MODULE 1: KLEIN-GORDON AND DIRAC EQUATIONS

Relativistic Quantum Mechanics

Bjorken & Drell: Relativistic QM (Vol. 1)

Sakurai : Advanced QM

Weinberg: Quantum Field Theory (Vol. 1)

Peskin & Schroeder: Introduction to QFT

$$\left.\begin{array}{l}\text{Non-relativistic QM} \\ \quad\text{(Heisenberg, Schrödinger)} \\ \text{Special Relativity} \\ \quad\text{(Tensor, Lorentz transformations)}\end{array}\right\}\ \text{Prerequisites}$$

$$x^0 = ct\,, \quad \vec{x} = x^i\,, \quad x^\mu = \{x^0, x^i\} = \{ct, \vec{x}\}$$

$$p^0 = \frac{E}{c}\,, \quad \vec{p} = p^i\,, \quad p^\mu = \{\tfrac{E}{c}, \vec{p}\} = \{p^0, p^i\}$$

$$g^{\mu\nu} = \begin{Bmatrix} 1 & & & 0 \\ & -1 & & \\ & & -1 & \\ 0 & & & -1 \end{Bmatrix} = g_{\mu\nu}$$: A constant (space-time independent)

$$A \cdot B = A_\mu B^\mu = g_{\mu\nu} A^\mu B^\nu$$

$$\sum_\mu A_\mu B^\mu \equiv A_\mu B^\mu$$: Einstein convention

$$\hbar = \frac{h}{2\pi}$$: Dirac $\qquad \not{p} = p_\mu \gamma^\mu$: Feynman

Choice of units : $\hbar = 1$, $c = 1$, $4\pi\epsilon_0 \to 1$, $\frac{\mu_0}{4\pi} \to 1$
(Dimensional analysis can recover them)

$$E^2 = p^2c^2 + m^2c^4$$ $\Rightarrow$ Relativistic when $pc \sim mc^2$

$$\lambda = \frac{h}{p}$$ $\qquad$ Scale $\sim \frac{\hbar}{mc}$ = Compton wavelength

$$E^2 = \vec{p}^2c^2 + m^2c^4 \implies E = \pm\sqrt{\vec{p}^2c^2 + m^2c^4}$$

Sign ambiguity is related to the fact that relativistic theories give rise to both particles and antiparticles.

$$E \to i\hbar\frac{\partial}{\partial t} \quad , \quad \vec{p} = \frac{\hbar}{i}\vec{\nabla}$$

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = -\hbar^2c^2\nabla^2\psi + m^2c^4\psi$$: Free particles

Schrödinger, Klein-Gordon

$$\Box = \partial_\mu\partial^\mu \quad : \quad \left[\Box + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0$$

Plane-wave solutions : $\psi = e^{-ip\cdot x/\hbar}$ with $p^2 = m^2c^2$.

Klein Gordon equation $\times$ multiply by ψ^*

subtract from it (K.G. eqn.)* $\times$ multiply by ψ

$$-\hbar^2\left(\psi^*\frac{\partial^2\psi}{\partial t^2}-\psi\frac{\partial^2\psi^*}{\partial t^2}\right)=-\hbar^2c^2\left(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*\right)$$

$$\therefore \frac{\partial}{\partial t}\Big[\underbrace{\frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right)}_{\rho}\Big]+\vec{\nabla}\cdot\Big[\underbrace{\frac{\hbar}{2im}\left(\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*\right)}_{\vec{j}}\Big]=0$$

$\therefore \quad \dfrac{\partial\rho}{\partial t}+\vec{\nabla}\cdot\vec{j}=0$: Continuity eqn.
Charge conservation eqn.

$$\int\rho\, d^3x = Q \Rightarrow \frac{dQ}{dt}=0$$

Schrödinger's eqn. has $\rho=|\psi|^2$.
ρ is real, but not necessarily positive.

$$j^\mu=(\rho c,\vec{j})=\frac{i\hbar}{2m}\left(\psi^*\frac{\partial}{\partial x_\mu}\psi-\psi\frac{\partial}{\partial x_\mu}\psi^*\right)\Rightarrow \partial_\mu j^\mu=0.$$

Stationary states : $\psi=e^{-iEt/\hbar}f(\vec{x})$

$$\Rightarrow \rho=\frac{E}{mc^2}\psi^*\psi$$

Lorentz contraction of volume by factor $\dfrac{E}{mc^2}$.

$$\rho_{number} = \rho_{charge} \quad : \text{Non-relativistic}$$

$$\rho_{number} \neq \rho_{charge} \quad : \text{Relativistic}$$

ρ from K.G. equation corresponds to charge density.

$E > 0$: Corresponds to particles with $\rho > 0$.

$E < 0$: Corresponds to antiparticles with $\rho < 0$.

In Fourier space,

$$\phi(t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dE \, e^{-iEt/\hbar} \, \tilde{\phi}(E)$$

For localised wavefunctions in time: $\phi(t) \sim \delta(t - t_0)$

In position space, localisation of particle to a region smaller than Compton wavelength, solutions with relativistic energy (and so $E<0$) are necessary.

K.G. equation describes charged scalar particles e.g. π^+ and π^-.

When the wavefunction is real, then $\rho = 0 = \vec{j}$.

That describes neutral scalar particles, e.g. π^0.

These are antiparticles of themselves.

They can be created/annihilated singly.

Two component framework:

$$\xi = \frac{1}{2}\left(\psi + \frac{i\hbar}{mc^2}\dot{\psi}\right)$$

$$\chi = \frac{1}{2}\left(\psi - \frac{i\hbar}{mc^2}\dot{\psi}\right)$$

Free particle at rest: $E = mc^2$

then $\xi = \psi$ and $\chi = 0$

Free antiparticle at rest.

$E = -mc^2$

then $\xi = 0$, $\chi = \psi$.

$$i\hbar \frac{\partial \xi}{\partial t} = \frac{i\hbar}{2}\left(\dot\psi + \frac{i\hbar}{mc^2}\ddot\psi\right)$$

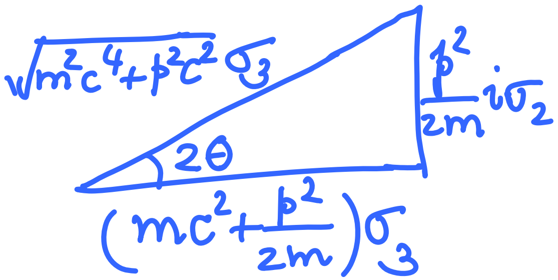
$$\frac{i\hbar\dot\psi}{mc^2} = \xi - \chi \quad , \quad -\hbar^2\ddot\psi = -\hbar^2c^2\nabla^2\psi + m^2c^4\psi, \quad \psi = \xi + \chi$$

$$i\hbar \frac{\partial \xi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2(\xi+\chi) + mc^2\xi$$

$$i\hbar \frac{\partial \chi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2(\xi+\chi) - mc^2\chi .$$

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\xi\\ \chi\end{pmatrix} = -\frac{\hbar^2}{2m}\underbrace{\begin{pmatrix}1 & 1\\ -1 & -1\end{pmatrix}}_{\sigma_3 + i\sigma_2}\nabla^2\begin{pmatrix}\xi\\ \chi\end{pmatrix} + mc^2\underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{\sigma_3}\begin{pmatrix}\xi\\ \chi\end{pmatrix}$$

Rotation about σ_1-direction by $\tanh^{-1}\dfrac{p^2/2m}{mc^2 + p^2/2m}$



Transformation is $\begin{pmatrix}\xi'\\ \chi'\end{pmatrix} = e^{iS}\begin{pmatrix}\xi\\ \chi\end{pmatrix}$

with $S = -\dfrac{i}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\tanh^{-1}\dfrac{p^2/2m}{mc^2+p^2/2m} = -S^\dagger .$

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\xi'\\ \chi'\end{pmatrix}=\begin{pmatrix}1&0\\0&-1\end{pmatrix}\sqrt{p^2c^2+m^2c^4}\begin{pmatrix}\xi'\\ \chi'\end{pmatrix}$$

$\Phi=\begin{pmatrix}\xi\\ \chi\end{pmatrix}$ Observables are bilinears in Φ.

$\Phi\to e^{iS}\Phi$, Observables transform as $O\to e^{iS}Oe^{-iS}$

Invariant bilinears are:

$\Phi^\dagger\eta\, O\,\Phi$ with $\eta=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$: e^{iS} is Hermitian

Prescription: Invariant observables are written in the form $\bar{\Phi}O\Phi$ when $\bar{\Phi}\equiv\Phi^\dagger\eta$.

Charge density ρ corresponds to $O=1$.

Various components of j^μ can be mapped to $O^\mu=\sigma^\mu$ with $\sigma^0=I$, $\vec{\sigma}$ are Pauli matrices.

<u>Electromagnetic coupling</u>:

$p^\mu\to p^\mu-\frac{e}{c}A^\mu$: Minimal coupling.

Electric potential eA_0 modifies time-derivative with coefficient $\mathbb{1}$. Coefficient of mc^2 is σ_3.

Energy is shifted in opposite direction for $E>0$ and $E<0$ solutions, when electric potential is introduced.

That confirms opposite values of charge for particle and antiparticle.

Particles and Antiparticles : Same mass,
But all charges are opposite.

K.G. equation coupled to electromagnetic fields

Minimal prescription: $p^\mu \longrightarrow p^\mu - \frac{e}{c} A^\mu$

$$\left[\left(i\hbar \frac{\partial}{\partial x_\mu} - \frac{e}{c} A^\mu\right)^2 - m^2c^2\right]\psi = 0$$

Magnetic field: $\vec{A} \neq 0$, $\vec{B} = \vec{\nabla} \times \vec{A}$, $A_0 = 0$.

$(c\vec{p} - e\vec{A})^2$ is the same operator as in Schrödinger equation

It gives $-\vec{\mu}\cdot\vec{B}$ term, with $\vec{\mu} = \frac{e}{2mc}\vec{L}$

Gyromagnetic ratio $g = 1$.

Electric field: Coulomb field $A_0 = -\frac{Ze}{r}$.

Central potential $\Rightarrow \vec{L}$ is conserved.

$$\Psi = R(r)\, Y_{lm}(\theta,\phi)$$

$\uparrow$ Solution of ∇^2 operator

$$\left[-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{r^2}\right]R = \frac{(E-eA_0)^2 - m^2c^4}{\hbar^2c^2}\,R$$

Non-rel. case:
$$\left[-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{r^2}\right]R = \frac{2m}{\hbar^2}(E-eA_0)\,R$$

R : $\quad l(l+1) - \left(\frac{Ze^2}{\hbar c}\right)^2 \qquad \frac{2EZe^2}{\hbar^2c^2} \qquad \frac{E^2-m^2c^4}{\hbar^2c^2}$

NR : $\quad \underbrace{l(l+1)}_{1/r^2} \qquad \underbrace{Ze^2\cdot\frac{2m}{\hbar^2}}_{1/r} \qquad \underbrace{E\cdot\frac{2m}{\hbar^2}}_{r\text{-independent}}$

Solutions are Associated Laguerre functions.

Behaviour as $r^{l'}$ near the origin, where

$$l'(l'+1) = l(l+1) - \left(\frac{Ze^2}{\hbar c}\right)^2 \Longrightarrow l' = -\frac{1}{2} + \frac{1}{2}\sqrt{(2l+1)^2 - 4Z^2\alpha^2}$$

Instability expected when $Z > \frac{137}{2}$.

Radial quantum number is n', a non-negative integer.

