cdot\vec{E}_{\vec{k}}^{p}=0$, $\vec{E}_{\vec{k}}^{p}\in\mathbb{C}^3$,
$W_{\vec{k}}=\{1\}$ if $n_1n_2n_3=0$ and $W_{\vec{k}}=\{1,2\}$ if $n_1n_2n_3\neq 0$.
Therefore (see Chap. Quantization of a electromagnetic field) the vacuum energy between the two plates, for the B domain with conducting boundary is

$$f(D)=\sum_{n1,n2,n3\in\mathbb{Z}^*}\hbar\,\omega_{\vec{k}}+\frac{1}{2}\sum_{\substack{n1,n2,n3\in\mathbb{Z}\\ n1n2n3=0}}\hbar\,\omega_{\vec{k}}\ .$$

The sums are obviously divergent . We take a cutoff of the k-domain by excluding

large $k=\|\vec{k}\|$ through a factor $\exp(-k/k_c)$ with $k_c \gg 1$. For large L we turn the sum over n_1, n_2 into an integral over k_1, k_2 and so (restoring $\hbar, c$) we obtain:

$$f(D)=\frac{\hbar c L^2}{\pi^2}\left(2\sum_{n3=1}^{\infty}\int\left(k_1^2+k_2^2+\frac{n_3^2\pi^2}{D^2}\right)^{1/2}\exp\left(\frac{-k}{k_c}\right)dk_1\,dk_2+\right.$$

$$\left.+\frac{1}{2}\int(k_1^2+k_2^2)^{1/2}\exp\left(\frac{-\kappa}{k_c}\right)dk_1\,dk_2\right) \quad \text{with } k=\left(k_1^2+k_2^2+\frac{n_3^2\pi^2}{D^2}\right)^{1/2} \quad , \quad \kappa=(k_1^2+k_2^2)^{1/2}$$

$$f(D)=\frac{\hbar c L^2}{\pi^2}\left(2\sum_{n=1}^{\infty}\int_{n\pi/D}^{\infty}2\pi k^2\exp(-k/k_c)\,dk+\frac{1}{2}\int_0^{\infty}2\pi\kappa^2\exp(-\kappa/k_c)\,d\kappa\right)$$

After some calculus we derive

$$f(D)=\frac{\hbar c L^2 k_c^3}{\pi}\left(a^2\frac{d^2}{da^2}\left(\frac{4}{1-\exp(-a)}\right)-a\frac{d}{da}\left(\frac{8}{1-\exp(-a)}\right)+\frac{8\exp(-a)}{1-\exp(-a)}+2\right)=$$

$$=\frac{2\hbar c\pi^2 L^2}{D^3}\widetilde{f}(a) \quad \text{where } a=\frac{\pi}{k_c D} \quad ,$$

$$\widetilde{f}(a)=\frac{2\exp(-a)(1+\exp(-a))}{a(1-\exp(-a))^3}+\frac{4\exp(-a)}{a^2(1-\exp(-a))^2}+\frac{1+3\exp(-a)}{a^3(1-\exp(-a))} \quad .$$

We can verify that $\lim_{a\to 0}\widetilde{f}(a)a^4=12$.

Let $\frac{a}{1-\exp(-a)}=w(a)$. We have that w is class C^{∞} in a neighbourhood of $a=0$ and we denote $f_q=\lim_{a\to 0}w^{(q)}(a)$ for $q=\overline{0,5}$ having therefore

$$f_0=1 \ , \ f_1=\frac{1}{2}$$

$$\left(\frac{a}{1-\exp(-a)}(1-\exp(-a))\right)^{(q)}=\delta_{1q} \text{ for } q\geq 1 \quad \text{and so}$$

$$\sum_{s=0}^{q}\binom{q}{s}((-1)^{s+1}+\delta_{0s})w^{(q-s)}(a)=\delta_{1q} \ ,$$

$$w^{(q)}(a)=\frac{1}{1-\exp(-a)}\left(\delta_{1q}+\sum_{s=1}^{q}\binom{q}{s}(-1)^s\exp(-a)w^{(q-s)}(a)\right)$$

Applying l'Hospital rule to the last relation we obtain

$$f_q=\frac{1}{1+q}(-1)^{q+1}\left(f_0+\sum_{s=1}^{q-1}\binom{q+1}{s}(-1)^s f_s\right) \quad \text{for } q>1 \qquad (8) \ .$$

We compute f_q for $q=\overline{0,5}$ using recurence formula (8) and then, succesively differentiating and having $(f_q)_{q=\overline{0,5}}$ we compute now

$\lim_{a\to 0}(w^3(a))^{(q)}$ and $\lim_{a\to 0}(w^2(a))^{(q)}$ for $q=\overline{0,5}$ and then with the relation

$\lim_{a\to 0}(\widetilde{f}(a)a^4)^{(q)}=$

$=\lim_{a\to 0}\sum_{s=0}^{q}(-1)^s\binom{q}{s}(2(w^3(a))^{(q-s)}(1+2^s)+4(w^2(a))^{(q-s)}+(\delta_{0s}+3)w^{(q-s)}(a))$ we can compute the coefficients $c_q=\lim_{a\to 0}(\widetilde{f}(a)a^4)^{(q)}$ for $q=\overline{0,5}$

Thus we obtain

$f_0=1, f_1=\frac{1}{2}, f_2=\frac{1}{6}, f_3=0, f_4=-\frac{1}{30}, f_5=0,$

$c_0=12, c_1=-1, c_2=0, c_3=0, c_4=-\frac{2}{15}, c_5=-28$,

$f(D)=\frac{2\hbar c\pi^2L^2}{D^3a^3}\left(\frac{12k_cD}{\pi}-1-\frac{\pi^3}{180k_c^3D^3}-\frac{7\pi^4}{30k_c^4D^4}+O(a^4)\right)=$

$=\frac{24\hbar cL^2}{\pi^2}k_c^4D-\frac{2\hbar cL^2}{\pi}k_c^3-\frac{\hbar c\pi^2L^2}{90D^3}-\frac{7\hbar c\pi^3L^2}{15k_cD^4}+\frac{2\hbar c\pi^2L^2}{D^3}O(\frac{\pi^2}{k_c^2D^2})$.

Hence for $k_c\gg 1$ we can approximate

$E(D)\approx\frac{24\hbar c}{\pi^2}L^2k_c^4L_1-\frac{4\hbar c}{\pi}k_c^3-\frac{\hbar c\pi^2}{90}L^2\left(\frac{1}{D^3}+\frac{1}{(L_1-D)^3}\right)$.

The force acting on the inner plate is therefore

$F(D)=-\frac{\partial E}{\partial D}\approx-\frac{1}{30}\hbar c\pi^2L^2\left(\frac{1}{D^4}-\frac{1}{(L_1-D)^4}\right)$ which for $L_1\gg D$ becomes

$F(D)\approx-\frac{\hbar c\pi^2L^2}{30D^4}$ and we conclude that there appears an attractive force between the plates when they are at distance D from each other, the attractive pressure being $p=\frac{1}{30}\frac{\hbar c\pi^2}{D^4}$.

39. Aharonov-Bohm effect

Aharonov-Bohm effect

An electron passing around a long solenoid would pick up a phase shift dependent on the magnetic field of the solenoid, even though the electrons themselves pass through a region of space which has a zero magnetic field. For an electron of charge *e* and mass *m* in an electromagnetic field Having the four-potential $(A_\alpha)_{\alpha=\overline{0,3}}=(\varphi,\vec{A})$ we have a Hamiltonian (see Chap. Electromagnetic four-potential …) :

$H=\frac{(\vec{p}+e\vec{A})^2}{2m}+e\varphi$. Therefore for the wave function (in the non-relativistic case) of the electron $\bar{\psi}=\bar{\psi}(t,\vec{x})$ we have $\bar{\psi}(t,\vec{x})=\exp(-\frac{i}{\hbar}\hat{H}t)\psi(\vec{x})$ with $\psi=\psi(\vec{x})$ satisfying the time-independent Schroedinger equation $\hat{H}\psi=E\psi$ for energy levels $E\in\mathbb{R}$ that is:

$\frac{1}{2m}(-i\hbar\nabla+e\vec{A})^2\psi(\vec{x})=E\psi(\vec{x})$ (1) when we take the Coulomb gauge with $\varphi=0$.

Equation (1) is equivalent to :

$$\nabla^2\psi+\frac{2ei}{\hbar}\vec{A}\cdot\nabla\psi+\frac{ei}{\hbar}(\nabla\cdot\vec{A})\psi+\left(\frac{2m}{\hbar^2}E-\frac{e^2}{\hbar^2}\vec{A}^2\right)\psi=0 \qquad (2)$$

Let $\psi_0=\psi_0(\vec{x})$ a solution of (1) for $\vec{A}=0$: $\nabla^2\psi_0+\frac{2m}{\hbar^2}E\psi_0=0$.

Taking for each $\vec{x}\in\mathbb{R}^3$ paths $\Gamma(\vec{x})$ from $\vec{0}$ to $\vec{x}$ defining

$$\psi(\vec{x})=\psi_0(\vec{x})\exp(-\frac{ie}{\hbar}\int_{\Gamma(\vec{x})}\vec{A}\cdot d\vec{x})$$ we have

$$\nabla\psi=(\nabla\psi_0)\exp(-\frac{ie}{\hbar}\int_{\Gamma(\vec{x})}\vec{A}\cdot d\vec{x})-\frac{ie}{\hbar}\psi_0\vec{A}\exp(-\frac{ie}{\hbar}\int_{\Gamma(\vec{x})}\vec{A}\cdot d\vec{x})$$

$$\nabla^2\psi=(\nabla^2\psi_0-\frac{2ie}{\hbar}(\nabla\psi_0)\cdot\vec{A}-\frac{ie}{\hbar}\psi_0(\nabla\cdot\vec{A})-\frac{e^2}{\hbar^2}\psi_0\vec{A}^2)\exp(-\frac{ie}{\hbar}\int_{\Gamma(\vec{x})}\vec{A}\cdot d\vec{x})$$

and so $\psi=\psi(\vec{x})$ satisfies (2) .

We can take solutions $\psi_1=\psi_1(\vec{x})$, $\psi_2=\psi_2(\vec{x})$ corresponding respective to different choosing of paths $\Gamma_1=\Gamma_1(\vec{x})$, $\Gamma_2=\Gamma_2(\vec{x})$ and $\Gamma=\Gamma_1\vee(-\Gamma_2)$ the closed path from $\vec{0}$ to $\vec{x}$ and back from $\vec{x}$ to $\vec{0}$.

Between the solutions corresponding respectively to the two paths at the point with coordinate $\vec{x}$ appears a phase difference $\Delta\varphi=\frac{e}{\hbar}(\int_{\Gamma_1}\vec{A}\cdot d\vec{x}-\int_{\Gamma_2}\vec{A}\cdot d\vec{x})=\frac{e}{\hbar}\int_{\Gamma}\vec{A}\cdot d\vec{x}$.

By Stokes theorem we derive $\Delta\varphi=\frac{e}{\hbar}\int_{\Sigma}(\nabla\times\vec{A})\cdot\boldsymbol{n}\,d\sigma=-\frac{e}{\hbar}\int_{\Sigma}\vec{B}\cdot\boldsymbol{n}\,d\sigma=\frac{-e\Phi}{\hbar}$

where Σ with normal $\boldsymbol{n}$ is a surface surrounded by Γ.

The phase difference at a point is proportional to the flux of the magnetic field through a surface surrounded by the closed path containing the point.

The wave function will have a different phase depending on which path the electron is taking, left or right around the solenoid and so the double slit interference pattern is therefore modified by the phase difference (see fig.1) . Electrons emerging from S pass through two slits S_1 and S_2 interfering on an observation screen with the interference pattern shifted when a magnetic field changed.

The electromagnetic potential vector is $\vec{A}=B\left(-\frac{y}{\sqrt{x^2+y^2}},\frac{x}{\sqrt{x^2+y^2}},0\right)$,

the magnetic field is $\vec{B}=\left(0,0,\frac{B}{\sqrt{x^2+y^2}}\right)$ with B -constant, the coordinates (x,y,z) system origin being at the center of the solenoid .

The direction of the magnetic field is outward from the figure and the arrow shows the orientation of the vector potential.

P_0 -interference central maximum in absence of magnetic field.

P -interference maximum in presence of magnetic field.

At the interference maximum P on the observation screen the phase difference introduced by the path lenght difference $\|\overrightarrow{S_1P}\|-\|\overrightarrow{S_2P}\|$ wich for $l\ll D$ is $\frac{p}{\hbar}l\sin\theta$ must compensate the phase difference $\Delta\varphi$ introduced by the presence of the magnetic field.

D is the distance between the plane of the slits and the observation screen plane , which planes are parallel and parallel to the z -axis, the magnetic field direction.

l is the distance between slits $\|\overrightarrow{S_1S_2}\|$ and θ is the angle between $\overrightarrow{S_1P}$ and $\overrightarrow{SP_0}$, S is situated behind the slits at equal distances from them.

Thus the path difference compensation leads to

$\frac{p}{\hbar}(\|\overrightarrow{S_1P}\|-\|\overrightarrow{S_2P}\|)=\Delta\varphi=-\frac{e\Phi}{\hbar}+2n\pi$ with $n\in\mathbb{Z}$ and in $O(\varepsilon^2)$ approximation

where $\varepsilon=\frac{l}{D}$ (see Chap. Wave propagation) $p=\|\vec{p}\|=\frac{\hbar}{\lambda}$,

λ -de Broglie wavelenght of the electron.

we will have $\|\overrightarrow{S_1P}\|-\|\overrightarrow{S_2P}\|\approx l\sin\theta$, $\|\overrightarrow{P_0P}\|\approx\left|D\tan\theta-\frac{l}{2}\right|\approx\left|D\sin\theta-\frac{l}{2}\right|$

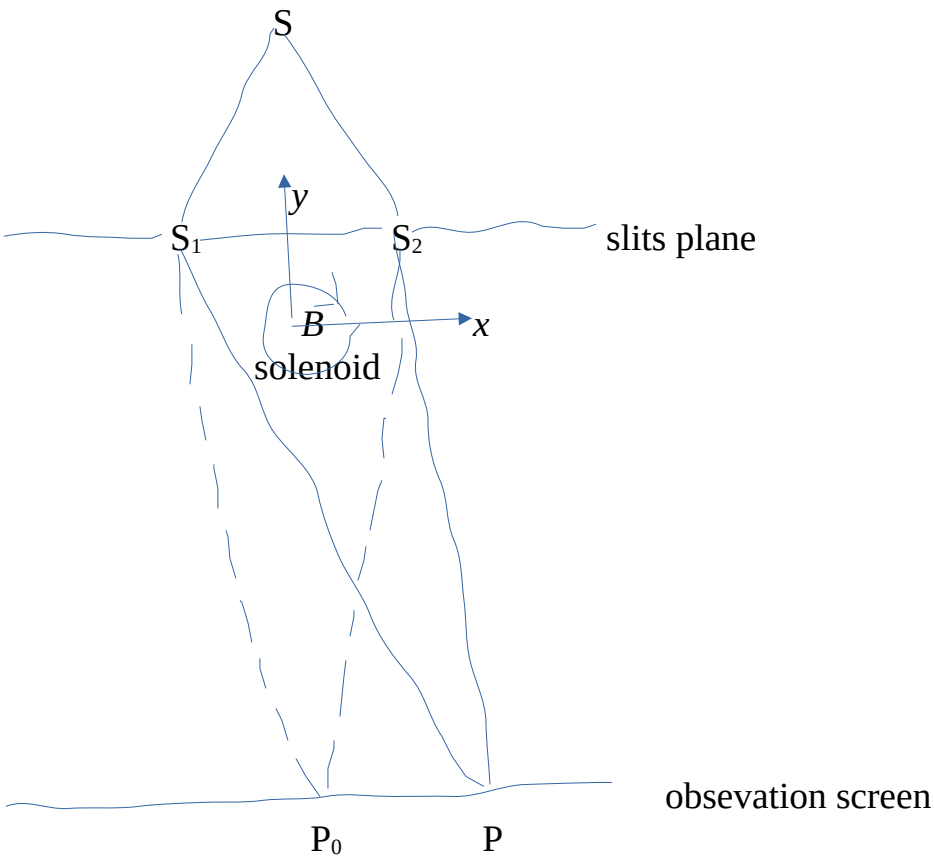
Taking S_0 the middle of the segment S_1S_2 and considering α the angle between $\overrightarrow{S_0P}$ and $\overrightarrow{S_0P_0}$ we obtain

$|\alpha|\approx\frac{\|\overrightarrow{P_0P}\|}{D}$, $\alpha\approx\frac{-e\Phi+2n\pi\hbar}{pl}-\frac{l}{2D}$, $\theta\approx\frac{-e\Phi+2n\pi\hbar}{pl}$.

Obviously the closest to P_0 interference maximum is obtained for

$n=\left\lfloor\frac{2e\Phi D+pl^2}{4\pi\hbar D}+\frac{1}{2}\right\rfloor$ and is determined by the corresponding value of α .

(see fig.2)



$\Gamma_1 = S\ S_1\ P$ $\Gamma_2 = S\ S_2\ P$ $\Gamma = S\ S_1\ P\ S_2\ S$

fig.1

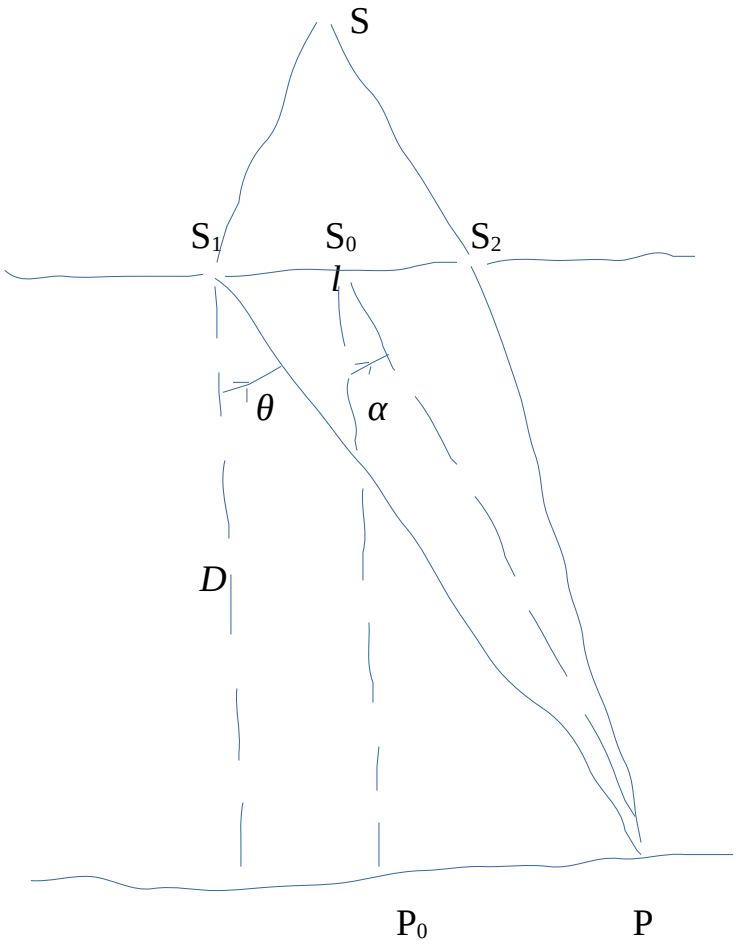


fig.2

40. Mott scattering. Spin Hall effect

Mott scatering. Scattering of a spin ½ particle on a spinless charged particle. Spin Hall effect

As before we take the speed of light in vacuum constant $c = 1$, reduced Planck constant $\hbar = 1$, electric permittivity of vacuum $\varepsilon = 1$ (by suitable choosing of measuring units for time , length and electric charge).
Let p be the incoming four-momentum of the charged spin ½ particle with charge q_1 and mass m and k the incoming four-momentum of the spinless particle having charge q_2 and mass μ . The mass μ is supposed to be much larger than the mass m and so we can consider the scattering in the mass center frame of the particles which in this case can be assimilated to the lab frame where the heavier particle is at rest. Then according to Feynman rules (see Chap. Feynman amplitudes and lattice gauge theory) , the Feynman amplitude of the scattering process at $q_1\, q_2$ first order is

$$A=(2\pi)^4 M\,\delta^4(p+k-p'-k')\ ,$$

$$M=-i\,q_1 q_2\,\bar{u}(p')\,\gamma^{\mu}u(p)\frac{1}{(p-p')^2}(k+k')_{\mu}\ ,$$

where p', k' are the outgoing four-momenta of the fermion respective the spinless particle.

In the center of mass frame we have $\vec{p}+\vec{k}=\vec{p}'+\vec{k}'=0$ and energy conservation leads to $E=p_0+k_0=p'_0+k'_0$, $\|\vec{p}\|=\|\vec{k}\|=\|\vec{p}'\|=\|\vec{k}'\|=r$,

$r=\frac{1}{2E}\left((E^2-(m+\mu)^2)(E^2-(\mu-m)^2)\right)^{1/2}$ with $p_0=p'_0=\sqrt{r^2+m^2}$, $k_0=k'_0=\sqrt{r^2+\mu^2}$.

According to Chap. Canonical quantization of a scalar field, decay rate and cross section, taking as in Chap. Feynman amplitudes and lattice gauge theory, for the electron field the normalization E_p/m instead of $2\omega(p)$ in the cross section formula, we will have a differential cross section given by

$$\frac{d\sigma}{d\Omega}=\frac{1}{|v_1-v_2|}\frac{4m^2}{4k_0p_0}\frac{1}{(2\pi)^2}\frac{2(k_0+p_0)r}{8(k_0+p_0)^2}|M|^2$$

where in the mass center frame $v_1=\frac{r}{p_0}$, $v_2=-\frac{r}{k_0}$ and so

$$\frac{d\sigma}{d\Omega}=\frac{m^2}{E^2}\frac{1}{(4\pi)^2}|M|^2\ .$$

As we proved in Chap. Anomalous magnetic moment of the electron we have the Gordon decomposition

$\bar{u}(p')\gamma^{\mu}u(p)=\frac{1}{2m}\bar{u}(p')((p'+p)^{\mu}+i\,\sigma^{\mu\nu}(p'-p)_{\nu})u(p)$ where $\sigma^{\mu\nu}=\frac{1}{2}i[\gamma^{\mu},\gamma^{\nu}]$.

Thus

$$M=\frac{-i\,q_1 q_2}{2m}\bar{u}(p')((p'+p)(k'+k)+i(p'-p)_{\nu}(k'+k)_{\mu}\sigma^{\mu\nu})u(p)\frac{1}{(p'-p)^2}\ .$$

In the mass center frame we have

$(p'+p)(k'+k)=(p'+p)(2k+p-p')=2k(p+p')=4k_0p_0+2\vec{p}(\vec{p}+\vec{p}')=$

$=4k_0p_0+4r^2\cos^2(\theta/2)$ considering that $p^2=p'^2=m^2$ and θ is the scattering deflection angle between $\vec{p}$ and $\vec{p}'$: $\vec{p}\cdot\vec{p}'=r^2\cos(\theta)$, $\vec{p}\times\vec{p}'=e_3r^2\sin(\theta)$, where $e_j=(\delta_{ij})_{i=\overline{1,3}}$ for $j=\overline{1,3}$.

$i(p'-p)_\nu(k+k')_\mu\sigma^{\mu\nu}=-((p'-p)_\nu(k+k')_0-(p'-p)_0(k+k')_\nu)\gamma^0\gamma^\nu-$

$-i((\vec{p}'-\vec{p})\times(\vec{k}+\vec{k}'))\cdot\vec{\Sigma}=$

$=2k_0(\gamma^0\not{p}-\not{p}'\gamma^0)-4k_0p_0-2i(\vec{p}\times\vec{p}')\cdot\vec{\Sigma}$, where as usual $\not{p}=\gamma^\nu p_\nu$,

$\vec{\Sigma}=\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}$, $\vec{\sigma}=(\sigma_i)_{i=\overline{1,3}}$ are the Pauli matrices.

$(p'-p)^2=2m^2-2(m^2+r^2)+2r^2\cos(\theta)=-4r^2\sin^2(\theta/2)$.

Because $\bar{u}(p')\not{p}'=m\bar{u}(p')$, $\not{p}u(p)=mu(p)$ we obtain

$$M=\frac{iq_1q_2}{m}\Big(2mk_0\bar{u}(p')\gamma^0u(p)+$$

$$+2r^2\cos^2(\theta/2)\bar{u}(p')u(p)-ir^2\sin(\theta)\bar{u}(p')\Sigma_3u(p)\Big)\frac{1}{4r^2\sin^2(\theta/2)}\ .$$

Consider now a flat conductor plate in which exists a flux of electrons $\vec{j}$ and we always measure the spin in direction $\vec{n}$. We have two relevant cases:

1) $\vec{n}=e_3$, $\vec{j}\|e_1$ and (e_1,e_2) is the plane of the conductor plate;

2) $\vec{n}=e_3$, the conductor plate plane is (e_2,e_3) and $\vec{j}\|(0,\cos(\varphi),\sin(\varphi))$.

In the 1) case we measure the spin normal to the motion of electrons and in 2) case we measure the spin along a direction contained in the plane in which the electrons are constrained to move.

Let $\varepsilon,\varepsilon'\in\{\pm\}$ the spin polarizations of the incoming respective outgoing electron in the scattering process. The charge carriers (electrons with mass *m* and charege *e* = - |*e*|) have spin up or down states along e_3 and can scatter on impurities from the cristal lattice grid, impurities that build a network of heavy charged diffusion centers in the way of motion for the electrons. A diffusion center is considered to have charge *q* and mass μ .

For a scattering on a diffusion center, the $\vec{p}'$ outgoing moment of the electron is constrained to be in the (e_1 , e_2) plane in the 1) case and in the (e_2 , e_3) plane in the 2) case and we will have $\vec{p}\times\vec{p}'\|e_3$, $\vec{p}\|e_1$ in the 1) case and $\vec{p}\times\vec{p}'\|e_1$, $\vec{p}=r(0,\cos(\varphi),\sin(\varphi))$ in the 2) case.

We take first the 1) case:

Let $B=B(\chi,e_1)=\begin{pmatrix}\cosh\chi & -\sinh\chi & 0 & 0\\ -\sinh\chi & \cosh\chi & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}=\exp(-\chi K_1)$

where $p=(p_0,-r,0,0)=(p^\alpha)_\alpha$ as a column vector with

$B\begin{pmatrix}m\\0\\0\\0\end{pmatrix}=p$, $\sinh\chi=\frac{r}{m}$, $\cosh\chi=\frac{p_0}{m}$

$R=R(\theta,e_3)=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \cos\theta & -\sin\theta & 0\\ 0 & \sin\theta & \cos\theta & 0\\ 0 & 0 & 0 & 1\end{pmatrix}=\exp(\theta J_3)$,

K_l, J_l , $l=\overline{1,3}$ Lorentz group generators.

(see Chap. Representations of the rotations group and of the restricted Lorentz group)

Then for $P=\cosh(\frac{\chi}{2})\boldsymbol{I}+\sinh(\frac{\chi}{2})\gamma^1\gamma^0$,

$Q=\cos(\frac{\theta}{2})\boldsymbol{I}-i\sin(\frac{\theta}{2})\Sigma_3=\cos(\frac{\theta}{2})\boldsymbol{I}+\sin(\frac{\theta}{2})\gamma^1\gamma^2$,

$u_\varepsilon=\begin{pmatrix}w_\varepsilon\\0\\0\end{pmatrix}$, $w_+=\begin{pmatrix}1\\0\end{pmatrix}$, $w_-=\begin{pmatrix}0\\1\end{pmatrix}$ we will have:

$u(p)=Pu_\varepsilon$, $u(p')=QPu_{\varepsilon'}$.

To compute *M* for the ε , ε' spin polarizations of the incoming respective outgoing electrons we have to compute

$\bar{u}(p')\gamma^0u(p)=u^+_{\varepsilon'}P^+Q^+Pu_\varepsilon=H$,

$\bar{u}(p')u(p)=u^+_{\varepsilon'}P^+Q^+\gamma^0Pu_\varepsilon=G$,

$\bar{u}(p')\Sigma_3u(p)=u^+_{\varepsilon'}P^+Q^+\gamma^0\Sigma_3Pu_\varepsilon=K$.

After some calculus we obtain :

$$H=\delta_{\varepsilon\varepsilon'}(\cos(\frac{\theta}{2})\cosh\chi+i\varepsilon\sin(\frac{\theta}{2}))\ ,$$

$$G=\delta_{\varepsilon\varepsilon'}(\cos(\frac{\theta}{2})+i\varepsilon\sin(\frac{\theta}{2})\cosh\chi)\ ,$$

$$K=\delta_{\varepsilon\varepsilon'}(\varepsilon\cos(\frac{\theta}{2})\cosh\chi+i\sin(\frac{\theta}{2}))\ ,$$

$M=\frac{ieq}{2mr^2\sin^2(\theta/2)}\delta_{\varepsilon\varepsilon'}((k_0p_0+r^2)\cos(\frac{\theta}{2})+i\varepsilon mk_0\sin(\frac{\theta}{2}))$,

$\frac{d\sigma}{d\Omega}=\left(\frac{\alpha}{2E}\right)^2\frac{1}{r^4\sin^4(\theta/2)}((k_0p_0+r^2)^2\cos^2(\frac{\theta}{2})+m^2k_0^2\sin^2(\frac{\theta}{2}))$.

$$(k_0 p_0 + r^2)^2 \cos^2(\frac{\theta}{2}) + m^2 k_0^2 \sin^2(\frac{\theta}{2}) = k_0^2 p_0^2 - k_0^2 r^2 \sin^2(\frac{\theta}{2}) + 2 r^2 k_0 p_0 \cos^2(\frac{\theta}{2}) +$$
$$+ r^4 \cos^2(\frac{\theta}{2}) \ .$$

For $\frac{r}{m}, \frac{m}{\mu} \in O(\epsilon)$ in a non-relativistic approach we have $\frac{r^2 k_0 p_0}{(k_0 p_0)^2} = \frac{r}{m} \frac{r}{p_0} \frac{m}{k_0} \in O(\epsilon^3)$ and so disposing of the $O(\varepsilon^3)$ terms we obtain

$$\frac{d\sigma}{d\Omega} = \left(\frac{\alpha k_0 p_0}{2E} \right)^2 \frac{1}{r^4 \sin^4(\theta/2)} (1 - v^2 \sin^2(\frac{\theta}{2})) = \left(\frac{d\sigma}{d\Omega} \right)_{\text{Rutherford}} (1 - v^2 \sin^2(\frac{\theta}{2}))$$ with

$v = \frac{r}{p_0}$ the incoming velocity and $\alpha = \frac{e q}{4\pi}$.

As we can see, in the 1) case spin flipping is not allowed during the scattering process and the amplitude depends on the incoming spin polarization but the cross section does not depend on spin polarizations (since $\varepsilon^2 = 1$).

However if there is a spin-orbit coupling between the electron and the diffusion center we expect the differential cross section to be spin polarization dependent since the spin-orbit coupling involves the magnetic moment of the electron and so different spin polarization electrons will be scattered at different angles. This fact can arise by higher order scattering Feynman diagrams since the amplitudes have to be added with the first order diagrams amplitudes and so ε comes in in the squared absolute amplitude.

In the case 2) we take

$$B = \exp(-\chi K_2) \ , \ R = \exp(\theta J_1) \ , \ S = \exp(\varphi J_1) \ ,$$
$$P = \cosh(\frac{\chi}{2}) \boldsymbol{I} + \sinh(\frac{\chi}{2}) \gamma^2 \gamma^0 \ , \ Q = \cos(\frac{\theta}{2}) \boldsymbol{I} - i \sin(\frac{\theta}{2}) \Sigma_1 = \cos(\frac{\theta}{2}) \boldsymbol{I} + \sin(\frac{\theta}{2}) \gamma^2 \gamma^3 \ ,$$
$$C = \cos(\frac{\varphi}{2}) \boldsymbol{I} - i \sin(\frac{\varphi}{2}) \Sigma_1 = \cos(\frac{\varphi}{2}) \boldsymbol{I} + \sin(\frac{\varphi}{2}) \gamma^2 \gamma^3$$

having $u(p) = C P u_\varepsilon$, $u(p') = Q C P u_{\varepsilon'}$ and we have to compute

$$\bar{u}(p') \gamma^0 u(p) = u_{\varepsilon'}^+ P^+ C^+ Q^+ C P u_\varepsilon = u_{\varepsilon'}^+ P^+ Q^+ P u_\varepsilon = \widetilde{H}$$
$$\bar{u}(p') u(p) = u_{\varepsilon'}^+ P^+ C^+ Q^+ \gamma^0 C P u_\varepsilon = u_{\varepsilon'}^+ P^+ Q^+ \gamma^0 P u_\varepsilon = \widetilde{G}$$
$$\bar{u}(p') \Sigma_1 u(p) = u_{\varepsilon'}^+ P^+ C^+ Q^+ \gamma^0 \Sigma_1 C P u_\varepsilon = u_{\varepsilon'}^+ P^+ Q^+ \gamma^0 \Sigma_1 P u_\varepsilon = \widetilde{K} \ .$$

We obtain

$$\widetilde{H} = \delta_{\varepsilon\varepsilon'} \cos(\frac{\theta}{2}) \cosh\chi + i \, \delta_{-\varepsilon'\varepsilon} \sin(\frac{\theta}{2})$$
$$\widetilde{G} = \delta_{\varepsilon\varepsilon'} \cos(\frac{\theta}{2}) + i \, \delta_{-\varepsilon'\varepsilon} \sin(\frac{\theta}{2}) \cosh\chi$$
$$\widetilde{K} = \delta_{-\varepsilon\varepsilon'} \cos(\frac{\theta}{2}) \cosh\chi + i \, \delta_{\varepsilon'\varepsilon} \sin(\frac{\theta}{2})$$

$$M=\frac{ieq}{2mr^2\sin^2(\frac{\theta}{2})}\left(\delta_{\varepsilon\varepsilon'}(p_0k_0\cos(\frac{\theta}{2})+r^2\cos(\frac{\theta}{2}))+\delta_{-\varepsilon'\varepsilon}imk_0\sin(\frac{\theta}{2})\right)$$

$$\frac{d\sigma}{d\Omega}=\left(\frac{\alpha}{2E}\right)^2\frac{1}{r^4\sin^4(\frac{\theta}{2})}\left(\delta_{\varepsilon\varepsilon'}(k_0p_0+r^2)^2\cos^2(\frac{\theta}{2})+\delta_{-\varepsilon'\varepsilon}m^2k_0^2\sin^2(\frac{\theta}{2})\right)$$

Considering again the non-relativistic case $\frac{r}{m},\frac{m}{\mu}\in O(\epsilon)$ and disposing of all the $O(\epsilon^3)$ smaller terms we will have:

$$\frac{d\sigma}{d\Omega}=\left(\frac{\alpha k_0p_0}{2E}\right)^2\frac{1}{r^4\sin^4(\frac{\theta}{2})}\left(\delta_{\varepsilon\varepsilon'}\cos^2(\frac{\theta}{2})+\delta_{-\varepsilon'\varepsilon}\sin^2(\frac{\theta}{2})-\delta_{-\varepsilon'\varepsilon}v^2\sin^2(\frac{\theta}{2})\right).$$

Averaging over incomong spin polarizations (unpolarized incoming current) and summing over outgoing spin polarizations (outgoing spin polarization is not measured) we obtain the same differential cross section formula as in the 1) case, as expected.

We notice that at larger scattering angles appears spin flipping during the scattering process in the case 2) when the spin orientation is in the motion plane.

As in Chap. Perturbation theory for the two-component Dirac equation, since the electron scatters in a Coulomb field we will have a spin-orbit interaction with a Larmor interaction energy given by

$\Delta H_L=-g_S\frac{\alpha}{2m^2r^3}\vec{L}\cdot\vec{S}$ with $\vec{L}=m\vec{x}\times\vec{v}$ the angular momentum, $g_S\approx 2$ the gyromagnetic ratio and $\alpha=\frac{eq}{4\pi}$, $\vec{x}$ the position vector of the electron pointing from the diffusion center, $\vec{v}=\frac{d\vec{x}}{dt}$, $r=\|\vec{x}\|$.

We have also a Thomas precession with an instantaneous rotation of the electron ret frame angular velocity

$\vec{\omega}_T=-\frac{1}{2}\vec{v}\times\vec{a}$ where $\vec{a}=\frac{d\vec{v}}{dt}$ is the acceleration of the electron.

In the classical Coulomb scattering we have an acceleration

$\vec{a}=\frac{1}{m}\frac{\alpha}{r^3}\vec{x}$ and so $\vec{\omega}_T=\frac{1}{2m^2}\frac{\alpha}{r^3}\vec{L}$, $\frac{d\vec{a}}{dt}=-\frac{3\alpha}{mr^5}(\vec{x}\cdot\vec{v})\vec{x}+\frac{1}{m}\frac{\alpha}{r^3}\vec{v}$.

For the Thomas precession contribution to the energy we have to consider the inertial forces acting on the spinning ball to which we approximate the electron in its rest frame, having a uniformly distributed mass with density ρ and spinning angular velocity ω.

In the electron rest frame R', which has an instantaneous rotation of angular velocity ω_T (see Chap. Perturbation theory for the two-component Dirac equation) we have

the Euler inertial forces field with density $-\rho\frac{d\vec{\omega}_T}{ds'}\times\vec{x}'$ ($(s',\vec{x}')$ time-space coordinates in R') $\frac{dt}{ds'}=\gamma\approx 1$, $\gamma=\frac{1}{\sqrt{1-v^2}}$,

$\frac{d\vec{\omega}_T}{ds'}\approx\frac{d\vec{\omega}_T}{dt}=-\frac{1}{2}\vec{v}\times\left(\frac{3\alpha}{mr^5}(\vec{x}\cdot\vec{v})\vec{x}\right)=\frac{3\alpha}{2m^2r^5}(\vec{x}\cdot\vec{v})\vec{L}$.

In the cassical Coulomb scattering, when the electron is in the proximity of the diffusion centre, the distance *r* is near to its minimum and so $\vec{x}\cdot\vec{v}=\frac{1}{2}\frac{d}{dt}r^2\approx 0$.

Therefore we can neglect the influence of the Euler force on the scattering process.

The centrifugal forces field is $F_{cf}=-\rho\vec{\omega}_T\times(\vec{\omega}_T\times\vec{x}')$ and has an energy $E_{cf}=\frac{4\pi\rho R^5}{15}\omega_T^2=\frac{1}{5}R^2\omega_T^2 m$ where $R=\frac{3}{5}\frac{e^2}{4\pi m}$ is the estimated radius of the electron (see Chap. Perturbation theory for the two-component Dirac equation) .

Thus with $\frac{e^2}{4\pi}=\frac{\alpha}{Z}$ we have $E_{cf}=\frac{9}{500}\frac{\alpha^4}{Z^2m^5r^6}\vec{L}^2$.

Since in the classical Coulomb scattering $\vec{L}$ is constant we take the centrifugal forces energy contribution as a potential $W=W(r)\propto\frac{1}{r^6}$.

If we consider a scattering of electrons on impurities in a crystal lattice grid we can determine *Z* as the electric charge of one impurity node in the lattice grid which is the difference between the number of valence electrons of the impurity atom and the number of valence electrons of the majority atom of the lattice grid (*Z* can be positive or negative and has the same sign as α) .

The Coriolis inertial forces field is $F_{cor}=-2\rho(\vec{\omega}_T\times(\vec{\omega}\times\vec{x}'))$.

As we noticed in Chap. Perturbation theory for the two-component Dirac equation , for the spin angular momentum we must have $\vec{S}=\frac{2}{5}mR^2\vec{\omega}$ and so

$F_{cor}=-\frac{5}{mR^2}\rho(\vec{\omega}_T\times(\vec{S}\times\vec{x}'))=\frac{125}{18}\frac{Z^2}{\alpha}\frac{\rho}{mr^3}((\vec{L}\cdot\vec{S})\vec{x}'-(\vec{L}\cdot\vec{x}')\vec{S})$.

If $\vec{L}\|\vec{S}$ (which is the situation in the 1) case), the Coriolis forces field is is conservative and we have a corresponding energy $E_{cor}=\int_B\left(\int_{\Gamma(\vec{x}')}-2\rho(\vec{\omega}_T\times(\vec{\omega}\times\vec{x}''))d\vec{x}''\right)d^3\vec{x}'$ where B is the electron ball of radius R , $\Gamma(\vec{x}')$ is a path from the origin to $\vec{x}'\in B$.

Thus in the 1) case we have

$E_{cor}=\frac{8\pi\rho}{15}R^5\vec{\omega}\cdot\vec{\omega}_T=\frac{\alpha}{2m^2r^3}\vec{L}\cdot\vec{S}$.

In the 2) case we take the conservative part of the Coriolis force field which can be $\widetilde{F}_{cor}(\vec{x}')=\frac{125}{18}\frac{Z^2}{\alpha}\frac{\rho}{mr^3}((\vec{L}\cdot\vec{S})\vec{x}'-(L_i x'_i S_i)_{i=\overline{1,3}})$ and

$E_{cor}=\int_B(\int_{\Gamma(\vec{x}')}\widetilde{F}_{cor}(\vec{x}'')d\vec{x}'')d^3\vec{x}'=\frac{\alpha}{2m^2r^3}\vec{L}\cdot\vec{S}$.

The dissipation generated by the non-conservative part of the Coriolis force field in the 2) case on a closed path Γ in the *R'* frame is according tho Stokes theorem proportional to the flux of $\vec{S}\times\vec{L}$ through the surface surrounded by Γ and since $\vec{L}$ is constant in the classical Coulomb scattering
and as we will see the motion equations determined with the conservative part potential additional spin-orbit interaction energy are in the 2) case not dependendent on spin, to compensate this dissipation we will have the flipping of the spin angular momentum $\vec{S}$ during the scattering process in the 2) case.
Hence we have a spin-orbit interaction energy

$\Delta H=\Delta H_L+W+E_{cor}=-\frac{(g_S-1)\alpha}{2m^2r^3}\vec{L}\cdot\vec{S}+\frac{9}{500}\frac{\alpha^4}{Z^2}\frac{1}{m^5r^6}\vec{L}^2$.

As in the classical Coulomb scattering (see I. Ința, S. Dumitru Complemente de fizică) , we consider a shock parameter ρ (do not confuse with the density of the electron ball above) which is the distance between the initial motion line and the axis parallel to the incoming moment $\vec{p}$ with $\|\vec{p}\|=mv_\infty$ through the spinless heavy diffusion center so that we have $\vec{L}_\infty=-\rho mv_\infty e_3$ in the 1) case and $\vec{L}_\infty=-\rho mv_\infty e_1$ in the 2) case and in both cases we take $W=W(r)=\frac{9}{500}\frac{\alpha^4}{Z^2}\frac{1}{m^3r^6}\rho^2v_\infty^2$, $r=\|\vec{x}\|$.