Total quantum no: $n_R = n' + l' + 1$.

$$n_R = \frac{2EZe^2}{\hbar^2 c^2} \cdot \frac{1}{2} \frac{\hbar c}{\sqrt{|E^2 - m^2c^4|}} = \frac{E\alpha Z}{\sqrt{|E^2 - m^2c^4|}}, \quad \alpha = \frac{e^2}{\hbar c}.$$

Compare: $n_{NR} = \frac{Ze^2 \cdot 2m}{\hbar^2} \cdot \frac{1}{2} \frac{\hbar}{\sqrt{2m|E|}} = \frac{Ze^2}{\hbar}\sqrt{\frac{m}{2|E|}} = n' + l + 1$

$$R: \underbrace{E = mc^2\left(1 + \frac{Z^2\alpha^2}{n_R^2}\right)^{-1/2}}_{\text{Includes relativistic kinetic energy}} \qquad NR: \underbrace{E = mc^2\left(-\frac{Z^2\alpha^2}{2n_{NR}^2}\right)}_{\text{Rydberg formula}}$$

$$n_R = n' + \frac{1}{2}\sqrt{\left(l+\frac{1}{2}\right)^2 - Z^2\alpha^2} = n_{NR} - \frac{Z^2\alpha^2}{2l+1} + \dots$$

$$E = mc^2 - \frac{mZ^2e^4}{2\hbar^2 n_R^2} + \frac{3}{8}\frac{mZ^4e^8}{\hbar^4 c^2 n_R^4} - \dots$$

Fine structure of energy levels : $\frac{mZ^4e^8}{\hbar^4 c^2 n_{NR}^4}\left(\frac{3}{8} - \frac{n_{NR}}{2l+1}\right)$

Sommerfeld's formula : Replaces by $2k$ (k positive integer)

Can be obtained also by including the correction to Kinetic Energy (e.g. $-\frac{p^4}{8m^3c^2}$) in perturbation theory.

From expansion of $\sqrt{p^2c^2 + m^2c^4}$

Bohr-Sommerfeld quantisation:

Action-angle variables and phase space.

For canonically conjugate variables, the period is quantised in units of Planck's constant.

Adiabatic invariants: $\oint p_i \, dq_i = n_i h$

(Separation of variables necessary)

Classical behaviour is recovered when $n_i \to \infty$.

Bohr: Circular orbits

$$\frac{mv^2}{r} = \frac{Ze^2}{r^2}, \quad \oint p_\phi \, d\phi = 2\pi m v r = nh$$

$$\Rightarrow E = -\frac{mZ^2e^4}{2n^2\hbar^2}, \quad (n = 1, 2, 3, \ldots)$$

Sommerfeld: Elliptic orbits allowed.

$$\oint p_r \, dr = n' h \quad (\text{with } n' = 0, 1, 2, \ldots)$$

$$E = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} - \frac{Ze^2}{r}, \quad p_\phi = n\hbar, \quad \frac{1}{r} = a(1+\epsilon\cos\theta)$$

$$a = \frac{mZe^2}{n^2\hbar^2}, \quad \epsilon = \sqrt{1 + \frac{2En^2\hbar^2}{mZ^2e^4}}.$$

$$\oint p_r \, dr = \oint p_r \cdot \frac{(dr/dt)}{(d\phi/dt)} d\phi = \oint \frac{p_r^2 r^2}{p_\phi} d\phi$$

$$= \oint \left(2mE - \frac{n^2\hbar^2}{r^2} + 2m\frac{Ze^2}{r}\right) \frac{r^2}{n\hbar} d\phi$$

$$= \oint \frac{m^2Z^2e^4}{n^2\hbar^2} \epsilon^2 (1 - \cos^2\phi) \cdot \frac{n^3\hbar^3}{m^2Z^2e^4} \cdot \frac{d\phi}{(1+\epsilon\cos\phi)^2}$$

$$= \oint \frac{n\hbar\,\epsilon^2 \sin^2\phi}{(1+\epsilon\cos\phi)^2} d\phi$$

$$\oint \frac{\epsilon^2\sin^2\phi}{(1+\epsilon\cos\phi)^2} d\phi = \oint \epsilon\sin\phi \, d\left(\frac{1}{1+\epsilon\cos\phi}\right) = \oint -\frac{\epsilon\cos\phi}{1+\epsilon\cos\phi} d\phi$$

$$= -2\pi + \oint \frac{d\phi}{1+\epsilon\cos\phi}$$

$$\therefore (n+n')h = n\hbar \oint \frac{dz}{iz} \cdot \frac{1}{1+\frac{\epsilon}{2}(z+\frac{1}{z})} = 2\pi \frac{n\hbar}{\sqrt{1-\epsilon^2}}$$

$$(z = e^{i\phi})$$

$$\Longrightarrow \quad E = -\frac{mZ^2e^4}{2(n+n')^2\hbar^2} \quad : \quad \begin{array}{l} n-1 \longrightarrow l \\ n' \longrightarrow n_r \end{array}$$

In Schrödinger's solution

Zeeman splitting : Orbital plane can make only certain discrete angles w.r.t. direction of the magnetic field.

$$\oint p_\phi \, d\phi = mh \quad \text{with} \quad m = +n, \ldots, 0, \ldots, -n$$

<u>Relativistic generalisation</u> :

p_ϕ , E are constants of motion.

$$\frac{1}{r} = \bar{a}(1+\epsilon\cos\gamma\phi) \quad , \quad \gamma^2 = 1-\left(\frac{Ze^2}{p_\phi c}\right)^2 = 1-\left(\frac{Z\alpha}{n}\right)^2$$

ϕ is periodic with 2π , r is periodic with $\frac{2\pi}{\gamma}$.

$$\bar{a} = \frac{mZe^2}{\gamma^2 p_\phi^2}\left(\frac{E}{mc^2}\right) = \frac{mZe^2}{\gamma n^2\hbar^2\sqrt{1-\epsilon^2(1-\gamma^2)}}$$

$$E = \sqrt{p^2c^2+m^2c^4} - \frac{Ze^2}{r} = \frac{\gamma mc^2}{\sqrt{1-\epsilon^2(1-\gamma^2)}} = \frac{\gamma mc^2}{\sqrt{1-(\epsilon Z\alpha/n)^2}}$$

Circular orbits : $\epsilon = 0$, $E = \gamma mc^2$

$$\oint p_r\,dr = \oint m\left(\frac{d(\frac{1}{r})}{d\phi}r^2\dot{\phi}\right)^2 dt = \int_0^{2\pi/\gamma} p_\phi r^2\left(\frac{d(\frac{1}{r})}{d\phi}\right)^2 d\phi$$

$$= \int_0^{2\pi/\gamma} n\hbar\,\frac{\epsilon^2\gamma^2\sin^2\gamma\phi}{(1+\epsilon\cos\gamma\phi)^2}\,d\phi$$

$$\Rightarrow \quad \frac{n'}{\gamma} + n = \frac{n}{\sqrt{1-\epsilon^2}}$$

Then $$E = mc^2\left[1+\frac{Z^2\alpha^2}{(n'+\gamma n)^2}\right]^{-1/2}$$

$$= mc^2\left[1+\frac{Z^2\alpha^2}{(n'+\sqrt{n^2-Z^2\alpha^2})^2}\right]^{-1/2}$$: Instability expected for $Z > 137$

Semiclassical quantisation needs correction from topological features of the orbit. (Maslov index)

Closed orbits with turning points should have $n_i \longrightarrow n_i + \frac{1}{2}$.

Spin $\frac{1}{2}$ cancels this shift by $\frac{1}{2}$, and Sommerfeld's formula agrees with experiment.

Einstein-Brillouin-Keller prescription.

Quantum statistical mechanics:

Phase space area is quantised in units of Planck's constant.

Dirac: $[x, p] = i\hbar \longleftrightarrow \{x, p\}_{PB} = 1$

Dirac equation:

First order equation in time.

Dispersion relation: $E = \vec{\alpha}\cdot\vec{p}\,c + \beta m c^2$

It has to be consistent with

$$E^2 = p^2c^2 + m^2c^4$$
$$= (\vec{\alpha}\cdot\vec{p}\,c + \beta m c^2)^2$$

That requires:

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij}\ , \quad \beta^2 = 1, \quad \beta\alpha_i + \alpha_i\beta = 0.$$

4-vector notation: $\alpha_\mu = (\beta, \alpha_i)$

$\alpha_\mu\alpha_\nu + \alpha_\nu\alpha_\mu = 2\delta_{\mu\nu}$: Clifford algebra

Hermitian Hamiltonian:

α_i, β are Hermitian (square) matrices.

$\alpha_\mu^2 = 1 \Rightarrow$ Eigenvalues are ± 1.

$$\mathrm{Tr}(\alpha_i) = \mathrm{Tr}(\alpha_i \beta^2) = \mathrm{Tr}(-\beta\alpha_i\beta) = \mathrm{Tr}(-\alpha_i\beta^2)$$
$$= -\mathrm{Tr}(\alpha_i)$$

$\therefore \mathrm{Tr}(\alpha_i) = 0$ and ± 1 eigenvalues occur with equal frequency.

Dimension of matrices is even.

In d space-time dimensions:

$2^{[d/2]}$ dimensional matrices are needed to describe $m \neq 0$ particles.

$2^{[(d-1)/2]}$ dim. matrices for $m=0$ particles.

$$\left(i\hbar\frac{\partial}{\partial t} + i\hbar c\,\vec{\alpha}\cdot\vec{\nabla} - \beta mc^2\right)\psi = 0$$

$\gamma^0 = \beta$ and $\gamma^i = \beta\alpha_i$

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$$

γ^0 is Hermitian, γ^i are anti-Hermitian

$$\left(i\hbar\gamma^\mu\frac{\partial}{\partial x^\mu} - mc\right)\psi = 0 \quad : \text{Covariant form}$$

$$\gamma^\mu A_\mu \equiv \cancel{A} = \gamma^0 A^0 - \vec{\gamma}\cdot\vec{A}$$

$$\left(i\cancel{\nabla} - \frac{mc}{\hbar}\right)\psi = 0 \quad \text{or} \quad (\cancel{p} - mc)\psi = 0$$

ψ is a multi-component object (spinor).

$\bar{\psi} \equiv \psi^\dagger\gamma^0$ takes care of $\vec{\gamma}^\dagger = -\vec{\gamma}$ in taking Hermitian conjugate of the equation

$$-i\hbar \frac{\partial \psi^\dagger}{\partial t} - i\hbar c(\vec{\nabla}\psi^\dagger)\cdot\vec{\alpha} - \psi^\dagger \beta mc^2 = 0$$

$$\Rightarrow -i\hbar \frac{\partial \overline{\psi}}{\partial t}\gamma^0 - i\hbar c(\vec{\nabla}\overline{\psi})\cdot\vec{\gamma} - \overline{\psi} mc^2 = 0$$

$$\Rightarrow -i\hbar \frac{\partial \overline{\psi}}{\partial x^\mu}\gamma^\mu - mc\overline{\psi} = 0$$

$$\Rightarrow \overline{\psi}\left(i\overleftarrow{\not{\nabla}} + \frac{mc}{\hbar}\right) = 0 \quad \text{or} \quad \overline{\psi}(\overleftarrow{\not{p}} + mc) = 0$$

<u>Dirac basis</u>: $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$, $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \gamma^0$

$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

4 components correspond to particle/antiparticle and up/down spin values.

$$\psi^\dagger i\hbar \frac{\partial \psi}{\partial t} + i\hbar \frac{\partial \psi^\dagger}{\partial t}\psi + \psi^\dagger i\hbar c\,\vec{\alpha}\cdot\vec{\nabla}\psi + i\hbar c(\vec{\nabla}\psi^\dagger)\cdot\vec{\alpha}\,\psi = 0$$

$$\therefore\quad i\hbar \frac{\partial}{\partial t}\underbrace{(\psi^\dagger\psi)}_{\rho} + i\hbar c\,\vec{\nabla}\cdot\underbrace{(\psi^\dagger\vec{\alpha}\,\psi)}_{\vec{j}} = 0$$

$$\rho \geq 0 \quad , \quad \vec{j} = c\,\psi^\dagger\vec{\alpha}\,\psi \quad \Rightarrow \quad j^\mu = c\,\overline{\psi}\gamma^\mu\psi$$

$c\vec{\alpha}$ can be interpreted as the velocity operator.