The work done by spin-orbit interaction forces to time moment *t* is

$\Delta H=W(r)-\frac{g_S-1}{2mr^3}\alpha(q\times\dot{q})\cdot\vec{S}-H_0$ where H_0 is a zero point energy and

$q=\vec{x}$ are the position coordinates.

Therefore since $\Delta H=\int_0^t\left(\frac{\partial(\Delta H)}{\partial\dot{q}}\ddot{q}+\frac{\partial(\Delta H)}{\partial q}\dot{q}\right)dt$

and for $T=\frac{1}{2}m\dot{q}^2$ kinetic energy and $V=\frac{\alpha}{r}$ the Coulomb potential we must have

$\int_0^t\left(\frac{\partial T}{\partial\dot{q}}\ddot{q}-\frac{\partial T}{\partial q}\dot{q}\right)dt=\int_0^t-\frac{\partial V}{\partial q}\dot{q}\,dt-\Delta H$ on solutions with $\dot{q}(0)=\dot{q}(t)=0$

and integrating by parts we obtain

$$\int_0^t\left(\frac{d}{dt}\left(\frac{\partial T}{\partial\dot{q}}\right)\dot{q}-\frac{\partial T}{\partial q}\dot{q}+\frac{\partial V}{\partial q}\dot{q}-\frac{d}{dt}\left(\frac{\partial(\Delta H)}{\partial\dot{q}}\right)\dot{q}+\frac{\partial(\Delta H)}{\partial q}\dot{q}\right)dt=0$$

we conclude that the Lagrangian of the system is

$L=L(q,\dot{q})=T-V-\Delta H=\frac{m\dot{q}^2}{2}-A(r)-m\frac{M}{r^3}(q\times\dot{q})\cdot\vec{S}$ where $A(r)=\frac{\alpha}{r}+W(r)$,

$M=-\frac{(g_S-1)\alpha}{2m^2}$, $r=\sqrt{q^2}$.

Introducing the generalized moment coordinates

$p=\frac{\partial L}{\partial\dot{q}}=m\dot{q}-m\frac{M}{r^3}\vec{S}\times q$ we have a Hamiltonian

$H=p\dot{q}-L=\frac{p^2}{2m}+A(r)+\frac{M}{r^3}\vec{S}\cdot(q\times p)+\frac{1}{2}m\frac{M^2}{r^6}(\vec{S}\times q)^2$

The Hamilton-Jacobi system is

$\dot{q}=\frac{\partial H}{\partial p}=\frac{p}{m}+\frac{M}{r^3}\vec{S}\times q$

$\dot{p}=-\frac{\partial H}{\partial q}=-A'(r)\frac{q}{r}+3\frac{M}{r^5}(\vec{S}\cdot(q\times p))q+\frac{M}{r^3}(\vec{S}\times p)+3\frac{mM^2}{r^8}(\vec{S}\times q)^2q-$

$-\frac{mM^2}{r^6}(\vec{S}^2q-(\vec{S}\cdot q)\vec{S})$

In the 1) case, we notice from the system that if $q(0),\dot{q}(0)$ are in the (e_1,e_2) plane , then the entire solution (q , p) remains in the (e_1 , e_2) plane. Thus we have to consider only the (q_1 , q_2 , p_1 , p_2) variables and in the 1) case we will have

$$q\times p\|\vec{S}\|e_3 \ , \ \vec{S}\cdot q=0 \ , \ \vec{S}\cdot p=0 \ , \ \dot{q}\times p+q\times\dot{p}=0 \ .$$

Hence in the 1) case $q\times p$ is conserved in time and also H is conserved in time.

Therefore we have $q\times p=\vec{\Lambda}=\Lambda e_3=-\rho m v_\infty e_3$,

$\frac{p^2}{2m}+A(r)+\frac{1}{8}\frac{M^2}{r^4}+\frac{M}{r^3}\vec{S}\cdot(q\times p)=E=\frac{1}{2}mv_\infty^2$ during the motion in the 1) case.

with $\vec{S}=\frac{1}{2}\varepsilon e_3$, $\varepsilon\in\{\pm1\}$.

From the HamiltonJacobi system we derive the motion equations

$m\ddot{q}=\frac{\alpha}{r^3}q-\frac{W'(r)}{r}q+3\frac{M}{r^5}(\vec{S}\cdot(q\times p))q+\frac{3mM^2}{r^8}(\vec{S}^2q-(\vec{S}\cdot q)^2\vec{S})-$

$-\frac{3mM}{r^5}(q\cdot\dot{q})(\vec{S}\times q)+\frac{2mM}{r^3}(\vec{S}\times\dot{q})$

In the 2) case we write the motion equations as $m\ddot{q}_i = F_i$, $i = \overline{1,3}$ and have the bounding $x = 0$ choosing the generalized coordinates (q_2, q_3) with

$x = 0$, $y = q_2$, $z = q_3$ and therefore the generalized forces are

$$Q_2 = F_1 \frac{\partial x}{\partial q_2} F_2 \frac{\partial y}{\partial q_2} + F_3 \frac{\partial z}{\partial q_2} = F_2$$

$$Q_3 = F_1 \frac{\partial x}{\partial q_3} + F_2 \frac{\partial y}{\partial q_3} + F_3 \frac{\partial z}{\partial q_3} = F_3 \ .$$

Thus in the 2) case we have

$$q = (0, q_2, q_3) \ , \ \vec{S} \times q = \frac{1}{2} \varepsilon (-q_2, 0, 0) \ ,$$

$$p = m\dot{q} - m\frac{M}{r^3}(\vec{S} \times q) = \left(\frac{\varepsilon m M}{2r^3} q_2, m\dot{q}_2, m\dot{q}_3 \right) \ , \ (\vec{S} \times q) \cdot p = -\frac{mM}{4r^3} q_2^2 \ ,$$

$Q_2 = \left(\frac{\alpha}{r^3} - \frac{W'(r)}{r} \right) q_2$, $Q_3 = \left(\frac{\alpha}{r^3} - \frac{W'(r)}{r} \right) q_3$ and the motion equations are

$$m\ddot{y} = \left(\frac{\alpha}{r^3} - \frac{W'(r)}{r} \right) y$$

$$m\ddot{z} = \left(\frac{\alpha}{r^3} - \frac{W'(r)}{r} \right) z$$

We notice that in the 2) extreme case, with the spin angular momentum in the motion plane we have no spin dependence of the motion equations. However we have proved that in the 2) case spin flipping appears. Thus in an intermediate case with the spin angular momentum having an arbitrary direction and electrons confined to move in the flat conductor plane we expect differentiate scattering to the left or right of the charge current direction depending on spin polarization as we will see in the 1) case and also spin flipping during the scattering process.

Considering now the 1) case, we have

$$e_r = (\cos\theta, \sin\theta) \ , \ e_\theta = (-\sin\theta, \cos\theta) \ ,$$

$$q = r e_r \ , \ \dot{q} = \dot{r} e_r + r\dot{\theta}\, e_\theta \ , \ \ddot{q} = \ddot{r} e_r + 2\dot{r}\dot{\theta}\, e_\theta - r\dot{\theta}^2 e_r + r\ddot{\theta}\, e_\theta$$

$$\Lambda = mr\left(r\dot{\theta} + \frac{\varepsilon\alpha}{4m^2 r^2} \right) \ , \ \frac{1}{2} m\dot{r}^2 = E - B(r) \ ,$$

$$B(r) = \frac{\alpha}{r} + W(r) - \frac{\alpha}{4} \frac{1}{m^2 r^3} \varepsilon\Lambda + \frac{1}{32} \frac{\alpha^2}{m^3 r^4} + \frac{\Lambda^2}{2mr^2} \qquad (1)$$

$$\left(\frac{d\theta}{dr} \right)^2 = \frac{\dot{\theta}^2}{\dot{r}^2} = \frac{\left(\Lambda - \frac{\varepsilon\alpha}{4mr} \right)^2}{2mr^4 (E - B(r))}$$

For $\bar{\alpha}=\left|\frac{\alpha}{Z}\right|=\frac{e^2}{4\pi}\approx\frac{1}{137}$ we will require $\left|\frac{\Lambda}{\bar{\alpha}}\right|<1$ and also, since the electron is as a well defined particle on mass shell we must consider that r is greater than half the reduced Compton wavelenght (see Chap. Relativistic dynamics... Compton wavelenght) and so $mr>\frac{1}{2}$.

Thus $\left|\frac{\alpha}{4}\frac{1}{m^2r^3}\right|=2m|Z|O(\bar{\alpha}^2)$ and $\left|W(r)/\left(\frac{\alpha}{4}\frac{1}{m^2r^3}\Lambda\right)\right|=|Z|\frac{288}{500}O(\bar{\alpha}^4)$ and so in $O(\bar{\alpha}^4)$ approximation we can drop the $W(r)$ term in the $B(r)$ expression, leaving us with $B(r)=\frac{\alpha}{r}+\frac{\Lambda^2}{2mr^2}-\frac{\alpha}{4}\frac{1}{m^2r^3}\varepsilon\Lambda+\frac{1}{32}\frac{\alpha^2}{m^3r^4}$.

For $F(r)=E-B(r)$ the equation $F(r)=0$ has at least one positive root, since $F(\infty)=E>0$ and $F(0)=-\infty$. Considering the (1) relations it follows that from $t=-\infty$ when $\theta(-\infty)=\pi$ (we consider $\Lambda<0$) and $r(-\infty)=\infty$ to $t=0$ when $\theta(0)=\theta_0$ and $r(0)=r_m$, the function $r=r(t)$ is decreasing until at $t=0$ it reaches the minimum value r_m where r_m is the greatest positive root of $F(r)=0$ (the equation $F(r)=0$ is a quartic equation in $\frac{1}{r}$) . From $t=0$ to $t=\infty$ when $\theta(\infty)=\varphi$ where φ is the scattering angle and $r(\infty)=\infty$ the function $r=r(t)$ is increasing. $\dot{r}=\dot{r}(t)$ changes sign only at $t=0$ since r_m must be the greatest positive root of $F(r)=0$.

Therefore $\dot{r}(t)=-\sqrt{\frac{2}{m}F(r)}$ for $t<0$, $\dot{r}(t)=\sqrt{\frac{2}{m}F(r)}$ for $t>0$ and from (1) follows now $\theta(r(t))-\theta_0=(\operatorname{sign}t)\int_{r_m}^{r(t)}\frac{\Lambda-\frac{\varepsilon\alpha}{4rm}}{r^2\sqrt{2m}\sqrt{E-B(r)}}dr$

The unicity of solutions for the differential equations system in $r = r(t)$, $\theta = \theta(t)$ for $r(0)=r_m$, $\theta(0)=\theta_0$ leads to $\theta(t)-\theta_0=\theta_0-\theta(-t)$, $r(t)=r(-t)$ and so taking $\chi=-\int_{r_m}^{\infty}\frac{\Lambda-\frac{\varepsilon\alpha}{4rm}}{r^2\sqrt{2m}\sqrt{E-B(r)}}dr$ we will have $\varphi+2\chi=-\operatorname{sign}\Lambda\,\pi$

We have $E-B(r)=\frac{1}{E^3r^4}G(Er)$ where

$$G(x)=x^4-\alpha x^3-\frac{\Lambda^2}{2}\frac{E}{m}x^2+\frac{\varepsilon\alpha\Lambda}{4}\left(\frac{E}{m}\right)^2x-\frac{\alpha^2}{32}\left(\frac{E}{m}\right)^3 ,$$

$$\int_{r_m}^{\infty}\frac{\Lambda-\frac{\varepsilon\alpha}{4rm}}{r^2\sqrt{2m}\sqrt{E-B(r)}}dr=\int_{Er_m}^{\infty}\sqrt{\frac{E}{2m}}\frac{\Lambda-\frac{\varepsilon\alpha}{4x}\frac{E}{m}}{\sqrt{G(x)}}dx .$$

We consider $\alpha>0$. Taking $A=-\alpha$, $B=-\frac{\Lambda^2}{2}\frac{E}{m}$, $C=\frac{\varepsilon\alpha\Lambda}{4}\left(\frac{E}{m}\right)^2$,

$D=-\frac{\alpha^2}{32}\left(\frac{E}{m}\right)^3$, $a=-\frac{3}{8}A^2+B$, $b=\frac{A^3}{8}-AB+C$, $c=-\frac{3}{256}A^4+\frac{A^2B}{16}-\frac{AC}{4}+D$,

$p=-\frac{a^2}{12}-c$, $q=-\frac{a^3}{108}+\frac{ac}{3}-\frac{b^2}{8}$ after some calculus , for $\frac{E}{m}=O(\epsilon)$,

$\epsilon\to 0$, $\left|\frac{\Lambda}{\alpha}\right|<1$ we obtain

$b\neq 0$, $27q^2+4p^3>0$ and solutions of the equation $G(x)=0$ can be expressed as

$u(C,D)=-\frac{A}{4}+\frac{1}{2}(-\delta\sqrt{2y-a}\pm\sqrt{-2y-a+4\delta\sqrt{y^2-c}})$ with $\delta\in\{\pm 1\}$,

$y=\frac{a}{6}+w-\frac{p}{3w}$, $w=\sqrt[3]{-\frac{q}{2}+\sqrt{\frac{q^2}{4}+\frac{p^3}{27}}}$ and we have

$u(C,D)=u(0,0)+O(\epsilon^2)$.

Thus in $O(v_\infty^4)$ approximation we can ignore the C,D terms in the expression of G so we can take $B(r)\approx\frac{\alpha}{r}+\frac{\Lambda^2}{2mr^2}$. (2)

Considering (2) and the case $\alpha>0$, $\left|\frac{\Lambda}{\alpha}\right|<1$, $v_\infty\ll 1$ we will have

$$mr_m v_\infty^2=\frac{\kappa^2 v_\infty^3}{-\alpha+\sqrt{\alpha^2+\kappa^2 v_\infty^3}}\approx 2\alpha \text{ where } \kappa^2=\rho^2 m^2 v_\infty .$$

Therefore $\frac{\alpha}{4mr|\Lambda|}\leq\frac{\alpha}{4mr_m|\Lambda|}<\frac{1}{8}\frac{v_\infty}{|\rho|m}<\frac{1}{4}v_\infty\ll 1$ if $|\rho|$ is greater than half the reduced Compton wavelenght.

Hence $\operatorname{sign}(\theta-\theta_0)=\operatorname{sign}\Lambda$ for $t>0$ if $|\rho|$ exceeds half the reduced Compton wavelenght and $\left|\frac{\Lambda}{\alpha}\right|<1$ and $v_\infty\ll 1$.

If $\left|\frac{\Lambda}{\alpha}\right|<1$, $v_\infty<\alpha$, $v_\infty\ll 1$ we will have

$\vec{v}^2=\dot{q}^2=\dot{r}^2+(r\dot{\theta})^2=\frac{2}{m}(E-B(r))+\left(\frac{\Lambda}{mr}-\frac{\alpha}{4(mr)^2}\right)^2<v_\infty^2+2\frac{\Lambda^2}{(mr_m)^2}+\frac{1}{8}\frac{\alpha^2}{(mr_m)^4}<$

$<v_\infty^2+\frac{1}{2}\left(\frac{\Lambda}{\alpha}\right)^2 v_\infty^4+\frac{1}{128}\left(\frac{v_\infty}{\alpha}\right)^2 v_\infty^6\ll 1.$

We remain therefore, for the $\alpha > 0$ case, in the non-relativistic application domain during the entire motion of the electron.

Integrating with (2) expression for $B(r)$ we obtain

$$(\operatorname{sign} t)(\theta-\theta_0)=\int_{1/r}^{1/r_m}\frac{\Lambda-\frac{\varepsilon\alpha}{4m}\tau}{\sqrt{2m}\sqrt{E-\alpha\tau-\frac{\Lambda^2}{2m}\tau^2}}d\tau=$$

$$=(\operatorname{sign}\Lambda)\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\left(\frac{\pi}{2}-\arcsin\frac{\frac{\Lambda^2}{r}+\alpha m}{\sqrt{2\Lambda^2Em+\alpha^2m^2}}\right)-\frac{\varepsilon\alpha v_\infty}{4\Lambda^2}\sqrt{1-\frac{2\alpha}{mrv_\infty^2}-\frac{\rho^2}{r^2}}\ .$$

$$\varphi=-(\operatorname{sign}\Lambda)\pi+2(\operatorname{sign}\Lambda)\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\left(\frac{\pi}{2}-\arcsin\frac{\alpha m}{\sqrt{2\Lambda^2Em+\alpha^2m^2}}\right)-\frac{\varepsilon\alpha}{2\Lambda^2}v_\infty\ .$$

We consider further that $\alpha>0$, $v_\infty<\alpha$, $\frac{|\Lambda|}{\alpha}<1$ and it follows:

$$-(\operatorname{sign}\Lambda)\varphi=\pi-2\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\arctan\frac{|\Lambda|v_\infty}{\alpha}+(\operatorname{sign}\Lambda)\frac{\varepsilon\alpha}{2\Lambda^2}v_\infty=\pi-2\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\left(\frac{|\Lambda|}{\alpha}v_\infty+\right.$$

$$\left.-\frac{|\Lambda|^3}{\alpha^3}\frac{v_\infty^3}{3}+\frac{|\Lambda|^5}{\alpha^5}\frac{v_\infty^5}{5}-\ldots\right)+(\operatorname{sign}\Lambda)\frac{\varepsilon\alpha v_\infty}{2\Lambda^2}=\pi-2\arctan\frac{|\Lambda|v_\infty}{\alpha}+\frac{2}{3}\frac{\varepsilon v_\infty^3}{\alpha}\operatorname{sign}\Lambda+O(v_\infty^4).$$

$$\varphi\approx-(\operatorname{sign}\Lambda)\pi+2\arctan\frac{\Lambda v_\infty}{\alpha}-\frac{2}{3}\frac{\varepsilon v_\infty^3}{\alpha}\ . \quad (3)$$

We notice that in absence of spin effects ($\varepsilon = 0$) we obtain

$\cot^2\frac{\varphi}{2}=\frac{\Lambda^2v_\infty^2}{\alpha^2}$ which is the dependence of the scattering angle φ on ρ from the classical Rutherford non-relativistic Coulomb scattering (see I. Inţa , S. Dumitru , Complemente de fizică).

The relation (3) defines the dependence of the diffusion angle φ on the shock parameter ρ (since $\Lambda=-\rho m v_\infty$) when a flux of particles are scattered on the same diffusion center.

Let the number of particles having shock parameter in the interval (ρ , $\rho+d\rho$) , that are scattered in an unit of time be *dN*. These particles are scattered in the angular interval (φ , $\varphi+d\varphi$) . If *j* is the flux of incoming particles (the number of particles passing in an unit of time through a normal to motion direction unit surface element) we must have $dN=j2\pi|\rho d\rho|=j\pi|d\rho^2|$ and if $d\sigma$ is the differential cross section we have $dN=j\,d\sigma$. Thus $d\sigma=\pi|d\rho^2|$.

Since the conduction electrons in the flat conductor plate are restricted to move in direction $\vec{j}$ parallel to the (e_1,e_2) plane ($\vec{j}\|e_1$) we have to consider the number of electrons passing a normal section of height *b* and width *d y* parallel to the (e_2 , e_3) in an unit of time as $dN=j\,b\,dy$ and we can define the bidimensional flux $\tilde{\vec{j}}=\frac{dN}{dy}e_1=\vec{j}\,b$ and subsequently the bidimensional cross section $\tilde{\sigma}=\frac{1}{b}\sigma$ for the scattering in the (e_1,e_2) plane.

As we proved, if $A=(2\pi)^4 M\,\delta^4(p+k-p'-k')$ is a total scattering amplitude, then the differential cross section is

$$d\sigma=\frac{k_0 p_0}{(k_0+p_0)r}\frac{4m^2}{4k_0p_0}\frac{1}{(2\pi)^2}\frac{d^3\vec{k}'}{2\omega(k')}\frac{d^3\vec{p}'}{2\omega(p')}|M|^2\delta^4(k+p-k'-p')=$$

$$=\frac{1}{(4\pi)^2}\frac{m^2}{(k_0+p_0)^2}|M|^2 d\Omega \text{ with } \omega(k')=\sqrt{\vec{k}'^2+\mu^2}\ ,\ \omega(p')=\sqrt{\vec{p}'^2+m^2}$$

Introducing cilindrical coordinates $(\bar{r},\bar{\theta},\bar{p})$, $\bar{\theta}\in(-\pi,\pi)$ with

$$x_1=\bar{r}\cos\bar{\theta}\ ,\ x_2=\bar{r}\sin\bar{\theta}\ ,\ x_3=\bar{p}\ ,\ r'=\sqrt{\bar{r}^2+\bar{p}^2}\ ,$$

$E=k_0+p_0=\sqrt{r'^2+\mu^2}+\sqrt{r'^2+m^2}$ leads to $r'=\frac{1}{2E}((E^2-(m+\mu)^2)(E^2-(\mu-m)^2))^{1/2}$.

Taking $I=\frac{d^3\vec{k}'}{2\omega(k')}\frac{d^3p'}{2\omega(p')}\delta^4(p+k-p'-k')$

with $\vec{p}+\vec{k}=0$ in the mass-center frame we derive

$$I=\frac{1}{2\omega(k')}\frac{1}{2\omega(p')}r'^2\sin\psi\, d\bar{\theta}\, d\psi\,\delta\left(E-\sqrt{r'^2+\mu^2}-\sqrt{r'^2+m^2}\right)dr'$$

where $\|\vec{k}'\|=\|\vec{p}'\|=r'$, $\frac{dr'}{dE}=\frac{\sqrt{r'^2+\mu^2}\sqrt{r'^2+m^2}}{Er'}$, $\psi\in(0,\pi)$.

Therefore the number of electrons scattered in an unit of time in directions defined by $\bar{\theta}\in(\theta,\theta+d\theta)$ is $dN=j\left(\int_0^{\pi}\int\frac{r'}{4E'}\sin\psi\,\delta(E'-E)|M|^2 dE'\,d\psi\right)\frac{m^2}{r(k_0+p_0)}\frac{1}{(2\pi)^2}d\bar{\theta}$

where we have $|M|^2=|M|^2(r,\bar{\theta},\varepsilon)$, $r'=r'(E')=r(E')$ defined above.

Hence $dN=j\frac{1}{2E^2}\frac{m^2}{(2\pi)^2}|M|^2 d\bar{\theta}$.

According to the interpretation of the bidimensional flux and cross section we have

$dN=\tilde{j}\,d\tilde{\sigma}$ and so $dN=j\,d\sigma=\tilde{j}\,d\tilde{\sigma}=j\frac{1}{2E^2}\frac{m^2}{(2\pi)^2}|M|^2 d\bar{\theta}$

and since $\tilde{j}=jb$ we obtain $\frac{d\tilde{\sigma}}{d\bar{\theta}}=\frac{1}{b}\frac{1}{2E^2}\frac{m^2}{(2\pi)^2}|M|^2=\frac{2}{b}\frac{d\sigma}{d\Omega}$

Considering the flux of electrons that are scatteredby the same diffusion center when the motion of electrons is constrained to the (e_1 , e_2) plane we have the shock parameter $\bar{\rho}$ which is the distance between the trajectory of an incoming electron and the axial plane through the diffusion center, parallel to the flux vector $\vec{j}$ and perpendicular to the plate. Then the number of particles which have the shock parameter in the interval $(\bar{\rho},\bar{\rho}+d\bar{\rho})$ and are deflected in an unit time interval is $dN=\tilde{j}|d\bar{\rho}|$. The dN particles will be deflected in the scattering angle interval $(\bar{\theta},\bar{\theta}+d\bar{\theta})$ having $\bar{\rho}$ as a function of $\bar{\theta}$ and $d\tilde{\sigma}=\frac{dN}{\tilde{j}}=|d\bar{\rho}|$ (4) .

Thus $d\tilde{\sigma}=\frac{d\tilde{\sigma}}{d\bar{\theta}}d\bar{\theta}=\frac{2}{b}\frac{d\sigma}{d\Omega}(r,\theta)d\theta=|d\bar{\rho}|$.

If $\frac{d\sigma}{d\Omega}$ not depends on the angle ψ between $\vec{S}$ and the incoming moment (that is it depends only on incoming moment norm r)integrating with $d\Omega=\sin\psi d\bar{\theta}d\psi$ we obtain $\sigma=\int\frac{d\sigma}{d\Omega}d\Omega=2\int\frac{d\sigma}{d\Omega}d\bar{\theta}=b\int\frac{d\tilde{\sigma}}{d\bar{\theta}}d\bar{\theta}=b\tilde{\sigma}$ and we verify $\tilde{\sigma}=\frac{\sigma}{b}$.

In the (e_1,e_2) plane we have $\vec{x}(r,\theta,\psi)=\vec{x}(\bar{r},\bar{\theta},\bar{p})$, $\psi=\frac{\pi}{2}$, $\bar{p}=0$, $\theta=\bar{\theta}$, $r=\bar{r}$ where $\vec{x}(r,\theta,\psi)=(r\cos\theta,r\sin\theta\sin\psi,r\sin\theta\cos\psi)$ and therefore for the bidimensional approach $\theta=\bar{\theta}$ in the spherical coordinate argument of $\frac{d\sigma}{d\Omega}$.

In the motion plane , the tridimensional scattering angle can be identified with the plane scattering angle ($\theta=\bar{\theta}=\varphi$) and also the tridimensional shock parameter ρ can be identified with the bidimensional shock parameter $\bar{\rho}$.

The determination of $\frac{d\tilde{\sigma}}{d\bar{\theta}}$ is made in the supposition that the spin angular momentum is normal to the motion plane. We cannot extend the relation $\frac{d\tilde{\sigma}}{d\bar{\theta}}=\frac{2}{b}\frac{d\sigma}{d\Omega}$ to the entire tridiensional solid angle since this relation, as we proven may be valid for $\psi=\frac{\pi}{2}$ but the motion plane changes if we vary ψ and the spindirection is no more normal to the motion plane and as we have seen in the derivation for the 2) case equations, the motion becomes spatial and we have a dependence on ψ of the tridimensional cross section (r,θ,ψ) spherical coordinates. So we have $\frac{d\tilde{\sigma}}{d\bar{\theta}}=\frac{2}{b}\frac{d\sigma}{d\Omega}$ only in the $\psi=\frac{\pi}{2}$ plane.

For the situation we consider (a Copper with Iridium impurities plate) we have $Z\geq 1$ (Copper has one valence electron and Iridium has to nine valence electrons) and so $\alpha>0$ and $|\bar{\rho}|$ must be considered smaller than half the minimum distance between impurity nodes in the plate crystal lattice grid (measured normal to charge current direction) which we denote a / 2 where a is a lattice grid constant.

v_∞ is the drift velocity of the electrons determined by the charge current $e\vec{j}$.

Therefore we will have $\frac{|\Lambda|}{\bar{\alpha}}<1$, $v_\infty<\alpha$, $v_\infty\ll 1$ and since $\Lambda=-\bar{\rho}mv_\infty$, considering (3) we obtain

$$d\bar{\rho}=-\frac{\alpha}{2mv_\infty^2}\frac{1}{\sin^2\left(\frac{\varphi}{2}+\frac{\varepsilon v_\infty^3}{3\alpha}\right)}d\varphi$$

with $\varphi=\bar{\theta}$ as the scattering angle in (e_1,e_2) plane,

$$\varphi\in(\varphi_+^1(\varepsilon),\varphi_+^2(\varepsilon))\cup(\varphi_-^1(\varepsilon),\varphi_-^2(\varepsilon)) \quad \text{where}$$

$$\varphi_+^1(\varepsilon)=-\pi-\frac{2\varepsilon v_\infty^3}{3\alpha}\ ,\ \varphi_+^2(\varepsilon)=-\pi+2\arctan\left(\frac{amv_\infty^2}{2\alpha}\right)-\frac{2\varepsilon v_\infty^3}{3\alpha}\ ,$$

$$\varphi_-^1(\varepsilon)=-\varphi_+^2(-\varepsilon)\ ,\ \varphi_-^2(\varepsilon)=-\varphi_+^1(-\varepsilon)\ .$$

From (4) follows now that the bidimensional differential cross section is

$$\frac{d\tilde{\sigma}_\varepsilon}{d\varphi}(\varphi)=\begin{cases}\dfrac{\alpha}{2mv_\infty^2}\dfrac{1}{\sin^2\left(\dfrac{\varphi}{2}+\dfrac{\varepsilon v_\infty^3}{3\alpha}\right)} & \text{if } \varphi\in(\varphi_+^1(\varepsilon),\varphi_+^2(\varepsilon))\cup(\varphi_-^1(\varepsilon),\varphi_-^2(\varepsilon)) \\ 0 & \text{else}\end{cases}$$

and we can verify that $\frac{d\tilde{\sigma}_\varepsilon}{d\varphi}(\varphi)=\frac{d\tilde{\sigma}_{-\varepsilon}}{d\varphi}(-\varphi)$ (5) .

The number of up-spin electrons that are deflected to the left of the incoming flux direction ($e_3\times\vec{j}$ gives the left side direction of the flux vector direction) is

$$n_l(+1)=\tilde{j}\int_{\varphi_+^1(+1)}^{-\pi}\frac{d\tilde{\sigma}_+}{d\varphi}d\varphi+\tilde{j}\int_{\varphi_-^1(+1)}^{\varphi_-^2(+1)}\frac{d\tilde{\sigma}_+}{d\varphi}d\varphi=\tilde{j}\frac{\alpha}{mv_\infty^2}\left(\tan\left(\frac{v_\infty^3}{3\alpha}\right)+\frac{amv_\infty^2}{2\alpha}\right)$$

and the number of up-spin electrons that are deflected to the right of the incoming flux direction in an unit of time is

$$n_r(+1)=\tilde{j}\int_{-\pi}^{\varphi_+^2(+1)}\frac{d\tilde{\sigma}_+}{d\varphi}d\varphi=\tilde{j}\frac{\alpha}{mv_\infty^2}\left(-\tan\left(\frac{v_\infty^3}{3\alpha}\right)+\frac{amv_\infty^2}{2\alpha}\right)$$

We notice that $n_l(+1)>n_r(+1)$ and so we can see that up-spin electrons are deflected mostly to the left of the incoming flux direction or equivalent to the right of the charge current direction, since electrons carry negative charge and in the same way we conclude that down-spin electrons are deflected mostly to the left of the charge current direction (as we proved, in the considered 1) case, spin flipping during the scattering process is not allowed so up-spin will accumulate on the right edge of the plate with respect to charge current direction and down-spin will accumulate on the left edge of the plate).

In the bidimensional approach, we will have a mean free path of the electrons that are moving in the conductor plate plane given by $l=\frac{1}{\tilde{n}\tilde{\sigma}}$ (see Chap. Feynman amplitudes and lattice gauge theory), where $\tilde{n}$ is the areal concentration of impurity nodes in the plate and $\tilde{\sigma}$ is the total bidimensional cross section $\tilde{\sigma}=\int\frac{d\tilde{\sigma}}{d\varphi}d\varphi=a$.

The number of electrons scattered in an unit of time by a diffusion center at angles in the interval $(\varphi,\varphi+d\varphi)$ and having spin polarization ε is (spin flipping is not allowed as we noticed) :

$d n_{\varepsilon}=\tilde{j}\frac{d\tilde{\sigma}_{\varepsilon}}{d\varphi}(\varphi)d\varphi$ which gives a particles bidimensional flux vector

$$\vec{\tilde{j}}_{\varepsilon}=\frac{d n_{\varepsilon}}{l d\varphi}(\varphi)(\cos\varphi,\sin\varphi)$$

Hence we will have a total bidimensional spin flux vector given by

$\vec{\tilde{j}}_{s}=\frac{1}{2}\int(\vec{\tilde{j}}_{+}(\varphi)-\vec{\tilde{j}}_{-}(\varphi))d\varphi=\frac{\tilde{j}}{2l}\int\left(\frac{d\tilde{\sigma}_{+}}{d\varphi}-\frac{d\tilde{\sigma}_{-}}{d\varphi}\right)(\cos\varphi,\sin\varphi)d\varphi$.

From (5) follows that in the (e_1 , e_2) plane we have:

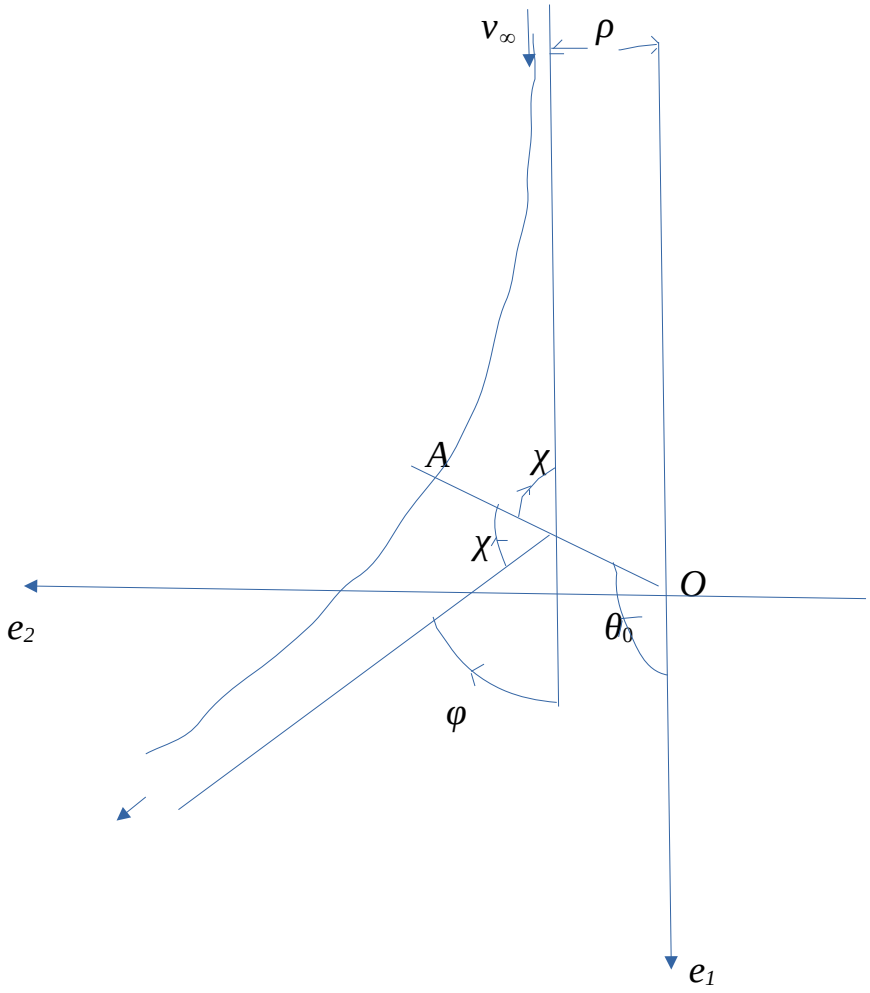
$$\vec{\tilde{j}}_{s}\cdot e_1=0 \quad \text{and} \quad \vec{\tilde{j}}_{s}\cdot e_2=\frac{\tilde{j}}{l}\int\frac{d\tilde{\sigma}_{+}}{d\varphi}\sin\varphi d\varphi=$$

$$=\frac{\tilde{j}}{l}\frac{\alpha}{2m v_{\infty}^2}\int_{\pi-2\arctan\left(\frac{a m v_{\infty}^2}{2\alpha}\right)}^{\pi}\frac{1}{\sin^2(\frac{\varphi}{2})}\left(\sin\left(\varphi-\frac{2v_{\infty}^3}{3\alpha}\right)-\sin\left(\varphi+\frac{2v_{\infty}^3}{3\alpha}\right)\right)d\varphi=$$

$$=-\frac{\tilde{j}}{l}\frac{\alpha}{m v_{\infty}^2}\int_{\pi-2\arctan\left(\frac{a m v_{\infty}^2}{2\alpha}\right)}^{\pi}\sin\left(\frac{2v_{\infty}^3}{3\alpha}\right)\left(\frac{1}{\sin^2(\frac{\varphi}{2})}-2\right)d\varphi=$$

$$=\left(-\tilde{j}\frac{a}{l}+4\frac{\tilde{j}}{l}\frac{\alpha}{m v_{\infty}^2}\arctan\left(\frac{a m v_{\infty}^2}{2\alpha}\right)\right)\sin\left(\frac{2v_{\infty}^3}{3\alpha}\right)$$

We verify that $\frac{a m v_{\infty}}{2\alpha}<1$ and $v_{\infty}\ll 1$ and so since $\lim_{x\to 0}\frac{\arctan x}{x}=1$ we derive that $\vec{\tilde{j}}_{s}\cdot e_2>0$. Therefore we have a spin current in the flat conductor plane that is normal to the charge current and is oriented to the right of the charge current direction (again we notice that the charge current has opposite orientation to the particles flux vector since electrons have negative charge). The apparition of the spin current pointing to the normal right direction of the charge current in a flat conductor sample is known as direct spin Hall effect.



For this figure we have $\Lambda=-\rho m v_\infty<0$, $\varphi+2\chi=\pi$, $\|O A\|=r_m$.

We assumed above conditions like $\frac{|\Lambda|}{\bar{\alpha}}<1$, $v_\infty<\bar{\alpha}$, $v_\infty\ll 1$ with $\bar{\alpha}=\frac{1}{137}$, so we have to verify that the conditions (formulated in Planck units since we have already considered $\hbar=1$, $c=1$) :
$\frac{2\bar{\alpha}}{am}>v_\infty$, $v_\infty<\bar{\alpha}$, $v_\infty\ll 1$ (6) are experimentally available.

Time reversal not changes the spin-orbit coupling
$\vec{L}\cdot\vec{S}$ since $\vec{L},\vec{S}$ being angular momenta are both odd under time reversal.

Thus considering the time reversed inverse spin Hall effect, inverse spin Hall effect in which spin dependent skew scattering of spin carriers from an injected pure spin current on impurities in a crystal lattice grid, for example, generates a charge current giving a measurable inverse spin Hall effect signal ISHE of intensity I_C with a inverse spin Hall effect induced voltage U_{ISHE} , we will obtain a process equivalent to the direct spin Hall effect in which the drift velocity of electrons corresponding to the signal current intensity I_C is the scattering initial velocity v_∞ generating as described above the normal to its direction spin current.
We use the inverse spin Hall effect experiments data (from references [1], [2]) to illustrate a spin-orbit coupling influenced scattering of electrons on diffusion centers as presented above and verify that (6) assumptions are indeed experimentally available.
The experiments used a Copper with Iridium impurities plate of width $w = 10^{-7}$ m , height $b = 10^{-7}$ m . The Copper crystal lattice constant is $d = 3{,}6\ 10^{-10}$ m .
When V is the volume of the plate and c is the fraction of Iridium atoms from the total number of atoms in the sample we estimate the minimum distance between Iridium atoms in the lattice grid as a , having

$c=\frac{\frac{V}{a^3}}{\frac{V}{d^3}+\frac{V}{a^3}}$ and so $\frac{V}{a^3}=\frac{V}{d^3}\frac{c}{1-c}$, $a=d\sqrt[3]{\frac{1-c}{c}}$.

Copper has a density $\rho = 8{,}94\ 10^3$ kg / m^3 and a atomic mass $A = 63{,}5\ 10^{-3}$ kg / mol.
The concentration of atoms for Copper is $n = N_A \rho / A$ where
$N_A = 6{,}023\ 10^{23}$ atoms / mol is the Avogadro number.
The measured ISHE voltages are in a range $U_{ISHE}\in(0,10^{-5})$ V (Volt) .
The inverse spin Hall effect resistances are in a range $|R_{ISHE}|\in(0,5\cdot10^{-5})\Omega(\text{Ohm})$ at $10\,K(\text{Kelvin})$ for a concentration $c=9\%$ and $|R_{ISHE}|\in(0,3\cdot10^{-5})\Omega$ for $c=6\%$.
The occurred flux of electrons is $j=\frac{I_C}{w\,b\,e}$ where $e=-1{,}6\cdot10^{-19}$C (Coulomb) is the electron charge and $I_C=\frac{U_{ISHE}}{R_{ISHE}}$ (the R_{ISHE} values are controlled through an applied magnetic field).
The Copper has one free electron per atom and so the concentration of conduction electrons is equal to n and the drift velocity of electrons that occurs is $v=\frac{j}{n}=\frac{U_{ISHE}}{R_{ISHE}}\frac{A}{N_A\rho}\frac{1}{w\,b\,e}$. Taking the maximal values for voltage and resistance we compute after dividing the value in m/s of v with the speed of light constant $3\cdot10^8$ m / s to obtain the value in Planck units :

$$v_\infty=3.4\cdot10^{-6} \text{ for } c=9\% \text{ and } v_\infty=5.66\cdot10^{-6} \text{ for } c=6\%.$$

We have the Planck lenght $l_P=1.6\cdot10^{-35}\,\mathrm{m}$ the Planck mass $m_P=2.17\cdot10^{-8}\,\mathrm{kg}$ and the electron mass $m=9.1\cdot10^{-31}\,\mathrm{kg}$ and so in Planck units we compute

$$am=\frac{d\sqrt[3]{\frac{1-c}{c}}m}{l_P m_P}\ ,\ am=1.91\cdot10^3 \text{ for } c=9\% \text{ and } am=2.21\cdot10^3 \text{ for } c=6\%.$$

We can verify that for both considered Iridium concentrations we have $\frac{2\bar{\alpha}}{am}>v_\infty$ and so the (6) assumptions are satisfied.

As we proved for $\frac{|\Lambda|}{\bar{\alpha}}<1$, $v_\infty\ll1$, $0<\alpha$ we have the trajectory of the electron in the scattering process on a diffusion centre given by

$$\theta-\theta_0=(\operatorname{sign}\Lambda)\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\left(\frac{\pi}{2}-\arcsin\frac{\frac{\Lambda}{r}+\alpha m}{\sqrt{2\Lambda^2E+\alpha^2m^2}}\right)-\frac{\varepsilon\alpha v_\infty}{4\Lambda^2}\sqrt{1-\frac{\rho^2}{r^2}-\frac{2\alpha}{mrv_\infty^2}}$$

for $t>0$ with $\theta(-t)-\theta_0=\theta_0-\theta(t)$ relation that can be written as

$$\theta-\theta_0=(\operatorname{sign}\Lambda)\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\arcsin\frac{|\Lambda|v_\infty y}{\sqrt{\Lambda^2v_\infty^2+\alpha^2}}-\frac{\varepsilon\alpha v_\infty}{4\Lambda^2}y \quad \text{for} \quad t>0\ ,$$

where $y=\sqrt{1-\frac{\Lambda^2v_\infty^2}{z^2}-\frac{2\alpha}{z}}$, $z=mrv_\infty^2$, $z>z_m$, $z_m=\frac{\Lambda^2v_\infty^2}{-\alpha+\sqrt{\Lambda^2v_\infty^2+\alpha^2}}\approx2\alpha$

and we have $y=y(z)$, $y(z_m)=0$, $y(\infty)=1$, $y\in(0,1)$, $z\in(z_m,\infty)$.