Its eigenvalues are $\pm c$.

Equation of motion for position:

$$\frac{d\vec{r}}{dt} = \frac{i}{\hbar}[H, \vec{r}\,] = [c\vec{\alpha}\cdot\vec{\nabla}, \vec{r}\,] = c\vec{\alpha} \equiv \vec{v}_{op}$$

free particle

$$\frac{d\vec{p}}{dt} = \frac{i}{\hbar}[H, \vec{p}\,] = 0 \quad , \quad \text{but} \quad \frac{d\vec{v}_{op}}{dt} = \frac{i}{\hbar}[H, c\vec{\alpha}\,] \neq 0$$

even for a free particle

$$\{H, \frac{d\vec{r}}{dt}\} = c^2\{\vec{\alpha}\cdot\vec{p}, \vec{\alpha}\} = 2c^2\vec{p}$$

For eigenstates of H, we have $\langle \vec{v}_{op} \rangle = \frac{\langle c^2\vec{p} \rangle}{E}$.

Commutation rules for $\vec{v}_{op}$ are different compared to $\vec{p}$ and $\vec{r}$.

Equation of motion for angular momentum:

$\vec{L} = \vec{r} \times \vec{p}$ is not conserved even for a free particle.

$$\frac{d\vec{L}}{dt} = \frac{i}{\hbar}[H, \vec{L}] = \frac{ic}{\hbar}[\vec{\alpha}\cdot\vec{p}, \vec{r}\times\vec{p}] = c[\vec{\alpha}\cdot\vec{\nabla}, \vec{r}\times\vec{p}] = c\vec{\alpha}\times\vec{p}$$

Define $\vec{J} = \vec{L} + \vec{S}$ is conserved.

Extra contribution is the spin of the particle.
(Intrinsic angular momentum)

$$\vec{S} = \frac{\hbar}{2}\begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$$

Eigenstates of $\vec{\sigma}$ are the up/down spin states.

$$\frac{d\vec{S}}{dt} = \frac{i}{\hbar} \cdot \frac{c\hbar}{2}\left[\begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \cdot \vec{p}\,,\, \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}\right]$$

$$= \frac{ic}{2}\begin{pmatrix} 0 & [\vec{\sigma}\cdot\vec{p}, \vec{\sigma}] \\ [\vec{\sigma}\cdot\vec{p}, \vec{\sigma}] & 0 \end{pmatrix}$$

$$= -c\begin{pmatrix} 0 & \vec{\sigma}\times\vec{p} \\ \vec{\sigma}\times\vec{p} & 0 \end{pmatrix}$$

$$\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$$

$$= -c\,\vec{\alpha}\times\vec{p}$$

Together, $\dfrac{d\vec{J}}{dt} = \dfrac{d}{dt}(\vec{L}+\vec{S}) = 0$

Eigenvalues of $\vec{S}$ are $\pm\frac{\hbar}{2}$.

(spin-half particles)

Helicity $= \vec{J}\cdot\hat{p} = \vec{S}\cdot\hat{p}$ is conserved for free particles. So the solutions of free Dirac equation are labeled by signs of helicity and energy.

Free particle solutions:

These are plane waves with 4 spinor components.

$$\psi^r(x) = \omega^r(0)\, e^{i(\vec{p}\cdot\vec{r}-Et)/\hbar} \quad : \; r=1,2,3,4$$

$$\Rightarrow \left(E - c\vec{\alpha}\cdot\vec{p} - \beta mc^2\right)\omega^r = 0$$

$$\Rightarrow \begin{pmatrix} E-mc^2 & -c\vec{\sigma}\cdot\vec{p} \\ -c\vec{\sigma}\cdot\vec{p} & E+mc^2 \end{pmatrix}\begin{pmatrix}\phi \\ \chi\end{pmatrix} = 0 \qquad \omega^r = \begin{pmatrix}\phi \\ \chi\end{pmatrix}$$

Determinant $= E^2 - m^2c^4 - c^2p^2 = 0$ as necessary

$$E_\pm = \pm\sqrt{p^2c^2 + m^2c^4}$$

Positive energies : $\omega_+^r = A\begin{pmatrix} \phi \\ \dfrac{c\vec{\sigma}\cdot\vec{p}}{E_+ + mc^2}\phi \end{pmatrix}$

with $\phi = \begin{pmatrix}1\\0\end{pmatrix}$ or $\begin{pmatrix}0\\1\end{pmatrix}$

Negative energies : $\omega_-^r = A\begin{pmatrix} \dfrac{c\vec{\sigma}\cdot\vec{p}}{E_- - mc^2}\chi \\ \chi \end{pmatrix}$

with $\chi = \begin{pmatrix}1\\0\end{pmatrix}$ or $\begin{pmatrix}0\\1\end{pmatrix}$

They have well-defined limits as $\vec{p}\to 0$ (rest frame).

$\psi^\dagger\psi = \dfrac{|E|}{mc^2}$ to follow Lorentz contractions

$$|A|^2 \times \left[1 + \frac{c^2 p^2}{(|E| + mc^2)^2} \right] = \frac{|E|}{mc^2}$$

$$\therefore \quad |A|^2 \times \left[\frac{|E|^2 + 2|E| \cdot mc^2 + m^2c^4 + p^2c^2}{(|E| + mc^2)^2} \right] = \frac{|E|}{mc^2}$$

$$\therefore \quad |A| = \sqrt{\frac{|E| + mc^2}{2mc^2}}$$: Fixes normalisation.

It follows that $\bar{\psi}\psi = \pm 1$ is Lorentz invariant.

Electromagnetic interactions:

$$i\hbar \frac{\partial}{\partial x^\mu} \longrightarrow i\hbar \frac{\partial}{\partial x^\mu} - \frac{e}{c} A_\mu \quad : \text{Minimal prescription}$$

$$\Rightarrow \quad i\hbar \frac{\partial \psi}{\partial t} = \left[c\, \vec{\alpha} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) + \beta m c^2 + e\Phi \right] \psi$$

$E > 0$ and $E < 0$ solutions are shifted in opposite directions by $e\Phi$. This is a consequence of opposite charges of particle and antiparticle

Non-relativistic limit : K.E., P.E. $\ll mc^2$

Then $\chi \ll \phi$, $E \approx mc^2 \Rightarrow \chi \approx \dfrac{\vec{\sigma} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right)}{2mc} \phi$

$$i\hbar \frac{\partial \phi}{\partial t} = \left(\frac{\left[\vec{\sigma} \cdot \left(\vec{p} - \frac{e}{c} \vec{A} \right) \right]^2}{2m} + e\Phi + mc^2 \right) \phi$$

: Pauli equation.

$$\sigma_i \sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$$

$$\Rightarrow i\hbar \frac{\partial \phi}{\partial t} = \Big[\underbrace{\frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m} + e\Phi + mc^2}_{\text{Schrödinger's equation terms}} + \underbrace{\frac{i\vec{\sigma}}{2m}\cdot(\vec{p} - \frac{e}{c}\vec{A})\times(\vec{p} - \frac{e}{c}\vec{A})}_{\text{Spin term}} \Big]\phi$$

$$= \Big[\frac{\vec{p}^2}{2m} - \frac{e}{2mc}(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}) + \frac{e^2}{2mc^2}\vec{A}^2 + e\Phi + mc^2 - \frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{B} \Big]\phi$$

Gyromagnetic ratio for spin term is $g = 2$. $\left(\vec{S} = \frac{\hbar}{2}\vec{\sigma}\right)$

Gyromagnetic ratio for orbital term is $g = 1$

$\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p} \longrightarrow \vec{L}\cdot\vec{B}$ in constant $\vec{B}$.

Magnetic moment $\vec{\mu} = -\frac{e}{2mc}(\vec{L} + 2\vec{S})$

$$D^\mu = \partial^\mu + \frac{ie}{\hbar c} A^\mu \quad , \quad F^{\mu\nu} = \frac{\hbar c}{ie}[D^\mu, D^\nu] = \partial^\mu A^\nu - \partial^\nu A^\mu$$

$$\Rightarrow \left(i\cancel{D} + \frac{mc}{\hbar}\right)\left(i\cancel{D} - \frac{mc}{\hbar}\right)\psi = 0$$

$$\gamma^\mu \gamma^\nu = \frac{1}{2}\{\gamma^\mu, \gamma^\nu\} + \frac{1}{2}[\gamma^\mu, \gamma^\nu]$$

$$= g^{\mu\nu} - i\Sigma^{\mu\nu} \quad \left(\Sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu]\right)$$

Hermitian

Then, $\left[\left(\partial^\mu + \frac{ie}{\hbar c} A^\mu\right)^2 - \frac{e}{2\hbar c}\Sigma^{\mu\nu} F_{\mu\nu} + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0$

Klein-Gordon equation terms

$$\Sigma^{\mu\nu} F_{\mu\nu} = 2\vec{\Sigma}\cdot\vec{B} - 2i\vec{\alpha}\cdot\vec{E} \qquad \left(\vec{S} = \frac{\hbar}{2}\vec{\Sigma}\right)$$

spin-dipole spin-orbit

Lorentz force: $\vec{E} = -\vec{\nabla}\Phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$, $\vec{B} = \vec{\nabla}\times\vec{A}$

$$\frac{d}{dt}\left(\vec{p} - \frac{e}{c}\vec{A}\right) = \frac{i}{\hbar}\left[H, \vec{p} - \frac{e}{c}\vec{A}\right] - \frac{e}{c}\frac{\partial \vec{A}}{\partial t}$$

$$= \frac{i}{\hbar}\left[c\vec{\alpha}\cdot\vec{p}, -\frac{e}{c}\vec{A}\right] + \frac{i}{\hbar}\left[-e\vec{\alpha}\cdot\vec{A} + e\Phi, \vec{p}\right] - \frac{e}{c}\frac{\partial \vec{A}}{\partial t}$$

$$= -e(\vec{\alpha}\cdot\vec{\nabla})\vec{A} + e\vec{\nabla}(\vec{\alpha}\cdot\vec{A}) - e\vec{\nabla}\Phi - \frac{e}{c}\frac{\partial \vec{A}}{\partial t}$$

$$= e\vec{E} + e\vec{\alpha}\times\vec{B}$$

$$= e\left(\vec{E} + \frac{\vec{v}_{op}}{c}\times\vec{B}\right)$$

Spin-precession: $\vec{S} = \frac{\hbar}{2}\vec{\Sigma}$, $\frac{d\vec{\Sigma}}{dt} = -\frac{2c}{\hbar}\vec{\alpha}\times\vec{p}$

Equation of motion is simple for eigenstates of H

$$\left\{H, \frac{d\vec{\Sigma}}{dt}\right\} = \frac{2c^2}{\hbar}\left\{\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right), -\vec{\alpha}\times\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right\}$$

(with $\Phi = 0$)

$$\alpha_i \alpha_j = \delta_{ij} + i\epsilon_{ijk}\Sigma_k$$

$$\Rightarrow \left\{H, \frac{d\vec{\Sigma}}{dt}\right\} = -i\frac{2c^2}{\hbar}\epsilon_{lmn}\epsilon_{ilj}\Sigma_j\left[\left(\vec{p}-\frac{e}{c}\vec{A}\right)_i, \left(\vec{p}-\frac{e}{c}\vec{A}\right)_m\right]$$

$$= 2ec\,\epsilon_{lmn}\epsilon_{ilj}\Sigma_j\,\epsilon_{imk}B_k$$

$$= 2ec\left(\delta_{il}\delta_{nk} - \delta_{in}\delta_{kl}\right)\epsilon_{ilj}\Sigma_j B_k$$

$$= 2ec\,\vec{\Sigma}\times\vec{B} \quad : \text{Larmor precession}$$

Analogue of $\frac{d\vec{S}}{dt} = \frac{e}{mc}\vec{S}\times\vec{B}$ in classical electrodynamics, with $g=2$. $(H \approx mc^2)$

Hydrogen atom problem : $\Phi(r) = -\frac{Ze}{r}$

Symmetries : Rotational $\Rightarrow$ Ang. Mom. Conserved

Time indep. $\Rightarrow$ Energy conserved.