The scattering angle is $\varphi=-\operatorname{sign}\Lambda\,\pi-2\chi$ with $\theta=\theta(r)$, $\chi=(\theta_0-\theta)(\infty)$

and so $\varphi=-\operatorname{sign}\Lambda\,\pi+2\left(1+\frac{\varepsilon\alpha^2}{4\Lambda^3}\right)\arctan\frac{\Lambda v_\infty}{\alpha}-\frac{\varepsilon\alpha v_\infty}{2\Lambda^2}$

having also $\theta_0+\chi=-\operatorname{sign}\Lambda\,\pi$ as it follows from the figure.

We notice that if $(r,\theta(r))_r$ is the trajectory in polar coordinates for $(\operatorname{sign}\Lambda,\varepsilon)=(f,e)\in\{\pm1\}\times\{\pm1\}$ then $(r,-\theta(r))_r$ is the trajectory for $(\operatorname{sign}\Lambda,\varepsilon)=(-f,-e)$ with the same $|\Lambda|, v_\infty$.

We take $\operatorname{sign}\Lambda=-1$, $\Lambda=-\rho mv_\infty$, $\rho m>\frac{1}{2}$, $|\Lambda|<\bar{\alpha}$, $v_\infty\ll1$.

Since for $t>0$ we have $\theta-\theta_0=\int_{r_m}^{r}\frac{\Lambda-\frac{\varepsilon\alpha}{4mr}}{r^2\sqrt{2m}\sqrt{E-B(r)}}dr$ and with the considered assumptions as we proved $\operatorname{sign}\left(\Lambda-\frac{\varepsilon\alpha}{4mr}\right)=\operatorname{sign}\Lambda$ we obtain that for $t>0$, θ is a decreasing function of r and $\theta-\theta_0<0$, $\theta(r_m)=\theta_0$.

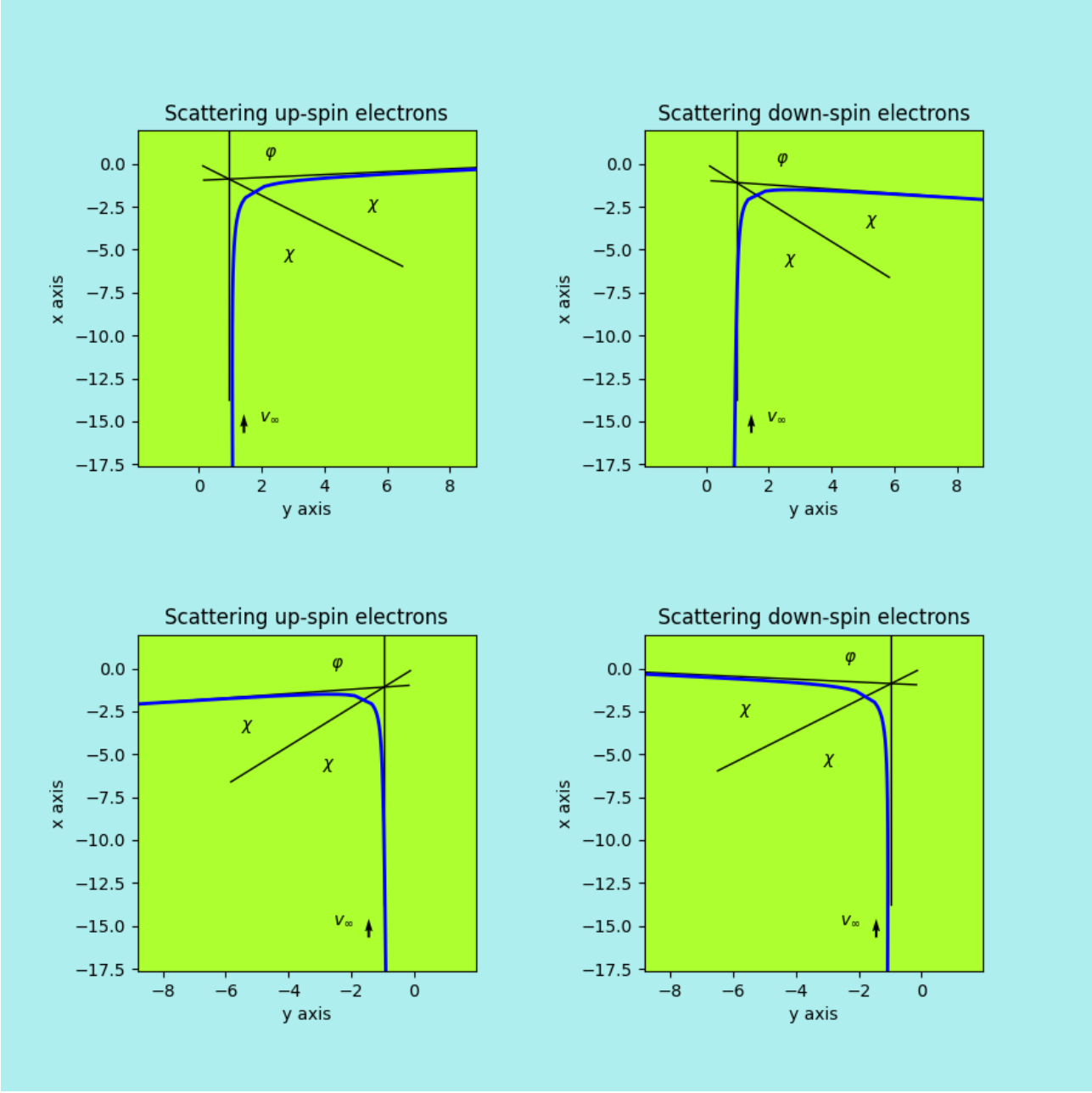
Therefore considering θ as a function of y we have that $\theta_0-\theta$ is a increasing function of y .

For getting a relevant graphic representation of the trajectory in polar coordinates $r=r(\theta)$ we have $0<\theta_0-\theta<\chi=(\theta_0-\theta)(1)$ (we consider further $\theta=\theta(y)$) .

We want an upper limitation for y (or equivalently for z or r) when $\theta_0-\theta\in(0,\chi-\delta)$ with $\delta>0$.
Because $\theta_0-\theta$ is increasing of y we derive that if $(\theta_0-\theta)(\bar{x})=\chi-\delta$ then for $y\in(0,\bar{x})$ we will have $(\theta_0-\theta)(y)\in(0,\chi-\delta)$.
Reminding that we have taken $\Lambda<0$, we have
$(\theta_0-\theta)'(y)=\left(1-\frac{\varepsilon\alpha^2}{4|\Lambda|^3}\right)\frac{1}{\sqrt{h^2-y^2}}+\frac{\varepsilon\alpha v_\infty}{4\Lambda^2}$ where $h=\sqrt{1+\frac{\alpha^2}{\Lambda^2 v_\infty^2}}$.
We have also $\frac{\alpha^2}{4|\Lambda|^3}=\frac{1}{4\alpha}\left(\frac{\alpha}{|\Lambda|}\right)^3>1$ and so $(\theta_0-\theta)'$ is increasing of y if $\varepsilon=-1$ and decreasing of y if $\varepsilon=1$ and obviously we have $(\theta_0-\theta)'>0$ in both cases.
Hence if $\varepsilon=-1$ we obtain $\delta=(\theta_0-\theta)(1)-(\theta_0-\theta)(\bar{x})<(\theta_0-\theta)'(1)(1-\bar{x})=$
$=\frac{|\Lambda|v_\infty}{\alpha}(1-\bar{x})$, $\bar{x}<1-\frac{\delta\alpha}{|\Lambda|v_\infty}$
In this case we have $\chi=\left(1+\frac{\alpha^2}{4|\Lambda|^3}\right)\arctan\frac{|\Lambda|v_\infty}{\alpha}-\frac{\alpha v_\infty}{4\Lambda^2}>$
$>\frac{|\Lambda|v_\infty}{\alpha}-\frac{1}{3}\frac{|\Lambda|^3 v_\infty^3}{\alpha^3}-\frac{v_\infty^3}{12\alpha}$. If we take v_∞ sufficiently small $v_\infty<\frac{1}{2}$ since already $\rho m>\frac{1}{2}$ and $|\Lambda|<\alpha$ we derive $\chi>\frac{1}{6}\frac{|\Lambda|v_\infty}{\alpha}$ and we can take $\delta=\left(\frac{\Lambda v_\infty}{\alpha}\right)^2\ll\chi$
obtaining $\bar{x}<1-\frac{|\Lambda|v_\infty}{\alpha}$
If $\varepsilon=1$ we have $\delta<(\theta_0-\theta)'(0)(1-\bar{x})=\left(\left(1-\frac{\alpha^2}{4|\Lambda|^3}\right)\frac{|\Lambda|v_\infty}{\sqrt{\Lambda^2 v_\infty^2+\alpha^2}}+\frac{\alpha v_\infty}{4\Lambda^2}\right)(1-\bar{x})$
If further $\alpha<\frac{1}{4}$ since $\rho m>\frac{1}{2}$, $|\Lambda|<\alpha$ we derive
$\delta<\left(\left(1-\frac{\alpha^2}{4|\Lambda|^3}\right)\frac{|\Lambda|v_\infty}{\alpha+\frac{1}{2}\alpha v_\infty^2}+\frac{\alpha v_\infty}{4\Lambda^2}\right)(1-\bar{x})=$
$=\left(\frac{|\Lambda|v_\infty}{\alpha}+\frac{\alpha v_\infty}{8(\rho m)^2}\frac{1}{1+\frac{1}{2}v_\infty^2}\right)<\left(\frac{|\Lambda|v_\infty}{\alpha}+\frac{1}{2}\alpha v_\infty\right)(1-\bar{x})$
Because $\alpha<\frac{1}{4}$ in this case we have $\chi=\left(1-\frac{\alpha^2}{4|\Lambda|^3}\right)\arctan\frac{|\Lambda|v_\infty}{\alpha}+\frac{\alpha v_\infty}{4\Lambda^2}>\frac{|\Lambda|v_\infty}{\alpha}$.
If $\frac{1}{2}\alpha v_\infty<\frac{|\Lambda|v_\infty}{\alpha}$ we can take $\delta=2\left(\frac{\Lambda v_\infty}{\alpha}\right)^2\ll\chi$ and if $\frac{|\Lambda|v_\infty}{\alpha}<\frac{1}{2}\alpha v_\infty$ we can take $\delta=\alpha v_\infty\frac{|\Lambda|v_\infty}{\alpha}\ll\chi$ in both situations
obtaining $\bar{x}<1-\frac{|\Lambda|v_\infty}{\alpha}$.

For $\bar{x}=\sqrt{1-\frac{\Lambda^2 v_\infty^2}{z^2}-\frac{2\alpha}{z}}$ we obtain the upper limitation for z as $\frac{1}{z}>\frac{1}{\alpha}\frac{-1+\sqrt{1+2\kappa^3-\kappa^4}}{\kappa^2}\approx\frac{1}{\alpha}\left(\kappa-\frac{1}{2}\kappa^2\right)$ where $\kappa=\frac{|\Lambda| v_\infty}{\alpha}$.

The figure below shows the limit case $|\Lambda|=v_\infty=\alpha=0.98$.



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41. Steepest descent approximation
Classical limit of Schroedinger equation

Steepest descent approximation

For a given real Lagrangian density
$\mathscr{L}=\mathscr{L}(\varphi,\partial\varphi)$ with $\varphi=\varphi(t,x)$, $(t,x)=(x^{\mu})_{\mu}\in\mathbb{R}^4$, $\mu=\overline{0,3}$, $x^0=t$, $x=(x^i)_{i=\overline{1,3}}$
$\left|(\varphi(0,x))_x\right\rangle=|\psi_I\rangle$, $\left|(\varphi(T,x))_x\right\rangle=|\psi_F\rangle$, $\varphi(t,x)=0_n$ for any $x\in\mathbb{R}^3\setminus D, t\in\mathbb{R}\setminus[0,T]$,
$\varphi(t,x)\in\mathbb{R}^n$ for any $(t,x)\in\mathbb{R}^4$, the action $S(\varphi)=\int\mathscr{L}(\varphi,\partial\varphi)\,dt\,d^3x$ by taking a discretization Γ of the φ -space $\varphi\to(q_1,...,q_N)=q\in\mathbb{R}^N$ can be written in the form $S=S(q)=S(a)+\frac{1}{2}(q-a)^T A(q-a)+O(\|q-a\|^3)$ with $(q-a)$ as a column vector and $A\in M_{N\times N}(\mathbb{R})$, $A=A^T$, $A=S''(a)$ with $S'(a)=0$, A depending only on the spacing of the discretization.
For computing the transition amplitude from state ψ_I to state ψ_F we will have (see Chap. … Path integral formalism …) :

$$\langle\psi_F|\exp(-\frac{i}{\hbar}\hat{H}T)|\psi_I\rangle=\int D\varphi\exp(\frac{i}{\hbar}\int\mathscr{L}(\varphi,\partial\varphi)\,dt\,d^3x)=$$

$$=C\int dq_1...dq_N\exp(\frac{i}{\hbar}S(q))$$ with C a discretization dependent constant.

Normalizing the field φ such that $O(\|q-a\|^2)=O(\hbar)$ (*) we obtain

$$\langle\psi_F|\exp(-\frac{i}{\hbar}\hat{H}T)|\psi_F\rangle=C\exp(\frac{i}{\hbar}S(a))\left(\frac{(2\pi i\hbar)^N}{\det A}\right)^{1/2}\exp(iO(\hbar^{1/2}))$$ for $N\to\infty$

(where C, A obviously depend on the discretization and so on N).
Thus in the limit $\hbar\to 0$ we can consider

$$\langle\psi_F|\exp(-\frac{i}{\hbar}\hat{H}T)|\psi_I\rangle=C\exp(\frac{i}{\hbar}\int\mathscr{L}(\varphi_s,\partial\varphi_s)\,dt\,d^3x)$$ where C is a constant

and $\left(d_\mu\left(\frac{\partial\mathscr{L}}{\partial(\partial_\mu\varphi)}\right)-\frac{\partial\mathscr{L}}{\partial\varphi}\right)(\varphi_s,\partial\varphi_s)=0$ (which corresponds to $S'(a)=0$)

Then if $\mathscr{L}=\frac{1}{2}(\partial\varphi)^2-V(\varphi)+J\cdot\varphi$ with $J=J(t,x)\in\mathbb{R}^n$ a source field and taking

$$S(\varphi)=\int(\frac{1}{2}(\partial\varphi)^2-V(\varphi))\,dt\,d^3x$$, $Z(J)=\exp(\frac{i}{\hbar}W(J))=\langle 0|\exp(-\frac{i}{\hbar}\hat{H}T)|0\rangle$

we will have :

$$Z(J)=\exp(\frac{i}{\hbar}(S(\varphi_s)+J\varphi_s))\int D\varphi\exp(-\frac{i}{\hbar}\int\frac{1}{2}\varphi(\partial^2+V''(\varphi_s))\varphi\,dt\,d^3x)$$

where $\partial^2\varphi_s+V'(\varphi_s)=J$ and we denoted $J\varphi_s=\int J(t,x)\cdot\varphi_s(t,x)\,dt\,d^3x$
Since $\det A=\exp(\mathrm{tr}(\log A))$ we can derive

$$W(J)=S(\varphi_s)+J\varphi_s+i\frac{\hbar}{2}\mathrm{tr}(\log(\partial^2+V''(\varphi_s)))+\hbar O(\hbar^{1/2})$$.

Classical limit of Schroedinger equation

As we have seen in Chap. … Path integral formalism … we can consider a discretized system described by generalized momentum and respective coordinates operators $\hat{p}=(\hat{p}_i)_{i=\overline{1,N}}=(-i\hbar\nabla_{qi})_{i=\overline{1,N}}$, $\hat{q}=(\hat{q}_i)_{i=\overline{1,N}}$ with wavefunctions $\psi=\psi(t,q)$, $q=(q_i)_{i=\overline{1,N}}$ -spatial coordinates , t -time coordinate and a Hamiltonian operator $\hat{H}(\hat{p},\hat{q})=\frac{\hat{p}^2}{2m}+V(\hat{q})$.

If we consider an initial state $|q_I\rangle=\psi_I$ and a final state $\langle q_F|=\psi_F$ then a system particle, starting at $t=0$ from q_I has a wave function $\psi(t)=\exp(-\frac{i}{\hbar}\hat{H}t)\,\psi_I$ and $\psi(t,q_F)=\langle q_F|\psi(t)\rangle=\langle q_F|\exp(-\frac{i}{\hbar}\hat{H}t)|q_I\rangle$ with the $|q\rangle$ states normalized as $\langle q|q'\rangle=\delta^N(q-q')$, $\int\delta^N(q-q')d^Nq=1$.

Therefore according to Chap. … Path integral formalism … we have $\psi(t,q_F)=\int Dq\exp(\frac{i}{\hbar}\int_0^t L(q,\dot{q})d\tau)$ where $\int Dq...$ means integration over all paths $q=q(\tau)$ with $q(0)=q_I$, $q(t)=q_F$ and $L(q,\dot{q})=p\dot{q}-H(p,q)$ (1)

$\dot{q}=\frac{\partial H}{\partial p}$ (2) (as we can easily derive , with the (1) definition the (2) relation is equivalent to $p=\frac{\partial L}{\partial\dot{q}}$ (3) .

For $\hbar$ approaching 0 we can consider (see Steepest descent approximation) for any q_I a family of paths $(\widetilde{q}=(q(\tau))_\tau)_{\widetilde{q}}$ defined by the motion equations $\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}_i}\right)-\frac{\partial L}{\partial q_i}=0$, $i=\overline{1,N}$ and $q(0)=q_I$ such that for any q_F there is a path $\widetilde{q}=(q(\tau))_\tau$ in the family with $q_F\in\widetilde{q}$, $q_F=q(t)$ and we can have well defined $S=S(t,q_F)=\int_0^t L(q(\tau),\dot{q}(\tau))d\tau$, $\psi(t,q_F)\approx\psi_0\exp(\frac{i}{\hbar}S)$ with ψ_0 a constant.

Under reasonable assumptions upon L , studying the bilocal problem represented by the motion equations and the conditions $q(0)=q_I$, $q(t)=q_F$ we conclude that we can take a infinitesimal variation $\delta q=\delta q(\tau)$ of $\widetilde{q}$ such that $\delta q(0)=0$, $\delta q(t)$ has an arbitrary direction and $q+\delta q$ remains in the $(\widetilde{q})_{\widetilde{q}}$ family of paths. The corresponding infinitesimal variation of S at (t,q_F) will be $\delta S=\frac{\partial S}{\partial q_F}(t,q_F)\,\delta q(t)$ and we have also $\delta S=\int_0^t\left(\frac{\partial L}{\partial q}\,\delta q(\tau)+\frac{\partial L}{\partial\dot{q}}\,\delta\dot{q}(\tau)\right)d\tau=$

$=\int_0^t\left(\frac{\partial L}{\partial q}-\frac{d}{d\tau}\left(\frac{\partial L}{\partial\dot{q}}\right)\right)\delta q(\tau)d\tau+\frac{\partial L}{\partial\dot{q}}\,\delta q(t)$

Thus since on the $\tilde{q}$ path the motion equations are satisfied and the infinitesimal $\delta(t)$ can have arbitrary direction it follows $\frac{\partial S}{\partial q}(t,q(t))=\frac{\partial L}{\partial \dot{q}}(q(t),\dot{q}(t))=p$ with $q=q(\tau)$ the $\tilde{q}$ path in the motion trajectories family that satisfies $q(0)=q_I$, $q(t)=q_F$.

With the same notations we obviously have :

$\frac{dS}{dt}(t,q(t))=L(q(t),\dot{q}(t))$, $\frac{dS}{dt}=\frac{\partial S}{\partial t}+\frac{\partial S}{\partial q}\dot{q}$ and so

$\frac{\partial S}{\partial t}(t,q)=L-p\dot{q}=-H(p,q)$

therefore on the motion trajectories we have $\frac{\partial S}{\partial q}(t,q(t))=p(t)$ (4) ,

$\frac{\partial S}{\partial t}(t,q(t))=-H(p(t),q(t))$ (5) with $p=\frac{\partial L}{\partial \dot{q}}(q,\dot{q})$, $H(p,q)=p\dot{q}-L$.

Taking for simplification $q_I=0_N$ it follows from (4) and (5) that if on the assumed trajectory the momentum $p=\frac{\partial L}{\partial \dot{q}}(q,\dot{q})$ and the energy $E=H(p,q)$ are well defined constant measurable quantities, then $S=pq-Et$ and so the wave function will be as expected $\psi=\psi_0\exp(\frac{i}{\hbar}(pq-Et))$

Plugging the $\psi(t,q)=\psi_0\exp(\frac{i}{\hbar}S(t,q))$ relation for the wave function into the Schroedinger equation $i\hbar\partial_t\psi(t,q)=\hat{H}\psi(t,q)=-\frac{\hbar^2}{2m}\nabla^2\psi(t,q)+V(q)\psi(t,q)$ we obtain $-\frac{\partial S}{\partial t}=-i\frac{\hbar}{2m}\nabla^2 S+\frac{1}{2m}(\nabla S)^2+V$ and with the (4) relation, this equation becomes in the $\hbar\to 0$ limit $-\frac{\partial S}{\partial t}=\frac{p^2}{2m}+V(q)$ which is precisely (5).

The limit $\hbar\to 0$ corresponds in fact to $\lambda=\frac{h}{p}\to 0$ that is a small wavelenght scale.

The classical limit solution represented by the classical solutions of (4) , (5) implies therefore the Schroedinger equation in the case of small wavelenghts in comparison to spatial dimensions which we consider, the numerical value of the Planck constant defining according to the (*) normalization in “Steepest descent approximation” the scale of lenghts.

42. Symmetry breaking. Effective potential

Symmetry breaking. Effective potential

Consider first a system described by generalized coordinates $(q_j)_{j=\overline{1,n}}$ and a Lagrangian $L=\frac{1}{2}m\dot{q}^2-V(q)$.

The Euler-Lagrange equations are $m\ddot{q}=-V'(q)$ and the system has stable equilibrium points at the minimum points q^s of the potential energy $V=V(q)$, having $V'(q^s)=\left(\frac{\partial V}{\partial q_l}(q^s)\right)_{l=\overline{1,n}}=0_n$.

At low energy we choose one of the minima at q^s and study small oscillations around that minimum.

For example, if $V(q)=-\frac{1}{2}q^2+\frac{\lambda}{4}(q^2)^2$ we have minima at $\|q^s\|=v=\sqrt{\frac{k}{\lambda}}$ if $k,\lambda>0$.

commuting to one of the minima $\|q^s\|=\sqrt{k/\lambda}$ breaks the reflection symmetry $q\to -q$ of the system, or if $n>1$, the $O(n)$ orthogonal group symmetry of the system.

In quantum mechanics, the particle can tunnel between the minima, the tunneling barrier being $V(0)$ - $V(q^s)$. The probability of being in one of the minima must be equal , thus respecting the symmetry of the Hamiltonian $H=\frac{p^2}{2m}+V(q)$.

In particular, the ground state wave function respects the symmetry and is of the form $\psi=\psi(\|q\|)$. However, in quantum field theory, for a generic scalar field $\varphi=\varphi(t,\vec{x})$, with $(t,\vec{x})=x\in\mathbb{R}^4$ and Lagrangian density $\mathscr{L}=\frac{1}{2}(\partial_0\varphi)^2-\frac{1}{2}(\nabla\varphi)^2-V(\varphi)$ we again have to find the the minimum of the potential energy $\int d^3\vec{x}\left(\frac{1}{2}(\nabla\varphi)^2+V(\varphi)\right)$.

In particular for the example $V(\vec{\varphi})=-\frac{1}{2}\mu^2\vec{\varphi}^2+\frac{\lambda}{4}(\vec{\varphi}^2)^2$ we will have minima at $\vec{\varphi}_s^2=\frac{\mu^2}{\lambda}$. The tunneling barrier is now $(V(\vec{0})-V(\vec{\varphi}_s))\int d^3\vec{x}$ and hence infinite (or more precisely extensive with the volume of the system). Tunneling is shut down and the ground state wave function is concentrated around one of the states $\vec{\varphi}_s$. It does not matter which $\vec{\varphi}_s=(\varphi_{js})_{j=\overline{1,n}}$ state we choose. The physics will be the same because of the $O(n)$ symmetry of the Lagrangian. For $n=1$ the reflection symmetry $\varphi\to-\varphi$ is broken and for $n\geq 2$ the continuous $O(n)$ symmetry is broken by commuting to one of the $\vec{\varphi}_s$ solutions to minima of the potential energy. This is the spontaneous symmetry breaking of a symmetric quantum field system.

In quantum field theory the ground state is also known as the vacuum, in which the field is " at rest " with no particles present. The value assumed by φ in the ground state is known as the vacuum expectation value of φ .
Upon spontaneous symmetry breaking we will observe the emergence of a massless boson.

Construct for example the complex field $\varphi=\frac{1}{\sqrt{2}}(\varphi_1+i\,\varphi_2)$ so that the Lagrangian density $\mathscr{L}=\frac{1}{2}((\partial\vec{\varphi})^2+\mu^2\vec{\varphi}^2)-\frac{\lambda}{4}(\vec{\varphi}^2)^2$ can be written as $\mathscr{L}=(\partial\varphi)^+(\partial\varphi)+\mu^2\varphi^+\varphi-\lambda(\varphi^+\varphi)^2$ which is manifestly invariant under $U(1)$ (the groups $O(2)$ and $U(1)$ are locally isomorphic) .
We parametrize the field by $\varphi(x)=\rho(x)\exp(i\,\theta(x))$ with $\rho(x)\in\mathbb{R}_+$, $\theta(x)\in\mathbb{R}$ and we have $\mathscr{L}=\rho^2(\partial\theta)^2+(\partial\rho)^2+\mu^2\rho^2-\lambda\rho^4$.

Spontaneous symmetry breaking means setting $\rho=v+\chi$ with $v=\sqrt{\frac{\mu^2}{2\lambda}}$ obtaining

$$\mathscr{L}=\frac{\mu^4}{4\lambda}+v^2(\partial\theta)^2+((\partial\chi)^2-2\mu^2\chi^2-4\sqrt{\frac{\mu^2\lambda}{2}}\chi^3-\lambda\chi^4)+(\sqrt{\frac{2\mu^2}{\lambda}}\chi+\chi^2)(\partial\theta)^2.$$

The $\frac{\mu^4}{4\lambda}$ term is just $-V(\varphi)\Big|_{\varphi=v}$. If we are only interested in the scattering of the mesons associated with χ this term does not enter at all: we are free to add an arbitrary constant to $\mathscr{L}$ to begin with. The same situation appears in quantum mechanics. In the discussion of the quantum harmonic oscillator the zero point energy $\frac{1}{2}\hbar\omega$ is not observable; only transitions between energy levels are physical.
We recognize in the phase θ (x) the massless field . The second term in the above expression is the kinetic energy of the massless field θ , the third term corresponds to the kinetic energy and potential energy of the massive field χ , which has the mass $\sqrt{2}\mu$ and the fourth term corresponds to the interaction between θ and χ fields.
In the same way, spontaneous breaking with parametrization $\varphi_1=v+\varphi'_1$, $v=\sqrt{\frac{\mu^2}{\lambda}}$, $\varphi_2=\varphi'_2$ we obtain a theory with a massive field φ'_1 and a massless field φ'_2 and Lagrangian density $\mathscr{L}=\frac{\mu^4}{4\lambda}+\frac{1}{2}((\partial\varphi'_1)^2+(\partial\varphi'_2)^2)-\mu^2\varphi'^2_1+O(\varphi'^3)$ the field φ'_1 having mass $\sqrt{2}\mu$.
Generally we will have Goldstone's theorem which states that whenever a continuous symmetry is spontaneously broken, massless fields, known as Nambu-Goldstone bosons emerge.
With every continuous symmetry, according to Noether theorem , a conserved charge

$\hat{Q}$ can be associated. That $\hat{Q}$ generates a symmetry is stated as $[\hat{H},\hat{Q}]=0$ (indeed according to Chap. Quantum statistical ensemble , with $\hat{Q}$ not depending explicit on time we have $\frac{d}{dt}\langle\hat{Q}\rangle_t=i\langle[\hat{H},\hat{Q}]\rangle_t$ expressing the conservation in time of $\hat{Q}$) .
With $|0\rangle$ the ground state, by adding an appropiate constant to the Hamiltonian, we can always write $\hat{H}|0\rangle=0$
Normally the vacuum is invariant under the symmetry transformation $\exp(i\theta\hat{Q})$ in other words $\exp(i\theta\hat{Q})|0\rangle=|0\rangle$, $\hat{Q}|0\rangle=0$.
Suppose the symmetry is spontaneously broken so that $\hat{Q}|0\rangle\neq 0$.
The Noether current to the conserved charge is $(J^{\mu})_{\mu=\overline{0,3}}$ so that we have $Q=\int d^3\vec{x}\,J^0(t,\vec{x})$. Conservation of the charge says that the integral can be evaluated at any time. Consider the state $|s\rangle=\int d^3\vec{x}\exp(-i\vec{k}\cdot\vec{x})\hat{J}^0(t,\vec{x})|0\rangle$ which has a spatial momentum $\vec{k}$. As $\vec{k}$ goes to $\vec{0}$ the state $|s\rangle$ goes to $\hat{Q}|0\rangle$ which has zero energy since $\hat{H}\hat{Q}|0\rangle=\hat{Q}\hat{H}|0\rangle=0$. Thus as the momentum of the state $|s\rangle$ goes to $\vec{0}$ its energy goes to zero. In a relativistic theory this means that $|s\rangle$ describes a massless particle.
Indeed for $\hat{\varphi}=\hat{\varphi}(x)$ field operator function we have
$\hat{\varphi}(x+a)=\exp(i\hat{p}a)\hat{\varphi}(x)\exp(-i\hat{p}a)$ and so $\hat{J}(x+a)=\exp(i\hat{p}a)\hat{J}(x)\exp(-i\hat{p}a)$
(with $\hat{p}$ -the four momentum field operator, see Chap. Spin-statistics theorem)
$\hat{J}(x+a)-\hat{J}(x)=i[\hat{p},\hat{J}(x)]+O(a^2)$, $-i\partial_l\hat{J}(x)=[\hat{p}_l,\hat{J}(x)]$ and since $\hat{p}_l|0\rangle=0$
we will have $\hat{p}_l|s\rangle=\int d^3\vec{x}\exp(-i\vec{k}\cdot\vec{x})[\hat{p}_l,\hat{J}^0(t,\vec{x})]|0\rangle=$
$=\int d^3\vec{x}(-ik_l)\exp(-i\vec{k}\cdot\vec{x})\hat{J}^0(t,\vec{x})|0\rangle=k_l|s\rangle$.
We see that the number of Nambu-Goldstone bosons is clearly equal to the number of conserved charges that do not leave the vacuum invariant, that is do not anihilate $|0\rangle$. In general, if the Lagrangian is left invariant by a symmetry group G with n (G) generators but the vacuum is left invariant by only a subgroup H of G with n (H) generators then there are n (G) – n (H) Nambu-Goldstone bosons.

Consider now the scalar field theory defined by the Lagrangian density
$\mathscr{L}=\frac{1}{2}(\partial\varphi)^2-V(\varphi)$, $\varphi=\varphi(t,\vec{x})\in\mathbb{R}$
(for example we can take $V(\varphi)=-\frac{1}{2}\mu^2\varphi^2+\frac{\lambda}{4!}\varphi^4$)
The action is $S(\varphi)=\int d^4x\,\mathscr{L}(\varphi,\partial\varphi)$.
For $\mu^2>0$ the action is minimized at some $\varphi_{min}\neq 0$ and the symmetry is broken.
For $\mu^2<0$ the action is minimized at $\varphi=0$ and quantizing the small fluctuations around $\varphi=0$ we obtain scalar particles that scatter of each other.
If we take in consideration quantum fluctuations, to absorb cutoff dependence (as we show in Chap. Path integral formalism . Theory renormalization) we have to include counterterms as indicated, taking a Lagrangian density

$\mathscr{L}(\varphi,\partial\varphi)+A(\partial\varphi)^2+B\varphi^2+C\varphi^4$ and we will see that the $\mu=0$ theory is posed on the edge of symmetry breaking and quantum fluctuations ought push it over the brink.

The amplitude in presence of the field sources $J=J(t,\vec{x})$ defining the scalar field theory (see Chap. Path integral formalism) is

$\langle 0|\exp(-\frac{i}{\hbar}\widehat{H}T)|0\rangle=Z(J)=\exp(\frac{i}{\hbar}W(J))=\int D\varphi\exp(\frac{i}{\hbar}(S(\varphi)+J\varphi))$

where we dropped a discretization dependent factor $Z(J=0)$ adopted the shorthand $J\varphi=\int d^4x J(x)\varphi(x)$ and $\widehat{H}$ is the Hamiltonian operator corresponding to a Lagrangian density $\widetilde{\mathscr{L}}(\varphi,\partial\varphi)=\mathscr{L}(\varphi,\partial\varphi)+J(x)\varphi(x)$:

$H=\int d^3\vec{x}\left(\frac{\partial\mathscr{L}}{\partial(\partial_0\varphi)}\partial_0\varphi-\widetilde{\mathscr{L}}(\varphi,\partial\varphi)\right)$ while T is the considered time interval of the action.

As we know, by differentiating *W* with respect to the source *J* (*x*) repeatedly we can obtain any scattering amplitude we want.

As a particular case of the relation derived in Chap. Feynman amplitudes … we have:

$\langle 0|\exp(-i\widehat{H}T)\hat{\varphi}(x)|0\rangle=\int D\varphi\exp(\frac{i}{\hbar}(S(\varphi)+J\varphi))\varphi(x)$ and so since the ground state can be considered a $\widehat{H}$ eigenstate we conclude that

$$\varphi_c(x)=\frac{\delta W}{\delta J(x)}=\frac{1}{Z(J)}\int D\varphi\exp(\frac{i}{\hbar}(S(\varphi)+J\varphi))\varphi=\langle 0|\hat{\varphi}(x)|0\rangle \qquad (1)$$

The relation (1) determines the vacuum expectation value of the field operator function which is φ_c as a functional of the source field *J* .

Taking the Legendre transform of W we obtain a functional of φ_c through the implicit dependence of J on φ_c :

$\Gamma(\varphi_c)=W(J)-\int d^4x J(x)\varphi_c(x)$ and we have

$$\frac{\delta\Gamma(\varphi_c)}{\delta\varphi_c(y)}=\int d^4x\frac{\delta J(x)}{\delta\varphi_c(y)}\frac{\delta W(J)}{\delta J(x)}-\int d^4x\frac{\delta J(x)}{\delta\varphi_c(y)}\varphi_c(x)-J(y)=-J(y) \qquad (2)$$

We can expand $\Gamma(\varphi_c)$ in the form

$$\Gamma(\varphi_c)=\int d^4x(-V_{eff}(\varphi_c(x))+K(\varphi_c(x))(\partial\varphi_c(x))^2+...) \qquad (3)$$

where $(...)$ indicates higher and higher powers of ∂.

$V_{eff}=V_{eff}(\varphi_c)$ is the effective potential and we notice that if J and φ_c not depend on x the relation (2) reduces to $V'(\varphi_c)=J$. In other words, the vacuum expectation value of $\hat{\varphi}$ in the absence of an external source is determined by minimizing $V_{eff}(\varphi_c)$.

As we proved in Chap. Steepest descent approximation we have for a proper normalization according to the distances scale that

$$W(J)\approx S(\varphi_s)+J\varphi_s+\frac{i\hbar}{2}\operatorname{tr}\log(\partial^2+V''(\varphi_s)) \qquad (4)$$

where $\varphi_s=\varphi_s(x)$ is the steepest descent function satisfying $\left.\frac{\delta(S(\varphi)+J\varphi)}{\delta\varphi(x)}\right|_{\varphi=\varphi_s}=0$

or more explicitly $\partial^2\varphi_s(x)+V'(\varphi_s(x))=J(x)$ (5)

so that φ_s as a solution of (5) is to be regarded as a function of J .

Therefore $\varphi_c(x)=\frac{\delta W}{\delta J(x)}\approx\frac{\delta(S(\varphi_s)+J\varphi_s)}{\delta\varphi_s}\frac{\delta\varphi_s}{\delta J}+\varphi_s+O(\hbar)=\varphi_s+O(\hbar)$.

To leading order in $\hbar$ the expectation value φ_c is equal to φ_s and we have

$$S(\varphi_c)+J\varphi_c=S(\varphi_s)+J\varphi_s+\int\frac{\delta(S(\varphi_s)+J\varphi_s)}{\delta\varphi_s}(\varphi_c-\varphi_s)d^4x+O(\hbar^2)=$$

$$=S(\varphi_s)+J\varphi_s+O(\hbar^2)$$ and so

$$\Gamma(\varphi_c)=W(J)-J\varphi_c\approx S(\varphi_c)+\frac{i\hbar}{2}\operatorname{tr}\log(\partial^2+V''(\varphi_c)) .$$

In practice it is impossible to evaluate the trace for arbitrary φ_c : we have to find all the eigenvalues of the operator $\partial^2+V''(\varphi_c)$ take their log and sum . However we can be content to study $\Gamma(\varphi)$ for φ independent of x in which case $V''(\varphi)$ is a constant and the operator $\partial^2+V''(\varphi)$ is translation invariant and easily treated in momentum space:

$$\operatorname{tr}\log(\partial^2+V''(\varphi))=\int d^4x\langle x|\log(\partial^2+V''(\varphi))|x\rangle=$$

$$=\int d^4x\int\frac{d^4k}{(2\pi)^4}\int\frac{d^4k'}{(2\pi)^4}\langle x|k\rangle\langle k|\log(\partial^2+V''(\varphi))|k'\rangle\langle k'|x\rangle=$$

$$=\int d^4x\int\frac{d^4k}{(2\pi)^4}\log(-k^2+V''(\varphi))$$

where we used $\int\frac{1}{(2\pi)^4}|k\rangle\langle k|=\boldsymbol{I}$, $\langle x|k\rangle=\exp(ikx)$

Therefore for φ_c not depending on x we have

$$V_{eff}(\varphi_c)\approx V(\varphi_c)-\frac{i\hbar}{2}\int\frac{d^4k}{(2\pi)^4}\log\left(\frac{k^2-V''(\varphi_c)}{k^2}\right) \qquad (5)$$

Note that we have added a φ_c independent constant to the potential to make the argument of the logarithm dimensionless.

The first term in (5) is the classical energy density contained in the background $\varphi=\varphi_c$ while the second term is the vacuum energy density of a scalar field with mass squared equal to $V''(\varphi_c)=-\mu^2+\frac{1}{2}\lambda\varphi_c^2$ (in natural units with $\hbar=1$, $c=1$).

Consider a fermion field described by the Dirac spinor field $\psi=\psi(x)$ interacting with the scalar field, adding to the Lagrangian density the term $\overline{\psi}(i\partial\!\!\!/-m-f\varphi)\psi$ with $p\!\!\!/=\gamma^\alpha p_\alpha$ for any $p=(p_\alpha)_{\alpha=\overline{0,3}}$, f -coupling constant and we will have the path integral

$$Z(J)=\exp\left(\frac{i}{\hbar}W(J)\right)=$$

$$=\int D\varphi D\overline{\psi}D\psi\exp\left(\frac{i}{\hbar}\int d^4x\left(\frac{1}{2}(\partial\varphi)^2-V(\varphi)+\overline{\psi}(i\partial\!\!\!/-m-f\varphi)\psi+J\varphi\right)\right)$$

Respecting the steps as above, considering that integrating over ψ variables first (see Chap. Feynman amplitudes … and Chap. Dirac equation … Fermion propagator)

$$Z(J)=\int D\varphi\exp\left(\frac{i}{\hbar}\int d^4x\left(\frac{1}{2}(\partial\varphi)^2-V(\varphi)+J\varphi\right)-i\hbar\,\mathrm{tr}\log(i\partial\!\!\!/-m-f\varphi)\right)\ ,$$

we find that for J , φ_c not depending on x , the fermion field contributes with

$$V_F(\varphi_c)=2i\hbar\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}\log\left(\frac{k^2-m^2(\varphi_c)}{k^2}\right)\quad\text{to } V_{eff}(\varphi_c)\ \text{ (where } m(\varphi_c)=m+f\varphi_c\ ),$$

which as we know is the vacuum energy density of a fermion field with mass m (φ_c) (in natural units $\hbar$ = 1 , c = 1) . (Notice the contrasting sign in $V_F(\varphi_c)$ of the integral compared to the sign of the integral term in (5) .)

To evaluate $I=i\int\frac{d^4k}{(2\pi)^4}\log\left(\frac{k^2-V''(\varphi_c)+i\varepsilon}{k^2+i\varepsilon}\right)$ we take a cutoff on $\vec{k}$ -space $\|\vec{k}\|<\Lambda$ and $\varepsilon>0$, $\varepsilon\to 0$ with $k=(\omega,\vec{k})$ integrating first over ω by parts and residues theorem obtaining

$$I=i\frac{\int d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega}{2\pi}\log\left(\frac{\omega^2-\omega_k^2+i\varepsilon}{\omega^2-\omega'^2_k+i\varepsilon}\right)=i\int\frac{d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega}{2\pi}\left(\frac{2\omega'^2_k}{\omega^2-\omega'^2_k+i\varepsilon}-\frac{2\omega_k^2}{\omega^2-\omega_k^2+i\varepsilon}\right)=$$

$$=-\int\frac{d^3\vec{k}}{(2\pi)^3}(\omega_k-\omega'_k)=-\frac{1}{2\pi^2}\int_0^\Lambda k^2\left(\sqrt{k^2-V''(\varphi_c)}-k\right)dk=$$

$$=\frac{\Lambda^4}{8\pi^2}-\frac{1}{2\pi^2}\int_a^\infty\frac{V''^2(\varphi_c)y^2}{(y^2-1)^3}dy=\Lambda^4\frac{1-a}{8\pi^2}-\frac{V''^2(\varphi_c)}{2\pi^2}\int_a^\infty\frac{1}{4(y^2-1)^2}dy=$$

$$=-\frac{1}{16\pi^2}\Lambda^2V''(\varphi_c)+\frac{1}{64\pi^2}V''^2(\varphi_c)-\frac{V''^2(\varphi_c)}{32\pi^2}\left(\frac{1}{a-1}+\frac{1}{a+1}+\log\frac{a-1}{a+1}\right)+O\left(\frac{1}{\Lambda^2}\right)=$$

$$=-\frac{1}{8\pi^2}\Lambda^2V''(\varphi_c)-\frac{1-4\log 2}{64\pi^2}V''^2(\varphi_c)+\frac{V''^2(\varphi_c)}{32\pi^2}\log\frac{\Lambda^2}{V''(\varphi_c)}+O\left(\frac{1}{\Lambda^2}\right)\ ,$$

where $\omega_k=\sqrt{\vec{k}^2+V''(\varphi_c)}$, $\omega'_k=\|\vec{k}\|$, $a=\sqrt{1+\frac{V''(\varphi_c)}{\Lambda^2}}$

and we used the Cebyshev substitution $y=\left(1+\frac{V''(\varphi_c)}{k^2}\right)^{1/2}$.