Parity : Discrete symmetry $\vec{r} \to -\vec{r}$, $t \to t$.

$P^2 = \mathbb{1} \Rightarrow$ Eigenvalues of P are ± 1.

Spherical harmonics $Y_{lm}(\theta,\phi)$ have parity $(-1)^l$.

$P\psi(\vec{r}) = \psi'(\vec{r}\,')$ with $\vec{r}\,' = -\vec{r}$.

Operators transform as $POP^{-1} = O'$.

} Unitary transformation

$H_{Dirac} = \vec{\alpha}\cdot\vec{p}c + \beta mc^2 + e\Phi(r)$: Central potential

It remains form invariant, provided P anticommutes with $\vec{\alpha}$, i.e. P is proportional to β.

Then $P\psi(\vec{r}) = \beta\psi(-\vec{r}) = \gamma^0\psi(-\vec{r})$.

Sometimes $e^{i\phi}\gamma^0$ is used instead of γ^0, because phase of ψ is unobservable.

Eigenstates are specified by eigenvalues (quantum numbers) of H, J^2, J_z, parity.

$\vec{J}$ is obtained as $\vec{L}+\vec{S} \Rightarrow j = l \pm \frac{1}{2}$.

Same j can be obtained from two states of l, corresponding to opposite parity.

$\vec{L}$ and $\vec{S}$ can be parallel or anti-parallel.

We separate the wavefunction into radial and angular parts : $\psi = R(r)\,\Theta(\theta,\phi)$.

$\vec{\alpha}\cdot\vec{p}$ needs to be rewritten in polar coordinates.

$$(\vec{\alpha}\cdot\vec{r})(\vec{\alpha}\cdot\vec{r})(\vec{\alpha}\cdot\vec{p})$$

$$r^2\,\vec{\alpha}\cdot\vec{p} = (\vec{\alpha}\cdot\vec{r})\left(\vec{r}\cdot\vec{p} + i\vec{\Sigma}\cdot(\vec{r}\times\vec{p})\right)$$

$$= r\,\alpha_r\left(-i\hbar r\frac{\partial}{\partial r} + i\vec{\Sigma}\cdot\vec{L}\right)$$

$$p_r \equiv \frac{1}{2}(\hat{r}\cdot\vec{p} + \vec{p}\cdot\hat{r}) = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}(r\ldots)$$

Then $\vec{\alpha}\cdot\vec{p} = \alpha_r\left[p_r + \frac{i}{r}(\vec{\Sigma}\cdot\vec{L} + \hbar)\right]$

$$(\vec{\Sigma}\cdot\vec{L}+\hbar) = \frac{1}{\hbar}\left(J^2+\frac{\hbar^2}{4}-L^2\right) = \hbar\underbrace{\left[j(j+1)+\frac{1}{4}-l(l+1)\right]}$$

$$\vec{J} = \vec{L}+\frac{\hbar}{2}\vec{\Sigma}$$

$$= \begin{cases} l+1 = j+\frac{1}{2} & \text{for } j=l+\frac{1}{2} \\ -l = -(j+\frac{1}{2}) & \text{for } j=l-\frac{1}{2} \end{cases}$$

$$(\vec{\Sigma}\cdot\vec{L}+\hbar)^2 = (\vec{\Sigma}\cdot\vec{L})^2 + 2\hbar\,\vec{\Sigma}\cdot\vec{L}+\hbar^2$$

$$= \vec{L}\cdot\vec{L} + i\vec{\Sigma}\cdot\underbrace{(\vec{L}\times\vec{L})}_{i\hbar\vec{L}} + 2\hbar\vec{\Sigma}\cdot\vec{L}+\hbar^2$$

$$= L^2 + \hbar\,\vec{\Sigma}\cdot\vec{L}+\hbar^2$$

$$= \left(\vec{L}+\frac{\hbar}{2}\vec{\Sigma}\right)^2 + \frac{\hbar^2}{4}$$

$$= J^2 + \frac{\hbar^2}{4}$$: Eigenvalues are $(j+\frac{1}{2})^2\hbar^2$.

$(\vec{\Sigma}\cdot\vec{L}+\hbar)$ commutes with $\vec{J}$.

The operator $\hbar K = \beta(\vec{\Sigma}\cdot\vec{L} + \hbar)$ commutes with H.

Eigenvalues are $\hbar k$, with $k = \pm(j+\frac{1}{2}) = \pm 1, \pm 2, \pm 3, \ldots$

Check: $[\vec{\alpha}\cdot\vec{p}, \beta(\vec{\Sigma}\cdot\vec{L}+\hbar)] \stackrel{?}{=} 0$

$$\alpha_i \Sigma_j = i\epsilon_{ijk}\alpha_k + (\text{symmetric})$$

$$\vec{p}\times\vec{L} + \vec{L}\times\vec{p} = 2i\hbar\vec{p}$$

Go back to the Hydrogen atom problem:

$$\left[c\alpha_r p_r + i\alpha_r\beta\frac{\hbar c k}{r} + \beta mc^2 + e\Phi\right]R(r) = E\,R(r)$$

Simpler 2×2 structure can be used

$$R = \frac{1}{r}\begin{pmatrix} G(r) \\ F(r) \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \alpha_r = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

Two first-order coupled equations (real):

$$\left(E - mc^2 + \frac{Ze^2}{r}\right) G + \hbar c \frac{\partial F}{\partial r} + \frac{\hbar c k F}{r} = 0$$

$$\left(E + mc^2 + \frac{Ze^2}{r}\right) F - \hbar c \frac{\partial G}{\partial r} + \frac{\hbar c k G}{r} = 0$$

General solutions are linear combinations of Confluent Hypergeometric functions.

(regular singularities at $r = 0, \infty$)

For $r \to \infty$, $\frac{Ze^2}{r}$ and $\frac{k}{r}$ drop out.

Solutions can be written as $e^{-\rho}$ with $\rho = \frac{\sqrt{m^2c^4 - E^2}}{\hbar c} r$,

so that $R \to 0$ as $r \to \infty$. (For bound states)

Factor out $F(\rho) = f(\rho)\, e^{-\rho}$ and $G(\rho) = g(\rho)\, e^{-\rho}$.

$$\left(\frac{d}{d\rho} - 1 + \frac{k}{\rho}\right) f - \left(\sqrt{\frac{mc^2-E}{mc^2+E}} - \frac{Z\alpha}{\rho}\right) g = 0$$

$$\left(\frac{d}{d\rho} - 1 - \frac{k}{\rho}\right) g - \left(\sqrt{\frac{mc^2+E}{mc^2-E}} + \frac{Z\alpha}{\rho}\right) f = 0$$

Solved near $r \to 0$, by power series method (Frobenius method).

$$f = \rho^s \sum_{\nu=0}^{\infty} f_\nu \rho^\nu, \quad g = \rho^s \sum_{\nu=0}^{\infty} g_\nu \rho^\nu, \quad f_0 g_0 \neq 0.$$

Equate coefficients of $\rho^{s+\nu-1}$ to zero.

$$(s+\nu+k) f_\nu - f_{\nu-1} + \frac{E-mc^2}{q} g_{\nu-1} + Z\alpha g_\nu = 0$$

$$(s+\nu-k) g_\nu - g_{\nu-1} - \frac{E+mc^2}{q} f_{\nu-1} - Z\alpha f_\nu = 0$$

(with $q = \sqrt{m^2c^4 - E^2} > 0$ for bound states with $E < mc^2$)

For $\nu = 0$ (indicial equation),

$$(s+k) f_0 + Z\alpha\, g_0 = 0 \quad , \quad (s-k) g_0 - Z\alpha\, f_0 = 0$$

For determinant of coefficients to vanish,

$$(s+k)(s-k) + Z^2\alpha^2 = 0 \implies s = \pm\sqrt{k^2 - Z^2\alpha^2}.$$

Only $s>0$ gives normalisable solutions.

Even then, solution is singular at the origin for $k^2=1$. But that solution is normalisable.

Instability expected when $Z\alpha > 1$ or $Z > 137$.

Also, $\dfrac{f_0}{g_0} = \dfrac{s-k}{Z\alpha}$ for the leading coefficients.

Multiply first eqn. by $(E+mc^2)$, second by q, and subtract

$$[(E+mc^2)(s+\nu+k) + qZ\alpha]\, f_\nu + [(E+mc^2)Z\alpha - q(s+\nu-k)]\, g_\nu = 0$$

For $\nu \to \infty$, $f_\nu \sim \frac{2}{\nu} f_{\nu-1}$ and $g_\nu \sim \frac{2}{\nu} g_{\nu-1}$.

That implies $f \sim e^{2\rho}$, $g \sim e^{2\rho}$, which gives back the asymptotic solution that was rejected.

So the series must terminate, say at $\nu = n' (=0,1,2,\dots)$, to produce a physical solution.

With $f_{n'+1} = 0 = g_{n'+1}$, the coefficients satisfy $f_{n'} = \frac{E-mc^2}{q} g_{n'}$.

Then energy eigenvalues satisfy,

$$\left[(E+mc^2)(s+n'+k) + qZ\alpha\right]\frac{E-mc^2}{q} + (E+mc^2)Z\alpha - q(s+n'-k) = 0$$

$$\therefore\ -q(s+n'+k) + (E-mc^2)Z\alpha + (E+mc^2)Z\alpha - q(s+n'-k) = 0$$

$$\therefore\ -2q(s+n') + 2EZ\alpha = 0$$

Thus $E > 0$, and $E = \dfrac{mc^2}{\left[1+\dfrac{Z^2\alpha^2}{(s+n')^2}\right]^{1/2}} = \dfrac{mc^2}{\left[1+\dfrac{Z^2\alpha^2}{\left(n'+\sqrt{(j+\frac{1}{2})^2 - Z^2\alpha^2}\right)^2}\right]^{1/2}}$

E depends on n' and j (but not on l or s)

It is equivalent to Sommerfeld's semi-classical result. ($j+\frac{1}{2}$ is an integer)

Expanding in powers of $Z\alpha$,

$$E = mc^2\left[1 - \frac{(Z\alpha)^2}{2(n'+j+\frac{1}{2})^2} + \frac{(Z\alpha)^4}{(n'+j+\frac{1}{2})^3}\underbrace{\left(\frac{3}{8(n'+j+\frac{1}{2})} - \frac{1}{2j+1}\right)}_{\text{Lifts degeneracy for same } n_{NR} \text{ but different } j} + O(Z\alpha)^6\right]$$

$$\Downarrow$$

$$n_{NR} \equiv n' + j + \frac{1}{2}$$

Further corrections (not present in Dirac equation)

(1) Finite nuclear mass

(2) Hyperfine interaction between electron's and nuclear magnetic moment.