Thus suppressing $\hbar$ (taking units such that $\hbar=1, c=1$) we will have

$$V_{eff}(\varphi)=V(\varphi)+\frac{1}{16\pi^2}V''(\varphi)\Lambda^2-\frac{1}{64\pi^2}V''^2(\varphi)\log\frac{\Lambda^2}{V''(\varphi)}+\frac{1-4\log 2}{128\pi^2}V''^2(\varphi)+ \quad (6)$$

$$+B\varphi^2+C\varphi^4 \ .$$

We were instructed to introduce counterterms $A(\partial\varphi)^2+B\varphi^2+C\varphi^4$ to absorb cutoff dependence (of which only $B\varphi^2+C\varphi^4$ are relevant since φ is independent of x).

Because $V''(\varphi)=-\mu^2+\frac{\lambda}{2}\varphi^2$ it follows that we have just enough counterterms in $B\varphi^2+C\varphi^4$ to absorb cutoff dependence in (6) and the theory is clearly renormalizable for first order in quantum fluctuations.

Supposing in contrast that V is a polynomial of degree 6 in φ we are allowed to have three counterterms $B\varphi^2 + C\varphi^4 + D\varphi^6$ but that is not enough since $(V''(\varphi))^2$ is now a polynomial of degree 8. This means that we should have started with V a polynomial of degree 8 but then V'' would be a polynomial of degree 12 , the process escalating into an infinite degree polynomial and having so a non-renormalizable theory.

In the renormalizable φ^4 theory, in Chap. Quantum field theory … Theory renormalization we fix the counterterms by imposing conditions on various scattering amplitudes. Here we would have to fix the coefficients B and C by imposing conditions on $V_{eff}(\varphi)$.

Consider the case $\mu = 0$, at the edge of symmetry breaking.

Thus $V(\varphi)=\frac{\lambda}{4!}\varphi^4 \quad , \quad V''(\varphi)=\frac{\lambda}{2}\varphi^2$,

$$V_{eff}(\varphi)=\left(\frac{1}{32\pi^2}\lambda\Lambda^2+B\right)\varphi^2+\left(\frac{1}{4!}\lambda+\frac{\lambda^2}{(16\pi)^2}\log\frac{\lambda\varphi^2}{2\Lambda^2}+C\right)\varphi^4+\frac{1-4\log 2}{2(16\pi)^2}\lambda^2\varphi^4 \ .$$

We see explicitly that the Λ dependence can be absorbed into B and C .

$\mu=0$ means $\left.\frac{d^2V}{d\varphi^2}\right|_{\varphi=0}=0$. To say that we have a $\mu=0$ theory means that we have to maintain a vanishing renormalized squared mass and thus we impose $\left.\frac{d^2V_{eff}}{d\varphi^2}\right|_{\varphi=0}=0$ and so we want $B=-\frac{\Lambda^2}{32\pi^2}\lambda$.

Similarly we would be to set $\left.\frac{d^4V_{eff}}{d\varphi^4}\right|_{\varphi=0}$ equal to some coupling, but differentiating the $\varphi^4\log\varphi^2$ term in V_{eff} four times we are going to get a term like $\log\varphi^2$ which is not defined at $\varphi=0$. We are forced to impose our condition on $\frac{d^4V_{eff}}{d\varphi^4}$ not at $\varphi=0$ but at φ equal to some arbitrarily chosen mass M.

(Recall that φ has the dimension of mass)

The second condition reads $\left.\frac{d^4 V_{eff}}{d\varphi^4}\right|_{\varphi=M} = \lambda(M)$.

After absorbing some φ independent constants into C we have :

$$V_{eff}(\varphi) = \left(\frac{\lambda}{4!} + \frac{\lambda^2}{(16\pi)^2}\log\frac{\varphi^2}{\Lambda^2} + C\right)\varphi^4$$

$$\frac{d^4 V_{eff}}{d\varphi^4} = \lambda + 4!C + \frac{\lambda^2}{(16\pi)^2}4!\log\frac{\varphi^2}{\Lambda^2} + \frac{25}{(8\pi)^2}\lambda^2$$

$$\lambda(M) = \lambda + 4!C + \frac{\lambda^2}{(16\pi)^2}4!\log\frac{M^2}{\Lambda^2} + \frac{25}{(8\pi)^2}\lambda^2$$

$$\lambda(M) = \lambda(M_0) + \frac{3}{(4\pi)^2}\lambda^2\log\frac{M}{M_0}$$

$$V_{eff}(\varphi) = \left(\frac{\lambda(M)}{4!} + \frac{\lambda^2}{(16\pi)^2}\log\frac{\varphi^2}{M^2} - \frac{25}{(8\pi)^2}\frac{\lambda^2}{4!}\right)\varphi^4$$

At some M_0 we must have $\lambda(M_0) = \lambda + O(\lambda^2)$ and so $\lambda(M) = \lambda + O(\lambda^2)$, $O(\lambda(M)) = O(\lambda)$, $\lambda^2 = (\lambda(M)) + O((\lambda(M))^3)$

$$V_{eff}(\varphi) = \left(\frac{\lambda(M)}{4!} + \frac{(\lambda(M))^2}{(16\pi)^2}\left(\log\frac{\varphi^2}{M^2} - \frac{25}{6}\right)\right)\varphi^4 + O((\lambda(M))^3) \quad (7)$$

As we can see from (7) , C and the cutoff Λ have both disappeared so we have a renormalizable theory.

Quantum fluctuations (for the $\mu = 0$ theory) generate a correction to the potential of the form $\varphi^4\log\varphi^2$.

$$\frac{dV_{eff}}{d\varphi} = \left(\frac{\lambda(M)}{6} + \frac{(\lambda(M))^2}{(8\pi)^2}\left(\log\frac{\varphi^2}{M^2} - \frac{11}{3}\right)\right)\varphi^3$$

$$\frac{d^2 V_{eff}}{d\varphi^2} = 3\left(\frac{\lambda(M)}{6} + \frac{(\lambda(M))^2}{(8\pi)^2}\left(\log\frac{\varphi^2}{M^2} - 3\right)\right)\varphi^2$$

$$\log\frac{\varphi_{min}^2}{M^2} = \frac{11}{3} - \frac{(8\pi)^2}{6\lambda(M)} \quad , \quad \frac{d^2 V_{eff}}{d\varphi^2}(\varphi_{min}) = 2\frac{(\lambda(M))^2}{(8\pi)^2}\varphi_{min}^2 > 0$$

Therefore $\varphi_{min} \neq 0$ defined by (8) is a minimizing point for V_{eff} which means that quantum fluctuations break the discrete symmetry $\varphi \to -\varphi$ pushing over the brink, as we announced the edge of symmetry breaking $\mu = 0$.

43. Anderson-Higgs mechanism

The Anderson-Higgs mechanism

Consider a $U(1)$ invariant theory with a complex scalar field $\varphi=\varphi(t,\vec{x})$, $(t,\vec{x})=x\in\mathbb{R}^4$, described by a Lagrangian density $\mathscr{L}=(\partial\varphi)^+(\partial\varphi)+\mu^2\varphi^+\varphi-\lambda(\varphi^+\varphi)^2$.

We gauge the theory, replacing ∂_ν with $D_\nu=\partial_\nu+ie A_\nu$, $A_\nu=A_\nu(x)$, $\nu=\overline{0,3}$.

Parametrizing the field in polar coordinates $\varphi=\rho(x)\exp(i\theta(x))$ the gauged theory expresses a Lagrangian density

$\mathscr{L}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\rho^2(\partial\theta+e A)^2+(\partial\rho)^2+\mu^2\rho^2-\lambda\rho^4$ with $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$.

Under a gauge transformation $\varphi\to\exp(i\alpha)\varphi$, $\alpha=\alpha(x)$ we have $\theta\to\theta+\alpha$, $e A_\mu\to e A_\mu-\partial_\mu\alpha$ and so the combination

$B_\mu=A_\mu+\frac{1}{e}\partial_\mu\theta$ is gauge invariant.

Upon spontaneous symmetry breaking, allowing φ a vacuum expectation value

$\langle\varphi\rangle=\frac{v}{\sqrt{2}}\in\mathbb{R}_+$, $v=\sqrt{\frac{\mu^2}{\lambda}}\neq 0$ we write $\rho=\frac{1}{\sqrt{2}}(v+\chi)$

(see Chap. Symmetry breaking) and we have

$\mathscr{L}=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\frac{1}{2}M^2B^2+e^2v\chi B^2+\frac{1}{2}e^2\chi^2B^2+$

$+\frac{1}{2}(\partial\chi)^2-\mu^2\chi^2-\mu\sqrt{\lambda}\chi^3-\frac{\lambda}{4}\chi^4+\frac{\mu^4}{4\lambda}$

The theory now consists of a vector field $(B_\mu)_\mu$ with mass $M = |e|\,v$ interacting with a real scalar field χ with mass $\sqrt{2}\mu$. The phase field which would have been the Nambu-Goldstone boson in the ungauged theory has disappeared: the gauge field $(A_\mu)_\mu$ has eaten the Nambu-Goldstone boson.

More general, in a spontaneously broken non-abelian gauge theory derived from a Higgs field φ Lagrangian density invariant under $G = S\,U\,(N)$

$\mathscr{L}=\frac{1}{2}(\partial_\mu\varphi)\cdot(\partial^\mu\varphi)-V(\varphi\cdot\varphi)$ with a vacuum expectation value $\langle\varphi\rangle=v$,

where we replace ∂_μ with $D_\mu=\partial_\mu-ig A_\mu^a T^a$, $(T^a)_a$ the generators of the $SU(N)$ representation, if the symmetry is broken to a subgroup H of G with generators $(T^c)_c$ (the vacuum expectation value is left invariant under H), considering that the $n(G)-n(H)$ Nambu-Goldstone bosons are eaten by gauge bosons, we obtain the mass spectrum of the gauge bosons replacing φ by its vacuum expectation value in the kinetic term $\frac{1}{2}(D^\mu\varphi)\cdot(D_\mu\varphi)=\frac{1}{2}A^{a\nu}(\mu^2)^{ab}A^b_\nu$ and determining the eigenvalues of $\mu^2=((\mu^2)^{ab})_{a,b}$ where $(\mu^2)^{ab}=g^2(T^a v)\cdot(T^b v)$.

Obviously μ^2 is self-adjoint and positive definite and we can diagonalize it to obtain the masses of the gauge bosons. The eigenvectors tell us which linear combinations of $(A^a_\nu)_\nu$ correspond to mass eigenstates. $((\mu^2)^{ab})_{a,b}$ has $n(H)$ zero eigenvalues. (indeed, v is left invariant by H which means $T^c v=0$ for any T^c generator of H and hence the gauge boson associated with T^c remains massless)

As a useful aplication we consider a Higgs field φ transforming as the adjoin representation of $SU(5)$ (under $U\in G=SU(5)$ we have $\varphi\to U\varphi U^+$ with φ a traceless self-adjoint 5×5 matrix having vacuum expectation value $\langle\varphi\rangle=\mathrm{diag}(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3},\frac{1}{2},\frac{1}{2})$.

We have $D_\mu\varphi=\partial_\mu\varphi-ig A^a_\mu[T^a,\varphi]$, $(\mu^2)^{ab}=g^2\,\mathrm{tr}([T^a,\langle\varphi\rangle][\langle\varphi\rangle,T^b])$, $a,b=\overline{1,24}$

The gauge bosons A^a for which T^a commute with $\langle\varphi\rangle$ remain massless, while the other bosons acquire mass, that is the $SU(5)$ symmetry is broken to $SU(3)\times SU(2)\times U(1)$ since generators of the form $\begin{pmatrix}C & 0\\ 0 & 0\end{pmatrix}$ or $\begin{pmatrix}0 & 0\\ 0 & B\end{pmatrix}$ or the generator $\mathrm{diag}(2,2,2,-3,-3)$ commute with $\langle\varphi\rangle$ where $C=C^+\in M_{3\times 3}(\mathbb{C})$, $B=B^+\in M_{2\times 2}(\mathbb{C})$, $\mathrm{tr}\,C=\mathrm{tr}\,B=0$.

44. Chiral anomaly

Chiral anomaly

Consider the theory of a single massless fermion with Lagrangian density $\mathscr{L}_0(\psi,\partial\psi)=\overline{\psi}i\gamma^\mu\partial_\mu\psi$ where $\psi=\psi(x)$, $x\in\mathbb{R}^4$ is the fermion Dirac spinor field. As we noticed in Chap. Fermion charge conserved current ... $\mathscr{L}_0$ is invariant under the separate transformations $\psi\to\exp(i\theta)\psi$ and $\psi\to\exp(i\theta\gamma^5)\psi$, corresponding according to Noether theorem to the conserved current $(J^\mu)_\mu=(\overline{\psi}\gamma^\mu\psi)_\mu$ and respective the conserved axial current $(J_5^\mu)=(\overline{\psi}\gamma^\mu\gamma^5\psi)_\mu$.
From the equations of motion (Euler-lagrange equations derived from the Lagrangian) follows immediately $\partial_\mu J^\mu=0$ (1) and $\partial_\mu J_5^\mu=0$ (2).
Now we want to check if relations (1) and (2) continue to hold under quantum fluctuations for massless fermions in a gauged quantum electrodynamics theory that involve photons, that is a Lagrangian density

$$\mathscr{L}(\psi,\partial\psi,A,\partial A)=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\overline{\psi}i\gamma^\mu\partial_\mu\psi-e\overline{\psi}\gamma^\mu A_\mu\psi=$$
$$=\mathscr{L}_1(\psi,\partial\psi,A,\partial A)-eJ^\mu A_\mu$$

with $(A_\mu)_\mu$ electromagnetic four-potential as photon field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, and *e* -electron charge.
As we prove in Chap. *SO*(10) unification, relation (1) continues to hold under quantum fluctuations, since otherwise we would have no gauge invariance of the amplitudes.
To check if (2) is violated under quantum fluctuations we have to consider an infinite number of Feynman diagrams that produces the expectation value $\langle 0|\partial_\mu\hat{J}_5^\mu(x)|0\rangle$, computable in Lattice gauge theory for the Lagrangian density $\mathscr{L}(\psi,\partial\psi,A,\partial A)$ that is (see Chap. Feynman amplitudes and lattice gauge theory): $\langle 0|\partial_\mu\hat{J}_5^\mu(x)|0\rangle=\int D\overline{\psi}D\psi DA\exp(i\int\mathscr{L}(\psi,\partial\psi,A,\partial A)d^4w)\partial_\mu J_5^\mu(x)$.
The zero and first order in *e* diagrams produce
$\int D\overline{\psi}D\psi DA\exp(i\int\mathscr{L}_1(\psi,\partial\psi,A,\partial A)d^4w)\partial_\mu J_5^\mu(x)$ and respective
$\int D\overline{\psi}D\psi DA\exp(i\int\mathscr{L}_1(\psi,\partial\psi,A,\partial A)d^4w)\partial_\mu J_5^\mu(x)\int d^4y\,eJ^\lambda(y)A_\lambda(y)$
and these expressions vanish since the first is $\partial_\mu(\gamma^\mu_{\alpha\beta}\gamma^5_{\beta\delta}iD^{fer}_{\delta\alpha}(x-x))=0$ and the second vanishes because the integrand is odd in the $A(y)$ path integration variables.
The second order in *e* diagrams are the chiral anomaly diagrams from fig.1.
Hence in *O* (e^3) approximation we have :

$$\int\langle 0|\partial_\mu\hat{J}_5^\mu(x)|0\rangle\exp(-iqx)d^4x=i\int\langle 0|\hat{J}_5^\mu(x)|0\rangle q_\mu\exp(-iqx)d^4x=$$
$$=i\int d^4x\exp(-iqx)\int D\overline{\psi}D\psi DA\exp(i\int\mathscr{L}_1(\psi,\partial\psi,A,\partial A)d^4w)$$
$$(-e^2)\int d^4y\,d^4z\,J_5^\mu(x)J^\lambda(y)J^\nu(z)A_\lambda(y)A_\nu(z)=$$

$$=e^2\int q_\mu \mathrm{tr}\left(\gamma^\mu\gamma^5\frac{1}{\not p-\not q}\gamma^\nu\frac{1}{\not p-\not k_1}\gamma^\lambda\frac{1}{\not p}+\gamma^\mu\gamma^5\frac{1}{\not p-\not q}\gamma^\lambda\frac{1}{\not p-\not k_2}\gamma^\nu\frac{1}{\not p}\right)\delta^4(q-k_1-k_2)$$

$$\frac{1}{(2\pi)^8}A_\lambda(k_1)A_\nu(k_2)d^4k_1d^4k_2d^4p=$$

$$=e^2\int i\Delta^{\mu\lambda\nu}(k_1,k_2)q_\mu\delta^4(q-k_1-k_2)A_\lambda(k_1)A_\nu(k_2)d^4k_1d^4k_2 \qquad (3)$$

where $A_\lambda(x)=\frac{1}{(2\pi)^4}\int\exp(ikx)A_\lambda(k)d^4k$ we have an extra (-) sign for the fermion loop and Bose statistics for the two photons and we defined

$$\Delta^{\mu\lambda\nu}(k_1,k_2)=\int\mathrm{tr}\left(\gamma^\mu\gamma^5\frac{1}{\not p-\not q}\gamma^\nu\frac{1}{\not p-\not k_1}\gamma^\lambda\frac{1}{\not p}+\gamma^\mu\gamma^5\frac{1}{\not p-\not q}\gamma^\lambda\frac{1}{\not p-\not k_2}\gamma^\nu\frac{1}{\not p}\right)\frac{i^3}{(2\pi)^8}d^4p=$$

$$=(2\pi)^{-4}\int D\overline{\psi}D\psi DA\exp\left(i\int\mathscr{L}_1(\psi,\partial\psi,A,\partial A)d^4w\right)\int J_5^\mu(0)J^\lambda(y)J^\nu(z)$$

$\exp(ik_1y)\exp(ik_2z)d^4yd^4z$ with $q=k_1+k_2$.

The charge $Q=\int d^3\vec{x}J^0(t,\vec{x})$ counts the number of fermions and must be a conserved in time quantity, which happens if $\partial_\mu J^\mu=0$ (since $\frac{dQ}{dt}=\int\nabla\cdot\vec{J}d^3\vec{x}=$

$=\lim_{R\to0}\int_{S(\vec{0},R)}\vec{J}\cdot\boldsymbol{n}d\sigma=0$) .

We can see, as in Chap. *SO*(10) unification that we must have $k_{1\lambda}\Delta^{\mu\lambda\nu}(k_1,k_2)=k_{2\nu}\Delta^{\mu\lambda\nu}(k_1,k_2)=0$ since otherwise fermion number conservation and also gauge invariance are violated.

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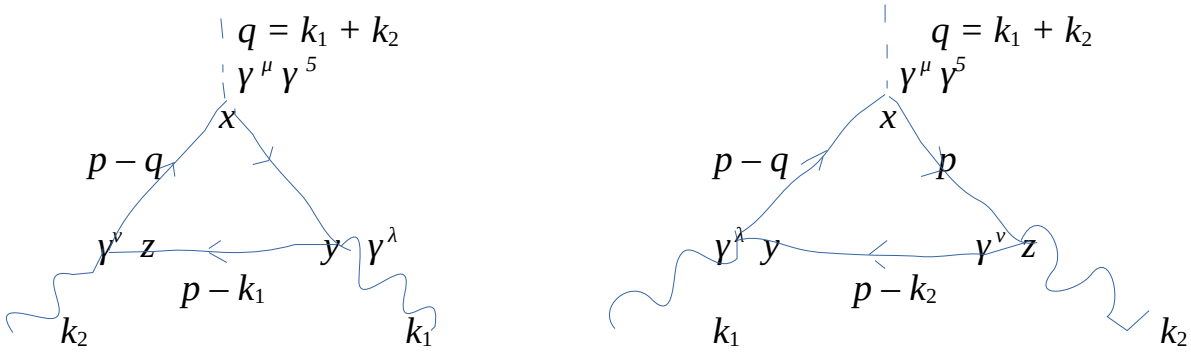

fig.1

Writing $\not k_1=\not p-(\not p-\not k_1)$ in the first term and $\not k_1=\not p-\not k_2-(\not p-\not q)$ in the second term of $k_{1\lambda}\Delta^{\mu\lambda\nu}(k_1,k_2)$ we obtain

$$k_{1\lambda}\Delta^{\mu\lambda\nu}(k_1,k_2)=-i\int\frac{d^4p}{(2\pi)^8}\mathrm{tr}\left(\gamma^\mu\gamma^5\frac{1}{\not p-\not q}\gamma^\nu\frac{1}{\not p-\not k_1}-\gamma^\mu\gamma^5\frac{1}{\not p-\not k_2}\gamma^\nu\frac{1}{\not p}\right)$$

Therefore $k_{1\lambda}\Delta^{\mu\lambda\nu}(k_1,k_2)=-\frac{i}{(2\pi)^8}\int(f(p+a)-f(p))d^4p$,

where $f(p)=\mathrm{tr}\left(\gamma^\mu\gamma^5\frac{1}{\not p-\not k_2}\gamma^\nu\frac{1}{\not p}\right)$, $a=-k_1$.

If the integral $\int f(p)d^4p$ is convergent or even logarithmically divergent, we can shift integration variable, leading to $\int(f(p+a)-f(p))d^4p=0$.

In our case the integral has superficial degree of divergence 2 and so we can't shift integration variables.

Further we will consider the k_1 , k_2 photons on mass shell , $k_1^2=0$, $k_2^2=0$ and we will take a,k_1^0,k_2^0 as small quantities which approach 0. Thus excepting a small range of $\|\vec p\|$ on which the integral is negligible under the assumptions we made, integrating over p_0 using residues theorem, we have that the poles of $f(p)$ and $f(p+a)$ as functions of $p_0\in\mathbb{C}$ with, $f(p)=\frac{\mathrm{tr}(\gamma^\mu\gamma^5(\not p-\not k_2)\gamma^\nu\not p)}{((p-k_2)^2+i\varepsilon)(p^2+i\varepsilon)}$, $\varepsilon>0$, $\varepsilon\to0$, are of the form $c-id$ with $c,d\in\mathbb{R}$, $cd>0$ and so (as in Chap. ... Georgi-Glashow model. Renormalization) we can perform a Wick rotation to euclidean four-dimensional space:

$I(a)=\int d^4p(f(p+a)-f(p))=i\int d_E^4p(f((ip_0,\vec p)+a)-f(ip_0,\vec p))=$

$=i\int d_E^4p(a_\lambda\partial^\lambda f(ip_0,\vec p)+...)\approx i\lim_{R\to\infty}-a^\lambda\frac{P_\lambda}{R}\widetilde f(P)2\pi^2R^3$ where $(P_\lambda)_\lambda=(ip_0,\vec p)$

and $P_\lambda\widetilde f(P)$ is understood as an average on the 3-dimensional spherical surface with radius R , $\|P\|=p_0^2+\vec p^2$, $S_R=\{p\in\mathbb{R}^4\,|\,\|P\|=R\}$ of $P_\lambda f(P)$.

We have $\mathrm{tr}(\gamma^\mu\gamma^5(\not p-\not k_2)\gamma^\nu\not p)=\mathrm{tr}(\gamma^5(\not p-\not k_2)\gamma^\nu\not p\gamma^\mu)=4i\epsilon^{\rho\nu\sigma\mu}k_{2\rho}p_\sigma$

where $\epsilon^{\rho\nu\sigma\mu}$ is the completely antisymmetric symbol with $\epsilon^{0123}=1$

and so we obtain $k_{1\lambda}\Delta^{\mu\lambda\nu}(k_1,k_2)=\frac{1}{(2\pi)^8}\lim_{R\to\infty}k_1^\delta\frac{P_\delta P_\sigma}{R^2}4i\epsilon^{\rho\nu\sigma\mu}k_{2\rho}2\pi^2$.

By a symmetry argument the averaged $\frac{P_\delta P_\sigma}{R^2}$ is $-\frac14\eta^{\delta\sigma}$ and we conclude

$$k_{1\lambda}\Delta^{\mu\lambda\nu}(k_1,k_2)=\frac{1}{(2\pi)^4}\frac{1}{8\pi^2}\epsilon^{\mu\nu\sigma\rho}k_{1\sigma}k_{2\rho} \quad , \qquad (4)$$

$$k_{2\nu}\Delta^{\mu\lambda\nu}(k_1,k_2)=\frac{1}{(2\pi)^4}\frac{1}{8\pi^2}\epsilon^{\mu\lambda\sigma\rho}k_{2\sigma}k_{1\rho}$$

For having fermion number conservation and gauge invariance not violated by those not vanishing expressions, we choose to shift integration variable in the linearly

divergent integral $\Delta^{\mu\lambda\nu}(k_1,k_2)$ by an arbitrary four-vector a defining

$$\Delta^{\mu\lambda\nu}(a,k_1,k_2)=i^3\int\frac{d^4p}{(2\pi)^8}\mathrm{tr}\left(\gamma^\mu\gamma^5\frac{1}{\not p+\not q-\not q}\gamma^\nu\frac{1}{\not p+\not q-\not k_1}\gamma^\lambda\frac{1}{\not p+\not a}+\right.$$
$$\left.+[\lambda,k_1\leftrightarrow\nu,k_2]\right)$$

and we will choose a such that $k_{1\lambda}\Delta^{\mu\lambda\nu}(a,k_1,k_2)$ and $k_{2\nu}\Delta^{\mu\lambda\nu}(a,k_1,k_2)$ vanish.

We take $f(p)=\mathrm{tr}\left(\gamma^\mu\gamma^5\frac{1}{\not p-\not q}\gamma^\nu\frac{1}{\not p-\not k_1}\gamma^\lambda\frac{1}{\not p}\right)$ and in the same way as above we will have $\Delta^{\mu\lambda\nu}(a,k_1,k_2)-\Delta^{\mu\lambda\nu}(k_1,k_2)=-\frac{i}{(2\pi)^8}\int d^4p(f(p+a)-f(p))=$

$$=\frac{1}{(2\pi)^8}\lim_{R\to\infty}a^\omega\frac{P_\omega}{R}\frac{\mathrm{tr}(\gamma^\mu\gamma^5\not P\gamma^\nu\not P\gamma^\lambda\not P)}{R^6}2\pi^2R^3+[\lambda,k_1\leftrightarrow\nu,k_2]=$$
$$=\frac{1}{(2\pi)^4}\frac{1}{8\pi^2}ia_\sigma\epsilon^{\mu\lambda\nu\sigma}+[\lambda,k_1\leftrightarrow\nu,k_2]$$

We can take $a=\alpha(k_1+k_2)+\beta(k_1-k_2)$ and so we obtain

$$\Delta^{\mu\lambda\nu}(a,k_1,k_2)=\Delta^{\mu\lambda\nu}(k_1,k_2)+\frac{i\beta}{(2\pi)^4\,4\pi^2}\epsilon^{\mu\lambda\nu\sigma}(k_1-k_2)_\sigma\ . \qquad (5)$$

Thus with $\beta=-\frac{1}{2}$,considering (4) we will have

$$k_{1\lambda}\Delta^{\mu\lambda\nu}(a,k_1,k_2)=k_{2\nu}\Delta^{\mu\lambda\nu}(a,k_1,k_2)=0$$

With this shifted integration choice of $\Delta^{\mu\lambda\nu}(a,k_1,k_2)$ replacing $\Delta^{\mu\lambda\nu}(k_1,k_2)$ for not violation of fermion number conservation and gauge invariance, according to (3) , in $O(e^3)$ approximation we have $\int\langle 0|\partial_\mu\hat J_5^\mu(x)|0\rangle\exp(-iqx)d^4x=$

$$=e^2\int iq_\mu\Delta^{\mu\lambda\nu}(a,k_1,k_2)\delta^4(q-k_1-k_2)A_\lambda(k_1)A_\nu(k_2)d^4k_1d^4k_2=$$
$$=e^2\int\left(iq_\mu\Delta^{\mu\lambda\nu}(k_1,k_2)+\frac{\epsilon^{\mu\lambda\sigma\nu}k_{1\mu}k_{2\sigma}}{(2\pi)^4\,4\pi^2}\right)\delta^4(q-k_1-k_2)A_\lambda(k_1)A_\nu(k_2)d^4k_1d^4k_2$$

Writing $\not q=\not p-(\not p-\not q)$ we obtain after some calculus as above :

$$q_\mu\Delta^{\mu\lambda\nu}(k_1,k_2)=-\frac{i}{(2\pi)^8}\int d^4p\,\mathrm{tr}\left(\gamma^5\frac{1}{\not p-\not q}\gamma^\nu\frac{1}{\not p-\not k_1}\gamma^\lambda-\gamma^\lambda\gamma^5\frac{1}{\not p-\not k_2}\gamma^\nu\frac{1}{\not p}\right)+$$
$$+[\lambda,k_1\leftrightarrow\nu,k_2]=k_{1\mu}\Delta^{\lambda\mu\nu}(k_1,k_2)+k_{2\mu}\Delta^{\nu\lambda\mu}(k_1,k_2)=\frac{i\epsilon^{\lambda\nu\mu\sigma}k_{1\mu}k_{2\sigma}}{(2\pi)^4\,4\pi^2}\ .$$

It follows now that

$$\int\langle 0|\partial_\mu\hat J_5^\mu(x)|0\rangle\exp(-iqx)d^4x=\int\frac{e^2\epsilon^{\nu\lambda\mu\sigma}k_{1\mu}k_{2\sigma}}{(2\pi)^8\,2\pi^2}\exp(-iqx)\exp(ik_1x)\exp(ik_2x)$$
$$A_\lambda(k_1)A_\nu(k_2)d^4xd^4k_1d^4k_2=\int\frac{e^2\epsilon^{\mu\lambda\sigma\nu}\exp(-iqx)}{2\pi^2}\partial_\mu A_\lambda(x)\partial_\sigma A_\nu(x)d^4x\ ,$$

$$\langle 0|\partial_\mu \hat{J}^\mu_5(x)|0\rangle = \frac{e^2}{8\pi^2}\,\epsilon^{\mu\lambda\sigma\nu}F_{\mu\lambda}(x)F_{\sigma\nu}(x)\ .$$

Hence under quantum fluctuations, the axial current of a massless fermion field is not conserved and its divergence is an operator capable of producing two photons (according to the fig.1 diagram) and having $\partial_\mu J^\mu_5 = \frac{e^2}{8\pi^2}\,\epsilon^{\mu\lambda\sigma\nu}F_{\mu\lambda}F_{\sigma\nu}$.

Writing the Lagrangian density in terms of left and right handed fields

$\psi_L = \frac{1}{2}(I - \gamma^5)\psi$ and $\psi_R = \frac{1}{2}(I + \gamma^5)\psi$, introducing

$J^\mu_R = \overline{\psi}_R\,\gamma^\mu\,\psi_R$, $J^\mu_L = \overline{\psi}_L\,\gamma^\mu\,\psi_L$ we have

$$\partial_\mu J^\mu_R = \frac{1}{2}\partial_\mu J^\mu + \frac{1}{2}\partial_\mu J^\mu_5 = \frac{e^2}{16\pi^2}\,\epsilon^{\mu\lambda\sigma\nu}F_{\mu\lambda}F_{\sigma\nu}\ ,$$

$$\partial_\mu J^\mu_L = \frac{1}{2}\partial_\mu J^\mu - \frac{1}{2}\partial_\mu J^\mu_5 = -\frac{e^2}{16\pi^2}\,\epsilon^{\mu\lambda\sigma\nu}F_{\mu\lambda}F_{\sigma\nu}$$

We can think of the left handed and right handed fermions running around the loop in fig.1 contributing oppositely to the anomaly.

Coupling the fermion field to a scalar field by adding $f\,\varphi\,\overline{\psi}\,\psi$ to the lagrangian density or as already done coupling it to the electromagnetic field, higher order diagrams such as the three loop diagram in fig.2 arise .

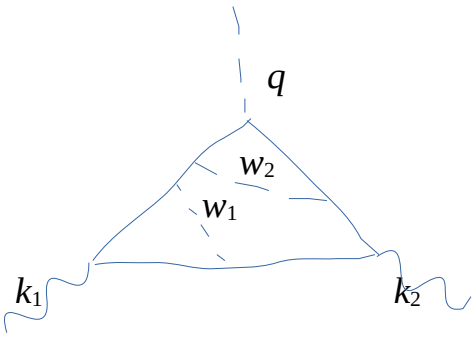

fig.2

Before we integrate over the momenta of the propagators labeled by w_1 , w_2 in fig.2 the Feynman integrand has seven fermion propagators and thus is more than sufficiently convergent so that we can shift integration variables. Thus before we integrate over w_1 and w_2 , all the appropiate current conservation identities are satisfied, for instance
$q_\lambda\,\Delta^{\lambda\mu\nu}{}_{3\,loop}(k_1, k_2, w_1, w_2) = 0$. Hence we encounter the non-renormalization of the anomaly so that higher order diagrams not contribute to the anomaly.

Having the $\psi \to \exp(i\theta\gamma^5)\psi$ symmetry with the associated conserved charge $Q=\int d^3\vec{x}J_5^0(t,\vec{x})$ the anomaly allowing for the charge $\hat{Q}$ a non-zero vacuum expectation value so that $\hat{Q}|0\rangle \neq 0$ and $\hat{Q}$ satisfying $[\hat{H},\hat{Q}]=0$ since generates a symmetry ($\hat{H}$ the Hamiltonian operator of the fermion field system) , following the considerations in Chap.Symmetry breaking , the Goldstone theorem leads to a Nambu-Goldstone boson $|s\rangle=\int d^3\vec{x}\exp(-i\vec{k}\cdot\vec{x})J_5^0(t,\vec{x})|0\rangle$ which describes the masless particle known as the pion having momentum $\vec{k}$.

The pseudovector spin 1 meson π^0 (pion) is made of a confined quark and antiquark, color-anticolor combination $\psi_M=(\psi_M^\mu(x_1,x_2))_\mu=(\overline{\psi}^a(x_1)\gamma^\mu\gamma^5\psi^a(x_2))_\mu$ (with summation over color index *a*) which at a location $x = x_1 = x_2$ in space-time has a pseudovectorial spin 1 particle of effective mass m_π equivalent Lorentz pseudovector field operator function (a pseudovector transforms as a Lorentz vector under the restricted Lorentz group and changes sign under parity transformation ; see Chap. Fermion charge … CPT transformations) $\hat{\varphi}=(\hat{\varphi}_\mu(t,\vec{x}))_\mu$ so that for $\hat{F}^\mu(x)=\psi_M^\mu(x,x)$ the propagator of the π^0 meson is $D_{\mu\lambda}(x-y)=-i\langle 0|T(\hat{F}_\mu(x)\hat{F}_\lambda(y))|0\rangle=-i\langle 0|T(\hat{\varphi}_\mu(x)\hat{\varphi}_\lambda(y))|0\rangle$ (with a pion Lagrangian density $\frac{1}{2}(\partial_\mu\varphi_\nu)(\partial^\mu\varphi^\nu)-m_\pi^2\varphi_\mu\varphi^\mu$; see Chap. Feynman amplitudes and lattice gauge theory … Meson and barion masses).

If $|k\rangle$ is the pion with four momentum k state, then Lorentz invariance tells us that $\langle 0|\hat{J}_5^\mu(0)|k\rangle=f k^\mu$.

As in Chap. Spin-statistics theorem we have $\langle 0|\hat{J}_5^\mu(x)|k\rangle=\langle 0|\exp(i\hat{p}x)\hat{J}_5^\mu(0)\exp(-i\hat{p}x)|k\rangle=\langle 0|\hat{J}_5^\mu(0)|k\rangle\exp(-ikx)=$ $=f k^\mu\exp(-ikx)$ where $\hat{p}$ is the four-momentum operator, acting on the states Hilbert space and so $\langle 0|\partial_\mu\hat{J}_5^\mu(x)|k\rangle=-if k^2\exp(-ikx)=-if m_\pi^2\exp(-ikx)$

So if the pion is massless as a Nambu-Goldstone boson to the spontaneously broken chiral symmetry in an ideal world , the axial current is conserved.

In the unified *S U*(3) x *S U*(2) x *U*(1) theory we can consider the decay of the π^0 pion into two photons $\pi^0 \to \gamma+\gamma$ and the corresponding amplitude which can be computed in lattice gauge theory

$-e^2\int\langle 0|a(k_1)a(k_2)T(\hat{A}_\nu(z)\hat{A}_\lambda(y)\hat{J}^\nu(z)\hat{J}^\lambda(y)\hat{J}_5^\mu(x))|0\rangle d^4y\,d^4z$ (6)

with $a = a(k)$ anihilation operator for the photon of four momentum *k* and k_1 , k_2 four-momenta of the outgoing photons . In first approximation, the Fourier transform of (6) in four-momentum *q* space of the incoming pion is (to multiplication with incoming and outgoing states normalization connstants) equal with:

$\frac{\varepsilon_\lambda(k_1)\varepsilon_\nu(k_2)}{\sqrt{2\omega_{k1}}\sqrt{2\omega_{k2}}}e^2\Delta^{\mu\lambda\nu}(a,k_1,k_2)\delta^4(q-k_1-k_2)$ where $\varepsilon(k_1),\varepsilon(k_2)$ are the photon polarization four-versors and *a* is taken as above respecting the necessity of gauge invariance and fermion number conservation (vector current conservation under fluctuations) (see also Chap. Feynman amplitudes and lattice gauge theory).

The integrand in (6) can be written as a sum
$\sum_k \langle 0|a(k_1)a(k_2)\hat{A}_\nu(z)\hat{A}_\lambda(y)\hat{J}^\nu(z)\hat{J}^\lambda(y)|k\rangle\langle k|\hat{J}_5^\mu(x)|0\rangle$
over all k -four-momentum states which states must be pion states, so that $\langle k|\hat{J}_5^\mu(x)|0\rangle$ not vanishes.
Since $\langle k|\hat{J}_5^\mu(x)|0\rangle = f^* k^\mu \exp(ikx)$ and $\langle 0|\partial_\mu \hat{J}_5^\mu(x)|k\rangle = -if m_\pi^2 \exp(-ikx)$ it follows that if the axial current is conserved and $m_\pi \neq 0$ then $f=0$ and the pion decay cannot occur. Therefore, since pion decay is observed we conclude that the real pion has an effective non-zero mass.

The strong interaction (Quantum chromodynamics) path integration theory allows computations (in lattice gauge theory for example) of amplitudes of processes in which hadrons interact by exchanging pions , for example schematically a proton $u^a u^b d^c$ (a,b,c -different color indices, u -up quarks , d -down quarks) on proton scattering through exchanging a pion $\bar{d}^a d^a$ involves an amplitude $\int \langle 0|P(\bar{x})P(\bar{y})\bar{d}^c(x)d^c(x)\bar{d}^c(y)d^c(y)\overline{P}(\bar{w})\overline{P}(\bar{z})|0\rangle d^4x\, d^4y$ where we denoted
$P(\bar{x}) = u^a(x_1)u^b(x_2)d^c(x_3), \overline{P}(\bar{w}) = \bar{u}^a(w_1)\bar{u}^b(w_2)\bar{d}^c(w_3),$
$P(\bar{y}) = u^a(y_1)u^b(y_2)d^c(y_3), \overline{P}(\bar{z}) = \bar{u}^a(z_1)\bar{u}^b(z_2)\bar{d}^c(z_3)$ with $x_j, y_j, w_j, z_j \in \mathbb{R}^4$
and generally we can construct a theory of nucleons interacting by exchanging pions. (see Chap. Feynman amplitudes and lattice gauge theory) .

45. Non-abelian gauge theory

Non-abelian gauge theory

We begin with a quantum field theory defined by a field $\varphi=\varphi(t,\vec{x})$, $x=(t,\vec{x})\in\mathbb{R}^4$ and a Lagrangian density $\mathscr{L}=\mathscr{L}(\varphi,\partial\varphi)$ which is invariant under an unitary Lie group G of field transformations.
(for the sake of definiteness we let $\varphi=(\varphi_1,\varphi_2,...,\varphi_N)$, $G=SU(N)$ and $\mathscr{L}=(\partial\varphi)^+(\partial\varphi)-V(\varphi^+\varphi)$)
We make then the transformations $U\in G$, $UU^+=\boldsymbol{I}$ to vary from place to place in space-time: $U=U(x)\in G$.
Clearly $\varphi^+\varphi$ is still invariant but under a transformation $\varphi(x)\to U(x)\varphi(x)$, $\partial_\mu\varphi$ transforms as $\partial_\mu\varphi\to\partial_\mu(U\varphi)=U(\partial_\mu\varphi+(U^+\partial_\mu U)\varphi)$.
To cancel the unwanted term $(U^+\partial_\mu U)\varphi$ we generalize the ordinary derivative ∂_μ to a covariant derivative D_μ with $D_\mu\varphi(x)=\partial_\mu\varphi(x)-ig\,A_\mu(x)\varphi(x)$ with g a coupling constant and $(A^\mu)_\mu$ transforming as a Lorentz vector under a $x\to\Lambda x$, $\Lambda\in SO^+(3,1)$ coordinates transform, where the field $(A_\mu)_\mu$ is called a gauge potential in direct analogy with electromagnetism.
We see that under a $\varphi(x)\to U(x)\varphi(x)$ gauge transformation we will have $D_\mu\varphi(x)\to U(x)D_\mu\varphi(x)$ so that the Lagrangian density $\mathscr{L}(\varphi,\partial\varphi)=(D_\mu\varphi)^+(D^\mu\varphi)-V(\varphi^+\varphi)$ remains invariant, if $A=(A_\mu)_\mu$ transforms as $gA_\mu\to gUA_\mu U^+-i(\partial_\mu U)U^+=gUA_\mu U^+ +iU\partial_\mu U^+$. (1)
Clearly A_μ have to be N x N matrices and the condition $A_\mu = A^+{}_\mu$ is preserved by the gauge transformation (1) and thus is consistent to take A_μ to be hermitean.
Writing $U=\exp(i\theta^a T^a)$ (with summation over a index) where $(T^a)_a$ are the the generators of G and $\theta^a=\theta^a(x)\in\mathbb{R}$ we have the infinitesimal form of (1) $gA_\mu\to gA_\mu+ig\,\theta^a[T^a,A_\mu]+\partial_\mu\theta^a T^a+O(\theta^2)$. (2)
The Lie algebra of the group G is defined by the structure constants $(f^{abc})_{a,b,c}$ with $[T^b,T^c]=if^{abc}T^a$ (for $G=SU(N)$ the $(T^a)_a$ are N^2-1 linear independent hermitean traceless matrices (see Chap. On the rotations group and the restricted Lorentz group)).
We notice that if $G = U(1)$ we have only one generator, which is a real constant number and (2) is a gauge transformation of a gauge potential familiar from electromagnetism, G being abelian.
Since $(T^a)_a$ are hermitean generators and A_μ is hermitean we can write $A_\mu=A^a_\mu T^a$ and if T^a are traceless we see from (2) that the trace of A_μ does not transform and so if T^a are traceless we can take A_μ traceless and we have $A_\mu=A^a_\mu T^a$ with $A^a_\mu=A^a_\mu(x)\in\mathbb{R}$, real functions.
We can construct the Lorentz invariant 1-form $A=A_\mu dx^\mu$.

In order to define a Lagrangian density for the non-abelian gauge potential $(A_\mu)_\mu$ which is an analog of the electromagnetism Lagrangian density $-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$,

we find our task in constructing a Lorentz invariant 2-form $F=\frac{1}{2}F_{\mu\nu}dx^\mu dx^\nu$ from A.

From A we can construct two possible 2-forms : $dA=\frac{1}{2}(\partial_\nu A_\mu-\partial_\mu A_\nu)dx^\nu dx^\mu$

and $A^2=A_\mu A_\nu dx^\mu dx^\nu=\frac{1}{2}[A_\mu,A_\nu]dx^\mu dx^\nu$.

Under a $U=\exp(i\theta^a T^a)$ transformation we have:

$A\to UAU^+ +\frac{1}{g}iU\,dU^+$ (3) where $dU=\partial_\mu U\,dx^\mu$.

Applying d to (3) we obtain

$dA\to U(dA)U^+ +(dU)AU^+ -UAdU^+ +\frac{1}{g}i\,dU\,dU^+$.

Also we have $A^2\to UA^2U^+ +\frac{1}{g}iUAdU^+ -\frac{1}{g}i(dU)AU^+ +\frac{1}{g^2}dU\,dU^+$

(where we used $U\,dU^+=-(dU)U^+$ since $UU^+=\boldsymbol{I}$).

Hence $dA-igA^2\to U(dA-igA^2)U^+$ and taking $F=dA-igA^2=\frac{1}{2}F_{\mu\nu}dx^\mu dx^\nu$,

we have that $-\frac{1}{2}\mathrm{tr}(F_{\mu\nu}F^{\mu\nu})$ is Lorentz invariant and invariant under the $U=U(x)$ transformation and
$F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu-ig[A_\mu,A_\nu]$.

Normalizing the $(T^a)_a$ such that $\mathrm{tr}(T^aT^b)=\frac{1}{2}\delta_{ab}$ we have $F_{\mu\nu}=F^a_{\mu\nu}T^a$ with

$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu+gf^{abc}A^b_\mu A^c_\nu$.

With the Yang-Mills Lagrangian density defined as

$$\mathscr{L}((A^a_\mu,\partial A^a_\mu)_{a,\mu})=-\frac{1}{2}\mathrm{tr}(F_{\mu\nu}F^{\mu\nu})=-\frac{1}{4}(\partial_\mu A^a_\nu-\partial_\nu A^a_\mu)(\partial^\mu A^{a\nu}-\partial^\nu A^{a\mu})-$$

$$-\frac{1}{2}g(\partial_\mu A^a_\nu-\partial_\nu A^a_\mu)f^{abc}A^{b\mu}A^{c\nu}-\frac{1}{4}g^2f^{abc}f^{ade}A^b_\mu A^c_\nu A^{d\mu}A^{e\nu}$$

we have a Yang-Mills quantum field theory for the $((A^a_\mu)_\mu)_a$ gauge vector bosons.
We can consider that the gauge bosons have masses $(M_a)_a$ and so we add to the Yang-Mills Lagrangian density terms like $\frac{1}{2}M_a^2A^a_\mu A^{a\mu}$.

When we give that way masses to the gauge bosons we see that the quadratic part of the Yang-Mills Lagrangian density is equivalent to

$\frac{1}{2}\sum_a A^a_\mu((\partial^2+M_a^2)\eta^{\mu\nu}-\partial^\mu\partial^\nu)A^a_\nu$ and so we can verify that the propagator for the $(A^a_\mu)_\mu$ gauge boson is $(D^a_{\nu\lambda})_{\nu,\lambda}$ given in the coordinates space by

$D^a_{\nu\lambda}(x)=\int \frac{d^4k}{(2\pi)^4}D^a_{\nu\lambda}(k)\exp(ikx)$ with the momentum space propagator

$$D^a_{\nu\lambda}(k)=\frac{-\eta^{\nu\lambda}+\frac{k_\nu k_\lambda}{M_a^2}}{k^2-M_a^2+i\varepsilon} \text{ with } \varepsilon\to 0\ ,\ \varepsilon>0,$$

showing that we have made the right choice of mass term.

Following the path of Fadeev-Popov method exposed in Chap…Quantum electrodynamics , for massless gauge bosons we write

$S(A)=\int d^4x(-\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}+J^{a\mu}A^a_\mu)$,

$I=\int DA\exp(iS(A))=\int D\theta\int DA\exp(iS(A))\Delta(A)\delta(f(A_\theta))=$

$=\int D\theta\int DA\exp(iS(A))\delta(f(A))$ (4)

where $A\to A_\theta$ stands for the gauge transformation $A\to A_g$, $g\in G$ (do not confuse $g\in G$ with the coupling constant g)

$A_{\theta\mu}=A_\mu+i\theta^a[T^a,A_\mu]+\frac{1}{g}\partial_\mu\theta^aT^a$, $\theta=(\theta^a)_a$, $f(A)=\partial^\mu A_\mu-\sigma=\partial A-\sigma$,

$A^a_{\theta\mu}=A^a_\mu-f^{abc}\theta^bA^c_\mu+\frac{1}{g}\partial_\mu\theta^a$, $\sigma^a=\sigma^a(x)\in\mathbb{R}$, $\sigma=\sigma^aT^a$

$$\Delta(A)=\left(\int D\theta\delta((\partial A^a-\sigma^a-\partial^\mu(f^{abc}\theta^bA^c_\mu-\frac{1}{g}\partial_\mu\theta^a))_a\right)^{-1} \quad (5)$$

Since in (4) $\Delta(A)$ is multiplied with $\delta(f(A))$ we can take in (5) $\partial A^a-\sigma^a=0$

We have $\partial^\mu(f^{abc}\theta^b(x)A^c_\mu(x)-\frac{1}{g}\partial_\mu\theta^b(x))=\int d^4yK^{ab}(x,y)\theta^b(y)$

$K^{ab}(x,y)=\partial^\mu(f^{abc}A^c_\mu(x)-\frac{1}{g}\partial_\mu\delta^{ab})\delta^4(x-y)$

and $(K^{ab}(x,y))_{(a,x),(b,y)}$ as a matrix K so that in (4) we can take

$\Delta(A)=\left(\int D\theta\delta(K\theta)\right)^{-1}=\det K$

We can take $c_a=c_a(x)$ so called ghost fields with $(c_a(x))_{a,x}$, $(c^+_a(x))_{a,x}$ independent sets of anticommuting Grassmann variables and we have to multipication with independent normalization constants that

$\det K=\int DcDc^+\exp(iS_{ghost}(c^+,c))$

where $S_{ghost}(c^+,c)=\int d^4xd^4yc^+(x)K^{ab}(x,y)c_b(y)=$

$=\int d^4x(\frac{1}{g}(\partial c^+_a(x))(\partial c_a(x))-\partial^\mu c^+_a(x)f^{abc}A^c_\mu(x)c_b(x))$

Defining $D_\mu c = \partial_\mu c - i g A^a_\mu [T^a, c] = (\partial_\mu c_a - g f^{abc} c_b A^c_\mu) T^a = (D_\mu c_a) T^a$,

we will have $S_{ghost}(c^+, c) = \frac{1}{g} \int d^4 x \, \partial^\mu c^+_a D_\mu c_a$

Therefore factoring out $\int D\theta$ and $\int D\sigma \exp(-(i/(2\xi)) \int d^4 x (\sigma(x))^2)$ since I is independent of σ we obtain

$I = \widetilde{C} \int D\sigma \exp(\frac{-i}{2\xi} \int d^4 x \, \sigma^2) \int D A \, D c \, D c^+ \exp(i(S(A) + S_{ghost}(c^+, c))) \delta(\partial A - \sigma)$

with $\widetilde{C}$ an independent constant.

Thus $I = \widetilde{C} \int D A \, D c \, D c^+ \exp(i S_{eff}(A, c^+, c))$ where

$S_{eff}(A, c^+, c) = \int d^4 x (\mathscr{L}_0 + \mathscr{L}_1)$,

$$\mathscr{L}_0 = -\frac{1}{4} \sum_a (\partial_\mu A^a_\nu - \partial_\nu A^a_\mu)(\partial^\mu A^{a\,\nu} - \partial^\nu A^{a\,\mu}) - \frac{1}{2\xi} \sum_{\bar{a}} (\partial^\mu A^{\bar{a}}_\mu)^2 + \sum_a \frac{1}{g} \partial^\mu c^+_a \partial_\mu c_a +$$

$+ \sum_b \frac{1}{2} M^2_b A^b_\mu A^{b\mu}$ (we take the $\bar{a}$ index summation over all massless gauge bosons and the b index summation over all massive gauge bosons)

$$\mathscr{L}_1 = -\frac{g}{2} (\partial_\mu A^a_\nu - \partial_\nu A^a_\mu) f^{abc} A^{b\mu} A^{c\,\nu} - \frac{g^2}{4} f^{abc} f^{ade} A^b_\mu A^c_\nu A^{d\mu} A^{e\,\nu} - \partial^\mu c^+_a f^{abc} c_b A^c_\mu$$

From the form of $\mathscr{L}_0$ we derive the propagator for massless gauge bosons as

$$D^a_{\nu\lambda}(k) = \left(-\eta^{\nu\lambda} + (1-\xi) \frac{k_\nu k_\lambda}{k^2} \right) \frac{1}{k^2}$$

(in the R_ξ gauge, with $\xi \in \mathbb{R}$ the gauge parameter)

and the ghost fields propagator as $D^{ghost}_{ab}(k) = \frac{g}{k^2} \delta_{ab}$

From the form of $\mathscr{L}_1$ we derive couplings as follows:

a) $g f^{abc} (\eta^{\mu\nu}(k_1 - k_2)^\lambda + \eta^{\nu\lambda}(k_2 - k_3)^\mu + \eta^{\lambda\mu}(k_3 - k_1)^\nu)$ for a cubic gauge bosons interaction, where k_1, k_2, k_3 label respective the incoming four-momenta to the interaction vertex a, b, c indexed bosons;

b) $-ig^2 \left(f^{abc} f^{ade} (\eta^{\mu\lambda} \eta^{\nu\varepsilon} - \eta^{\mu\varepsilon} \eta^{\nu\lambda}) + f^{adc} f^{abe} (\eta^{\mu\lambda} \eta^{\nu\varepsilon} - \eta^{\lambda\varepsilon} \eta^{\mu\nu}) + \right.$

$\left. + f^{abd} f^{ace} (\eta^{\nu\mu} \eta^{\lambda\varepsilon} - \eta^{\nu\varepsilon} \eta^{\mu\lambda}) \right)$ for a quartic gauge bosons interaction verttex;

c) $f^{abc} k^\mu$ for a ghost fields - gauge boson interaction vertex where k labels the outgoing ghost particle four-momentum indexed with a and b is the incoming ghost particle index , c is the incoming boson index.

Note that the c_a and c^+_a are known as ghost fields because they violate spin-statistics connection: Though scalar , they are treated as anticommuting. This 'violation' is acceptable because they are not associated with physical particles and are introduced merely to represent $\Delta(A)$ in a convenient form.

46. Electroweak unification. Quantum chromodynamics Georgi-Glashow model

Electroweak unification. Quantum chromodynamics
Georgi-Glashow model

We will denote further the $SU(N)$ canonical representation $SU(N)\ni U=(U^i_j)_{i,j=\overline{1,N}}:\mathbb{C}^N\ni(\varphi^i)_i\to(U^i_j\varphi^j)_i\in\mathbb{C}^N$ by N .

A field $\varphi=(\varphi^i)_i$ will be denoted transforming as (N_1,N_2,r) (that is belongs to a (N_1,N_2,r) representation of $SU(3)\times SU(2)\times U(1)$ if it transforms as a N_1 representation under $SU(3)$ as a N_2 representation under $SU(2)$ ($N_1\in\{1,3\}$, $N_2\in\{1,2\}$ with 1 meaning the identity representation) and as $\varphi\to\exp(i\theta\frac{Y}{2})\varphi$ (with $\frac{Y}{2}\varphi=r\varphi$, $r\in\mathbb{R}$ and Y a self-adjoint operator), under $\exp(i\theta)\in U(1)$.

The generators of $SU(N)$ are self-adjoint traceless matrices $(T^a)_{a=\overline{1,N^2-1}}$ and we have $f^{abc}\in\mathbb{R}$ with $a,b,c=\overline{1,N^2-1}$, $[T^b,T^c]=if^{abc}T^a$ (with summation over a index). Considering the generators normalized so that $\mathrm{tr}(T^aT^b)=\frac{1}{2}\delta_{ab}$ we will have $if^{abc}=2\,\mathrm{tr}(T^a[T^b,T^c])$ leading to $f^{abc}=-f^{acb}=f^{cab}$ for any a,b,c.

As we noticed in Chap. Fermion charge… Majorana neutrino . Chirality , the weak interaction occurs only with participation of the left handed fields, so we put the left handed neutrino field ν_L and the left handed electron field e_L into a 2 representation of SU (2) and the right handed electron filed e_R into a 1 representation of $SU(2)$: $\psi_L=\begin{pmatrix}\nu\\ e\end{pmatrix}_L$, e_R where ν_L and e_L are left handed Dirac spinor fields and e_R is a right handed spinor field.

To include electromagnetism with a massless boson field which would turn out to be the photon, we extend the gauge symmetry to $SU(2)$ x $U(1)$, denoting the generator of $U(1)$ by $\frac{Y}{2}$, called the hypercharge, so that we have a covariant derivative

$D_\mu=\partial_\mu-igW^a_\mu T^a-ig'B_\mu\frac{Y}{2}$ with $T^i=\frac{1}{2}\sigma^i$, σ^i -the Pauli matrices , $i=\overline{1,3}$.

To generate a mass term for the electron we introduce a Higgs field $\varphi=\begin{pmatrix}\varphi^1\\ \varphi^0\end{pmatrix}$ transforming as a 2 under $SU(2)$ and having a vacuum expectation value $\langle\varphi\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v\end{pmatrix}$ with $v\in\mathbb{R}$ which couples to ψ_L and e_R in the interaction terms

$-f\,\overline{\psi}_L\varphi e_R-f\,\overline{e}_R\varphi^+\psi_L=-\frac{1}{\sqrt{2}}fv\overline{e}_Le_R-\frac{1}{\sqrt{2}}fv\overline{e}_Re_L$

giving to the electron a mass $m=\frac{1}{\sqrt{2}} f\, v$.

We can verify that upon spontaneous symmetry breaking of the Higgs field Lagrangian density symmetry (see Chap. Symmetry breaking) from the *SU*(2) x *U*(1) group to the *U*(1) group by setting the potential energy minimum point at the vacuum expectation value $\langle \varphi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}$ (for example a Higgs field Lagrangian density $(\partial_\mu \varphi^j)^+ (\partial^\mu \varphi^j) + \mu^2 \varphi^{j+} \varphi^j - \lambda (\varphi^{j+} \varphi^j)^2$ with $v = \sqrt{\frac{\mu^2}{\lambda}}$) three of the four degrees of freedom for the Higgs field (since φ^0, φ^1 are complex) are the resulting Nambu-Goldsone bosons and they are eaten by the three $(W^a)_{a=\overline{1,3}}$ bosons and it remains one real degree of freedom which corresponds to the Higgs particle.

The T^a generators are normalized by the commutation relations $[T^a, T^b] = i\, \epsilon_{abc} T^c$ and $\mathrm{tr}\, T^{a2} = \frac{1}{2}$ to $T^a = \frac{1}{2} \sigma^a$, $a = 1,2,3$.

The normalization of the $\frac{Y}{2}$ operator is not fixed and so is not the normalization of the gauge coupling *g*' . By construction we want spontaneous symmetry breaking to leave invariant a linear combination of T^3 and $\frac{Y}{2}$ to be identified as the generator the massless photon couples to, namely the charge operator $Q = T^3 + \frac{Y}{2}$.

For e_L to have charge -1 (we choose g, g' to be positive), the doublet ψ_L must have $\frac{Y}{2} \psi_L = -\frac{1}{2} \psi_L$. The field e_R must have $\frac{Y}{2} e_R = -1$ since $T^3 e_R = 0$.

The invariance of the $f\, \overline{\psi}_L \varphi e_R$ forces the field φ to have $\frac{Y}{2} \varphi = \frac{1}{2} \varphi$. Also for $\varphi = \langle \varphi \rangle$ we have $T^3 \varphi = -\frac{1}{2} \varphi$.

Through spontaneous symmetry breaking (see Chap. Anderson-Higgs mechanism) we have $\varphi \to \langle \varphi \rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v \end{pmatrix}$ leading to

$$(D_\mu \varphi)^+ (D^\mu \varphi) \to \frac{g^2}{2} W_\mu^a W^{b\mu}(0,v) T^a T^b \begin{pmatrix} 0 \\ v \end{pmatrix} + g\, g' W_\mu^a B^\mu (0,v) T^a \frac{Y}{2}\begin{pmatrix} 0 \\ v \end{pmatrix} +$$

$$+ \frac{g'^2}{2} B_\mu B^\mu (0,v) \left(\frac{Y}{2}\right)^2 \begin{pmatrix} 0 \\ v \end{pmatrix} = \frac{g^2}{8} v^2 W_\mu^+ W^{-\mu} +$$

$$+ \frac{1}{2}\left(g W_\mu^3 T^3 \varphi + g' B_\mu \frac{Y}{2}\varphi\right)^+ \left(g W^{3\mu} T^3 \varphi + g' \frac{Y}{2}\varphi\right) = \frac{g^2}{8} v^2 W_\mu^+ W^{-\mu} +$$

$$+ \frac{v^2}{8}\left(g W_\mu^3 - g' B_\mu\right)\left(g W^{3\mu} - g' B^\mu\right) \qquad \text{where } W^\pm = W^1 \mp i W^2 \ .$$

Therefore defining $\tan\theta = \frac{g'}{g}$ we will have massive W bosons W^1, W^2 with mass squared $\frac{v^2}{4} g^2 = M_W^2$, a massive Z boson $Z = W^3 \cos\theta - B \sin\theta$ with mass squared $M_Z^2 = \frac{M_W^2}{\cos^2\theta} = \frac{v^2}{4}(g^2 + g'^2)$ while the orthogonal combination $A = W^3 \sin\theta + B\cos\theta$ remains massless and will be identified with the photon.

We include quarks in the theory by taking doublets $q_L^\alpha = \begin{pmatrix} u^\alpha \\ d^\alpha \end{pmatrix}_L$ transforming as 2 under $SU(2)$ and singlets u_R^α, d_R^α transforming as 1 under $SU(2)$ where $\alpha = \overline{1,3}$ denotes the color index, u_L^α, d_L^α are the left handed and u_R^α, d_R^α are the right handed up- respective down- quark Dirac spinor fields. The up-quarks have charge 2/3 and the down quarks have charge -1/3 and so u_R^α must have hypercharge $\frac{Y}{2} u_R^\alpha = \frac{2}{3} u_R^\alpha$, d_R^α must have hypercharge $\frac{Y}{2} d_R^\alpha = -\frac{1}{3} d_R^\alpha$ and q_L^α must have hypercharge $\frac{Y}{2} q_L^\alpha = \frac{1}{6} q_L^\alpha$.

Taking $B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$, $W_{\mu\nu}^a = \partial_\mu W_\nu^a - \partial_\nu W_\mu^a + g\, \epsilon_{abc} W_\mu^b W_\nu^c$ (see Chap. Non-abelian gauge theory) ,

$$(\psi^\beta)_\beta = ((\nu, e), (u^\alpha, d^\alpha)_\alpha) = (\psi^{\lambda 1}, \psi^{\lambda 2})_\lambda \ , \ \psi^\lambda = \begin{pmatrix} \psi^{\lambda 1} \\ \psi^{\lambda 2} \end{pmatrix} \ , \ \overline{\psi}^\lambda = (\overline{\psi}^{\lambda 1}, \overline{\psi}^{\lambda 2}) \ ,$$

the electroweak Lagrangian density (we can also include the other families of leptons and quarks (see Chap. Feynman amplitudes and lattice gauge theory)) can be written

as $\mathscr{L}=\sum_{\beta}\overline{\psi}^{\beta}(i\partial\!\!\!/-m_{\beta})\psi^{\beta}+\sum_{\lambda}(\frac{g}{2}W_{\mu}^{-}\overline{\psi}_{L}^{\lambda 2}\gamma^{\mu}\psi_{L}^{\lambda 1}+\frac{g}{2}W_{\mu}^{+}\overline{\psi}_{L}^{\lambda 1}\gamma^{\mu}\psi_{L}^{\lambda 2})+$

$+\sum_{\lambda}\frac{g}{\cos\theta}Z_{\mu}(\frac{1}{2}(\overline{\psi}_{L}^{\lambda 1}\gamma^{\mu}\psi_{L}^{\lambda 1}-\overline{\psi}_{L}^{\lambda 2}\gamma^{\mu}\psi_{L}^{\lambda 1})-J_{em\,\lambda}^{\mu}\sin^{2}\theta)+\sum_{\lambda}g\sin\theta A_{\mu}J_{em\,\lambda}^{\mu}+$

$+\frac{1}{2}M_{Z}^{2}Z_{\mu}Z^{\mu}+\frac{1}{2}M_{W}^{2}W_{\mu}^{+}W^{-\mu}-\frac{1}{4}B_{\mu\nu}B^{\mu\nu}-\frac{1}{4}W_{\mu\nu}^{a}W^{a\mu\nu}$

where $J_{em\,\lambda}^{\mu}=(\overline{\psi}^{\lambda 1},\overline{\psi}^{\lambda 2})\gamma^{\mu}Q\begin{pmatrix}\psi^{\lambda 1}\\ \psi^{\lambda 2}\end{pmatrix}$ is the electromagnetic current with $Q=T^{3}+\frac{Y}{2}$

an we take $Y\ \nu_{R}=0,$ following that we must have the charge of the electron $e=-g\sin\theta$.

We can see that the exchange of a W boson generates the Fermi weak interaction term $-\frac{g^{2}}{2M_{W}^{2}}\overline{\nu}_{L}\gamma^{\mu}e_{L}\overline{e}_{L}\gamma_{\mu}\nu_{L}$.

(Indeed, since the $W_{\mu}^{1}(x)W_{\nu}^{2}(y)$ and $W_{\mu}^{2}(x)W_{\nu}^{1}(y)$ terms in a $W^{-}(x)W^{+}(y)$ W boson exchange of order g^{2} Feynman diagram path integration vanish because they are odd in integration variable the corresponding amplitude reduces to

$-i\frac{g^{2}}{4}\overline{\nu}_{L}(p)\gamma^{\mu}e_{L}(q)\overline{e}_{L}(r)\gamma^{\nu}\nu_{L}(s)(D_{\mu\nu}^{1}(p-q)+D_{\mu\nu}^{2}(p-q))(2\pi)^{4}\delta^{4}(p+r-s-q)$

where the boson propagator is $D_{\mu\nu}^{1}(k)=D_{\mu\nu}^{2}(k)=\frac{1}{k^{2}-M_{W}^{2}+i\varepsilon}\left(-\eta_{\mu\nu}+\frac{k_{\mu}k_{\nu}}{M_{W}^{2}}\right)$

and as we learned in Chap.Feynman amplitudes and lattice gauge theory we can dispose of the $k_{\mu}k_{\nu}$ term, since $k=p-q$ with p,q on mass shell in the amplitude expression. Also because the boson mass is much larger than the fermion masses we approximate $k^{2}-M_{W}^{2}\approx-M_{W}^{2}$ and so the above equivalent interaction term can express the Fermi weak interaction between electrons an neutrinos.

We can write the Z boson coupling as $\frac{g}{\cos\theta}Z_{\mu}(J_{leptons}^{\mu}+J_{quarks}^{\mu})$ and the exchange of a Z boson generates, in asimilar way as for the W boson, a neutral current interaction between leptons and quarks

$-\frac{g^{2}}{M_{W}^{2}}(J_{leptons}+J_{quarks})^{\mu}(J_{leptons}+J_{quarks})_{\mu}$. Studying various processes described by this interaction we can determine θ and then estimate g from $e=g\sin\theta$.

$J_{quarks}^{\mu}=\frac{1}{2}(\overline{u}_{L}\gamma^{\mu}u_{L}-\overline{d}_{L}\gamma^{\mu}d_{L})-(\frac{2}{3}\overline{u}\gamma^{\mu}u-\frac{1}{3}\overline{d}\gamma^{\mu}d)\sin^{2}\theta$

$J_{leptons}^{\mu}=\frac{1}{2}(\overline{\nu}_{L}\gamma^{\mu}\nu_{L}-\overline{e}_{L}\gamma^{\mu}e_{L})+\overline{e}\gamma^{\mu}e\sin^{2}\theta$

We can also write, considering that $T^{a}\psi_{R}^{\lambda}=0$ the electroweak Lagrangian density as

$$\mathscr{L}=\sum_{\beta}\overline{\psi}^{\beta}(i\partial\!\!\!/-m_{\beta})\psi^{\beta}+\sum_{\lambda}g\,\overline{\psi}^{\lambda}\gamma^{\mu}W_{\mu}^{a}T^{a}\psi^{\lambda}+\sum_{\lambda}g'\,\overline{\psi}^{\lambda}\gamma^{\mu}B_{\mu}\frac{Y}{2}\psi^{\lambda}+\frac{1}{2}M_{Z}^{2}Z_{\mu}Z^{\mu}+$$
$$+\frac{1}{2}M_{W}^{2}W_{\mu}^{-}W^{+\mu}-\frac{1}{4}B_{\mu\nu}B^{\mu\nu}-\frac{1}{4}W_{\mu\nu}^{a}W^{a\mu\nu}\quad .$$

As we mentioned we have three families of leptons and quarks (see Chap. Feynman amplitudes and lattice gauge theory) :
(ν_e,e^-) neutrino and electron -first generation;
(ν_μ,μ^-) muon neutrino and muon -second generation;
(ν_τ,τ^-) tau neutrino and tauon -third generation;
(u^α,d^α) up quark and down quark -first generation;
(c^α,s^α) charm quark and strange quark -second generation;
(t^α,b^α) top quark and bottom quark -third generation;
$\alpha=1,2,3$ -color index ;
The $u^\alpha,c^\alpha,t^\alpha$ have electric charge $\frac{2}{3}|e|$;
The $d^\alpha,s^\alpha,b^\alpha$ have electric charge $-\frac{1}{3}|e|$;
The neutrinos have neutral electric charge;
The e^-,μ^-,τ^- have charge $e=-|e|$.
A generation makes a family of leptons and quarks and *u,c,t,d,s,b* are the quark flavors, ν_e , e^- , ν_μ , μ^- , ν_τ , τ^- are the leptons.

The W bosons interaction part of the Lagrangian density ,
$$\frac{g}{2}W_{\mu}^{+}\overline{u}_{L}^{\alpha}\gamma^{\mu}d_{L}^{\alpha}+\frac{g}{2}W_{\mu}^{-}\overline{d}_{L}^{\alpha}\gamma^{\mu}u_{L}^{\alpha}+\frac{g}{2}W_{\mu}^{+}\overline{\nu}_{L}\gamma^{\mu}e_{L}+\frac{g}{2}W_{\mu}^{-}\overline{e}_{L}\gamma^{\mu}\nu_{L}\ ,$$
allows the β -decay in which for example (β^- -decay) in a neutron ,which is a color singlet *udd* (see Chap. Feynman amplitudes and lattice gauge theory), a down quark becomes a up quark emitting a W boson which then decays into an electron and a antineutrino so that the neutron becomes a proton *uud* by emission of an electron and a antineutrino according to the coupling (see fig. 1)
$$-\frac{g^2}{4}\overline{u}_{L}^{\alpha}\gamma^{\mu}d_{L}^{\alpha}W_{\mu}^{+}(x)W_{\nu}^{-}(y)\overline{e}_{L}\gamma^{\nu}\nu_{L}\ .$$
We can also have a β^+ decay in which a proton becomes a neutron by emission of a positron and a neutrino. In β^- decay the weak interaction converts an atomic nucleus into a nucleus with atomic number increased by one while emitting an electron and an antineutrino. In β^+ decay the weak interaction converts an atomic nucleus into a nucleus with atomic number decreased by one while emitting a positron and a neutrino. β^- decay occurs in neutron rich nuclei and β^+ decay occurs in proton rich nuclei . In all cases where β^+ decay is allowed energetically , also electron capture is possible in which a nucleus captures one of its atomic electrons resulting the emission of a neutrino: a up quark from a proton *uud* interacts with the electron exchanging a

W boson and becomes a down quark emitting a neutrino according to coupling (see fig. 2)

$$-\frac{g^2}{4}\bar{d}_L^{\alpha}\gamma^{\mu}u_L^{\alpha}W_{\mu}^{-}(x)W_{\nu}^{+}(y)\bar{\nu}_L\gamma^{\nu}e_L\ .$$

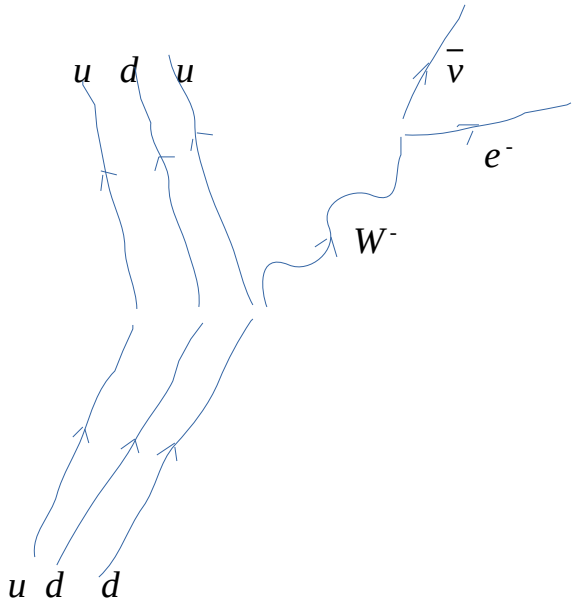

fig.1

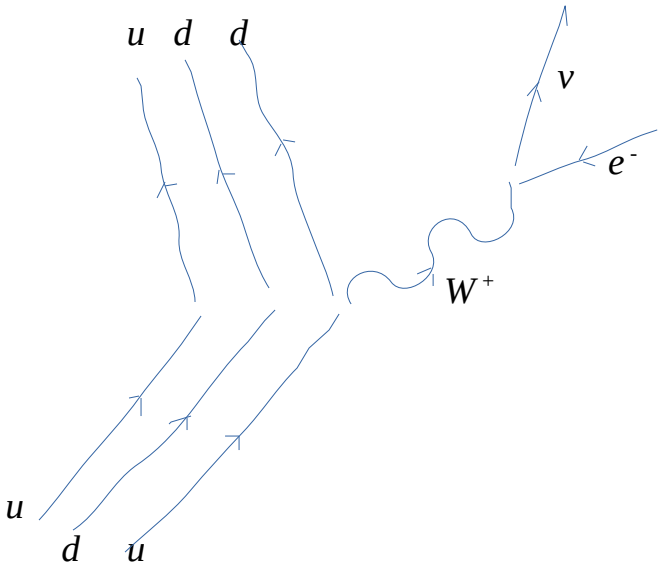

fig.2

The Δ^{++} baryon, consisting of three up quarks which have no orbital angular momentum has a total spin of 3/2 (each quark contributes with spin angular momentum 1 / 2) . Therefore the Δ^{++} baryon must be a fermion and have an antisymmetrical wave function. For the tensorial product of three identical up quark wave functions leading to an antisymmetrical state we must have at least three discrete degrees of freedom for the up quark wave function. Hence we derive for the quark the existence of color degree of freedom. The quarks come in three colors and we define the *SU*(3) invariance by color transformations and the 8 color charges

$(\rho^a)_{a=\overline{1,8}}$ of the color quark $(\psi^{\alpha})_{\alpha=\overline{1,3}}$, ψ^{α} a Dirac spinor function ,

$\rho^a=\bar{\psi}^{\alpha}\frac{1}{2}\lambda^a_{\alpha\beta}\psi^{\beta}$, $\lambda^a, a=\overline{1,8}$ -the Gell-Mann matrices , generators of $SU(3)$.

(see Chap. Feynman amplitudes and lattice gauge theory) .

The Quantum chromodynamics is therefore a *SU*(3) gauge group non-abelian gauge theory described by a Lagrangian density

$\mathscr{L}=\sum_{\text{flavors}}\bar{\psi}^{\alpha}(i\gamma^{\mu}(\delta_{\alpha\beta}\partial_{\mu}-ig A^a_{\mu}T^a_{\alpha\beta})-m\delta_{\alpha\beta})\psi^{\beta}-\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}$ where $(A^a_{\mu})_{\mu,a}$ is the gauge field known as gluon field and

$F^a_{\mu\nu}=\partial_{\mu}A^a_{\nu}-\partial_{\nu}A^a_{\mu}+g f^{abc}A^b_{\mu}A^c_{\nu}$, $T^a=\frac{1}{2}\lambda^a$, $[T^b,T^c]=i f^{abc}T^a$.

Note that quarks of different flavors can have different masses *m*.
As we proved in Chap. Feynman amplitudes and lattice gauge theory , the potential energy of a quark-antiquark system or that of a baryonic three quark system grows with the (square of) separation distance if the momentum range of the quarks is small enough, so that, due the strong coupling constant g , at small energies, the quarks are confined in quark-antiquark particles or three quark particles as protons (*u u d*) or neutrons (*u d d*) or other hadrons. As we will show, the strong coupling constant flows to zero in the large momentum limit and so at high energies we have asymptotic freedom of quarks, with quarks interacting as isolated particles.
The perturbative calculation of the renormalization group flow (for the dependence of the coupling constant on momentum range parameter), since the coupling g becomes ever stronger down to the momentum scale, requires higher order in g approximations and becomes finally inadequate.Nevertheless it is plausible that g goes to infinity with decreasing to zero momentum scale and that the gluons keep the quarks and themselves in permanent confinement. To calculate the amplitudes of various processes in the non-perturbative approach for low momentum scale we can use lattice gauge theory (see Chap. Feynman amplitudes and lattice gauge theory) and provide the order parameter for confinement (below from which the higher order terms in g become significant).

Further we can consider a theory which includes Electroweak interaction and strong Quantum chromodynamics interaction.
The left handed up and down quarks are in a doublet $\begin{pmatrix} u^{\alpha} \\ d^{\alpha} \end{pmatrix}_L$ with hypercharge $\frac{Y}{2}=\frac{1}{6}$. We denote this $(3,2,\frac{1}{6})_L$ with the three numbers indicating how these fields transform under *SU*(3)x*SU*(2)x*U*(1) . Similarly the right handed up quark is $(3,1,\frac{2}{3})_R$, the right handed down quark is $(3,1,-\frac{1}{3})_R$. The leptons $\begin{pmatrix} \nu \\ e \end{pmatrix}_L$ and e_R are $(1,2,-\frac{1}{2})_L$ and respective $(1,1,-1)_R$ where 1 in the first entry indicates that these fields do not participate in the strong interaction.
All the quarks and leptons of each family are placed in
$(3,2,\frac{1}{6})_L$, $(3,1,\frac{2}{3})_R$, $(3,1-\frac{1}{3})_R$, $(1,2,-\frac{1}{2})_L$, $(1,1,-1)_R$ (*) .
Since gauge transformations commute with the Lorentz group, the gauge transformations cannot change left handed fields to right handed fields. The charge conjugation changes left handed fields to right handed fields and viceversa. So by charge conjugation of the right handed fields, instead of (*) we can write
$(3,2,\frac{1}{6})$, $(3^*,1,-\frac{2}{3})$, $(3^*,1,\frac{1}{3})$, $(1,2,-\frac{1}{2})$, $(1,1,1)$ (**)
with all fields left handed.

(where N^* denotes the representation of $SU(N)$ which transforms elements $(\varphi_i)_{i=\overline{1,N}} \in \mathbb{C}^N$ like $(\varphi^{i*})_{i=\overline{1,N}}$ with $(\varphi^j)_i$ transforming in the N representation. Thus under $U=(U^i_j)_{i,j} \in SU(N)$ we have $\varphi_i \to (U^i_j)^* \varphi_j = U^{+j}_i \varphi_j$)

The smallest *SU*(*N*) group that contains *SU*(3)x*SU*(2)x*U*(1) is *SU*(5) .

Of the 24 traceless self-adjoint matrices that generate *SU*(5) we have 8 which have the form $\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}$ with $A \in M_{3\times 3}(\mathbb{C})$ and 3 have the form $\begin{pmatrix} 0 & 0 \\ 0 & B \end{pmatrix}$ with $B \in M_{2\times 2}(\mathbb{C})$ so we can take $A=\frac{1}{2}\lambda^a$, $a=\overline{1,8}$, λ^a -the Gell-Mann matrices and $B=\frac{1}{2}\sigma^i$, $i=\overline{1,3}$, σ^i -the Pauli matrices and therefore $SU(3)$ and $SU(2)$ fit into $SU(5)$.

Furthermore the 5×5 self-adjoint traceless matrix $\frac{Y}{2}=\mathrm{diag}(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3},\frac{1}{2},\frac{1}{2})$ generates a $U(1)$. $\frac{Y}{2}$ is the hypercharge .

In other words we separate the index $(\alpha,i)_{\alpha=1,2,3;\, i=4,5}$. The three objects ψ^α transform as 3 under *SU*(3) and do not transform under *SU*(2) and hence each of them belong to a 1 singlet of *SU*(2) . Furthermore they carry hypercharge -1/3 .

So the $(\psi^\alpha)_\alpha$ transform as $(3,1,-\frac{1}{3})$ under $SU(3)\times SU(2)\times U(1)$.

The two objects ψ^i transform as 1 under $SU(3)$ and as 2 under $SU(2)$ and carry hypercharge 1/2 . Thus they transform as $(1,2,\frac{1}{2})$ and so the 5 of $SU(5)$ decomposes into representations of $SU(3)\times SU(2)\times U(1)$:

$5 \to (3,1,-\frac{1}{3}) \oplus (1,2,\frac{1}{2})$.

Taking the conjugate we see that

$5^* \to (3^*,1,\frac{1}{3}) \oplus (1,2^*,-\frac{1}{2})$ and therefore, identifying $2 \to 2^*$ through $(\nu,e) \to (e,-\nu)$ we decompose $5^* \to (3^*,1,\frac{1}{3}) \oplus (1,2,-\frac{1}{2})$ with the two composing parts appearing in the (**) list.

Consider now the antisymmetric tensor representation of *SU*(5) denoted as 10 defined by antisymmetric 5×5 matrices $(\psi^{\mu\nu})_{\mu\nu}$, $\psi^{\mu\nu}=-\psi^{\nu\mu}$ with $\mu,\nu=\overline{1,5}$ transforming under $U=(U^\mu_\nu)_{\mu,\nu} \in SU(5)$ as $\psi=(\psi^{\mu\nu})_{\mu,\nu} \to U\,\psi U^T$ with $U^T=(U^\nu_\mu)_{\mu,\nu}$. Thus a generator T^a of $SU(5)$ acts on ψ like $(T^a\psi)^{\mu\nu}=T^a_{\mu\delta}\psi^{\delta\nu}+\psi^{\mu\delta}T^a_{\nu\delta}$,

since $U\,\psi U^T=\exp(i\theta^a T^a)\,\psi\exp(i\theta^a T^{aT})=\psi+i\theta^a(T^a\psi+\psi T^{aT})+O(\theta^2)$.

We know already $5\rightarrow(3,1,-\frac{1}{3})\oplus(1,2,\frac{1}{2})$ and taking the antisymmetric tensorial product, after we identify $3\otimes_A 3\rightarrow 3^*$ by $3\otimes_A 3\ni(\varphi^{\alpha\beta})_{\alpha\beta}\rightarrow(\epsilon_{\alpha\beta\gamma}\varphi^{\beta\gamma})_\alpha\in 3^*$ we have

$(3,1,-\frac{1}{3})\otimes_A(3,1,-\frac{1}{3})\rightarrow(3^*,1,-\frac{2}{3})$

$(3,1,-\frac{1}{3})\otimes_A(1,2,\frac{1}{2})\rightarrow(3,2,\frac{1}{6})$

$(1,2,\frac{1}{2})\otimes_A(1,2,\frac{1}{2})=(1,1,1)$

and so we derive

$10=5\otimes_A 5\rightarrow(3,2,\frac{1}{6})\oplus(3^*,1,-\frac{2}{3})\oplus(1,1,1).$

Hence the known quark and lepton fields in a given family fit perfectly into the 5^* and 10 representations of $SU(5)$.

We write therefore 5^* as the column vector $(\psi_\mu)_\mu=\begin{pmatrix}\psi_\alpha\\ \psi_i\end{pmatrix}_{\alpha,i}=\begin{pmatrix}(d_c^\alpha)_\alpha\\ e\\ -\nu\end{pmatrix}$ where we denoted $\widetilde{d}$ -the down quark Dirac spinor field, $\widetilde{e}$ -the electron dirac spinor field, $\widetilde{\nu}$ -the neutrino Dirac spinor field, $d=\widetilde{d}_L=\frac{\boldsymbol{I}-\gamma^5}{2}\widetilde{d}$ -the left handed down quark field, $d_c=\gamma^2\widetilde{d}_R^*$ -charge conjugated right handed down quark $\widetilde{d}_R=\frac{\boldsymbol{I}+\gamma^5}{2}\widetilde{d}$, $e=\widetilde{e}_L=\frac{\boldsymbol{I}-\gamma^5}{2}\widetilde{e}$ -left handed electron field, $\nu=\widetilde{\nu}_L=\frac{\boldsymbol{I}-\gamma^5}{2}\widetilde{\nu}$ -left handed neutrino .

Obviously $((d_c^\alpha)_\alpha,0,0)$ transforms as $(3^*,1,\frac{1}{3})$ and $(0,0,0,e,-\nu)$ transforms as $(1,2^*,-\frac{1}{2})$.

We write 10 as the antisymmetric matrices

$(\psi^{\mu\nu})_{\mu,\nu}=(\psi^{\alpha\beta},\psi^{\alpha i},\psi^{j\alpha},\psi^{jj})_{\alpha,\beta,i,j}$ with $\alpha,\beta=\overline{1,3}$, $i,j=4,5$

$$(\psi^{\mu\nu})_{\mu,\nu}=\frac{1}{\sqrt{2}}\begin{pmatrix}0 & u_c & -u_c & u & d\\ -u_c & 0 & u_c & u & d\\ u_c & -u_c & 0 & u & d\\ -u & -u & -u & 0 & e_c\\ -d & -d & -d & -e_c & 0\end{pmatrix}$$ (where we suppressed the color index)

so that $\psi^{\alpha\beta}=\frac{1}{\sqrt{2}}\epsilon_{\alpha\beta\gamma}u_c^\gamma$, $\psi^{\alpha 4}=-\psi^{4\alpha}=\frac{u^\alpha}{\sqrt{2}}$, $\psi^{\alpha 5}=-\psi^{5\alpha}=\frac{d^\alpha}{\sqrt{2}}$,

$\psi^{45}=-\psi^{54}=\frac{1}{\sqrt{2}}e_c$ with $\widetilde{u}$ up quark , $u_c=\gamma^2\widetilde{u}_R^*$, $\widetilde{u}_R=\frac{\boldsymbol{I}+\gamma^5}{2}\widetilde{u}$,

$\tilde{e}_R=\frac{I+\gamma^5}{2}\tilde{e}$, $e_c=\gamma^2\tilde{e}_R^*$.