(3) Higher order QED effects, such as vacuum polarisation. e.g. Lamb shift which separates $2s_{1/2}$ and $2p_{1/2}$ energy levels.

These are calculated in perturbation theory.

For the ground state ($n'=0$):

$$E_0 = mc^2\sqrt{1-Z^2\alpha^2} \quad \text{and} \quad \rho_0 = Z\alpha\left(\frac{mc}{\hbar}\right)r = \frac{Zr}{a_{Bohr}}.$$

For a given n_{NR}, allowed $n'=0,1,\dots,n_{NR}-1$.

Largest value of j corresponds to $n'=0$.

For largest j, $k=j+\frac{1}{2}$ only.

For all other j's, $k=\pm(j+\frac{1}{2}) = \pm(n_{NR}-n')$.

Angular part of the wavefunction:

Eigenfunctions of $\hbar K = \hbar\begin{pmatrix} \vec{\sigma}\cdot\vec{L}+\hbar & 0 \\ 0 & -(\vec{\sigma}\cdot\vec{L}+\hbar) \end{pmatrix}$

or Eigenfunctions of $(\vec{\Sigma}\cdot\vec{L}+\hbar)$ with opposite sign eigenvalues for upper and lower components.

They can be obtained by combining $Y_{lm} \otimes \begin{pmatrix} \uparrow \\ \downarrow \end{pmatrix}$.

They give Clebsch-Gordon coefficients for $j = l \oplus \frac{1}{2}$.

$$\mathcal{Y}_l^{j=l\pm\frac{1}{2},m} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \pm\sqrt{l\pm m+\frac{1}{2}} & Y_{l,m-\frac{1}{2}} \\ \sqrt{l\mp m+\frac{1}{2}} & Y_{l,m+\frac{1}{2}} \end{pmatrix}, \quad Y_{l,m}^{*} = (-1)^m Y_{l,-m}.$$

$$\int \left(\mathcal{Y}_l^{jm}\right)^{\dagger} \mathcal{Y}_{l'}^{j'm'} \, d\Omega = \delta_{jj'} \delta_{ll'} \delta_{mm'}$$

These have to be combined to give 4-component spinors. That requires same j, but different l.

Operator changing l by one unit, and also behaving as a pseudoscalar is $\vec{\sigma} \cdot \hat{r}$.

$$\vec{\sigma} \cdot \hat{r} \; \mathcal{Y}_{j\mp\frac{1}{2}}^{jm} = -\mathcal{Y}_{j\pm\frac{1}{2}}^{jm}.$$

In Dirac basis, $\alpha_r = \begin{pmatrix} 0 & \vec{\sigma}\cdot\hat{r} \\ \vec{\sigma}\cdot\hat{r} & 0 \end{pmatrix}$.

$$k = j+\tfrac{1}{2} > 0 \; : \quad \psi = \frac{1}{r}\begin{pmatrix} G(r)\, \mathcal{Y}^{jm}_{j-\frac{1}{2}} \\ i F(r)\, \mathcal{Y}^{jm}_{j+\frac{1}{2}} \end{pmatrix}$$

$$k = -(j+\tfrac{1}{2}) < 0 \; : \quad \psi = \frac{1}{r}\begin{pmatrix} G(r)\, \mathcal{Y}^{jm}_{j+\frac{1}{2}} \\ i F(r)\, \mathcal{Y}^{jm}_{j-\frac{1}{2}} \end{pmatrix}$$

These are eigenstates of j, k, parity, Energy.

$\frac{F}{G} = O(Z\alpha) = O\left(\frac{v}{c}\right)$. Change in E is $O\left(\frac{v^2}{c^2}\right)$.

Non-relativistic reduction:

(Foldy-Wouthuysen transformation)

Perform a unitary change in basis, which rotates away the coupling between upper and lower components of the Hamiltonian.

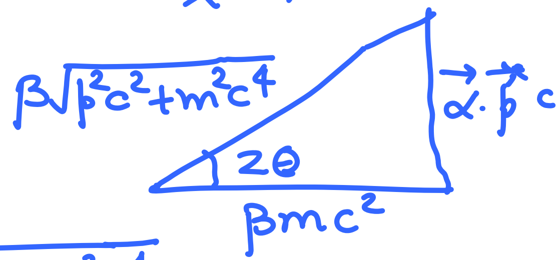
Free particle case: $H = \vec{\alpha}\cdot\vec{p}c + \beta mc^2$

Lorentz boost to the rest frame removes $\vec{\alpha}\cdot\vec{p}c$ term

$$\psi \longrightarrow e^{iS}\psi \quad , \quad H \longrightarrow e^{iS} H e^{-iS} \quad \text{(time independent)}$$

Similar to rotating $\sigma_x B_x + \sigma_y B_y$ to $\sigma_{x'} B_{x'}$.

$$\tan 2\theta = \frac{|\vec{p}|}{mc} = O\left(\frac{v}{c}\right)$$



$$e^{iS} = e^{\beta\vec{\alpha}\cdot\hat{p}\,\theta} \quad \text{gives} \quad H' = \beta\sqrt{p^2c^2+m^2c^4}.$$

Coulomb problem: $H = \underbrace{\beta mc^2 + e\Phi}_{\text{Diagonal}} + \underbrace{c\vec{\alpha}\cdot(\vec{p} - \frac{e}{c}\vec{A})}_{\text{Off-diagonal}}$

Let $\psi' = e^{iS}\psi$. S can be time-dependent.

$$i\frac{\partial}{\partial t}\left(e^{-iS}\psi'\right) = H\psi = He^{-iS}\psi' = e^{-iS}\left(i\frac{\partial\psi'}{\partial t}\right) + \left(i\frac{\partial}{\partial t}e^{-iS}\right)\psi'$$

$$\therefore\ i\frac{\partial\psi'}{\partial t} = \left[e^{iS}\left(H - i\frac{\partial}{\partial t}\right)e^{-iS}\right]\psi' = H'\psi'$$

Choose S to minimise off-diagonal terms in H'.

$$e^{i\lambda S}F\,e^{-i\lambda S} = \sum_{n=0}^{\infty}\frac{(i\lambda)^n}{n!}[S,[S,\dots,[S,F]\dots]]$$

One can keep terms up to desired order in $\frac{v}{c}$.

We will keep terms up to $O(\frac{v}{c})^4$, relative to mc^2.

We need commutators of type $[S,H]$ and $[S,\frac{\partial}{\partial t}]$.

$$H' = H + i[S,H] - \frac{1}{2}[S,[S,H]] - \frac{i}{6}[S,[S,[S,H]]]$$
$$+ \frac{1}{24}[S,[S,[S,[S,\beta mc^2]]]] - \dot{S} - \frac{i}{2}[S,\dot{S}] + \frac{1}{6}[S,[S,\dot{S}]]$$
$$+ \text{Higher orders}$$

First transformation is : $S^{(1)} = -i\beta\Theta/2mc^2$

with $\Theta = c\vec{\alpha}\cdot(\vec{p} - \frac{e}{c}\vec{A})$

$$i[S^{(1)}, H] = -\Theta + \frac{\beta}{2mc^2}[\Theta, e\Phi] + \frac{1}{mc^2}\beta\Theta^2$$
$$\frac{i^2}{2}[S^{(1)},[S^{(1)},H]] = -\frac{\beta\Theta^2}{2mc^2} - \frac{1}{8m^2c^4}[\Theta,[\Theta,e\Phi]] - \frac{1}{2m^2c^4}\Theta^3$$
$$\frac{i^3}{3!}[S^{(1)},[S^{(1)},[S^{(1)},H]]] = \frac{\Theta^3}{6m^2c^4} - \frac{1}{6m^3c^6}\beta\Theta^4$$
$$\frac{i^4}{4!}[S^{(1)},[S^{(1)},[S^{(1)},[S^{(1)},H]]]] = \frac{\beta\Theta^4}{24m^3c^6}$$

$$-\dot{S}^{(1)} = \frac{i\beta\dot{\mathcal{O}}}{2mc^2} \quad , \quad -\frac{i}{2}[S^{(1)}, \dot{S}^{(1)}] = -\frac{i}{8m^2c^4}[\mathcal{O}, \dot{\mathcal{O}}]$$

$$H^{(1)} = \beta\left(mc^2 + \frac{\mathcal{O}^2}{2mc^2} - \frac{\mathcal{O}^4}{8m^3c^6}\right) + e\Phi - \frac{1}{8m^2c^4}[\mathcal{O},[\mathcal{O},e\Phi]]$$

$$- \frac{i\hbar}{8m^2c^4}[\mathcal{O}, \dot{\mathcal{O}}] + \mathcal{O}' \leftarrow \text{off-diagonal}$$

$$\mathcal{O}' = \frac{\beta}{2mc^2}[\mathcal{O}, e\Phi] - \frac{\mathcal{O}^3}{3m^2c^4} + i\hbar\frac{\beta\dot{\mathcal{O}}}{2mc^2}$$

Transformation is first order in $\mathcal{O}$.

Effect on diagonal part of H is second order in $\mathcal{O}$.

Second transformation : $S^{(2)} = -\dfrac{i\beta\mathcal{O}'}{2mc^2}$

It produces $H^{(2)} = (\text{Diagonal part of } H^{(1)}) + \mathcal{O}''$

$$\mathcal{O}'' = \frac{\beta}{2mc^2}\left[\mathcal{O}', e\Phi - \frac{1}{8m^2c^4}[\mathcal{O},[\mathcal{O},e\Phi]] - \frac{i\hbar}{8m^2c^4}[\mathcal{O},\dot{\mathcal{O}}]\right]$$

$$+ \frac{i\hbar\beta\dot{\mathcal{O}}'}{2mc^2} + \beta\left(\frac{\mathcal{O}^2}{2mc^2} - \frac{\mathcal{O}^4}{8m^3c^6}\right)$$

Finally, $S^{(3)} = -\frac{i\beta O''}{2mc^2}$ gets rid of O'', leaving behind only diagonal part of $H^{(1)}$.

$$\frac{O^2}{2m} = \frac{\left(\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right)^2}{2m} = \frac{\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2}{2m} - \frac{e}{2mc}\vec{\sigma}\cdot\vec{B}$$

$$\frac{O^4}{8m^3} \approx \frac{p^4}{8m^3}$$ upto desired order.

$S^{(1)}$ and $c\vec{\alpha}\cdot\vec{p}$ are $O\left(\frac{v}{c}\right)$.

$e\Phi$ is the electrostatic energy $O\left(\frac{v^2}{c^2}\right)$.

$e\vec{A}$ is the magnetic part $O\left(\frac{v^3}{c^3}\right)$. $\longleftarrow$ Appears in $\dot{S}^{(1)}$.

$$[O, \mathcal{E}] + i\dot{O} = -i\vec{\alpha}\cdot\vec{\nabla}(e\Phi) - i\vec{\alpha}\cdot\dot{\vec{A}}\frac{e}{c} = ie\vec{\alpha}\cdot\vec{E}$$

$$\underbrace{\left[O, \frac{ie}{8m^2}\vec{\alpha}\cdot\vec{E}\right]}_{O\left(\frac{v}{c}\right)^4} = \frac{ie}{8m^2}\left[\vec{\alpha}\cdot\vec{p}c, \vec{\alpha}\cdot\vec{E}\right]$$

$$= \frac{iec}{8m^2}\left(\sum_{ij}\alpha_i\alpha_j\left(-i\frac{\partial E_j}{\partial x_i}\right) + 2i\vec{\Sigma}\cdot\vec{p}\times\vec{E}\right)$$

$$= \frac{ec}{8m^2}\vec{\nabla}\cdot\vec{E} + \frac{iec}{8m^2}\vec{\Sigma}\cdot\vec{\nabla}\times\vec{E} + \frac{ec}{4m^2}\vec{\Sigma}\cdot\vec{E}\times\vec{p}$$

Terms involving $\vec{\Sigma}$ are Hermitian when taken together.
For a central electrostatic potential, $\vec{E} \parallel \vec{r}$, $\vec{\nabla} \times \vec{E} = 0$.

$$H_{\text{spin-orbit}} = -\frac{e\hbar}{4m^2c^2}\vec{\Sigma}\cdot\left(-\frac{1}{r}\frac{\partial(e\Phi)}{\partial r}\vec{r}\times\vec{p}\right)$$

$$= \frac{e\hbar}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{\Sigma}\cdot\vec{L}$$

This is due to magnetic field seen by the electron in its rest frame. It includes Thomas precession, and shows that $g=1$ for orbital magnetic moment.