We add a $(1,1,0)$ field, ψ_0 , which transforms obviously as the identity 1 representation of $SU(5)$ corresponding to the antineutrino $\nu_c=\gamma^2\tilde{\nu}_R^*$ with $\tilde{\nu}_R=\frac{I+\gamma^5}{2}\tilde{\nu}$.

Therefore we have the grand unified $SU(3)$x$SU(2)$x$U(1)$ theory written in terms of $SU(5)$ representations Georgi-Glashow model $5^*\oplus 10\oplus 1$ with a Lagrangian density

$$\mathcal{L}=-\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}+\sum_\Phi\overline{\Phi}\ \gamma^\mu(i\partial_\mu-m_\Phi)\Phi+\sum_\psi g_3\overline{\psi}\cdot\gamma^\mu A^{a3}_\mu T^a_{(3)}[\psi]+$$

$$+\sum_\psi g_2\overline{\psi}\cdot\gamma^\mu A^{a2}_\mu T^a_{(2)}[\psi]+\sum_\psi g_1\overline{\psi}\cdot\gamma^\mu\sqrt{\frac{5}{3}}B_\mu T_{(1)}[\psi]+\frac{1}{2}(\mu^2)^{ab}A^a_\mu A^{b\mu} \qquad (1)$$

where $\Phi\in\{\tilde{\nu},\tilde{e},\tilde{u}^\alpha,\ \tilde{d}^\alpha|\alpha=\overline{1,3}\}$ (we can consider obviuously also the other families of quarks and leptons),

$\psi\in\{\psi_\mu,\psi^{\mu\nu},\psi_0|\mu,\nu=\overline{1,5}\}$

$T^a_{(3)}=\begin{pmatrix}A&0\\0&0\end{pmatrix}$, $A=\frac{1}{2}\lambda^a$, $a=\overline{1,8}$,

$T^a_{(2)}=\begin{pmatrix}0&0\\0&B\end{pmatrix}$, $B=\frac{1}{2}\sigma^a$, $a=\overline{1,3}$,

$T_{(1)}=\sqrt{\frac{3}{5}}\frac{Y}{2}$, $(T^a)_{a=\overline{1,12}}=((T^a_{(3)})_{a=\overline{1,8}},(T^a_{(2)})_{a=\overline{1,3}},T_{(1)})$,

$(A^a_\mu)_{a=\overline{1,12}}=((A^{a3}_\mu)_{a=\overline{1,8}},(A^{a2}_\mu)_{a=\overline{1,3}},B_\mu)$; $[T^b,T^c]=if^{abc}T^a$,

$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu+gf^{abc}A^b_\mu A^c_\nu$ with $g=g_3$ for $a=\overline{1,8}$, $g=g_2$ for $a=\overline{9,11}$;

For $(\psi,\varphi)=((\psi_\mu)_\mu,(\varphi_\mu)_\mu)$ we have defined $\gamma^\lambda\psi=(\gamma^\lambda\psi_\mu)_\mu$, $\overline{\psi}\cdot\varphi=\overline{\psi}_\mu\varphi_\mu$ and $T^a[\psi]=(-T^a_{\nu\mu}\psi_\nu)_\mu$;

For $(\psi,\varphi)=((\psi^{\mu\nu})_{\mu,\nu},(\varphi^{\mu\nu})_{\mu,\nu})$ we have defined $\gamma^\lambda\psi=(\gamma^\lambda\psi^{\mu\nu})_{\mu,\nu}$, $\overline{\psi}\cdot\varphi=\overline{\psi}^{\mu\nu}\varphi^{\mu\nu}$ and $T^a[\psi]=T^a\psi+\psi T^{aT}$.

To generate the mass terms in the Lagrangian density (1), represented by $-\sum_\Phi\overline{\Phi}m_\Phi\Phi$ we can introduce a Higgs field which transforms as a 5: $(\varphi^\mu)_{\mu=\overline{1,5}}$, $\varphi_\mu=\varphi^{\mu*}$ and has a vacuum expectation value $\langle\varphi\rangle=(\delta_{5\mu}v)_{\mu=\overline{1,5}}$ with $v\in\mathbb{R}$ considering the couplings $2\Re(\psi^T_\mu f\gamma^0\gamma^2\psi^{\mu\nu}\varphi_\nu+\psi^{\mu\nu}f\gamma^0\gamma^2\psi^{\lambda\rho}\varphi^\sigma\epsilon_{\mu\nu\lambda\rho\sigma})$.

The first coupling determines the mass of the down quarks and of the electron and the second coupling determines the mass of the up quark.

By the Anderson-Higgs mechanism, we obtain the mass operator $((\mu^2)^{ab})_{a,b}$ and the gauge mass spectrum as in the electroweak theory.

Thus we will have the corresponding massive W bosons $W^{\pm}_{\mu}=A^{12}_{\mu}\mp i\,A^{22}_{\mu}$, the massive Z boson $Z_{\mu}=A^{32}_{\mu}\cos\theta-B_{\mu}\sin\theta$ and the massless photon $A_{\mu}=A^{32}_{\mu}\sin\theta+B_{\mu}\cos\theta$ with $\tan\theta=\frac{g_1}{g_2}$, because as in the electroweak theory we have $\frac{Y}{2}\langle\varphi\rangle=\frac{1}{2}\langle\varphi\rangle$.
We have also $T^{a}_{(3)}\langle\varphi\rangle=0$ and so the $(A^{a3})_{a=\overline{1,8}}$ remain massless.

In a grand unified *SU*(5) theory we would have$(5/3)^{1/2}\,g_1 = g_2 = g_3 = g$ and 12 more gauge bosons that transform quarks into leptons and viceversa:
$W^{\pm}_{u\alpha}=W^{1}_{u\alpha}\pm i\,W^{2}_{u\alpha}$, $W^{\pm}_{d\alpha}=W^{1}_{d\alpha}\pm i\,W^{2}_{d\alpha}$, $\alpha=1,2,3$ corresponding to generators
$T^{1}_{u\alpha}=(\delta_{4\mu}\delta_{\alpha\nu}+\delta_{4\nu}\delta_{\alpha\mu})_{\mu,\nu}$, $T^{2}_{u\alpha}=(-i\,\delta_{\alpha\mu}\delta_{4\nu}+i\,\delta_{\alpha\nu}\delta_{4\mu})_{\mu,\nu}$
$T^{1}_{d\alpha}=(\delta_{5\mu}\delta_{\alpha\nu}+\delta_{5\nu}\delta_{\alpha\mu})_{\mu,\nu}$, $T^{2}_{d\alpha}=(-i\,\delta_{\alpha\mu}\delta_{5\nu}+i\,\delta_{\alpha\nu}\delta_{5\mu})_{\mu,\nu}$ with $\mu,\nu=\overline{1,5}$.
The grand unified *SU*(5) theory would allow a proton decay in which the down quark and a up quark of the proton $p = uud$ anihilate each other producing a $W^{+}{}_{d}$ boson which then decays into a positron e^{+} and a anti- up quark which forms with the remaining up quark of the incoming proton a outgoing pion $\pi^{0} = u\bar{u}$ according to interaction term $\overline{\psi}_{\alpha\beta}\gamma^{\mu}\psi_{5\beta}W^{-}_{d\alpha\mu}(x)W^{+}_{d\alpha\lambda}(y)\overline{\psi}_{54}\gamma^{\lambda}\psi_{\alpha 4}$ and the Feynman diagram below in fig.3 .

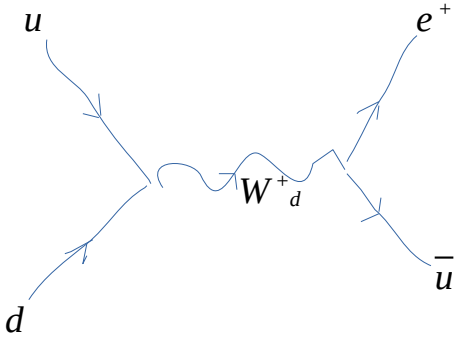

fig.3

Let M_X denote generically the masses of those gauge bosons transforming quarks into leptons and viceversa. Then the amplitude of proton decay is of order g^2 / M_X^2 and the proton decay rate Γ is given by $(g^2 / M_X^2)^2$ times a phase space factor controlled esentially by the proton mass since the pion and positron mass are negligible compared to the proton mass m_P . By dimensional analysis we determine that $\Gamma \sim (g^2 / M_X^2)^2\, m_P^5$. The decay rate determines the evolution of the $N = N(t)$ number of protons in a sample by the equation $\frac{dN}{dt}=-\Gamma N$ and so $N=N_0\exp(-\Gamma t)$ and

the mean lifetime of a proton is therefore $\tau = \frac{\int_0^\infty t N(t) dt}{\int_0^\infty N(t) dt} = \frac{1}{\Gamma}$.

We expect the world to be stable and so Γ has to be small and M_X has to be huge compared to the kind of energy scales we can reach experimentally.
The mass M_X is of the same order as the mass scale M_{GUT} at which the grand unified $SU(5)$ theory is spontaneously broken down to $SU(3)$x$SU(2)$x$U(1)$ as we already exemplified in Chap. Anderson-Higgs mechanism , considering a Higgs field φ transforming as a traceless self-adjoint 5x5 matrix in the adjoint representation of $SU(5)$ allowing for φ a vacuum expectation value

$\langle \varphi \rangle = \text{diag}(-\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}, \frac{1}{2}, \frac{1}{2})$.

As we move up in the mass or energy scale μ , we will show that the couplings $g_3(\mu)$ $g_2(\mu)$ are asymptotically free decreasing while $g_1(\mu)$ increases. Thus at some mass scale M_{GUT} they will meet and that is where the $SU(3)$x$SU(2)$x$U(1)$ theory is unified into $SU(5)$. We anticipate that the mass scale M_{GUT} will come out much higher than any scale we were used to.

We will determine now the renormalizations of the couplimg constants g_j , j = 1,2,3 under consideration of quantum fluctuations to order $O(g^2)$ in $SU(3)$x$SU(2)$x$U(1)$ theory with the (1) Lagrangian density considering the scattering process involving two particles interchanging bosons corresponding to generators which belong to one (j) of the three subrepresentations generators $(T^a_{(j)})_a$, $j=1,2,3$.
In the following m stands generically for the fermion masses involved in the interactions. We calculate the scattering process at energies high compared to the mass m and so we will set all quarks and leptons masses equal to one $m \to 0$, setting $m=0$ everywhere we can, such as in the numerator of an expression.
The order zero fluctuations Feynman diagram for a scattering process is fig.4 with s_1 and $s+q$ four-momenta on mass shell, which since as mentioned we consider $m \to 0$ leads to $q^2 = -\mu^2 \leq 0$ and μ^2 being the momentum transfer squared.

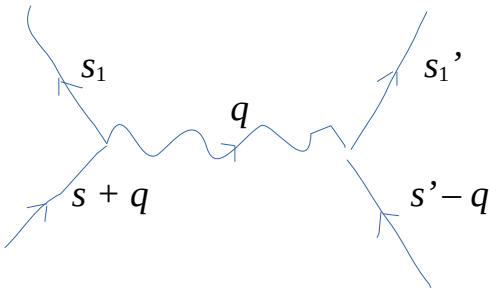

fig.4 $s_1 = s$, $s_1' = s'$

The q four-momentum virtual boson can fluctuate into a fermion and an antifermion according to fig.5 and fig.6 diagrams

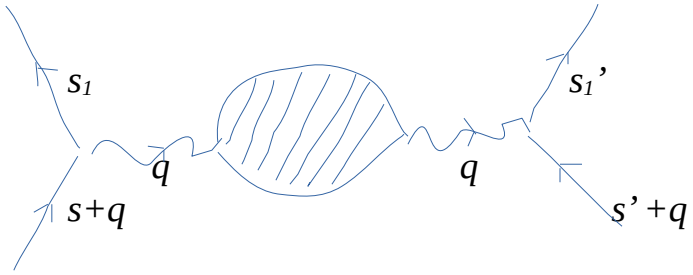

fig.5

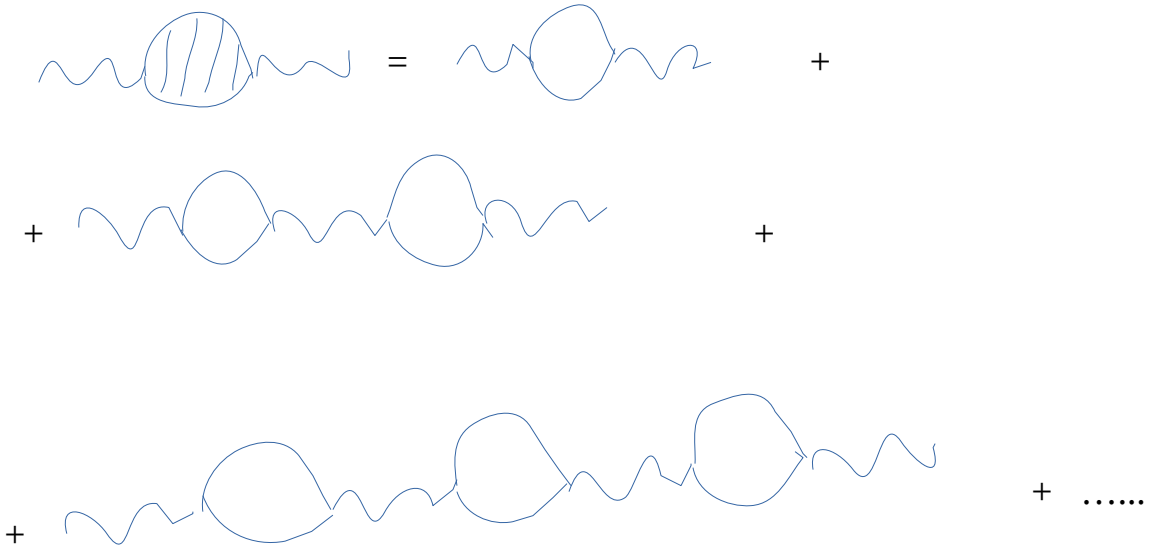

fig.6

The Feynman amplitude for fig.5 fig.6 Feynman diagram scattering process with consideration of fluctuations is

$(2\pi)^4 \boldsymbol{M}\,\delta^4(s_1+s'_1-s-s')$ with $s_1=s$, $s'_1=s'$,

$$\boldsymbol{M}=-g^2\bar{u}(s)\gamma^{\mu}u(s+q)\left|iD_{\mu\nu}(q)+iD_{\mu\lambda}(q)i\Pi_F^{\lambda\rho}(q)iD_{\rho\nu}(q)+\right.$$
$$\left.+iD_{\mu\lambda}(q)i\Pi_F^{\lambda\rho}(q)iD_{\rho\sigma}(q)i\Pi_F^{\sigma\kappa}(q)iD_{\kappa\nu}(q)+...\right|\bar{u}(s')\gamma^{\nu}u(s'-q)\,\mathrm{tr}(T^aT^a)$$

where we suppressed the spin index for the generical fermion Dirac spinor function u and we take the massless boson propagator

$$D_{\mu\nu}(q)=\left(-\eta_{\mu\nu}+(1-\xi)\frac{q_\mu q_\nu}{q^2}\right)\frac{1}{q^2}$$

(as we will notice the case of a massive boson propagator can be treated in the same way giving the same result since the momentum transfer being considered high compared to the boson mass for having a significant fluctuations contribution we can neglect the boson mass in the momentum space propagator denominator) and also , according to Feynman rules we will have

$$i\Pi_F^{\lambda\rho}(q)=\int \mathrm{tr}\left(-\frac{1}{(2\pi)^4} i g \gamma^\lambda \frac{i}{\not p-m+i\varepsilon} i g \gamma^\rho \frac{i}{\not p+\not q-m+i\varepsilon}\right) d^4 p\, \mathrm{tr}(T^a T^a)\ .$$

(Notice the minus sign for the fermion loop.)

We have $q_\lambda((\not p+\not q+m)\gamma^\lambda(\not p+m))_{\alpha\varepsilon}=4m^2 u_\alpha(p+q)\bar u(p+q)(\not p+\not q)u(p)\bar u_\varepsilon(p)-$
$-4m^2 u_\alpha(p+q)\bar u(p+q)\not p u(p)\bar u_\varepsilon(p)=4m^3\left(u_\alpha(p+q)\bar u(p+q)u(p)\bar u_\varepsilon(p)-\right.$
$\left.-u_\alpha(p+q)\bar u(p+q)u(p)\bar u_\varepsilon(p)\right)=0$ and so $q_\lambda\Pi_F^{\lambda\rho}(q)=0$ and similar $q_\rho\Pi_F^{\lambda\rho}(q)=0$.

Together with Lorentz invariance this requires that

$$i\Pi_F^{\lambda\rho}(q)=g^2(q^\lambda q^\rho-\eta^{\lambda\rho}q^2)i\Pi_F(q^2) \text{ and so } g^2\Pi_F(q^2)=-\frac{1}{3q^2}\eta_{\lambda\rho}\Pi_F^{\lambda\rho}(q)$$

obtaining $\boldsymbol{M}=g^2 i\,\eta_{\mu\nu}\bar u(s)\gamma^\mu u(s+q)\left(\frac{1}{1+g^2\Pi_F(q^2)}+\text{'}q_\mu q_\nu \text{ term'}\right)\bar u(s')\gamma^\nu u(s'-q)$.

We have $q_\mu\bar u(s)\gamma^\mu u(s+q)=\bar u(s)(\not s+\not q)u(s+q)-\bar u(s)\not s u(s+q)=0$
(since $\not k u(k)=m u(k)$) and so we can drop the $q_\mu q_\nu$ term in the above expression.

If there are no gluon self interacting fluctuations which is the case in Quantum electrodynamics or the subrepresentation is of $j = 1$, $g = g_1$ the effective coupling at momentum transfer squared $\mu^2=-q^2$ is $g(\mu)$ which comparing the resulted expression for $\boldsymbol{M}$ with the zero order in fluctuations amplitude , satisfies

$g^2(\mu)=\frac{g^2}{1+g^2\Pi_F(-\mu^2)}$ (2) and generally we will have a correction to $\frac{1}{g^2(\mu)}$ due to fermion loop fluctuations described by fig.5 diagrams given by

$\frac{1}{g^2(\mu)}=\frac{1}{g^2}+\Pi_F(-\mu^2)$ at momentum transfer squared $\mu^2=-q^2$ and in Quantum electrodynamics we have a electric charge renormalization $e^2(\mu)=\frac{e^2}{1+e^2\Pi_F(-\mu^2)}$.

Let $I(q^2,m)=\int \frac{d^4p}{(2\pi)^4}\mathrm{tr}\left(\gamma_\mu\frac{1}{\not p+\not q-m+i\varepsilon}\gamma^\mu\frac{1}{\not p-m+i\varepsilon}\right)$ (3)

We have $\Pi_F(q^2)=-\frac{i}{3q^2}I(q^2,m)\,\mathrm{tr}(T^aT^a)$.

Using the identity $\int_0^1 \frac{d\alpha}{\alpha x-(1-\alpha)y}=\frac{1}{xy}$ we obtain:

$$I(q^2,m)=\int_0^1\int\frac{d^4p}{(2\pi)^4}\frac{\mathrm{tr}\left(\gamma_\mu(\not p+(1-\alpha)\not q+m)\gamma^\mu(\not p-\alpha\not q+m)\right)}{(p^2-m^2+\alpha(1-\alpha)q^2+i\varepsilon)^2}=$$

$$=\int_0^1\int\frac{d^4p}{(2\pi)^4}\frac{-8p^2+8\alpha(1-\alpha)q^2-8(1-2\alpha)pq-8m^2}{(p^2-m^2+\alpha(1-\alpha)q^2+i\varepsilon)^2}=$$

$$=\int_0^1 d\alpha\int\int_{-\infty}^{\infty}H_\alpha(p_0,\vec p)\,dp_0\,d^3\vec p$$ where the poles of $H_\alpha(p_0,\vec p)$ as a complex (4)

function of p_0 are $z_\pm=\pm(a-ib)$ with $a,b\in\mathbb{R}_+$, $b\neq0$ and so

$$\int_{-\infty}^{\infty}H_\alpha(p_0,\vec p)\,dp_0=2\pi i\,\mathrm{Rez}(H_\alpha(\cdot,\vec p),z_-)=\int_{-i\infty}^{i\infty}H_\alpha(z,\vec p)\,dz=i\int_{-\infty}^{\infty}H_\alpha(iz,\vec p)\,dz\ ,$$

$$I(q^2,m)=i\int\frac{d\alpha}{(2\pi)^4}\int\frac{8k^2-8(m^2-\alpha(1-\alpha)q^2)}{(k^2+m^2-\alpha(1-\alpha)q^2)^2}d_E^4k \qquad (5)$$

Taking a cutoff $\|k\|_4<\Lambda$ we derive:

$$I(q^2,m)=i\int_0^1\frac{d\alpha}{(2\pi)^4}\int_0^{\Lambda^2}\pi^2k\frac{8k-8(m^2-\alpha(1-\alpha)q^2)}{(k+m^2-\alpha(1-\alpha)q^2)^2}dk=$$

$$=i\int_0^1\frac{d\alpha}{2\pi^2}\left(\Lambda^2-3(m^2-\alpha(1-\alpha)q^2)\log\frac{\Lambda^2+m^2-\alpha(1-\alpha)q^2}{m^2-\alpha(1-\alpha)q^2}-\frac{2(m^2-\alpha(1-\alpha)q^2)}{\Lambda^2+m^2-\alpha(1-\alpha)q^2}+\right.$$

$$\left.+2(m^2-\alpha(1-\alpha)q^2)\right)\ .$$

For $m_\nu^2\gg m^2$ the integrand of $I(q^2,m_\nu)$ according to (5) is $O(\frac{1}{m_\nu^2})$ and is

negligible compared to thre integrand of $I(q^2,m)$ and therefore we can take

$(m_\nu,c_\nu)_{\nu=\overline{1,3}}$, $c_\nu\in\mathbb{R}$, $m_\nu^2\gg m^2$ such that

$$\sum_\nu c_\nu=1\ ,\ \sum_\nu c_\nu m_\nu^2=m^2\ ,\ \sum_\nu c_\nu m_\nu^2\log m_\nu^2=m^2\log m^2$$ and

c_ν remaining bounded while $m_\nu\to\infty$ in the so called Paul-Villars regularization

$$I(q^2,m)\approx I(q^2,m)-\sum_\nu c_\nu I(q^2,m_\nu^2) \qquad (6)\ .$$

Thus for large Λ , $\Lambda\to\infty$ we have

$$I(q^2,m)\approx i\int_0^1\frac{d\alpha}{2\pi^2}3\sum_\nu c_\nu\left((m^2-\alpha(1-\alpha)q^2)\log(m^2-\alpha(1-\alpha)q^2)-\right.$$

$$\left.-(m_\nu^2-\alpha(1-\alpha)q^2)\log(m_\nu^2-\alpha(1-\alpha)q^2)\right)\ .$$

We have also

$$(m_\nu^2-\alpha(1-\alpha)q^2)\log(m_\nu^2-\alpha(1-\alpha)q^2)=(m_\nu^2-\alpha(1-\alpha)q^2)\log m_\nu^2-\alpha(1-\alpha)q^2+$$

$$+O(\frac{q^2}{m_\nu^2}).$$

Hence for $m_\nu^2\gg\mu^2$, taking $m\to0$ we obtain

$$I(q^2,m)\approx i\int_0^1 3\frac{d\alpha}{2\pi^2}(-\alpha(1-\alpha)q^2\log(-\alpha(1-\alpha)q^2)+\alpha(1-\alpha)q^2+\alpha(1-\alpha)\log\overline{M}^2)=$$

$$=iq^2 3\int_0^1 \frac{d\alpha}{2\pi^2}(\alpha(1-\alpha)\log\frac{\overline{M}^2}{\mu^2}+\alpha(1-\alpha)(1-\log(\alpha(1-\alpha))))$$

where $\log\overline{M}^2=\sum_\nu c_\nu\log m_\nu^2$ and taking $M>0$ such that

$\log M^2=\log\overline{M}^2+6\int_0^1 \alpha(1-\alpha)(1-\log(\alpha(1-\alpha)))d\alpha$ we have a parameter M so that at momentum transfer squared μ^2 with $m\to 0$ we have

$$I(\mu^2)=I(q^2,m)\approx 3iq^2\frac{1}{12\pi^2}\log\frac{M^2}{\mu^2}$$

$$\Pi_F(q^2)=\frac{1}{12\pi^2}\log\frac{M^2}{\mu^2}\mathrm{tr}(T^aT^a) \qquad (7)$$

The effective coupling in Quantum electrodynamics case is $g(\mu)=-e(\mu)$, $e(\mu)$ -effective electron charge and is given by $g^2(\mu)=\frac{g^2}{1+g^2a\log\frac{M^2}{\mu^2}}$,

$a=\frac{1}{12\pi^2}$, $\frac{1}{g^2(\mu)}=\frac{1}{g^2}+2a\log\frac{M}{\mu}$ and taking $t=\log\mu$ as a renormalization group flow parameter we have a renormalization group flow equation

$\frac{dg}{dt}=ag^3=\beta(g)$, $a>0$.

If a theory happens to have coupling constants g_i , $i=\overline{1,N}$ then we have $\frac{dg_i}{dt}=b_i(g_1,g_2,\dots g_N)$ .The $(g_1,g_2,\dots,g_N)$ is interpreted as the coordinate of a particle in N -dimensional space, t -as time and $b_i(g_1,g_2,\dots,g_N)$, $i=\overline{1,N}$ as a position dependent velocity field. As we increase t(or μ) we study how the particle moves or flows. We will denote $(g_1,g_2,\dots,g_N)$ as g . Those couplings g^* at which $(b_i(g^*))_{i=\overline{1,N}}$ vanish are fix points. If the velocity field around a fix point is such that the particle moves toward the point (and once reaching it, it stays there since its velocity is now zero) , the fix point is known as attractive or stable.

Thus to study the asymptotic behaviour of a quantum field theory at high energies we have to find all its attractive fix points under the renormalization group flow. We can tipically see that some couplings are flowing toward larger values while other are flowing to zero.

The asymptotic or high energy behaviour of the theory on the sign of b_i. In the case of Quantum chromodynamics and Electroweak theory (couplings g_3 and g_2) we will notice a renormalization group flow with $\beta < 0$ (because of the gluon self-interaction fluctuations as we will show below) and so $g = 0$ is an attractive fix point at high energies (the coupling goes to zero as μ goes to infinity) and we have asymptotic

freedom of Quantum Chromodynamics and Electroweak theory causing the weakening of strong interaction and weak interaction at high energies (and low distances) , the quarks being no more confined at high energies.

In the $SU(3)\times SU(2)\times U(1)$ and $SU(5)$ theories the $\mathrm{tr}(T^aT^a)$ factor in (7) must be considered for both 5^* and 10 representations. For the 5^* representation the factor is $\mathrm{tr}(T^aT^a)$ and for the 10 representation we have to consider all summations $\sum_{\mu,\nu,\alpha,\beta}\overline{\psi}^{\mu\nu}\gamma^{\rho}(T^a_{\mu\alpha}\psi^{\alpha\nu}+T^a_{\nu\beta}\psi^{\mu\beta})\overline{\psi}^{\alpha\beta}\gamma^{\sigma}(T^a_{\alpha\mu}\psi^{\mu\beta}+T^a_{\beta\nu}\psi^{\alpha\nu})$ with $\mu,\nu,\alpha,\beta=\overline{1,5}$ which leads to a factor

$$T^a_R=\frac{1}{4}\sum_{\mu\neq\nu,\ \alpha\neq\beta}(T^a_{\mu\alpha}\delta_{\beta\nu}+T^a_{\nu\beta}\delta_{\alpha\mu})(T^a_{\alpha\mu}\delta_{\beta\nu}+T^a_{\beta\nu}\delta_{\alpha\mu})=\frac{1}{2}(3\,\mathrm{tr}(T^aT^a)+\sum_{\mu=\nu}T^a_{\mu\nu}T^a_{\nu\mu})$$

The generators are diagonal or have all diagonal elements equal to zero.

Therefore $T^a_R\in\left\{\frac{3}{2}\mathrm{tr}(T^aT^a),2\,\mathrm{tr}(T^aT^a)\right\}$, $\max_a T^a_R=2\,\mathrm{tr}(T^aT^a)$

and $\Pi_F(q^2)=\frac{1}{12\pi^2}(\mathrm{tr}(T^aT^a)+T^a_R)F\log\frac{M^2}{\mu^2}$

where F is the number of lepton-quark families.

The Higgs field φ transforming as a traceless selfadjoint matrix in the adjoint representation of $SU(5)$ has vacuum expectation value $\mathrm{diag}(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3},\frac{1}{2},\frac{1}{2})$ commuting with the $T^a_{(i)}$, $i=1,2,3$ generators and so when the $SU(5)$ symmetry is spontaneously broken to $SU(3)\times SU(2)\times U(1)$ all $SU(3)\times SU(2)\times U(1)$ gluons will be massless and for the renormalization of g_3 and g_2 at some momentum transfer squared μ^2 we have to consider gluon self-interactions as in fig.7 (a) , (b) and to ensure gauge invariance of the amplitude computations we must consider also gluon-ghost interactions diagrams to order $O(g^2)$ as in fig.7 (c) .

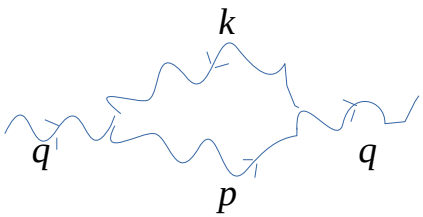

fig.7 (a)

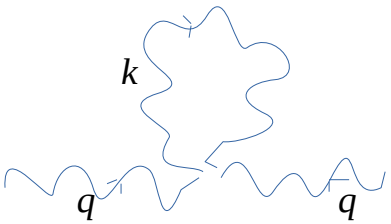

fig.7 (b)

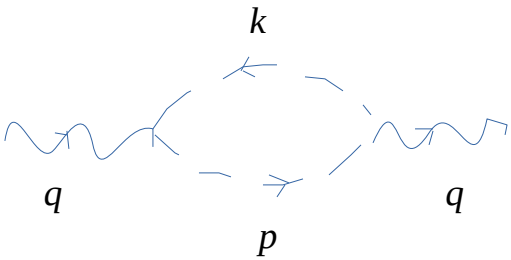

fig.7 (c)

where the (a) is the two three gluons self-interaction vertices loop *GT* , (b) is the four gluons self-interaction vertex loop *GF* and (c) is the two gluon-ghost field interaction vertices loop *GG*.

The Feynman amplitude for the fig.4 scattering under considering of fig.5 and fig. 7 fluctuations is $(2\pi)^4 \boldsymbol{M}\,\delta^4(s_1+s_1'-s-s')$ with

$$\boldsymbol{M}=-g^2\bar{u}(s)\gamma^{\mu}u(s+q)\left[iD_{\mu\lambda}(q)+iD_{\mu\rho}(q)i\Pi^{\rho\sigma}(q)iD_{\sigma\lambda}(q)+\right.$$
$$\left.+iD_{\mu\rho}(q)i\Pi^{\rho\sigma}(q)iD_{\sigma\kappa}(q)i\Pi^{\kappa\nu}(q)iD_{\nu\lambda}(q)+...\right]\bar{u}(s')\gamma^{\lambda}u(s'-q)\,\mathrm{tr}(T^aT^a) \qquad (8)$$

where $D_{\mu\lambda}(q)=\left(-\eta_{\mu\lambda}+(1-\xi)\frac{q_\mu a_\lambda}{q^2}\right)\frac{1}{q^2}$

$\Pi^{\rho\sigma}(q)=\Pi_F^{\rho\sigma}(q)+\Pi_{GT}^{\rho\sigma}(q)+\Pi_{GF}^{\rho\sigma}(q)+\Pi_{GG}^{\rho\sigma}(q)$ and according to Feynman rules:

$$i\Pi_{GT}^{\rho\sigma}(q)=\int\frac{d^4k\,d^4p}{2(2\pi)^4}iD_{\alpha\beta}(k)iD_{\eta\delta}(p)V_{\rho\alpha\eta}^{abc}(q,k,p)V_{\sigma\beta\delta}^{abc}(-q,-k,-p)\delta^4(q+k+p)$$

(with summation over *b* ,*c* indices and we notice the 1 / 2 symmetry factor)

$$i\Pi_{GF}^{\rho\sigma}(q)=\int\frac{d^4k}{2(2\pi)^4}iD_{\nu\delta}(k)W_{\rho\sigma\nu\delta}^{aabb}$$

(with summation over *b* index , noticing the 1 / 2 symmetry factor)

$$i\Pi_{GG}^{\rho\sigma}(q)=\int\frac{(-1)d^4k\,d^4p}{(2\pi)^4}iD_{fb}^{ghost}(p)iD_{ed}^{ghost}(k)H_{aeb}^{\rho}(p)H_{afd}^{\sigma}(k)\delta^4(q+p-k)$$

(with summation over *f* , *b* , *e* , *d* indices , noticing the minus sign from the ghost loop, since the ghost fields are treated as Grassmann variables)

where according to Chap. Non-abelian gauge theory we have

$H_{aeb}^{\rho}=p^{\rho}f^{bea}$ (ghost-gluon coupling)

$D_{fb}^{ghost}(p)=\frac{g}{p^2}\delta_{fb}$ (ghost field propagator)

$V_{\rho\alpha\eta}^{abc}(q,k,p)=gf^{abc}(\eta^{\rho\alpha}(q-k)^{\eta}+\eta^{\rho\eta}(p-q)^{\alpha}+\eta^{\alpha\eta}(k-p)^{\rho})$ (three gluon vertex coupling)

$W_{\rho\sigma\nu\delta}^{bcde}=-ig^2\left[f^{hbc}f^{hde}(\eta^{\rho\nu}\eta^{\sigma\delta}-\eta^{\rho\delta}\eta^{\sigma\nu})+f^{hdc}f^{hbe}(\eta^{\rho\nu}\eta^{\delta\sigma}-\eta^{\rho\sigma}\eta^{\delta\nu})+\right.$
$\left.+f^{hbd}f^{hce}(\eta^{\rho\sigma}\eta^{\nu\delta}-\eta^{\rho\delta}\eta^{\nu\sigma})\right]$ (four gluon vertex coupling)

We take the Feynman-'t Hooft gauge with ξ = 1 and so

$D_{\nu\delta}(k)=-\frac{\eta_{\nu\delta}}{k^2+i\varepsilon}$,

$i\Pi_{GF}^{\rho\sigma}(q)=-\frac{3\eta^{\rho\sigma}}{(2\pi)^4}f^{ahb}f^{ahb}\int\frac{d^4k}{k^2+i\varepsilon}$ (with summation over h,b) .

As we did for Π_F we have $I(m)=\int\frac{1}{k^2-m^2+i\varepsilon}d^4k=\int\frac{1}{k_0^2-\vec{k}^2-m^2+i\varepsilon}dk_0d^3\vec{k}=$

$$=\int_{-\infty}^{\infty}\frac{1}{k_0^2-\vec{k}^2-m^2+i\varepsilon}dk_0d^3\vec{k}=\int_{-i\infty}^{i\infty}\frac{1}{z^2-\vec{k}^2-m^2+i\varepsilon}dz\,d^3\vec{k}=\int\frac{-id_E^4k}{k^2+m^2-i\varepsilon}=$$

$=-i\pi^2\int_0^\infty \frac{k\,dk}{k+m^2-i\varepsilon}$ and therefore making the right cutoff $\|k\|_4<\Lambda$ we obtain

$I(m)=-i\pi^2(\Lambda^2-m^2\log\frac{\Lambda^2+m^2}{m^2})$. Taking $(m_\nu,c_\nu)_{\nu=\overline{1,3}}$, $m_\nu\gg m$ with $\sum_\nu c_\nu=1$, $\sum_\nu c_\nu m_\nu^2=m^2$, $\sum_\nu c_\nu m_\nu^2\log m_\nu^2=m^2\log m^2$ so that c_ν remain bounded as $m_\nu\to\infty$ we have in the Paul-Villars regularization $I(m)\approx I(m)-\sum_\nu c_\nu I(m_\nu)=0$.

Hence with $m\to 0$ in the Paul-Villars regularization we can consider $\Pi^{\rho\sigma}_{GF}(q)=0$. Further , after some calculus we obtain

$$i\Pi^{\rho\sigma}_{GT}(q)=-\frac{1}{2(2\pi)^4}g^2f^{abc}f^{abc}\int\frac{d^4k}{k^2(q+k)^2}\big(-10k^\rho k^\sigma+2q^\rho q^\sigma+7q^\rho k^\sigma+7q^\sigma k^\rho-$$
$$-\eta^{\rho\sigma}(5q^2+2k^2+2kq)\big)d^4k=\frac{g^2f^{abc}f^{abc}}{2(2\pi)^4}\int_0^1 d\alpha\int\frac{d^4k}{(k^2+\alpha(1-\alpha)q^2+i\varepsilon)^2}\big(10k^\rho k^\sigma+$$
$$+\eta^{\rho\sigma}((5-2\alpha(1-\alpha))q^2+2k^2)+\text{ '}q^\sigma q^\rho\text{ term'}\big)= \qquad (9)$$
$$=\frac{-ig^2f^{abc}f^{abc}}{2(2\pi)^2}\int_0^1 d\alpha\int\frac{d^4_Ek}{(k^2-\alpha(1-\alpha)q^2)^2}\Big(\eta^{\rho\sigma}\Big(\frac{9}{2}k^2-(5-2\alpha(1-\alpha))q^2\Big)+$$
$$+\text{ '}q^\sigma q^\rho\text{ term'}\Big)\quad\text{(with summation over } b,c \text{ indices)}$$

Since $q_\mu\bar u(s)\gamma^\mu u(s+q)=\bar u(s)(\not s+\not q)u(s+q)-\bar u(s)\not s u(s+q)=(m-m)\bar u(s)u(s+q)=0$ and similar $q_\lambda\bar u(s')\gamma^\lambda u(s'-q)=0$ in the (8) expression of the amplitude, we can drop any $q^\rho q^\sigma$ term from the $\Pi^{\rho\sigma}_{GF}(q)$ expression in (9)

Taking $I(q,m)=\int\frac{d^4_Ek}{(k^2-\alpha(1-\alpha)q^2+m^2)^2}\Big(\frac{9}{2}k^2-(5-2\alpha(1-\alpha))q^2\Big)$

for a cutoff $\|k\|_4<\Lambda$ we have for large Λ

$$I(q,m)\approx\pi^2\int_0^1 d\alpha\Big(\frac{9}{2}\Lambda^2-(9m^2+(5-11\alpha(1-\alpha))q^2)\log\frac{\Lambda^2}{m^2-\alpha(1-\alpha)q^2}+$$
$$+\frac{9}{2}m^2+(5-\frac{13}{2}\alpha(1-\alpha))q^2\Big)$$

In the same way as above we can take a Paul-Villars regularization with $(m_\nu,c_\nu)_{\nu=\overline{1,3}}$, $m_\nu^2\gg\mu^2=-q^2$, $m_\nu\gg m$, $m\to 0$, $\sum_\nu c_\nu=1$, $\sum_\nu c_\nu m_\nu^2=m^2$, $\sum_\nu c_\nu m_\nu^2\log m_\nu^2=m^2\log m^2$, c_ν remaining bounded while $m_\nu\to\infty$ so that

$$i\Pi^{\rho\sigma}_{GF}(q)=\frac{-g^2f^{abc}f^{abc}}{2(2\pi)^4}i\eta^{\rho\sigma}(I(q,m)-\sum_\nu c_\nu I(q,m_\nu))=$$
$$=\frac{19}{96\pi^2}ig^2\eta^{\rho\sigma}f^{abc}f^{abc}q^2\log\frac{M^2}{\mu^2} \qquad (10)$$

Where $M > 0$ is a parameter satisfying

$$\log M^2=\sum_\nu c_\nu \log m_\nu^2-\int_0^1 \frac{6}{19}\left(9\alpha(1-\alpha)+(11\alpha(1-\alpha)-5)\log(\alpha(1-\alpha))\right)d\alpha\ .$$

Also we have $i\Pi_{GG}^{\rho\sigma}(q)=\frac{-g^2 f^{abc}f^{abc}}{(2\pi)^4}\int \frac{k^\sigma(k-q)^\rho}{k^2(k-q)^2}d^4k=$

$$=\frac{ig^2 f^{abc}f^{abc}}{(2\pi)^4}\int_0^1 d\alpha\int \frac{d_E^4 k}{(k^2-\alpha(1-\alpha)q^2)^2}\left(\eta^{\rho\sigma}\frac{k^2}{4}+\text{'}q^\rho q^\sigma\text{ term'}\right)\ .$$

In the same way as above we know that we can drop any $q^\rho q^\sigma$ term and that we can take the Paul-Villars regularization with $(m_\nu,c_\nu)_{\nu=\overline{1,3}}$, $m_\nu^2\gg\mu^2=-q^2$, $m_\nu\gg m$, $m\to 0$, $\sum_\nu c_\nu=1$, $\sum_\nu c_\nu m_\nu^2=m^2$, $\sum_\nu c_\nu m_\nu^2\log m_\nu^2=m^2\log m^2$, c_ν remaining bounde while $m_\nu\to\infty$ (11) ,

$$i\Pi_{GG}^{\rho\sigma}(q)=\frac{i}{(2\pi)^4}f^{abc}f^{abc}\eta^{\rho\sigma}(I(q,m)-\sum_\nu c_\nu I(q,m_\nu))$$

where $I(q,m)=\int_0^1\int \frac{d_E^4 k}{(k^2-\alpha(1-\alpha)q^2+m^2)^2}\frac{k^2}{4}\approx$

$$\approx\frac{\pi^2}{4}\int_0^1 d\alpha\left(\Lambda^2-2(m^2-\alpha(1-\alpha)q^2)\log\frac{\Lambda^2}{m^2-\alpha(1-\alpha)q^2}+m^2-\alpha(1-\alpha)q^2\right)$$

and so $i\Pi_{GG}^{\rho\sigma}=\frac{1}{192\pi^2}ig^2\eta^{\rho\sigma}f^{abc}f^{abc}\log\frac{M^2}{\mu^2}$ with $M>0$ a parameter satisfying

$$\log M^2=\sum_\nu c_\nu\log m_\nu^2-3\int_0^1 2\alpha(1-\alpha)(\log(\alpha(1-\alpha))-1)d\alpha\ .$$

We can slghtly continuously variate $(m_\nu,c_\nu)_{\nu=\overline{1,3}}$ (for m_ν sufficienly large) in each case of Π_F , Π_{GT} , Π_{GG} calculation such that the (11) relations remain valid for all F,GT,GG situations and also the parameter M becomes the same for all F,GT,GG cases.

Thus we have a parameter $M>0$, $M^2\gg\mu^2=-q^2$ such that for any momentum transfer squared $\mu^2=-q^2$ we have

$\Pi^{\rho\sigma}(q)=-\eta^{\rho\sigma}q^2 g_j^2\Pi(q^2)$ with

$$\Pi(q^2)=\frac{1}{64\pi^2}\left(\frac{16}{3}\widetilde{T}_R^a F-13C_G^a\right)\log\frac{M^2}{\mu^2}\ ,\quad \widetilde{T}_R^a=\text{tr}(T^aT^a)+T_R^a\ ,$$

$C_G^a=f^{abc}f^{abc}$ (with summation over b,c) $C_G^a=2$ if $j=2$, $C_G^a=3$ if $j=3$, $C_G^a=0$ if $j=1$.

From (8) follows now

$\boldsymbol{M}=ig^2\bar{u}(s)\gamma^\mu u(s+q)\bar{u}(s')\gamma_\mu u(s'-q)\frac{1}{1+g^2\Pi(q^2)}\frac{1}{q^2}\text{tr}(T^aT^a)$ and hence the effective couplings at momentum transfer $\mu^2=-q^2$ are $g_j(\mu)$, $j=1,2,3$ with

$$g_{2,3}^2(\mu)=\frac{g_{2,3}^2}{1+g_{2,3}^2\Pi_{2,3}(\mu)}\ ,\ \frac{5}{3}g_1^2(\mu)=\frac{\frac{5}{3}g_1^2}{1+\frac{5}{3}g_1^2\Pi_1(\mu)}\quad \text{where}$$

$$\Pi_j(\mu)=\frac{1}{32\pi^2}\left(\frac{16}{3}\widetilde{T}_R^a F-13C_G^a\right)\log\frac{M}{\mu}\ .$$

Taking the maximum value for $\widetilde{T}_R^a$, since $\mathrm{tr}(T^aT^a)=\frac{1}{2}$ for any a we can write

$$\frac{3}{5}\frac{1}{g_1^2(\mu)}=\frac{3}{5}\frac{1}{g_1^2}+\frac{1}{32\pi^2}8F\log\frac{M}{\mu}\qquad (12)$$

$$\frac{1}{g_2^2(\mu)}=\frac{1}{g_2^2}+\frac{1}{32\pi^2}(8F-26)\log\frac{M}{\mu}\qquad (13)$$

$$\frac{1}{g_3^2(\mu)}=\frac{1}{g_3^2}+\frac{1}{32\pi^2}(8F-39)\log\frac{M}{\mu}\qquad (14)$$

With $t=\log\mu$ the renormalization group flow equations are $\frac{dg_j}{dt}=a_j g_j^3(t)$ with

$a_1=\frac{5}{3}\frac{1}{8\pi^2}F$, $a_2=\frac{4F-13}{32\pi^2}$, $a_3=\frac{8F-39}{64\pi^2}$ and since $F\le 3$ we have $a_1>0$, $a_{2,3}<0$ so as we announced , for the g_2,g_3 couplings we have asymptotic freedom behaviour at high momentum transfer (the couplings decrease to the attractive fix point zero as the energy increases).

The two asymptotically free couplings $g_3(\mu)$, $g_2(\mu)$ decrease while $\sqrt{\frac{5}{3}}g_1$ increases as we move up in the energy scale μ . At some mass scale M_{GUT} they will meet and that is where $SU(3)$x$SU(2)$x$U(1)$ is unified into $SU(5)$.

(we have a normalization factor of $\sqrt{\frac{5}{3}}$ since for $\sqrt{\frac{5}{3}}T_{(1)}=\frac{Y}{2}$ we will have $\mathrm{tr}(T_{(1)}T_{(1)})=\frac{1}{2}$)

At the unification mas scale we have $\sqrt{\frac{5}{3}}g_1(M_{GUT})=g_2(M_{GUT})=g_3(M_{GUT})=g_{GUT}$.

The strong coupling analog of the fine structure constant is $\alpha_S(\mu)=\frac{g_3^2(\mu)}{4\pi}$.

The weak coupling analog of the fine structure constant is $\alpha_W(\mu)=\frac{g_2^2(\mu)}{4\pi}$.

The fine structure constant is $\alpha(\mu)=\frac{e^2(\mu)}{4\pi}=\frac{g_2^2(\mu)\sin^2\theta(\mu)}{4\pi}$ with $\tan\theta(\mu)=\frac{g_1(\mu)}{g_2(\mu)}$.

Taking $\alpha_{GUT}=\frac{g_{GUT}^2}{4\pi}$ from (12) , (13) , (14) we obtain:

$$\frac{1}{\alpha_S(\mu)}=\frac{1}{\alpha_{GUT}}+\frac{1}{8\pi}(8F-39)\log\frac{M_{GUT}}{\mu} \qquad (15)$$

$$\frac{1}{\alpha_W(\mu)}=\frac{\sin^2\theta(\mu)}{\alpha(\mu)}=\frac{1}{\alpha_{GUT}}+\frac{1}{8\pi}(8F-26)\log\frac{M_{GUT}}{\mu} \qquad (16)$$

$$\frac{3}{5}\frac{\cos^2\theta(\mu)}{\alpha(\mu)}=\frac{1}{\alpha_{GUT}}+\frac{1}{8\pi}8F\log\frac{M_{GUT}}{\mu} \qquad (17)$$

The number of fermion families F contributes equally to (15) , (16) , (17) . This is as it should be since the fermions are effectively massless for the purpose of this calculation and do not 'know' that the unifying group has been broken into $SU(3)xSU(2)xU(1)$. These equations are derived assuming that all fermion masses are small compared to μ , plugging in measured values of α_S and α . With three equations we are able to determine the unification mass scale M_{GUT} and coupling α_{GUT} and we can predict θ . In other words, unless the ratio g_1 to g_2 is precisely right, the three lines of $g_2=g_2(\mu)$, $g_3=g_3(\mu)$, $\sqrt{\frac{5}{3}}g_1=\sqrt{\frac{5}{3}}g_1(\mu)$ graphics will not meet at one point.

Let $\frac{1}{\alpha_{GUT}}=X$, $\log\frac{M_{GUT}}{\mu}=Y$, $\frac{1}{8\pi}(8F-39)=A$, $\frac{1}{8\pi}(8F-26)=B$, $\frac{8F}{8\pi}=C$

and we have $\frac{1}{\alpha_S}=X+AY$, $\frac{\sin^2\theta}{\alpha}=X+BY$, $\frac{3}{5}\frac{\cos^2\theta}{\alpha}=X+CY$

$$\frac{\frac{1}{\alpha_S}-\frac{\sin^2\theta}{\alpha}}{A-B}=\frac{\frac{\sin^2\theta}{\alpha}-\frac{3}{5}\frac{\cos^2\theta}{\alpha}}{B-C} \quad ,$$

$$\sin^2\theta(\mu)=\frac{1}{6}+\frac{5}{9}\frac{\alpha(\mu)}{\alpha_S(\mu)} \qquad (18)$$

$$\frac{\sin^2\theta(\mu)}{\alpha(\mu)}=\frac{1}{\alpha_S(\mu)}+\frac{1}{8\pi}\log\frac{M_{GUT}}{\mu} \qquad (19)$$

$$\frac{1}{\alpha(\mu)}=\frac{8}{3}\frac{1}{\alpha_{GUT}}+\frac{1}{8\pi}\left(\frac{64}{3}F-26\right)\log\frac{M_{GUT}}{\mu} \qquad (20)$$

From (19) we obtain $\frac{1}{\alpha(\mu)}\geq\frac{1}{8\pi}13\log\frac{M_{GUT}}{\mu}$.

Therefore a lower bound on the proton life time (and hence on M_{GUT}) translates into an upper bound on the fine structure constant: The stability of the world implies the weakness of electromagnetism.

In a grand unified theory , A_μ couples to a generator of the grand unifying gauge group and we know that the generators of any group such as $SU(N)$ (that is not given by the direct product of U (1) with other groups) are forced by the non-trivial

commutation relations $[T^b,T^c]=if^{abc}T^a$ to assume quantized eigenvalues. For example the eigenvalues of T^3 in $SU(2)$ which depend on the representation of course, must be multiples of $1/2$. Within $SU(3)\times SU(2)\times U(1)$ we cannot understand charge quantization since the generator of $U(1)$ is not quantized. But upon grand unification into $SU(5)$ (or more generally any group without $U(1)$ factors) electric charge is quantized.

Considering the $SU(3)\times SU(2)\times U(1)$ theory with the couplings g_1,g_2,g_3 as the $5^*\oplus 10\oplus 1$ gauge group representation with (1) Lagrangian density theory as presented above we computed the (8) amplitude expression to derive renormalization formulas, taking the Feynman diagram according to fig.5 where the fluctuation of the scattering intermediating *q* four-momentum boson occurs as a succesion of fermion loops *F* , three gluon interaction loops *GT* , four gluon interaction loops *GF* and gluon-ghost interaction loops *GG* . We must show that this renormalization removes all possible divergences that may occur by boson fluctuations and so the theory is in fact renormalizable. To do this we write an effective Lagrangian density which includes ghost fields in the form
$\mathscr{L}=\mathscr{L}_0+\sum_k \mathscr{L}_k$ where $\mathscr{L}_0$ is the quadratic part and $\mathscr{L}_k$ are interaction terms and we normalize the ghost fields so that no coupling constants appear in the $\mathscr{L}_0$ expression (considering $\sqrt{g}\,c_a$ instead of the ghost field c_a-see Chap. Non-abelian gauge theory). The interaction terms involve a coupling constant c_k , fermion fields ψ , boson (gluon) fields φ , ghost fields κ and one degree differential operators ∂ : $\mathscr{L}_k=c_k(\partial)^{\delta k}(\varphi)^{bk}(\psi)^{fk}(\kappa)^{hk}$.

Counting inverse mass dimensions we have $0=4+\dim[c_k]-\delta_k-b_k-\frac{3}{2}f_k-h_k$ and from the (1) Lagrangian density we have $\dim[c_k]=0$. The gluon fields are all bosons and the quarks and leptons are all fermions.

For a Feynman diagram *G* we define :

n_k -the number of vertices corresponding to $\mathscr{L}_k$

N_B -the number of boson external lines

N_F -the number of fermion external lines

N_G -the number of ghost external lines

l -the number of loops (number of independent integrals in the amplitude computation for *G*)

n_B -the number of boson internal lines

n_F -the number of fermion internal lines

n_G -the number of ghost internal lines

The superficial degree of divergence for the corresponding to *G* Feynman integral is $d_G=4l-2n_B-n_F-2n_G+\sum_k n_k\delta_k$.

We have:

$2n_B+N_B=\sum_k n_k b_k$; $2n_F+N_F=\sum_k n_k f_k$; $2n_G+N_G=\sum_k n_k h_k$;

$l=n_B+n_F+n_G-\sum_k n_k+1$ and so

$$d_G=4+2(n_B+n_G)+3n_F+\sum_k n_k(\delta_k-4)=4+(\sum_k n_k f_k-N_F)+\sum_k n_k(b_k+f_k+h_k)-$$

$$-N_B-N_F-N_G-\sum_k n_k(b_k+\frac{3}{2}f_k+h_k)=4-N_B-N_G-\frac{3}{2}N_F$$

$$d_G=4-N_B-N_G-\frac{3}{2}N_F \ .$$

Considering the nature of interaction terms in the efective Lagrangian density we have that if $N_F\neq 0$ then $N_F\geq 2$ and if $N_F=0$ then $N_B+N_G\geq 2$.

Thus $d_G\leq 2$ and the number of external lines for Feynman amplitudes with overall divergences is bounded from above . Hence there is a posibility that the divergences may be removed by a finite number of renormalization constants and interaction parameters, the theory being renormalizable. For renormalization of the coupling constants we have to consider only Feynman diagrams with $N_B = 2$ and $d_G = 2$ that is precisely a succesion of fermion loops *F* , three gluon interaction loops *GT* , four gluon interaction loops *GF* and ghost-gluon interaction loops *GG* as we exposed in fig.5 , fig .6 , fig. 7 (a) , (b) , (c) .

47. Electron-positron anihilation

Electron-positron anihilation

An electron and a positron can meet and anihilate each other giving rise to two photons: $e^-(p_1)+e^+(p_2)\rightarrow \gamma(\varepsilon_1,k_1)+\gamma(\varepsilon_2,k_2)$,

p_1, p_2 -electron and respective positron four-momenta;

$\varepsilon_1, \varepsilon_2$ -polarization versors of the two outgoing photons;

k_1, k_2 -four momenta of the two outgoing photons.

(Anihilating into one photon that is physical and on mass shell is kinematically impossible)

The process is described to order $O(e^2)$ by Feynman diagrams fig.1 and fig.2

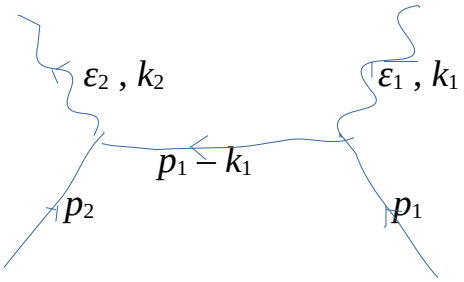

fig.1

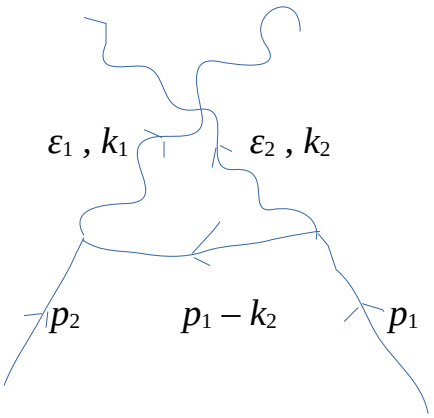

fig.2

The amplitude is (Bose statistics for the two photons):

$$A=A(k_1,\varepsilon_1,k_2,\varepsilon_2)+A(k_2,\varepsilon_2,k_1,\varepsilon_1) \quad \text{with}$$

$$A(k_1,\varepsilon_1,k_2,\varepsilon_2)=(2\pi)^4(ie)(ie)\bar{v}(p_2)\not{\varepsilon}_2\frac{i}{\not{p}_1-\not{k}_1-m}\not{\varepsilon}_1 u(p_1)\,\delta^4(p_1+p_2-k_1-k_2)$$

$$A=(2\pi)^4\boldsymbol{M}\,\delta^4(p_1+p_2-k_1-k_2)\ .$$

Averaging over initial spin polarizations through a similar calculus as in Chap. Scattering in Quantum electrodynamics . Electron-photon scattering , choosing the transverse gauge in the rest frame of the electron and so having

$$\varepsilon_1 p_1=\varepsilon_2 p_1=\varepsilon_1 k_1=\varepsilon_2 k_2=0\ ,\ \varepsilon_1^2=\varepsilon_2^2=-1 \text{ we derive}$$

$$|\boldsymbol{M}|^2=\frac{e^4}{8m^2}\left(\frac{p_1k_2}{p_1k_1}+\frac{p_1k_1}{p_1k_2}-4(\varepsilon_1\varepsilon_2)^2+2\right)=\frac{e^4}{8m^2}\left(\frac{\omega_1}{\omega_2}+\frac{\omega_2}{\omega_1}-4(\varepsilon_1\varepsilon_2)^2+2\right)$$

where $\omega_{1,2}$ are the pulsations of the photons in the electron rest frame and m is the mass of the electron and positron.

and we will have a differential cross section describing the distribution of the outgoing photons momenta in the electron rest frame (see Chap. Feynman amplitudes and lattice gauge theory) given by

$d\sigma=\frac{1}{(2\pi)^2}\frac{m}{\|\vec{p}_2\|}\frac{d^3\vec{k}_1}{2\omega_1}\frac{d^3\vec{k}_2}{2\omega_2}|\boldsymbol{M}|^2\delta^4(p_2+p_1-k_2-k_1)$.

We can take independent polarization directions $\varepsilon_1^1=\varepsilon_2^1=(0,\mathrm{vers}(\vec{k}_1\times\vec{k}_2))$, $\varepsilon_1^2=(0,\mathrm{vers}(\vec{k}_1\times\vec{\varepsilon}_1^1))$, $\varepsilon_2^2=(0,\mathrm{vers}(\vec{k}_2\times\vec{\varepsilon}_2^1))$ and with φ being the angle between $\vec{p}_2$ and $\vec{k}_1$ summing over final polarizations of the photons in the electron rest rest frame , we have $|\boldsymbol{M}|^2=\frac{e^4}{2m^2}\left(\frac{\omega_1}{\omega_2}+\frac{\omega_2}{\omega_1}+\sin^2\varphi\right)$

If in the electron rest frame we have $p_1+p_2=k_1+k_2$ and θ is the angle between $\vec{k}_1$ and $\vec{p}_2$ then $\sin\varphi=\|\vec{p}_2\|\frac{\sin\theta}{\omega_2}$, $\omega_2=E-\omega_1$ with $E=m+p_2^0$

$k_2^2=2mE-2\omega_1(E-\|\vec{p}_2\cos\theta\|)$

Also (see Chap. Canonical quantization of a scalar field) we have

$f(\omega_2)\frac{d^3\vec{k}_2}{2\omega_2}=\theta(k_2^0)\delta(k_2^2)d^4k_2$ (where θ is the Heaviside function and $\omega_2=\|\vec{k}_2\|$)

Thus with $d\Omega$ the infinitesimal solid angle of the outgoing k_1 photon directions with respect to incoming positron direction and

$p_2^0=\sqrt{\vec{p}_2^2+m^2}$, $\omega_2=E-\omega_1$, $E=m+p_2^0$, $\omega_1=\frac{mE}{E-\|\vec{p}_2\|\cos\theta}$ we obtain

$d\sigma=\frac{\alpha^2}{2m}\frac{\omega_1}{E-\|\vec{p}_2\|\cos\theta}\left(\frac{\omega_1}{\omega_2}+\frac{\omega_2}{\omega_1}+\frac{\vec{p}_2^2}{\omega_2^2}\sin^2\theta\right)d\Omega$

with $\alpha=\frac{e^2}{4\pi}$ the fine structure constant.

For the further considerations we can verify that for $\theta = \theta(t)$ the Heaviside function

$\theta(t)=\begin{cases}1 & \text{for } t>0\\ 0 & \text{for } t<0\end{cases}$ we have

$\theta(t)=-i\int\frac{d\omega}{2\pi}\frac{\exp(i\omega t)}{\omega-i\varepsilon}$, $\theta(-t)=i\int\frac{d\omega}{2\pi}\frac{\exp(i\omega t)}{\omega+i\varepsilon}$,

$\Im\left(\frac{1}{p^0-q^0-i\varepsilon}\right)=\pi\delta(p^0-q^0)$ where $\varepsilon>0$, $\varepsilon\to 0$.

Let $O=O(x)$, $x=(t,\vec{x})\in\mathbb{R}^4$ some field operator function acting on states of a quantum field theory with an unique vacuum state $|0\rangle$ and the unitary representation of the inhomogeneous Lorentz group $U=U(a,\Lambda)$ such that for any field operator function we have $O(\Lambda x+a)=U(a,\Lambda)O(x)U^+(a,\Lambda)$ where $x\to\Lambda x+a$ is a Poincare transformation , $a\in\mathbb{R}^4$, $\Lambda\in SO^+(3,1)$ is a restricted Lorentz transformation. We have $U(a,\boldsymbol{I})=\exp(i\hat{p}a)$, $U|0\rangle=|0\rangle$ with $\hat{p}$ -the four momentum operator acting on states .

(see Chap. Spin statistics theorem)

Consider the two point amplitude

$$iD(x-y)=\langle 0|T(O(x)O(y))|0\rangle=$$
$$=\theta(x^0-y^0)\langle 0|O(x)O(y)|0\rangle+\theta(y^0-x^0)\langle 0|O(y)O(x)|0\rangle \ .$$

We have $\langle 0|O(x)O(y)|0\rangle=$

$$=\sum_{\psi}\langle 0|\exp(i\hat{p}\,x)O(0)\exp(-i\hat{p}\,x)|\,\psi\rangle\langle\,\psi|\exp(i\hat{p}\,y)O(y)\exp(-i\hat{p}\,y)|0\rangle$$

where $(|\psi\rangle)_{\psi}$ is a complete orthonormal set of four-momentum eigenstates

$\hat{p}|\,\psi\rangle=p_{\psi}|\,\psi\rangle$, $p_{\psi}^0\geq 0$, $p_{\psi}^2\geq 0$.

Therefore $\langle 0|O(x)O(y)|0\rangle=\sum_{\psi}\exp(i\,p_{\psi}(y-x))|O_{0\,\psi}|^2$ where $O_{0\,\psi}=\langle 0|O(0)|\,\psi\rangle$.

Thus

$$iD(x-y)=\sum_{\psi}(\theta(x^0-y^0)\exp(i\,p_{\psi}(y-x))+\theta(y^0-x^0)\exp(i\,p_{\psi}(x-y)))\ ,$$

$$iD(q)=\int d^4x\exp(iqx)iD(x)=-i(2\pi)^3\sum_{\psi}|O_{0\,\psi}|^2\left(\frac{\delta^3(\vec{q}-\vec{p}_{\psi})}{p_{\psi}^0-q^0-i\,\varepsilon}+\frac{\delta^3(\vec{q}+\vec{p}_{\psi})}{p_{\psi}^0+q^0-i\,\varepsilon}\right)\ ,$$

$$\Im(2i\int d^4x\exp(iqx)\langle 0|T(O(x)O(y))|0\rangle)=$$
$$=(2\pi)^4\sum_{\psi}|O_{0\,\psi}|^2(\delta^4(q-p_{\psi})+\delta^4(q+p_{\psi}))\ .$$

For the anticommutator $\{O(x),O(y)\}=O(x)O(y)+O(y)O(x)$ we will have

$\int d^4x\exp(iqx)\langle 0|\{O(x),O(y)\}|0\rangle=(2\pi)^4\sum_{\psi}|O_{0\,\psi}|^2(\delta^4(q-p_{\psi})+\delta^4(q+p_{\psi}))$ and so

$$\int d^4x\exp(iqx)\langle 0|\{O(x),O(y)\}|0\rangle=\Im(2i\int d^4x\exp(iqx)\langle 0|T(O(x)O(y))|0\rangle).$$

Experimentally we can measure the cross section $\sigma(e^+e^-\rightarrow$ hadrons $)$ of positron-electron anihilation into hadrons (hadrons are made of confined quarks and antiquarks) in the mass center frame of the incoming particles according to fig.3 diagram as a function of the total mass center frame energy E .

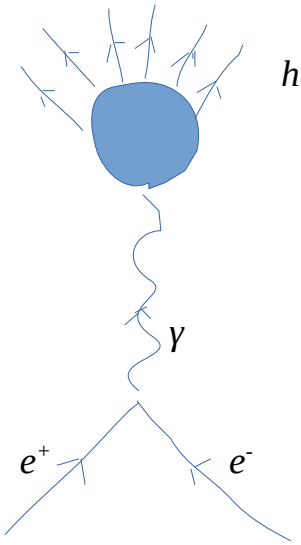

fig.3

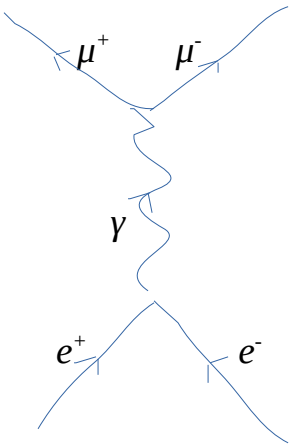

fig.4

The half of the diagram, involving the electron and positron lines and the photon propagator appears also in the Feynman diagram fig.4 of positron-electron anihilation in a muon-antimuon pair $e^+e^-\to\mu^+\mu^-$ and so we can determine experimentally the ratio $R(E)=\frac{\sigma(e^+e^-\to \text{hadrons})}{\sigma(e^+e^-\to\mu^+\mu^-)}$.

We perform the experiment at high energies E in a way that a beam of positrons of momentum $\vec{k}$ meets at the interaction point a similar beam of electrons of momentum $-\vec{k}$ and thus for each singular electron positron interaction the virtual photon (not on mass shell) has four-momentum $q=(E,0,0,0)$ giving a photon propagator $-\frac{\eta_{\mu\nu}}{E^2}$ and according to Feynman rules the amplitude of the process in which the virtual photon decays into a muon-antimuon pair or a quark-antiquark pair is defined by

$$A=(2\pi)^4\boldsymbol{M}\,\delta^4(q-p_1-p_2)\ ,\ \boldsymbol{M}=ie^2Q\bar{u}(p_1)\gamma^\mu v(p_2)\overline{v_e}(k_2)\gamma_\mu u_e(k_1)\frac{1}{E^2}$$

where Q is the muon that is -1 respective the quark charge factor , $k_1=(E/2,-\vec{k})$, $k_2=(E/2,\vec{k})$ and u,v are from the muon/quark Dirac spinor quantization and u_e,v_e are from the electron Dirac spinor quantization (see Chap.Quantization of a Dirac field , Chap. Electroweak unification and Chap. Feynman amplitudes and lattice ...)

We notice that the energy being high we have asymptotic freedom of Quantum chromodynamics and Electroweak theory and the resulting quarks can be considered free and on mass shell.

Since the energy E is high , that is quark and muon masses are negligible compared to the total energy E, these masses can be all considered equal to a value m which is taken zero in the limit, the u and v functions can be considered to be the same for all sorts of fermions that appear and also the muon and quark propagators will be the same. Thus we have a, generical for all lepton sorts, field operator function

$$\hat{\psi}=\hat{\psi}(x)=\int\frac{d^3\vec{p}}{(2\pi)^{3/2}(E_p/m)^{1/2}}(b(p)u(p)\exp(-ipx)+d^+(p)v(p)\exp(ipx))$$

where we suppressed spin index and b,d respective b^+,d^+ are anihilation and creation operators for a particle respective antiparticle , $E_p=\sqrt{\vec{p}^2+m^2}$, so that for $J^\mu(x)=\hat{\bar{\psi}}(x)\gamma^\mu\hat{\psi}(x)$, $|h\rangle=b^+(p_1)d^+(p_2)|0\rangle$ we have $[\hat{p}_\mu,\hat{\psi}(x)]=-i\partial_\mu\hat{\psi}(x)$ (see Chap. Symmetry breaking) and so $[\hat{p},b^+(k)]=kb^+(k)$, $[\hat{p},d^+(k)]=kd^+(k)$, $\hat{p}|h\rangle=(p_1+p_2)|h\rangle=p_h|h\rangle$

$$\bar{u}(p_1)\gamma^\mu v(p_2)=(2\pi)^3(E_{p1}/m)^{1/2}(E_{p2}/m)^{1/2}\langle h|J^\mu(0)|0\rangle,$$

$$|\boldsymbol{M}|^2=(2\pi)^6\frac{(E_{p1}E_{p2})^{1/2}}{16m^3E^4}e^4Q^2\,\mathrm{tr}((\not{k}_2-m)\gamma_\nu(\not{k}_1+m)\gamma_\mu)\langle 0|J^\mu(0)|h\rangle\langle h|J^\nu(0)|0\rangle\ .$$

Therefore we it will be real kinetical factors $K_{\mu\nu}$ such that

$$\sigma(e^+e^-\rightarrow \text{hadrons})=\left(3\sum_a Q_a^2\right)K_{\mu\nu}\sum_h (2\pi)^4\delta^4(q-p_h)\langle 0|J^\mu(0)|h\rangle\langle h|J^\nu(0)|0\rangle \ . \ (1)$$

where the sum over *a* index counts the squares of charges of the various quarks that contribute to the outcoming hadrons energy *E* with a factor of 3 accounting for color. The sum over *h* index considers the complete orthonormal system of $\frac{(2\pi)^3}{V}b^+(p_1)d^+(p_2)|0\rangle$ quark-antiquark pairs four-momentum eigenstates as normalized $|h\rangle$ states that can appear out of the electron-positron anihilation process.

Similar, with the same kinetical factors $K_{\mu\nu}$ we derive

$$\sigma(e^+e^-\rightarrow\mu^+\mu^-)=K_{\mu\nu}\sum_h (2\pi)^4\delta^4(q-p_h)\langle 0|J^\mu(0)|h\rangle\langle h|J^\nu(0)|0\rangle \ (2)$$

where in this case the $|h\rangle$ states are now muon-antimuon pairs four-momentum eigenstates.

We have $R^{\mu\nu}=\sum_h (2\pi)^4\delta^4(q-p_h)\langle 0|J^\mu(0)|h\rangle\langle h|J^\nu(0)|0\rangle=$

$=\sum_h\int d^4x\exp(iqx)\langle 0|\exp(i\hat{p}x)J^\mu(0)\exp(-i\hat{p}x)|h\rangle\langle h|J^\nu(0)|0\rangle=$

$=\int d^4x\exp(iqx)\langle 0|J^\mu(x)J^\nu(0)|0\rangle$, because the $(|h\rangle)_h$ being orthononormal and complete it follows $\sum_h |h\rangle\langle h|=\boldsymbol{I}$.

Also we have $\int d^4x\exp(iqx)\langle 0|J^\nu(0)J^\mu(x)|0\rangle=$

$=\sum_h\int d^4x\exp(iqx)\langle 0|J^\nu(0)|h\rangle\langle h|\exp(i\hat{p}x)J^\mu(0)\exp(-i\hat{p}x)|0\rangle=$

$=\sum_h (2\pi)^4\delta^4(q+p_h)\langle 0|J^\nu(0)|h\rangle\langle h|J^\mu(0)|0\rangle=0$, because $p_h^0=p_1^0+p_2^0>0$ and $q=(E,\vec{0})$ with $E>0$ and so $\delta^4(q+p_h)=0$.

Therefore from what we derived above we obtain

$R^{\mu\nu}=\int d^4x\exp(iqx)\langle 0|\{J^\mu(x)J^\nu(0)\}|0\rangle=$

$=\Im(2i\int d^4x\exp(iqx)\langle 0|T(J^\mu(x)J^\nu(0))|0\rangle)$

As we know from Chap. Feynman amplitudes and lattice gauge theory we have

$\langle 0|T(J^\mu(x)J^\nu(0))|0\rangle=\int DAD\overline{\psi}D\psi\exp(i\int \mathscr{L}(\psi,\partial\psi,A,\partial A)d^4w)J^\mu(x)J^\nu(0)$

where $\mathscr{L}$ is the $SU(3)\times SU(2)\times U(1)$ theory Lagrangian density .

(see Chap. Electroweak unification… Georgi-Glashow model)

To determine $R^{\mu\nu}$ for the purpose of (1) calculation we would have to calculate an infinite number of Feynman diagrams involving quarks and gluons like in fig.5 . Because the electroweak coupling constants are small compared to the strong coupling constant *g*(*E*) and the strong coupling constant gets smaller and smaller as *E* increases we will consider only the zero order diagram fig,6 (a) with no internal gluon lines and the second order in *g*(*E*) diagrams fig.6 (b) , (c) , (d) with only one strong interaction gluon internal line.

The diagram in fig.6 (a) is the same one that we must only consider to determine $R^{\mu\nu}$ for the purpose of (2) calculation since muons do not participate in strong interactions (we merely replace the quark propagator with the muon propagator which as we noticed can be considered the same) . At high energy E , we can neglect $(g(E))^2$ and so the leading term in $R(E)$ is $3\sum_a Q_a^2$ that is $\lim_{E\to\infty} R(E)=3\sum_a Q_a^2$.

The fact that the factor 3 comes out by experiment leads to the conclusion that we must have the quarks appearing in three colors.

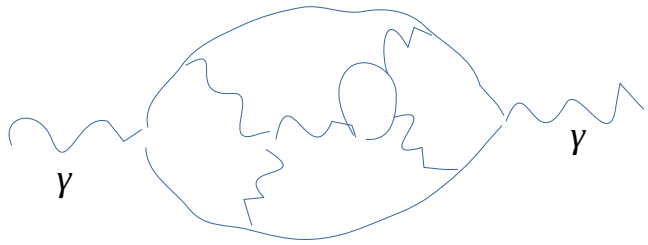

fig.5

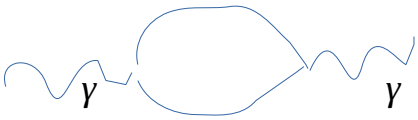

fig.6 (a)

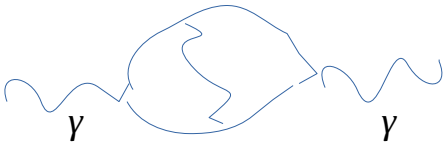

fig.6 (b)

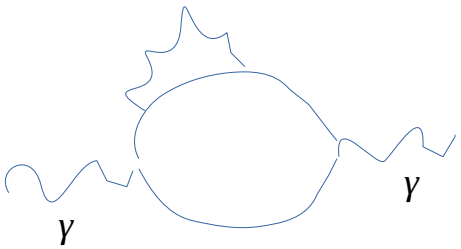

fig.6 (c)

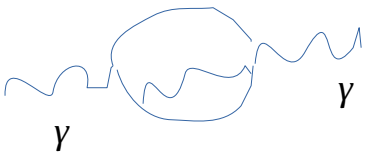

fig.6 (d)

We can add to the Lagrangian density an arbitrary constant and the physics not changes.

Hence we can consider that the vacuum energy is zero and therefore we have that the fig.6 (a) diagram contribution to $\int d^4x \exp(iqx)\langle 0|T(J^\mu(x)J^\nu(0))|0\rangle$ is

$I^{\mu\nu}(q)=$

$=\int d^4x \exp(iqx)\int DA\,D\overline{\psi}D\psi \exp\left(i\int \mathscr{L}_0 d^4w\right)\overline{\psi}(x)\gamma^\mu\psi(x)\overline{\psi}(0)\gamma^\nu\psi(0)$

where $\mathscr{L}_0$ is the Lagrangian density $\mathscr{L}$ without any interaction term and so

$I^{\mu\nu}(q)=Z_0\int d^4x \exp(iqx)(-1)\,\mathrm{tr}\left(iD^{fer}(-x)\gamma^\mu iD^{fer}(x)\gamma^\nu\right)=$

$$=Z_0\int\frac{d^4p}{(2\pi)^4}\left(\frac{1}{\not p-m+i\varepsilon}\gamma^\mu\frac{1}{\not p+\not q-m+i\varepsilon}\gamma^\nu\right)$$

With the assumption that *m* is negligible compared to *E* we have already computed $I^{\mu\nu}(q)$ in Chap. Electroweak unification ... and (considering that $\varepsilon > 0$) it turns out to be $I^{\mu\nu}(q)=(-q^\mu q^\nu+\eta^{\mu\nu}q^2)\frac{i}{12\pi^2}(i\pi+\log\frac{M^2}{q^2})$ with M an energy scale parameter. (where $Z_0=\int DA\,D\overline{\psi}D\psi\exp(i\int\mathscr{L}_0 d^4w)=1$ since we have considered the vacuum energy equal to zero)

The second order in $g(E)$ term of $\int d^4x\exp(iqx)\langle 0|T(J^\mu(x)J^\nu(0))|0\rangle$, given by the contribution of fig.6 (b) , (c) , (d) diagrams is

$G^{\mu\nu}(q)=$

$=(ig(E))^2\int d^4x\,d^4y\,d^4z\exp(iqx)\int DA\,D\overline{\psi}D\psi\exp(i\int\mathscr{L}_0 d^4w)\overline{\psi}(x)\gamma^\mu\psi(x)$

$\overline{\psi}(y)\gamma^\rho T^c\psi(y)\overline{\psi}(0)\gamma^\nu\psi(0)\overline{\psi}(z)\gamma^\sigma T^c\psi(z)A^c_\rho(y)A^c_\sigma(z)=$

$=-(g(E))^2\int d^4x\,d^4y\,d^4z\exp(iqx)(-1)\mathrm{tr}(iD^{fer}(-x)\gamma^\mu iD^{fer}(x)\gamma^\nu)$

$(-1)\mathrm{tr}(iD^{fer}(z-y)\gamma^\rho iD^{fer}(y-z)\gamma^\sigma)\mathrm{tr}(T^cT^c)iD^{bos}_{\rho\sigma}(y-z)$

where T^c are the $SU(3)$ generators with corresponding strong interaction gluon fields $(A^c_\lambda)_\lambda$.

After some calculus we obtain :

$G^{\mu\nu}(q)=i(g(E))^2I^{\mu\nu}(q)S\,\mathrm{tr}(T^cT^c)$

where $S=\int\frac{d^4r\,d^4s}{(2\pi)^4}\frac{1}{s^2+i\varepsilon}\mathrm{tr}\left(\frac{1}{\not r-m+i\varepsilon}\gamma^\rho\frac{1}{\not r+\not s-m+i\varepsilon}\gamma_\rho\right)\delta^4(0)$.

Let $I(q)=\frac{i}{12\pi^2}(i\pi+\log\frac{M^2}{q^2})$ and we have

$$R(E)=3\sum_a Q_a^2\left(1-4\frac{(g(E))^2}{\pi}\Im((\pi-i\log\frac{M^2}{q^2})S)\right)$$

At first approximation we can write

$$S=\int\frac{d^4s}{(2\pi^4)}\int d^4y\,d^4z(-1)\mathrm{tr}(iD^{fer}(y-z)\gamma^\rho iD^{fer}(z-y)\gamma_\rho)\frac{\exp(is(y-z))}{s^2+i\varepsilon}=$$

$$\approx\int\frac{d^4s}{(2\pi)^4}\frac{1}{s^2+i\varepsilon}\int d^4y\,d^4z\exp(is(y-z))\langle 0|T(J^\rho(y)J_\rho(z))|0\rangle=$$

$$=\int\frac{d^4s}{(2\pi)^4}\frac{1}{s^2+i\varepsilon}\int d^4y\,d^4z$$

$$\sum_h\exp(is(y-z))(\theta(y-z)\exp(ip_h(z-y))+\theta(z-y)\exp(ip_h(y-z)))O_{0h}O^*_{0h}=$$

$$=-2i(2\pi)^3\delta^4(0)\int\frac{d^4s}{s^2+i\varepsilon}\sum_h\frac{\delta^3(\vec{s}-\vec{p}_h)}{p_h^0-s^0-i\varepsilon}O_{0h}O_{0h}^*$$

where $O_{0h}O_{0h}^*=\langle 0|J^\rho(0)|h\rangle\langle h|J_\rho(0)|0\rangle$

$$S=-2i(2\pi)^3\delta^4(0)\sum_h\int\frac{ds_0}{(s_0^2-\vec{p}_h^2+i\varepsilon)(p_h^0-s_0-i\varepsilon)}O_{0h}O_{0h}^*=$$

$$=-(2\pi)^4\delta^4(0)\sum_h\frac{O_{0h}O_{0h}^*}{(\|\vec{p}_h\|-i\varepsilon)(p_h^0+\|\vec{p}_h\|-i\varepsilon)}$$

(we used residues theorem for integration over s_0)

We notice that since $p_h=p_1+p_2$ with p_1, p_2 on mass shell we have $p_h^0>0$, $p_h^2=p_h^{02}-\|\vec{p}_h\|^2\geq 0$ and we have also from relations we derived above

$$\delta^4(0)\sum_{h,\,p_h=p}O_{0h}O_{0h}^*=\int\frac{d^4x}{(2\pi)^4}\exp(ipx)\langle 0|J^\rho(x)J_\rho(0)|0\rangle=$$

$$=\int\frac{d^4x}{(2\pi)^4}2\Im(i\exp(ipx)\langle 0|T(J^\rho(x)J_\rho(0))|0\rangle)=\frac{1}{(2\pi)^4}\eta_{\mu\nu}2\Im(iI^{\mu\nu}(p))=$$

$$=-\frac{1}{(2\pi)^4}\frac{1}{4\pi}p^2$$. Considering that the 4 -volume element in momentum space is $\frac{1}{\delta^4(0)}=\frac{(2\pi)^4}{VT}$ we can turn the sum over h into an integral over p having

$$S=\frac{\delta^4(0)}{4\pi}\int_D\frac{d^4p}{\|\vec{p}\|}(p_0+\|\vec{p}\|)(p_0^2-\|\vec{p}\|)=\delta^4(0)\int_0^M\int_0^r p(r-p)\,dp\,dr=\delta^4(0)\frac{M^4}{24}$$

Where we naturally limited the possible p_h values to $D=\{p\in\mathbb{R}^4|0<p_0<M,\|\vec{p}\|<p_0\}$ since M is the leading energy scale parameter.

Therefore $R(E)=3\sum_a Q_a^2\left(1+\frac{1}{6}(g(E))^2\delta^4(0)M^4\log\frac{M^2}{E^2}\right)$. (*)

As we derived in Chap. Electroweak unification … Georgi-Glashow model we have :

$$(g(E))^2=\frac{g^2(\mu)}{1+\frac{g^2(\mu)}{32\pi^2}(8F-39)\log\frac{\mu}{E}}$$ and as E increases, the energy scale parameter M used to estimate the cuttoff integrals in the renormalization will be taken sufficiently large to allow $M\gg E$, but constant and we can see from (*) how fast Quantum Chromodynamics is turning off at high energies.

(μ is a finite energy range at which we have determined the strong coupling constant $g=g(\mu)$.

48. *SO*(10) unification

$SO(10)$ unification

For any $n\in\mathbb{N}^*$ we can find $2n$ $2^n\times 2^n$ matrices γ_j , $j=\overline{1,2n}$ tat satisfy the Clifford algebra relations $\{\gamma_i,\gamma_j\}=\gamma_i\gamma_j+\gamma_j\gamma_i=2\delta_{ij}$:

For $n=1$ we take $\gamma_1=\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\gamma_2=\tau_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $\tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$;

Given the $2n$ γ matrices $\left(\gamma_j^{(n)}\right)_{j=\overline{1,2n}}$ we construct the $2n+2$ γ matrices $\left(\gamma_j^{(n+1)}\right)_{j=\overline{1,2n+2}}$ as follows:

$\gamma_j^{(n+1)}=\gamma_j^{(n)}\otimes\tau_3=\begin{pmatrix}\gamma_j^{(n)}&0\\0&-\gamma_j^{(n)}\end{pmatrix}$ for $j=\overline{1,2n}$

$\gamma_{2n+1}^{(n+1)}=\boldsymbol{I}_{2^n}\otimes\tau_1=\begin{pmatrix}0&\boldsymbol{I}_{2^n}\\\boldsymbol{I}_{2^n}&0\end{pmatrix}$, $\gamma_{2n+2}^{(n+1)}=\boldsymbol{I}_{2^n}\otimes\tau_2=\begin{pmatrix}0&-i\boldsymbol{I}_{2^n}\\i\boldsymbol{I}_{2^n}&0\end{pmatrix}$.