The $\vec{\nabla}\cdot\vec{E}$ contribution is known as the Darwin term. It is due to the fact that a relativistic particle cannot be localised better than its Compton wavelength, and so it sees a smeared potential.

$$\langle \delta V \rangle = \langle V(\vec{r}+\delta\vec{r})\rangle - \langle V(\vec{r})\rangle$$

$$= \left\langle \delta\vec{r}\cdot\frac{\partial V}{\partial r}\hat{r} + \frac{1}{2}\sum_{i,j}\delta r_i\,\delta r_j\frac{\partial^2 V}{\partial r_i\,\partial r_j} + \dots \right\rangle$$

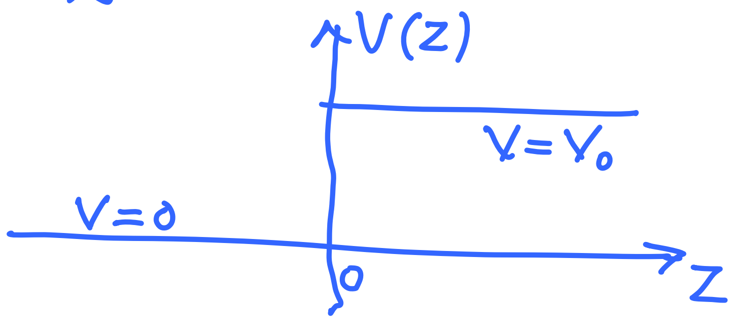
$$\simeq \frac{1}{6}(\delta\vec{r})^2\nabla^2 V, \quad \text{with } |\delta\vec{r}| \sim \frac{\hbar}{mc}$$

When there are large potentials (exceeding $2mc^2$), one cannot limit the discussion to a single particle theory. It is necessary to include processes of pair creation/annihilation.

Reflection from a potential barrier: (Klein paradox)

Consider a plane-wave incident on a step-function barrier, while moving along z-direction.

$V(z)$ is electromagnetic, but independent of spin.



Incident wave from left: $E > 0$, spin $\uparrow$

$$\psi_i = a\, e^{ip_1 z/\hbar} \begin{pmatrix} 1 \\ 0 \\ cp_1/(E+mc^2) \\ 0 \end{pmatrix} \quad : \quad E^2 = p_1^2 c^2 + m^2 c^4$$

Let $$\psi_r = b\, e^{-ip_1 z/\hbar} \begin{pmatrix} 1 \\ 0 \\ -cp_1/(E+mc^2) \\ 0 \end{pmatrix} + b'\, e^{-ip_1 z/\hbar} \begin{pmatrix} 0 \\ 1 \\ 0 \\ cp_1/(E+mc^2) \end{pmatrix}$$

$$\psi_t = d\, e^{ip_2 z/\hbar} \begin{pmatrix} 1 \\ 0 \\ cp_2/(E-V_0+mc^2) \\ 0 \end{pmatrix} + d'\, e^{ip_2 z/\hbar} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -cp_2/(E-V_0+mc^2) \end{pmatrix}$$

$$(E-V_0)^2 = p_2^2 c^2 + m^2 c^4$$

At the $z=0$ boundary, wavefunction has to be continuous, for all the spinor components.

$$(\psi_i + \psi_r)_{z=0_-} = (\psi_t)_{z=0_+}$$

$$a + b = d\,, \quad b' = d'\,, \quad (a-b)\frac{p_1}{E+mc^2} = \frac{d\,p_2}{E-V_0+mc^2}$$

$$b'\frac{p_1}{E+mc^2} = -d'\frac{p_2}{E-V_0+mc^2}$$

There is no spin-flip : $b' = 0 = d'$.

Let $\quad r = \dfrac{p_2}{p_1} \cdot \dfrac{E+mc^2}{E-V_0+mc^2}$. ($p_2$ can be imaginary)

Then, $\quad a = d\left(\dfrac{1+r}{2}\right)\,, \quad b = d\left(\dfrac{1-r}{2}\right)$.

Amount of reflection and transmission is characterised by the current $j_z = c\psi^\dagger \alpha_z \psi$.

$$\frac{(j_z)_r}{(j_z)_i} = \frac{|b|^2}{|a|^2} = \frac{|1-r|^2}{|1+r|^2}\,, \quad \frac{(j_z)_t}{(j_z)_i} = \frac{|d|^2}{|a^2|}\cdot \mathrm{Re}(r) = \frac{4\,\mathrm{Re}(r)}{|1+r|^2}$$

Continuity condition : $(j_z)_i = (j_z)_r + (j_z)_t$

(a) $E - mc^2 > V_0$: p_2 is real, $1 > r > 0 \Rightarrow j_r < j_i$, $j_t > 0$.

Partial transmission, similar to $E_{NR} > V_0$.

(b) $E + mc^2 > V_0 > E - mc^2$: p_2 is imaginary, r is imaginary

$$\Rightarrow j_r = j_i \ , \ j_t = 0 .$$

Total reflection, similar to $E_{NR} < V_0$.

(c) $V_0 > E + mc^2$: p_2 is real, $r < 0 . \Rightarrow j_r > j_i$, $j_t < 0$.

Resolution corresponds to pair creation at the barrier, and components of the pair going off in opposite directions. e.g. $e^- \longrightarrow \underbrace{e^- + e^-}_{\text{Reflected}} + \underbrace{e^+}_{\text{Transmitted}}$

Single particle description has to be given up in favour of many-body theory. (QM $\longrightarrow$ QFT)

Dirac equation thus indicates its own limitations

$-E - mc^2 > -V_0$ = Potential for e^+

For pair creation: ΔV at barrier $> 2mc^2$.

Range of this variation in $V \lesssim \frac{\hbar}{mc}$.

Quantum uncertainty allows $\Delta E \sim mc^2$ over regions of Compton wavelength. (Virtual pairs)

Large ΔV pulls virtual pairs apart creating real particle-antiparticle pairs.

This is a spontaneous process (e.g. possible with $j_i = 0$).

There is a feedback on the potential in reality. Taking out $2mc^2$ (energy) weakens potential height; that ultimately stops pair creation process.

Examples:

(1) QED: Large electric fields $|\vec{\nabla} V| > \frac{2m^2c^3}{\hbar}$.

For $Z\alpha \approx 1$, $E_0 \approx 0$ and $r_{Bohr} \approx \frac{\hbar}{mc}$.

More detailed estimates indicate $Z \gtrsim 170$ for spontaneous e^+e^- creation.

This situation can be realised in collisions of two heavy nuclei. Experimental realisation is messy because of collision dynamics and nuclear forces. (identification of source of pair creation is difficult)

(2) QCD : Potential binding quarks is confining. $q\bar{q}$ dynamical pair creation is possible when hadrons are excited sufficiently. Observed often in accelerator collisions. Rates are not easy to calculate, but qualitative expectations agree with experimental results.

(3) Gravity : Masses of particle and antiparticle are equal. The gravitational potential in Dirac equation is included by $\beta mc^2 \longrightarrow \beta(mc^2 + V_{grav})$.

For $V_{grav} > 0$: The case (c) gives $j_r = j_i$, $j_t = 0$ also (Total reflection, no pair creation)

But gravitational interaction is attractive; and pair creation is possible if V_{grav} drops sufficiently rapidly.

This is possible in case of black holes (Hawking radiation)

$$\frac{GM^2}{R} \sim Mc^2 \implies GM \sim Rc^2 \text{ for black holes}$$

Field produced by such an object is

$$V_{grav} = -\frac{GMm}{r} \sim -\frac{R}{r} mc^2 .$$

It can have $\Delta V \sim mc^2$, for $\Delta r \sim R$ at $r \sim R$.

Pairs are spontaneously produced provided $\lambda_{Compton} \gtrsim R$.

For $R \sim 10$ kms, essentially photons and gravitons are emitted. Feedback decreases M and R. Radiation loss speeds up, till black hole totally evaporates.

<u>Zitterbewegung</u>: $\vec{v}_{op} = c\vec{\alpha}$ has eigenvalues $\pm c$.

Size of the oscillations is of the order of Compton wavelength. Smearing of the trajectory leads to effects such as Darwin term in H-atom energy spectrum.

Free-particle : $\frac{d\vec{p}}{dt} = 0 \Rightarrow \vec{p} = \text{const}.$

$$\frac{d\vec{v}_{op}}{dt} = \frac{i}{\hbar}[H, c\vec{\alpha}] = \frac{2ic}{\hbar}(H\vec{\alpha} - c\vec{p}) = \frac{2i}{\hbar}(H\vec{v}_{op} - c^2\vec{p})$$

$$\therefore \vec{v}(t) = H^{-1}c^2\vec{p} + e^{2iHt/\hbar}(\vec{v}(0) - H^{-1}c^2\vec{p})$$

$$\therefore \vec{r}(t) = \vec{r}(0) + H^{-1}c^2\vec{p}\,t + \frac{\hbar}{2iH}(e^{2iHt/\hbar} - 1)(\vec{v}(0) - H^{-1}c^2\vec{p})$$

Classically, $\vec{v}_{cl} = \frac{\vec{p}c^2}{E}$, for point particle.

QM: Actual objects are wavepackets.
Spread of the wavefunction oscillates with frequency $\frac{2H}{\hbar}$.

These oscillations cannot be eliminated from any localised wavepacket. They contribute to physical quantities, e.g. $\vec{j} = c\psi^{\dagger}\vec{\alpha}\,\psi$.

A typical contribution to $\vec{j}$ couples upper and lower components of ψ (in Dirac basis).

$$\int d^3x \int \frac{d^3p'}{(2\pi)^3}\left[v(\vec{p}\,',s')\, e^{i(E't-\vec{p}\,'\cdot\vec{x})/\hbar}\right]^{\dagger} \vec{\alpha}$$

$$\times \int \frac{d^3p}{(2\pi)^3}\left[u(\vec{p},s)\, e^{-i(Et-\vec{p}\cdot\vec{x})/\hbar}\right]$$

$$= \int \frac{d^3p'}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3}\, v^{\dagger}(\vec{p}\,',s')\,\vec{\alpha}\, u(\vec{p},s)\, e^{-it(E+E')/\hbar} \cdot (2\pi)^3\delta^3(\vec{p}+\vec{p}\,')$$

$$= \int \frac{d^3p}{(2\pi)^3}\, v^{\dagger}(-\vec{p},s')\,\vec{\alpha}\, u(\vec{p},s)\, e^{-2iEt/\hbar}$$

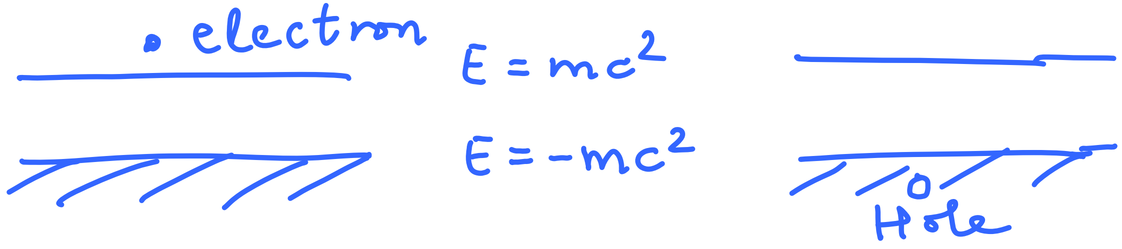
We cannot eliminate these oscillations, when using complete basis of states involving both positive and negative energy solutions.

Hole theory: Energy levels with arbitrary negative values make the theory unstable. (Nothing prevents decay to a lower energy state.)

Dirac took help of the exclusion principle, to define the vacuum state as one in which all the negative energy levels are filled. (Dirac sea)

Everything is measured w.r.t. the filled sea, the sea itself does not have observable consequences. (The absolute values $Q \to \infty$, $E \to \infty$ can be troublesome in trying to couple the quantum theory to gravity.)

A vacancy in the Dirac sea is called a hole.



Excitation from $E<0$ to $E>0$ is pair creation.
Decay from $E>0$ to $E<0$ is pair annihilation.

Absence of an electron $(Q=-e, E<0, \vec{p}, \vec{\sigma})$
$\equiv$ Presence of a positron $(Q=+e, E>0, -\vec{p}, -\vec{\sigma})$

This language is often used in condensed matter physics for describing electron bands.

Field theory quantisation needs many body language, where vacuum and operators are defined so as only positive energy excitations are available. (No sea is defined/used.)
Antiparticles are directly identified by their charge density, as in case of Klein-Gordon equation.
(Bosons cannot have a filled sea.)

Charge conjugation : Allows construction of solutions with opposite value of charge.

K.G. case : $\left[\left(i\hbar\frac{\partial}{\partial x_\mu} - \frac{e}{c}A^\mu\right)^2 - m^2c^2\right]\psi = 0$

$\Downarrow$ Complex conjugation

$$\left[\left(i\hbar\frac{\partial}{\partial x_\mu} + \frac{e}{c}A^\mu\right)^2 - m^2c^2\right]\psi^* = 0$$

Wavefunction transforms as $\psi_c = \psi^*$.

Dirac case : $\left[\left(i\hbar\not{\partial} - \frac{e}{c}\not{A}\right) - mc\right]\psi = 0$

After charge conjugation,

$$\left[\left(i\hbar\not{\partial} + \frac{e}{c}\not{A}\right) - mc\right]\psi_c = 0$$

Complex conjugation : $[(-i\hbar\partial_\mu - \frac{e}{c}A_\mu)(\gamma^\mu)^* - mc]\,\psi^* = 0$

Let $\psi_c = (C\gamma_0)\psi^*$ with $(C\gamma^0)(\gamma^\mu)^*(C\gamma^0)^{-1} = -\gamma^\mu$.

Dirac basis : γ^2 is imaginary, $\gamma^0, \gamma^1, \gamma^3$ are real.

Then $C\gamma_0 = i\gamma^2$ satisfies the requred condition.

Off-diagonal γ^2 interchanges upper and lower components of the Dirac spinor.

<u>Chirality</u> : The no. of $n\times n$ matrices obeying Clifford algebra is $n+1$.

$\gamma^5 = \gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ gives $\{\gamma^5, \gamma^\mu\} = 0$.

γ^5 is Hermitian and $(\gamma_5)^2 = 1$.

$\beta H + H\beta = 2mc^2$, $\gamma^5 H + H\gamma^5 = 2c\gamma_5 \vec{\alpha}\cdot\vec{p} = 2c\vec{\Sigma}\cdot\vec{p}$

Dirac basis : $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$, $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$, $\gamma^5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

$\vec{\Sigma}\cdot\hat{p}$ is the projection of spin along the direction of motion. It is called helicity. Also $\vec{\Sigma}\cdot\hat{p} = \vec{J}\cdot\hat{p}$.

We have, $\langle\beta\rangle = \frac{mc^2}{E}$ and $\langle\gamma^5\rangle = \langle\vec{\Sigma}\cdot\vec{p}\rangle\frac{c}{E}$.

So γ^5 is $\frac{v}{c}$ times the helicity operator, and measures the handedness of the particle.

In general, $\gamma^5 = \frac{i}{4!}\epsilon_{\mu\nu\lambda\sigma}\gamma^\mu\gamma^\nu\gamma^\lambda\gamma^\sigma$, and any 4×4 matrix can be expanded using the complete basis of 16 matrices :

$$\{\underset{1}{1}, \underset{+4}{\gamma^\mu}, \underset{+6}{\Sigma^{\mu\nu}}, \underset{+4}{\gamma^\mu\gamma^5}, \underset{+1}{\gamma^5}\}$$

They transform as $\{S, V, T, A, P\}$. : Lorentz group

γ_5 is a pseudoscalar, since $\gamma^0\gamma^5(\gamma^0)^{-1} = -\gamma^5$.

Projection operators : $\frac{1 \pm \gamma_5}{2}$ are projection operators for chirality.

Projection operator for energy is $\frac{1 \pm \gamma_0}{2}$ in the rest frame, where $p^0 = \frac{E}{c} = mc$, $\vec{p} = 0$.

Lorentz covariant form is : $\Lambda_\pm = \frac{\pm \not{p} + mc}{2mc}$.

Projection operator for spin is $\frac{1 \pm \sigma_z}{2}$ in the rest frame, with z-axis as the measurement direction.

$$\sigma_z \longrightarrow \Sigma_z = \gamma_5 \alpha_z = \gamma_5 \vec{\alpha} \cdot \hat{z} = \gamma_5 \gamma_z \gamma_0 = \gamma_5 \hat{\not{z}} \gamma_0$$

Then $\Sigma_\pm(\hat{z}) = \frac{1 \pm \gamma_5 \hat{\not{z}}}{2}$, with $E<0$ giving opposite spin compared to $E>0$.

In general Lorentz frame, spin $\vec{\Sigma}$ becomes s^μ, with $p_\mu s^\mu = 0$. So $\Sigma_\pm(s) = \frac{1 \pm \gamma_5 \not{s}}{2}$, with $s_\mu s^\mu = -1$.

<u>Weyl equation</u>: Projected from the Dirac equation for massless particles.

With no βmc^2 term in H, $\frac{1\pm\gamma_5}{2}$ commute with H.

Eigenvalues of γ_5 are ± 1. The two sectors decouple, and each can be described by a 2-component differential equation.

Weyl basis : $\gamma^5_W = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\gamma^0_W = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\vec{\alpha}_W = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix}$.

Decoupled equations : $H\Psi = \pm c\,\vec{\sigma}\cdot\vec{p}\,\Psi$

$\pm$ signs of helicity correspond to R and L particles.

This 2-component equation is useful in describing massless neutrinos.

$\vec{\sigma}$ and $-\vec{\sigma}$ are inequivalent representations, since $\sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k$ but $(-\sigma_i)(-\sigma_j) \neq i\epsilon_{ijk}(-\sigma_k)$

Experimentally, only ν_L and $\bar{\nu}_R$ are observed.

Separation of Dirac eqn. to Weyl eqn. projects according to helicity. But $\pm$ energy components remain in 2-component Weyl equation.

ν_L and $\bar{\nu}_R$ have helicities $-\frac{1}{2}$ and $+\frac{1}{2}$ respectively.

In Weyl representation, γ^0 (for parity) and γ^2 (for charge conjugation) are off-diagonal matrices. They couple L and R components of the Dirac spinor. For Weyl spinors, P and C are not good operations

$$\nu_L \xrightarrow{P} \nu_R \quad , \quad \nu_L \xrightarrow{C} \bar{\nu}_L \quad , \quad \nu_L \xrightarrow{CP} \bar{\nu}_R .$$

CP is a well-defined operation for Weyl spinors. Electromagnetic coupling of Weyl spinors cannot be defined (because EM interaction respects C). So Weyl fermions are electromagnetically neutral. Chiral gauge interactions (e.g. Weak interactions) are allowed for Weyl fermions.

Dirac fermions, in the limit $m \to 0$ or $E \gg mc^2$, behave as a pair of Weyl fermions. (e.g. ψ_L and ψ_R)

Since $\gamma_5 \left(\frac{1 \pm \gamma_5}{2}\right) = \pm \left(\frac{1 \pm \gamma_5}{2}\right)$, the operator $\bar{\psi}\gamma_5\psi$ measures the chiral charge.

Also $\psi \to e^{i\theta\gamma_5}\psi$ is an exact symmetry for massless Dirac fermion. It is called chiral symmetry, and is important in studying strong interactions. (It is broken by $m \neq 0$)

$m \neq 0$ couples ψ_L and ψ_R degrees of freedom.

Weyl and Dirac representations are related by a unitary transformation of the Clifford algebra basis.

Majorana representation: This is a choice where all γ-matrices are imaginary, and the Dirac equation is real. (Half the no. of degrees of freedom)

$$\hat{\alpha}_1 = -\alpha_1 , \ \hat{\alpha}_2 = \beta , \ \hat{\alpha}_3 = -\alpha_3 , \ \hat{\beta} = \alpha_2 \Rightarrow \hat{\gamma}_\mu^* = -\hat{\gamma}_\mu$$

Then $\left(\hbar \frac{\partial}{\partial t} + \hbar c \, \hat{\vec{\alpha}} \cdot \vec{\nabla} + i \hat{\beta} mc^2\right) \psi = 0$.

Parity can be defined using operator $i\hat{\beta}$.

Charge conjugation operation is $\psi_c = \psi^*$.

Majorana fermions are their own antiparticles.

Electromagnetic interactions ($\vec{p} \longrightarrow \vec{p} - \frac{e}{c} \vec{A}$), introduces imaginary operator in the equation.

Majorana fermions are therefore completely neutral.

Neutrinos can be Majorana particles (more correctly a mixture of Weyl and Majorana particles).

If so, there will be neutrinoless double β-decay possible.

Since neutrinos have been observed to mix, they can have Dirac/Majorana mass terms.

Majorana fermions have probability density/current, but no charge density/current. Their number is conserved only modulo 2.

The fermion statistics obeys:

$$c|0\rangle = |1\rangle, \quad c|1\rangle = |0\rangle, \quad c^2 = 1.$$

(Different from the exclusion principle)

Roughly c behaves as $a + a^\dagger$.

Whether or not Weyl + Majorana properties can be obeyed simultaneously, depends on dimension of theory. In $(3+1)$-dim., it is not possible.

<u>Time reversal</u>: It is a transformation that reverses the arrow of time. It can be a symmetry for a particular problem, e.g. $m\ddot{x} = F$.

Wigner's classification of symmetries in QM:

Symmetric transformation leaves all the transition probabilities invariant, i.e. $|\langle\phi|\psi\rangle|^2 = |\langle\phi'|\psi'\rangle|^2$.

Wigner showed that any such transformation is

(a) Unitary and linear: $\langle U\phi | U\psi\rangle = \langle\phi|\psi\rangle$

$$U(a\psi_1 + b\psi_2) = a\,U\psi_1 + b\,U\psi_2$$

(b) Antiunitary and antilinear: $\langle U\phi | U\psi\rangle = \langle\psi|\phi\rangle$

$$U(a\psi_1 + b\psi_2) = a^* U\psi_1 + b^* U\psi_2.$$

Most symmetries encountered in physical problems are unitary and linear. e.g. translation, rotation, gauge symmetry, parity, charge conjugation. These can be continuously connected to identity for continuous transformations.