This iterative construction yields for $SO(2n)$ the gamma matrices :

$\gamma_{2k-1}=\boldsymbol{I}\otimes\boldsymbol{I}\otimes\ldots\otimes\boldsymbol{I}\otimes\tau_1\otimes\tau_3\otimes\ldots\otimes\tau_3$,

$\gamma_{2k}=\boldsymbol{I}\otimes\boldsymbol{I}\otimes\ldots\otimes\boldsymbol{I}\otimes\tau_2\otimes\tau_3\otimes\ldots\otimes\tau_3$, $k=\overline{1,n}$

with $\boldsymbol{I}$ the 2×2 identity matrix appearing $k-1$ times

and τ_3 appearing $n-k$ times.

In analogy with the Lorentz group we define the $n(2n-1)$ independent hermitean matrices $\sigma_{ij}=\frac{i}{2}[\gamma_i,\gamma_j]=\begin{cases}i\gamma_i\gamma_j & \text{for } i\neq j\\ 0 & \text{for } i=j\end{cases}$

For $Q\in SO(2n)$ we have (see Chap. On the rotations group ...)

$Q=\exp(i\theta_{ij}J^{ij})$ with $\theta_{ij}=-\theta_{ji}\in\mathbb{R}$, $J^{ij}=-J^{ji}\in M_{2n\times 2n}(\mathbb{C})$ so that for $q<j$:

$J^{ij}_{kl}=i(\delta_{qk}\delta_{jl}-\delta_{ql}\delta_{jk})$, $q,j=\overline{1,2n}$ and it follows $[J^{qj},J^{jk}]=iJ^{qk}$ for $q<j<k$, (with no summation over j index)

$[\sigma_{qj},\sigma_{jk}]=2i\sigma_{qk}$. Hence the $\frac{1}{2}\sigma_{ij}$ represent the J^{ij} -s .

Consider now the unitary representation $U=U(Q)$, for $Q\in SO(2n)$ defined by

$U=\exp(\frac{1}{2}i\omega_{qj}\sigma_{qj})$ for $Q=\exp(i\omega_{qj}J^{qj})$, $\omega_{qj}=-\omega_{jq}\in\mathbb{R}$.

For ψ cosidered as a complex 2^n -dimensional column vector, under $\psi\to U\psi$ we have $\psi^+\gamma_k\psi\to\psi^+\exp(-\frac{1}{2}i\omega_{qj}\sigma_{qj})\gamma_k\exp(\frac{1}{2}i\omega_{qj}\sigma_{qj})=\psi^+\gamma_k\psi+$

$+\omega_{qj}\psi^+(\delta_{kj}\gamma_q-\delta_{kq}\gamma_j)\psi+O(\omega^2)$ and thus with $v_k=\psi^+\gamma_k\psi$ we have

$v_k\to v_k-\omega_{kj}v_j+\omega_{qk}v_q+O(\omega^2)=Q_{kl}v_l+O(\omega^2)$.

In complete analogy to $\overline{\psi}\gamma^\mu\psi$ transforming as a Lorentz vector under ψ transforming as Dirac spinor, v_k transforms as a vector under under $SO(2n)$ if ψ

transforms under the representation $U = U(Q)$ of $SO(2n)$.

We define $\gamma^{FIVE}=(-i)^n \gamma_1 \gamma_2 ... \gamma_{2n}$ and we have $\gamma^{FIVE}= \tau_3 \otimes \tau_3 \otimes ... \otimes \tau_3$ with τ_3 appearing n times and by analogy with the Lorentz group we define the left handed spinors $\psi_L=\frac{1}{2}(\boldsymbol{I}-\gamma^{FIVE})\,\psi$ and the right handed spinors $\psi_R=\frac{1}{2}(\boldsymbol{I}+\gamma^{FIVE})\,\psi$ having $\gamma^{FIVE}\,\psi_L=-\psi_L$, $\gamma^{FIVE}\,\psi_R=\psi_R$.

Since γ^{FIVE} commutes with σ_{qj} under $\psi \to U\,\psi$ we have $\psi_L \to U\,\psi_L$, $\psi_R \to U\,\psi_R$. The projection into left and right handed spinors cut the number of components into halves and we have in conclusion two irreducible representations of $SO(2n)$ with dimension 2^{n-1}: S^+-right handed spinors and S^--left handed spinors.

Consider the $2n$-dimensional real vectors $x=(x_1,...,x_n,y_1,...,y_n)$, $x'=(x_1',...,x_n',y_1',...,y_n')$. By definition $SO(2n)$ consists of linear transformations that leave $\sum_{j=1}^{n} x_j' x_j + y_j' y_j$ invariant. $U(n)$ acting on $z=(x_1+i\,y_1,...,x_n+i\,y_n)$ consists of the subset of linear transformations that leave invariant $\sum_{j=1}^{n} x_j' x_j + y_j' y_j$ and also $\sum_{j=1}^{n} x_j' y_j - y_j' x_j$.

So we have a natural embedding of $SU(n)$ in $SO(2n)$ and since $(x_1, \ldots, x_n, y_1, \ldots, y_n)$ can be rewritten as $(x_1+i\,y_1,...,x_n+i\,y_n,x_1-i\,y_1,...,x_n-i\,y_n)$ we have $2n=n\oplus n^*$ where $2n$ is the $2n$-dimensional real vector representation of $SO(2n)$ defined as $v_k \to Q_{kj} v_j$ for $Q=(Q_{kj})_{k,j=\overline{1,2n}} \in SO(2n)$ and n denotes the n-dimensional representation of $SU(n)$ defined as $w^k \to U^k_j w^j$ for $U=(U^k_j)_{k,j=\overline{1,n}} \in SU(n)$ and n^* is the n-dimensional representation of $SU(n)$ defined as $w_k \to U^{+j}_k w_j$ for $U=(U^k_j)_{k,j=\overline{1,n}} \in SU(n)$.

For $\otimes_A$ the antisymmetric tensorial product we consider the $2n \otimes_A 2n$ the antisymmetric real tensor representation of $SO(2n)$ denoted $n(2n-1)$ defined as $\psi^{ij} \to Q_{ik} Q_{jl} \psi^{kl}$ for $Q=(Q_{ij})_{i,j=\overline{1,2n}} \in SO(2n)$, $\psi=(\psi^{ij})_{i,j=\overline{1,2n}} \in M_{2n\times 2n}(\mathbb{R})$, $\psi^{ij}=-\psi^{ji}$ and we can verify

$2n \otimes_A 2n \to (n\oplus n^*)\otimes_A(n\oplus n^*)=(n^*\otimes_A n)\oplus(n\otimes_A n^*)\oplus(n\otimes_A n)\oplus(n^*\otimes_A n^*)$

$(n\otimes_A n^*)\oplus(n^*\otimes_A n) \to 1\oplus(n^2-1)$,

$n\otimes_A n \to n(n-1)/2$, $n^*\otimes_A n^* \to (n(n-1)/2)^*$

where 1 denotes the singlet representation of $SU(n)$:

$$v \to v \text{ for } U \in SU(n) .$$

n^2-1 denotes the adjoint representation of $SU(n)$:

$$\Phi \to U \Phi U^+ \text{ for } \Phi=(\Phi^i_j)_{i,j} \in M_{n\times n}(\mathbb{C}) , \operatorname{tr}\Phi=0 , U \in SU(n) . \qquad (1)$$

$n(n-1)/2$ denotes the antisymmetric tensor representation of $SU(n)$:

$$\psi \to U\,\psi U^T \text{ for } \psi=(\psi^{ij})_{i,j}\in M_{n\times n}(\mathbb{C})\ ,\ \psi=-\psi^T\ ,\ U\in SU(n). \qquad (2)$$

$(n(n-1)/2)^*$ denotes the antisymmetric covariant tensor representation of $SU(n)$:

$$\psi \to U^*\,\psi U^+ \text{ for } \psi=(\psi_{ij})_{i,j}\in M_{n\times n}(\mathbb{C})\ ,\ \psi=-\psi^T\ ,\ U\in SU(n). \qquad (3)$$

Hence $n(2n-1)=1\oplus(n^2-1)\oplus(n(n-1)/2)\oplus(n(n-1)/2)^*$

Any basis of $2n\otimes_A 2n$ is a generator system for the canonical $SO(10)$ ($n=5$) representation and so we have generators $1,(\Phi_i^j)_{i,j=\overline{1,5}}$, $(\psi^{ji})_{i,j=\overline{1,5}}$, $(\psi_{ji})_{i,j=\overline{1,5}}$ satisfying (1) , (2) , (3) as 5×5 matrices defining respective the $1,24,10,10^*$ invariant subspaces of the $45=2n\otimes_A 2n$ representation of $SO(10)$:

$45=1\oplus 24\oplus 10\oplus 10^*$.

Suppose the $S^+=16^+$ (for $n=5$) breaks into a bunch of representations of $SU(5)$.

Let $\hat{1},\hat{\Phi}_i^j$, $\hat{\psi}^{ji}$, $\hat{\psi}_{ji}$ representing the corresponding generators of $SO(10)$ in the 16^+ representation of $SO(10)$. Suppose the bunch of representations that S^+ breaks up into contains the singlet 1 of $SU(5)$. Then $(\hat{\psi}^{ji})_{i,j}$ acting on 1 gives the 10 representation of $SU(5)$ (an antisymmetric tensor of two indices with a tensor with no indices is an antisymmetric tensor with two indices).

$(\hat{\psi}^{ji})_{i,j}$ acting on 10 is a tensor with four upper indices which certainly contains the $[4]$ representation of $SU(5)$ given by $\psi^{ijkl}\to U^i_m U^j_p U^k_q U^l_r\,\psi^{mpqr}$ with ψ^{ijkl} antisymmetric in all indices , which is equivalent to $\epsilon_{wijkl}\,\psi^{ijkl}=U^{+s}_w\,\epsilon_{smpqr}\,\psi^{mpqr}$ so that we have $[4]=[1]^*\to 5^*$.

Thus to be an invariant subspace 16^+ must contain $1,10$ and 5^* but $1+10+5$ already add up to 16 and we conclude $16^+=1\oplus 10\oplus 5^*$ (4) :

The 10 and 5^* of $SU(5)$ fit inside the 16^+ of $SO(10)$.

The two spinor representations S^+ and S^- are conjugated each to other.

For C defined as $C^{(1)}=\tau_2$, $C^{(n+1)}=\begin{cases} C^{(n)}\otimes\tau_1 & \text{for } n\equiv 1 \pmod 2 \\ C^{(n)}\otimes\tau_2 & \text{for } n\equiv 0 \pmod 2 \end{cases}$

we will have $C\,\sigma_{ij}C^{-1}=-\sigma_{ij}^*$, $C\,\gamma_j C^{-1}=(-1)^n\gamma_j^*$, $C\,S^+\,C^{-1}=S^-$, $C^2=\boldsymbol{I}$.

The conjugate spinor S^- breaks into $16^-=1\oplus 10^*\oplus 5$ (5) .

If we introduce one more field transforming as 1 under *SU*(5) , that is a singlet under *SU*(5) and so under *SU*(3)x*SU*(2)x*U*(1) , this field describes a lepton with no electric charge and is not involved in the known weak interaction and can be identified as the antineutrino field ν_R^c which is equivalent by conjugation to the right handed neutrino field ν_R .

For $n=2$ we have the $(\sigma_{qj})_{q,j=\overline{1,4}}$, $\sigma_{qj}=i\,\gamma_q\gamma_j$ matrices and we define

$$\sigma_1=-\frac{1}{2}(\sigma_{12}-\sigma_{34})\ ,\ \sigma_2=-\frac{1}{2}(\sigma_{31}-\sigma_{24})\ ,\ \sigma_3=-\frac{1}{2}(\sigma_{23}-\sigma_{14})$$

having $\sigma_q\sigma_j=i\,\epsilon_{qjk}\sigma_k$, $\gamma^{FIVE}=-\gamma_1\gamma_2\gamma_3\gamma_4$, $\sigma_1^2=\sigma_2^2=\sigma_3^2=\frac{1}{2}(\boldsymbol{I}-\gamma^{FIVE})$,

$\sigma_q \frac{1}{2}(\boldsymbol{I}+\gamma^{FIVE})=0$ and for $\theta\in\mathbb{R}$, $\boldsymbol{n}=(n_i)_{i=\overline{1,3}}$, $\boldsymbol{n}^2=1$ we have

$\exp(\frac{1}{2} i\theta n_j \sigma_j)\frac{1}{2}(\boldsymbol{I}-\gamma^{FIVE})\psi = \frac{1}{2}(\boldsymbol{I}-\gamma^{FIVE})(\cos\frac{\theta}{2}+in_j\sigma_j\sin\frac{\theta}{2})\psi$ and so

$\exp(\frac{1}{2}\theta n_j\sigma_j)$ leaves invariant $S^-=2^-$ which has complex dimension 2 .

Therefore $(\sigma_j)_j$ represent the Pauli matrices of $SU(2)$ representation.

Given the product form of the gamma matrices γ_j and hence of σ_{ij} for $n\in\mathbb{N}^*$, we can write the states of the spinor epresentations as $|\varepsilon_1,\varepsilon_2,...,\varepsilon_n\rangle$ with $\varepsilon_i\in\{\pm 1\}$, $|+\ \rangle=\begin{pmatrix}1\\0\end{pmatrix}$, $|-\ \rangle=\begin{pmatrix}0\\1\end{pmatrix}$ and we will have

$$S^+=\mathrm{Sp}\{|\varepsilon_1,...,\varepsilon_n\rangle | \prod_{i=1}^n \varepsilon_i=1\} \quad , \quad S^-=\mathrm{Sp}\{|\varepsilon_1,...,\varepsilon_n\rangle | \prod_{i=1}^n \varepsilon_i=-1\}$$

For $n=2$ we have $\sigma_{12}=i(\tau_1\otimes\tau_3)(\tau_2\otimes\tau_3)=-\tau_3\otimes\boldsymbol{I}$, $\sigma_{34}=-\boldsymbol{I}\otimes\tau_3$,

$\sigma_3=\frac{1}{2}(\tau_3\otimes\boldsymbol{I}-\boldsymbol{I}\otimes\tau_3)$, $\sigma_3|+\ +\rangle=\sigma_3|-\ -\rangle=0$ and thus under $SU(2)$ the $|+\ +\rangle$ and the $|-\ -\rangle$ make two singlets and in a similar way, identifying $\sigma_i\to\tau_i$, $|+\ -\rangle\to\begin{pmatrix}1\\0\end{pmatrix}$, $|-\ +\rangle\to\begin{pmatrix}0\\1\end{pmatrix}$ we have that $|+\ -\rangle$ and $|-\ +\rangle$ make up a $SU(2)$ doublet.

Since $\prod_{i=1}^5 \varepsilon_i=1$ implies $\varepsilon_1\varepsilon_2=\varepsilon_3\varepsilon_4\varepsilon_5$ we have $16^+\to(2^+,4^+)\oplus(2^-,4^-)$.

In the same way as we derived $(4),(5)$ we obtain

$4^+\to 1\oplus 3^*$, $4^-\to 1\oplus 3$, $2^+\to 1\oplus 1$, $2^-\to 2$.

We identify the natural *SU*(2) subgroup of *SO*(4) as the *SU*(2) of the electroweak interaction and the natural *SU*(3) subgroup of *SO*(6) as the color *SU*(3) of the strong interaction. Thus (2^+, 4^+) are the *SU*(2) singlets while (2^-, 4^-) are the *SU*(2) doublets of the standard *SU*(3)x*SU*(2)x*U*(1) model.

Since $4^-=3\oplus 1$ upon restriction to color, u_L and d_L must fit in the 3 and so of the four states $|-\ -\ -\rangle$, $|+\ +\ -\rangle$, $|+\ -\ +\rangle$, $|-\ +\ +\rangle$ we take the $SU(2)$ doublets

$|u_L^\alpha\rangle=|-\ +\ +\ +\ -\rangle=|3\rangle$, $|-\ +\ +\ -\ +\rangle=|4\rangle$, $|-\ +\ -\ +\ +\rangle=|5\rangle$

$|d_L^\alpha\rangle=|+\ -\ +\ +\ -\rangle=|6\rangle$, $|+\ -\ +\ -\ +\rangle=|7\rangle$, $|+\ -\ -\ +\ +\rangle=|8\rangle$

$|\nu_L\ \rangle=|-\ +\ -\ -\ -\rangle=|1\rangle$, $|e_L\ \rangle=|+\ -\ -\ -\ -\rangle=|2\rangle$

By the same heuristic argument we take the *SU*(2) singlets

$\left|\nu_R^c\right\rangle=\left|+\,+\,+\,+\,+\right\rangle=\left|9\right\rangle$, $\left|e_R^c\right\rangle=\left|-\,-\,+\,+\,+\right\rangle=\left|10\right\rangle$

$\left|u_R^{\alpha c}\right\rangle=\left|+\,+\,-\,-\,+\right\rangle=\left|11\right\rangle$, $\left|+\,+\,-\,+\,-\right\rangle=\left|12\right\rangle$, $\left|+\,+\,+\,-\,-\right\rangle=\left|13\right\rangle$

$\left|d_R^{\alpha c}\right\rangle=\left|-\,-\,-\,-\,+\right\rangle=\left|14\right\rangle$, $\left|-\,-\,-\,+\,-\right\rangle=\left|15\right\rangle$, $\left|-\,-\,+\,-\,-\right\rangle=\left|16\right\rangle$.

The *SO*(10) unified Lagrangian density (see Chap. Non-abelian gauge theory) is

$$\mathscr{L}=\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}+\overline{\Phi}(i\gamma^\mu\partial_\mu-m_\Phi)\Phi+\frac{1}{2}(\mu^2)_{ab}A^{a\mu}A^a_\mu+g\,\overline{\psi}\gamma^\mu A^a_\mu T^a\psi \quad \text{where}$$

$\Phi=(\nu,e,(u^\alpha)_\alpha,(d^\alpha)_\alpha)$, $\psi=\sum_{j=1}^{16}\psi^j\left|j\right\rangle$, $(a)_a=(i\,j)_{i,j=\overline{1\,10},\,j>i}$

m_Φ is a quark and lepton mass diagonal matrix $m_\Phi=\mathrm{diag}(m_\nu,m_e,(m_u)_\alpha,(m_d)_\alpha)$

$((\mu^2)_{ab})_{a,b}$ is the boson squared mass matrix.

Under $Q\in SO(10)$, $Q=\exp(i\,\omega_{ij}J^{ij})$ we have the $S^+=16^+$ representation of $SO(10)$ such that $U=U(Q)=\exp(\frac{1}{2}i\,\omega_{ij}\sigma_{ij})\in SU(32)$,

$U\left|i\right\rangle=U_i^j\left|j\right\rangle$, $(\psi^j)_j=(\nu_L,e_L,(u_L^\alpha)_\alpha,(d_L^\alpha)_\alpha,\nu_R^c,e_R^c,(u_R^{\alpha c})_\alpha,(d_R^{\alpha c})_\alpha)$

ψ^j are left handed Dirac spinor fields transforming as $\psi^j\to U_i^j\psi^i$,

$T^a=\frac{1}{8}\sigma_{ij}$ such that $\mathrm{tr}(T^aT^a)=\frac{1}{2}$.

The electric charge operator $\hat{Q}$,when acting on a state $\left|\varepsilon_1,...,\varepsilon_5\right\rangle$ transforms as a singlet under $SU(3)$ so must have the value $Q=a\,\varepsilon_1+b\,\varepsilon_2+c(\varepsilon_3+\varepsilon_4+\varepsilon_5)$.

We must have $Q(\nu_L)=Q(\nu_R^c)=0$, $Q(e_L)=-1$ and so

$\hat{Q}\left|\varepsilon_1,...,\varepsilon_5\right\rangle=(-\frac{1}{2}\varepsilon_1+\frac{1}{6}(\varepsilon_3+\varepsilon_4+\varepsilon_5))\left|\varepsilon_1,...,\varepsilon_5\right\rangle$

We can verify $Q(u_L)=\frac{2}{3}$, $Q(d_L)=-\frac{1}{3}$, $Q(u_R^c)=-\frac{2}{3}$, $Q(d_R^c)=\frac{1}{3}$)

$\hat{Q}=\frac{1}{2}\sigma_{12}-\frac{1}{6}(\sigma_{56}+\sigma_{78}+\sigma_{910})$

The *SU*(3)x*SU*(2)x*U*(1) theory Lagrangian density correspondent in a *SO*(10) with the *SO*(6)x*SO*(4) subgroup is therefore

$$\mathscr{L}=\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}+\overline{\Phi}(i\gamma^\mu\partial_\mu-m_\Phi)\Phi+g_1\frac{1}{2}\sum_{i,j\le4}\overline{\psi}\gamma^\mu A^{ij}_\mu T^{ij}\psi+g_2\frac{1}{2}\sum_{i,j>4}\overline{\psi}\gamma^\mu A^{ij}T^{ij}\psi+$$

$$+\frac{1}{2}(\mu^2)_{ab}A^a_\mu A^{b\mu} \quad \text{where } A^{ij}=-A^{ji} \ , \ T^{ij}=-T^{ji}=\frac{1}{8}\sigma_{ij}$$

for $i\,j=a$, $i<j$, $i,j\le4$ or $i,j>4$.

The required mass term is

$$(\overline{\Phi}_L m_\Phi\Phi_R+\overline{\Phi}_R m_\Phi\Phi_L)=\Re\sum_{i=1}^{8}m_i(\psi^{i+8T}\gamma^0\gamma^2\psi^i-\psi^{iT}\gamma^0\gamma^2\psi^{i+8})$$

which can be generate by a Higgs field $H=(H_{ij})_{i,j=\overline{1,16}}$, $H_{ij}=-H_{ji}$ transforming as the 128^* of $SU(16)$:

Under $U=(U^i_j)_{i,j=\overline{1,16}}\in SU(16)$ we have $H_{ij}\to U^{+k}_i U^{+l}_j H_{kl}$, $H\to U^* H U^+$.
We allow to H having a vacuum expectation value
$\langle H_{ij}\rangle=v_i\delta_{ji+8}$ for $i<j$, $v_i\in\mathbb{R}$ for $i=\overline{1,8}$, $v_i=v$ for $i=\overline{1,2}$, $v_i=w$ for $i=\overline{3,8}$.
Then following Chap. Anderson Higgs mechanism we have
$(\mu^2)_{ab}=(T^a[\langle H\rangle])_{ij}(T^b[\langle H\rangle])^*_{ij}$ where $T^a[\langle H\rangle]=-T^{a*}\langle H\rangle-\langle H\rangle T^a$
The symmetry is spontaneosly broken to $SO(6)$x$SO(4)$.
It follows that the A^a boson remains massless if for $\frac{1}{8}\sigma=T^a$ we have
$\langle i|\sigma^*\langle H\rangle\sigma|j\rangle=-\langle H_{ij}\rangle$ for any $i,j=\overline{1,16}$
Considering the $SO(6)\times SO(4)$ theory we will have the cases
a) $\sigma=i\gamma_k\gamma_l$ with $k\neq l$, $k,l\in\{1,2,3,4\}$
b) $\sigma=i\gamma_k\gamma_l$ with $k\neq l$, $k,l\in\{5,6,7,8,9,10\}$
Then exists $\varepsilon\in\{\pm1,\pm i\}$ such that if $k\in\{1,2\}\cup\{9,10\}=A$ we have
$\varepsilon\sigma|k\rangle=|l\rangle$, $\varepsilon^*\sigma^*|k\rangle=|l\rangle$ with $l\in A$
and exists $\varepsilon\in\{\pm1,\pm i\}$ such that if $k\in\{3,4,5,6,7,8\}\cup(\{3,4,5,6,7,8\}+8)=B$
we have $\varepsilon\sigma|k\rangle=|l\rangle$, $\varepsilon^*\sigma^*|k\rangle=|l\rangle$ with $l\in B$.
We have $|i\pm8\rangle=K|i\rangle$ where $K=\tau_1\otimes\boldsymbol{I}\otimes\tau_1\otimes\tau_1\otimes\tau_1$.
If $|i\rangle\neq\alpha K|j\rangle$ for any $\alpha\in\mathbb{C}$ we have $\langle H_{ij}\rangle=0$, $\sigma^*|i\rangle\neq\sigma^*\alpha K|j\rangle$ for any $\alpha\in\mathbb{C}$.
Since $\sigma^*K=\pm K\sigma$ it follows $\sigma^*|i\rangle\neq\alpha K\sigma|j\rangle$ for any $\alpha\in\mathbb{C}$, we derive
$\langle i|\sigma^*\langle H\rangle\sigma|j\rangle=0=-\langle H\rangle$
We have $\sigma^*=\sigma^T$ since $\sigma=\sigma^+$.
Let m be the number of occurences of τ_2 in the tensorial product that defines σ .
Then $\sigma^T=(-1)^m\sigma$. Also we have $K\sigma=\kappa\sigma K$ with $\kappa\in\{\pm1\}$.
If $|j\rangle=K|i\rangle$ we obtain $\langle i|\sigma^*\langle H\rangle\sigma|j\rangle=\kappa(-1)^m\langle i|\sigma\langle H\rangle K\sigma|i\rangle=$
$=\kappa(-1)^{m+\rho}\langle i|\langle H\rangle|j\rangle=\kappa(-1)^{m+\rho}H_{ij}$
where $\rho=\begin{cases}1 & \text{if } \sigma=\chi\tau_q\otimes a\otimes b\otimes b\otimes d\ ,\ q\in\{1,2\}\ ,\ \chi\in\mathbb{C}\\ 0 & \text{else}\end{cases}$.
Therefore the generator $\frac{1}{8}\sigma$ boson will be massless if $\kappa(-1)^{m+\rho}=-1$.
We have $\rho=0$ in the b) case, $\rho=0$ for $\sigma\in\{\sigma_{12},\sigma_{34}\}$,
$\rho=1$ for $\sigma\in\{\sigma_{13},\sigma_{14},\sigma_{23},\sigma_{24}\}$
K commutes with γ_j for $j\in\{2,5,8\}=M$ and anticommutes with γ_j for $j\in N$,
$N=\{1,3,4,6,7,9,10\}$
$m\equiv1\pmod 2$ for $\sigma=\sigma_{ij}$, $ij\in\{24,13\}$ in the a) case
and $ij\in\{68,610,810,79,57,59\}$ in the b) case.
Hence massless bosons correspond to σ_{ij} with $ij\in\{12,24\}$ in the a) case and
$ij\in\{56,59,510,69,610,78,910\}$.
Considering the expression we derived for $\hat{Q}$ we can confirm that the photon is massless in the $SO(6)\times SO(4)$ theory.

As we mentioned before we introduced the $SU(5)$ singlet field $\nu_R^c = \gamma^2 \frac{1+\gamma^5}{2} \nu^*$ which is a left handed field and is assimilable by conjugation with the right handed neutrino while the left handed neutrino is a *SU*(2) doublet. Since the right handed neutrino is a *SU*(5) singlet we can give it a Majorana mass *M* (see Chap. Fermion charge… Majorana neutrino) without breaking *SU*(5). Hence we expect *M* to be larger than or of the same order of magnitude as the the mass scale $M_{GUT} \sim M_X$ at which *SU*(5) is broken to *SU*(3)x*SU*(2)x*U*(1) (or equivalently *SO*(10) is broken to *SO*(6)x*SO*(4)) which as we saw in Chap. … Georgi-Glashow model is of the same order as M_X -the mass of gluons that transform quarks in leptons and viceversa and much larger than the mass scales that we have been explored experimentally.

The Majorana mass term will be $M\Re(\nu_R^T \gamma^2 \gamma^0 \nu_R)$ with the specification that the Dirac spinor components $(\nu_{R\alpha})_{\alpha=\overline{0,3}}$ must be treated as anticommuting Grassmann variables.

With the presence of right handed and left handed neutrinos we can also have a Dirac mass term $m(\overline{\nu}_R \nu_L + \overline{\nu}_L \nu_R) = m\overline{\nu}\nu$. Since his term breaks $SU(2)\times U(1)$ just like the mass terms for quarks and leptons , we expect *m* to be of the same order of magnitude as the known quark and lepton masses and therefore $m << M$.

We have $-\overline{\nu}_R^c \nu^c = \overline{\nu}\nu_R = (\overline{\nu}_R \nu_L)^* = \overline{\nu}_L \nu_R$ and $-\overline{\nu}_R^c \nu_R = -\overline{\nu}_R^c \nu = \nu_R^T \gamma^2 \gamma^0 \nu_R$.

Thus the entire mass term can be written as

$$\Re(m(\overline{\nu}_R \nu_L + \overline{\nu}_L \nu_R) + M\ \nu_R^T \gamma^2 \gamma^0 \nu_R) = \Re((\overline{\nu}_R, -\overline{\nu}_R^c)\begin{pmatrix} 0 & m \\ m & M \end{pmatrix}\begin{pmatrix} \nu^c \\ \nu \end{pmatrix})$$

We can diagonalize the mass matrix $\overline{M} = \begin{pmatrix} 0 & m \\ m & M \end{pmatrix}$ having

$R(\theta)\overline{M}R^T(\theta) = \begin{pmatrix} \lambda_- & 0 \\ 0 & \lambda_+ \end{pmatrix}$ with $R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, $\tan\theta = -\frac{\lambda_-}{m}$, $\cot\theta = \frac{\lambda_+}{m}$,

$\lambda_- = \frac{M - \sqrt{M^2+4m^2}}{2} \approx -\frac{m^2}{M}$, $0 < -\lambda_- \ll m$, $\lambda_+ = \frac{M+\sqrt{M^2+4m^2}}{2} \approx M$,

$$\Re(m(\overline{\nu}_R \nu_L + \overline{\nu}_L \nu_R) + M\ \nu_R^T \gamma^2 \gamma^0 \nu_R) = \Re\left(\lambda_-(\overline{\nu}_R\cos\theta + \overline{\nu}_R^c \sin\theta)(\nu^c\cos\theta - \nu\sin\theta) + \right.$$
$$\left. + \lambda_+(\overline{\nu}_R\sin\theta - \overline{\nu}_R^c\cos\theta)(\nu^c\sin\theta + \nu\cos\theta)\right)$$

From the first term, corresponding to the small eigenvalue $\lambda_- \approx -\frac{m^2}{M}$ and the mass state $\nu^c\cos\theta - \nu\sin\theta$ we have $\Re(\lambda_- \overline{\nu}_R \nu^c)$ which is a (negative) Majorana mass term for the right handed neutrino and the remaining term is $\lambda_- \sin\theta\cos\theta(\overline{\nu}_L \nu_R + \overline{\nu}_R \nu_L)$ giving to the (observed) left handed neutrino a positive Dirac mass $m\sin^2\theta$.

Therefore a tiny Dirac mass is naturally generated for the observed neutrino , fact known as the seesaw mechanism in diagonalizing the (large Majorana mass) mass matrix to a very small eigenvalue and a large eigenvalue. The generated mass is suppressed relative to known quark and lepton masses *m* by a small factor of m/M .

We have in the *SU*(5) and *SO*(10) theories a Lagrangian density of the form
$\mathscr{L}=\mathscr{L}_0+g\,\overline{\psi}\gamma^{\mu}A^a_{\mu}T^a\psi$ with $\psi=(\psi_i)_i$, ψ_i -Dirac spinor fields ,
$T^a=(T^a_{ij})_{i,j}$ gauge group representation generator matrices,
$\mathscr{L}_0=\overline{\psi}(i\gamma^{\mu}\partial_{\mu}-m)\psi-\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}+\frac{1}{2}M_a^2A^a_{\mu}A^{a\mu}$.
By variation upon $\delta\overline{\psi}$ and $\delta\psi$ we obtain from the Lagrangian density the Euler-Lagrange motion equations for quarks and leptons:
$i\gamma^{\mu}\partial_{\mu}\psi_i+g\,\gamma^{\mu}A^a_{\mu}T^a_{ij}\psi_j=m_i\psi_i$ (6)
$i\partial_{\mu}\overline{\psi}_k\gamma^{\mu}-g\,\overline{\psi}_j\gamma^{\mu}A^a_{\mu}T^a_{jk}=-m_k\psi_k$ (7)
Multiplying (6) left with $\overline{\psi}_kT^b_{ki}$ and (7) right with $T^b_{ki}\psi_i$ if we set all quark and lepton masses equal to the same $m\to 0$ summing the multipied (6) and (7) we obtain $\partial_{\mu}(\overline{\psi}_i\gamma^{\mu}T^b_{ij}\psi_j)=0$ (8)
Consider the operator functions $\hat{J}^{a\mu}=\hat{\overline{\psi}}_i(x)\gamma^{\mu}T^a_{ij}\hat{\psi}_j(x)$, $x\in\mathbb{R}^4$.
From the path integration :
$F^{\mu\lambda\nu}(x,y,z)=\langle 0|T(\hat{J}^{a\mu}(x)\hat{J}^{b\lambda}(y)\hat{J}^{c\nu}(z)\hat{A}^a_{\mu}(x)\hat{A}^b_{\lambda}(y)\hat{A}^c_{\nu}(z))|0\rangle=$
$=\int D\overline{\psi}D\psi DA\exp(i\int\mathscr{L}d^4w)A^a_{\mu}(x)A^b_{\lambda}(y)A^c_{\nu}(z)J^{a\mu}(x)J^{b\lambda}(y)J^{c\nu}(z)$,
we expect $F^{\mu\lambda\nu}(x,y,z)$ to be gauge invariant since it is a coefficient in the expansion after g powers of $\int D\overline{\psi}D\psi DA\exp(i\mathscr{L}d^4w)$ which is gauge invariant.
Under a gauge transformation $U=\exp(i\theta^aT^a)$ we will have (see Chap. Non-abelian gauge theory) : $J^{a\mu}(x)A^a_{\mu}(x)\to J^{a\mu}(x)A^a_{\mu}(x)+i\,\overline{\psi}(x)[T^c,T^b]\gamma^{\mu}A^c_{\mu}(x)\theta^b(x)\psi(x)-$
$-\overline{\psi}(x)\gamma^{\mu}f^{abc}A^c_{\mu}(x)\theta^b(x)T^a\psi(x)+\frac{1}{g}\overline{\psi}\gamma^{\mu}T^a\psi(x)\partial_{\mu}\theta^a(x)+O(\|\theta\|^2+\|\partial\theta\|^2)=$
$=J^{a\mu}(x)A^a_{\mu}(x)+\frac{1}{g}\overline{\psi}(x)\gamma^{\mu}T^a\psi(x)\partial_{\mu}\theta^a(x)$ since $[T^c,T^b]=if^{ab}T^a$, $f^{acb}=-f^{abc}$.
Therefore gauge invariance leads to
$\int\langle 0|T(\hat{J}^{a\mu}(x)\partial_{\mu}\theta^a(x)\hat{J}^{b\lambda}(y)\hat{J}^{c\nu}(z)\hat{A}^b_{\lambda}(y)\hat{A}^c_{\nu}(z))|0\rangle d^4x=0$ (9) ,
$\theta=\theta(x)$ being an an arbitrary infinitesimal function.
Integratin in (9) by parts with θ arbitrary infinitesimal function it follows
$\langle 0|T(\partial_{\mu}\hat{J}^{a\mu}(x)\hat{J}^{b\lambda}(y)\hat{J}^{c\nu}(z)\hat{A}^b_{\lambda}(y)\hat{A}^c_{\nu}(z))|0\rangle=0$ (10)
This is consistent with the (8) relation and says that a current conservation law like (8) , if gauge invariance works, must hold even under quantum fluctuations as they are described for example, by the diagrams of a possible violating gauge invariance relation (11) anomaly below (see fig.) .

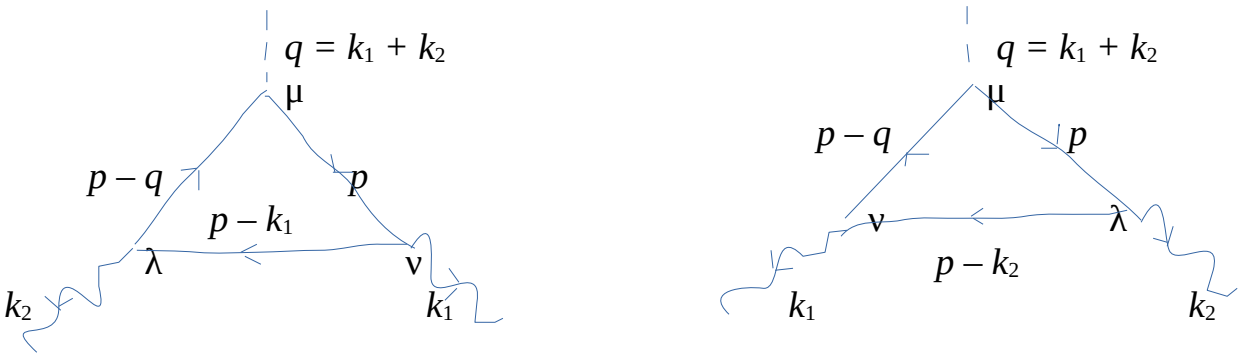

fig.

In the same way as above, gauge invariance invariance implies

$$0=\int d^4x\exp(-iqx)\langle 0|a^b(k_2)a^c(k_1)T(\partial_\mu \hat{J}^{a\mu}(x)\hat{J}^{b\lambda}(y)\hat{J}^{c\nu}(z)\hat{A}^b_\lambda(y)\hat{A}^c_\nu(z))|0\rangle=$$

$$=\int \frac{d^4x\, i\exp(-iqx)}{(2\pi)^3\sqrt{2\omega_{k1}2\omega_{k2}}}\exp(ik_2y)\exp(ik_1z)q_\mu\langle 0|T(\hat{J}^{a\mu}(x)\hat{J}^{b\lambda}(y)\hat{J}^{c\nu}(z))|0\rangle\varepsilon_{2\lambda}\varepsilon_{1\nu}$$

$\varepsilon_{2\lambda}=\varepsilon_\lambda(k_2)$, $\varepsilon_{1\nu}=\varepsilon_\nu(k_1)$ polarization versor components of the outgoing bosons. (even if we have two bosons coming out from the y , z vertices)

($a^{b+}(k_2), a^{c+}(k_1)$ creation operators for the A^b respective A^c bosons which are on mass shell , with $\omega_{k1}=k_1^0$, $\omega_{k2}=k_2^0$)

According to Feynman rules the anomaly amplitude

$$A=(2\pi)^4\boldsymbol{M}\,\delta^4(q-k_1-k_2)=$$

$$=\int \exp(-iqx)\langle 0|a^b(k_2)a^c(k_1)T(\hat{J}^{a\mu}(x)\hat{J}^{b\lambda}(y)\hat{J}^{c\nu}(z)\hat{A}^b_\lambda(y)\hat{A}^c_\nu(z))|0\rangle d^4x\,d^4y\,d^4z$$

considering that all fermion and quark masses have the same (small) value, so that the propagators are identical, is determined in first approximation by

$$\boldsymbol{M}=\frac{i}{(2\pi)^7\sqrt{2\omega_{k1}\omega_{k2}}}\sum_R A_{abc}(R)\int d^4p\,\mathrm{tr}\Big(\gamma^\mu D^{fer}(p)\gamma^\nu D^{fer}(p-k_1)\gamma^\lambda D^{fer}(p-q)+$$

$$+\gamma^\mu D^{fer}(p)\gamma^\lambda D^{fer}(p-k_2)\gamma^\nu D^{fer}(p-q)\Big)$$

where $D^{fer}(p)=\frac{1}{\not{p}-m+i\varepsilon}$ with m quark and fermion masses, $\not{p}=\gamma^\alpha p_\alpha$,

$A_{abc}(R)=\mathrm{tr}(T^aT^bT^c+T^aT^cT^b)$ with the trace evaluated in the R representation of the gauge group and the sum is taken over all representations that occur in the considered theory.

The anomaly is proportional to $\sum_R A_{abc}(R)$.

For the $SU(5)$ theory, calculating A_{abc} for all possible a,b,c we see that it suffices to set T^a, T^b, T^c all equal to $\mathrm{diag}(2,2,2,-3,-3)$ if we want to check $\sum_R A_{abc}(R)=0$.

We calculate $T^3\Big|_{5^*}=3(-2)^3+2(+3)^3=30$, $T^3\Big|_{10}=3(+4)^3+6(-1)^3+(-6)^3=-30$.

$\sum_R A_{abc}(R)=0$ and the anomaly vanishes in the $SU(5)$ theory.

For $SO(10)$ we have the generators $J^{sj}=i(\delta_{sk}\delta_{jl}-\delta_{sl}\delta_{jk})$

and for $Q=\exp(i\omega_{sj}J^{sj})$, $\omega_{sj}=-\omega_{js}$, $s,j=\overline{1,10}$ we have the representation

$U=U(Q)=\exp(\frac{1}{2}i\omega_{sj}\sigma_{sj})$ and $Q J^{sj} Q^T=Q_{ps}Q_{kj}J^{pk}$

$\exp(\frac{1}{2}i\omega_{sj}U\sigma_{sj}U^+)=U(Q\exp(i\omega_{sj}J^{sj})Q^T)=$

$=U(\exp(i\omega_{sj}Q_{ps}Q_{kj}J^{pk}))=\exp(\frac{1}{2}i\omega_{sj}Q_{ps}Q_{kj}\sigma_{pk})$,

$U\sigma_{sj}U^+=Q_{ps}Q_{kj}\sigma_{pk}$

The anomaly is proportional to $A^{sjklmn}=\mathrm{tr}(\sigma_{sj}\sigma_{kl}\sigma_{mn})$.

We have $A^{sjklmn}=\mathrm{tr}(U\sigma_{sj}U^+U\sigma_{kl}U^+U\sigma_{mn}U^+)=Q_{ps}Q_{rj}Q_{qk}Q_{hl}Q_{wm}Q_{vn}A^{sjklmn}$

Thus A^{sjklmn} is an invariant tensor antisymmetric in s-j , k-l , m-n .

We have $A^{sjklmn}=-i\,\mathrm{tr}(\gamma_s\gamma_j\gamma_k\gamma_l\gamma_m\gamma_n)$.

If $j=k$ it follows $A^{sjklmn}=-i\,\mathrm{tr}(\gamma_s\gamma_l\gamma_m\gamma_n)$ and if s,l,m,n are all distinct the trace vanishes since the gamma matrices anticommute. If $s=l$ it also vanishes since $\mathrm{tr}\,\sigma_{mn}=0$.Therefore we have to consider $(s=m$ and $l=n)$ or $(s=n$ and $l=m)$

Thus to determine A_{abc} if $j=k$ we have to sum $\mathrm{tr}(\sigma_{sj}\sigma_{jk}\sigma_{ks})+\mathrm{tr}(\sigma_{sj}\sigma_{ks}\sigma_{jk})=$

$i\,\mathrm{tr}(\sigma_{sk}\sigma_{ks}+\sigma_{sj}\sigma_{js})=0$.

Hence if $A_{abc}\neq 0$ we can consider all s,j,k,l,m,n distinct and so since the gamma matrices anticommute, we have $A^{sjklmn}=-A^{nsjklm}$.

Because $\mathrm{tr}(AB)=\mathrm{tr}(BA)$ for any matrices, it follows $A^{sjklmn}=A^{nsjklm}$ and so $A^{sjklmn}=0$ and so $A_{abc}\propto A^{sjklmn}+A^{sjmnkl}=0$.

We can conclude therefore that the *SU*(5) and *SO*(10) unified theories are free from anomaly.

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