Antiunitary symmetry has to be discrete. The important case is that of time reversal. The interchange of initial and final states produces complex conjugation for transition amplitudes.

For antiunitary operators, adjoint is defined by the rule, $\langle \phi | A^\dagger \psi \rangle = \langle \psi | A \phi \rangle$.

For time reversal, $t \to -t$, $\vec{x} \to \vec{x}$.

$$\vec{p} \to -\vec{p}, \quad \vec{S} \to -\vec{S}$$

$$\vec{A} \to -\vec{A}, \quad \Phi \to \Phi$$

K. G. equation: $[(i\hbar\partial_\mu - \frac{e}{c}A_\mu)^2 - m^2c^2]\,\psi = 0$

$\psi \to \psi^*$ (complex conjugation) transforms the wavefunction under time reversal.

Dirac equation: $\mathcal{T}\,\psi(\vec{x},t) = T\,\psi^*(\vec{x},-t)$

$$i\hbar\frac{\partial}{\partial t}\psi = H\,\psi = \left[\vec{\alpha}\cdot(\vec{p}-\frac{e}{c}\vec{A})c + \beta mc^2 + e\Phi\right]\psi$$

Given the changes of signs due to complex conjugation, we need $T\vec{\alpha}^*T^{-1} = -\vec{\alpha}$, $T\beta^*T^{-1} = \beta$.

In the Dirac basis, α_2 is imaginary, $\alpha_1, \alpha_3, \beta$ are real. T commutes with β and α_2, but anticommutes with α_1 and α_3. That implies $T = i\gamma^1\gamma^3$.

Applying time reversal twice should give back the original state.

PCT invariance: Property of quantum field theories in general. It relates particle and antiparticle properties.

K.G. eqn: $\mathcal{T}\psi(\vec{x},t) = \psi^*(\vec{x},-t)$

$$\mathcal{C}\mathcal{T}\psi(\vec{x},t) = \psi(\vec{x},-t)$$

$$P\mathcal{C}\mathcal{T}\psi(\vec{x},t) = \psi(-\vec{x},-t)$$

Antiparticle is a particle moving backward in space and time.

Dirac eqn: $\psi_{PCT}(x') \equiv P\mathcal{C}\mathcal{T}\psi(x)$

$$= P(C\gamma_0)(\mathcal{T}\psi(x))^*$$

$$= \gamma^0(i\gamma^2)(i\gamma^1\gamma^3)^*\psi(-x)$$

$$= i\gamma^5\psi(-x)$$

Particular internal components are projected by the operators $\frac{\pm \not{p} + m}{2m}$ and $\frac{1 \pm \gamma_5 \not{s}}{2}$.

ψ_{PCT} corresponds to opposite signs of energy and spin compared to ψ. (Consistent with hole theory)

This relation between particle and antiparticle leads to crossing symmetry in QFT.

(Particle in final state $\longleftrightarrow$ Antiparticle in initial state)

PCT invariance of QFT is a consequence of proper Lorentz invariance and spin-statistics connection. (PCT theorem)

Experimental checks of PCT need a QFT formulation going beyond the usual framework

PCT is antiunitary and relates any process to its inverse process. It relates dynamical properties of particles and antiparticles, e.g. they must have the same total decay rate. (partial decay rates may be different)

Strong, electromagnetic, gravitational interactions obey P, C, T individually.
Weak interactions violate P, C maximally, and T to a small extent.
In our experience, time is asymmetric, i.e. future is very different than past.
Causality, arrow of time, second law of thermodynamics.

In quantum theory, time is treated as a parameter, and not as an operator.

Time asymmetric boundary conditions enforce causality. (e.g. retarded propagators, $i\epsilon$-prescription, time-ordered products etc.)

In our universe, "big bang" provides the boundary conditions for time.

To create observed particle-antiparticle asymmetry, from an initially symmetric state, we need certain properties (Sakharov conditions).

(1) Baryon/Lepton number violating interaction.

(2) T/CP - violation.

Both exist at a tiny level in weak interactions.

(3) Out of equilibrium stage for the universe.

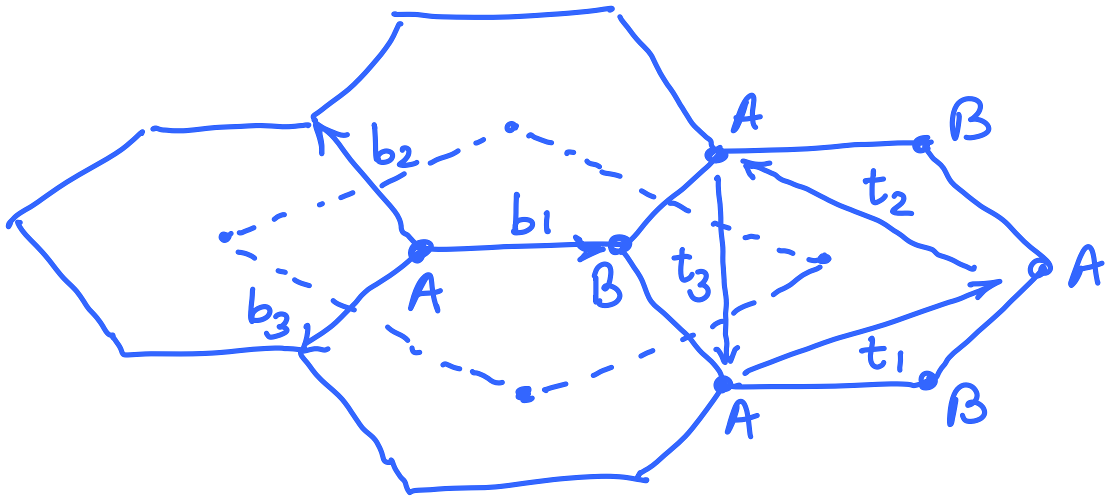
Provided by gravity.

Graphene: Condensed matter system obeying Dirac equation in 2+1 dimensions.

It is a layer of carbon atoms, arranged as a 2-dim hexagonal lattice.
Out of 4 valence electrons of carbon, 3 form bonds with sp^2 hybridisation. The fourth one is in π-orbital, and is responsible for dynamical properties at low energies.
In tight-binding approximation,

$$H = -t \sum_{\langle ij \rangle} a_i^\dagger a_j \ , \quad t > 0 \ , \quad \{a_i, a_j^\dagger\} = \delta_{ij} \ .$$

Choose units such that lattice spacing $= 1$.

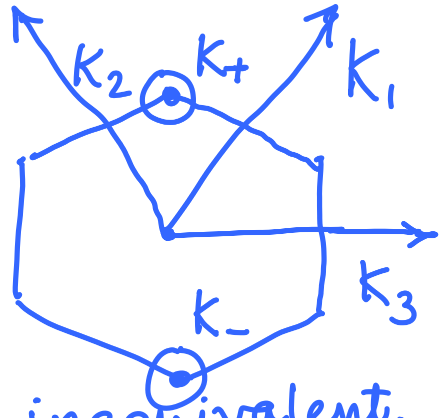


The type of site (A or B) is specified by pseudospin.
The unit cell contains both A and B sites.
The labels A and B can be interchanged by rotation of π along the axis normal to the layer.
Neighbours of A are: $\vec{b}_1 = (1,0)$, $\vec{b}_2 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$, $\vec{b}_3 = \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)$.
Neighbours of B are given by $-\vec{b}_i$.
Primitive translation vectors for unit cell are:
$\vec{t}_1 = \vec{b}_1 - \vec{b}_3$, $\vec{t}_2 = \vec{b}_2 - \vec{b}_1$, $\vec{t}_3 = \vec{b}_3 - \vec{b}_2$.

Use $\vec{t_1}$ and $\vec{t_2}$ as the basis vectors.
The reciprocal lattice vectors obey: $\vec{K_i} \cdot \vec{t_j} = 2\pi\,\delta_{ij}$

$$\vec{K_1} = \frac{4\pi}{3}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) = -\frac{4\pi}{3}\vec{b_3}\,,\quad \vec{K_2} = \frac{4\pi}{3}\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right) = \frac{4\pi}{3}\vec{b_2}.$$

Let $\vec{K_3} = \frac{4\pi}{3}\vec{b_1}$ as well.



The Brillouin zone is a hexagon, rotated by $\frac{\pi}{6}$ from the lattice.
It has opposite sides identified.
From the six corners, only two are inequivalent.
They can be chosen as $\vec{K_+} = \frac{1}{3}(\vec{K_1} + \vec{K_2}) = -\frac{4\pi}{9}\vec{t_3} = -\vec{K_-}$.

In the A-B basis, H is off-diagonal, and its Hermiticity makes it a linear combination of σ_1 and σ_2. (A σ_3-term can be added when energies of A and B sites are not equal, e.g. BN.)

$$H = -t \sum_{\substack{\text{unit}\\\text{cells}}} \begin{pmatrix} a_A^\dagger & a_B^\dagger \end{pmatrix} \begin{pmatrix} 0 & \sum_i e^{i\vec{k}\cdot\vec{b}_i} \\ \sum_i e^{-i\vec{k}\cdot\vec{b}_i} & 0 \end{pmatrix} \begin{pmatrix} a_A \\ a_B \end{pmatrix}$$

$$E^2 = t^2 \left| \sum_i e^{i\vec{k}\cdot\vec{b}_i} \right|^2 = t^2 \left(3 + 4\cos\frac{3k_x}{2} \cos\frac{\sqrt{3}k_y}{2} + 2\cos\sqrt{3}k_y \right)$$

For any k_y, E^2 is extremised at $\cos\frac{3k_x}{2} = \pm 1 \Rightarrow k_x = \frac{2\pi}{3} n$.

The extremal values are $E^2 = t^2 \left(1 \pm 2\cos\frac{\sqrt{3}k_y}{2}\right)^2$.

In particular, $E^2 = 0$ at $\left|\cos\frac{\sqrt{3}k_y}{2}\right| = \frac{1}{2}$.

$\therefore k_y = \pm \frac{2\pi}{3\sqrt{3}}$ for $k_x = \pm\frac{2\pi}{3}$, and $k_y = \pm\frac{4\pi}{3\sqrt{3}}$ for $k_x = 0$.

The corners of the Brillouin zone are given by $\pm\frac{4\pi}{9}\vec{t}_i$, where excitations can occur without energy gap.

With $\vec{t}_i \cdot \vec{t}_j = 3\vec{b}_i \cdot \vec{b}_j = \frac{9}{2}\delta_{ij} - \frac{3}{2}$, the phases $e^{\pm i\vec{k}\cdot\vec{b}_i}$ reduce to $\{1, \omega, \omega^2\}$, at these corners.

In the neighbourhood of $\vec{K}_+$: $\vec{k} = \vec{K}_+ + \vec{l}$.

Taylor expansion gives: $\sum_i e^{i\vec{k}\cdot\vec{b}_i} = \sum_i \omega^{i-1}\, \vec{l}\cdot\vec{b}_i$

$$= \frac{3}{2}(l_x + i l_y)$$

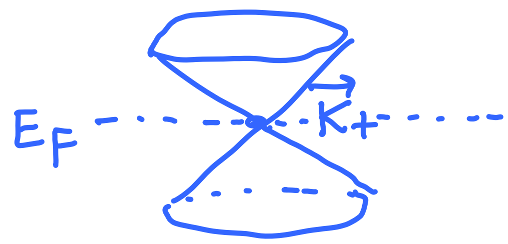
Thus, for low energy excitations, $H^{(+)}_{AB} = -\frac{3t}{2}\vec{\sigma}\cdot\vec{l}$.

In the neighbourhood of $\vec{K}_-$: $H^{(-)}_{AB} = +\frac{3t}{2}\vec{\sigma}\cdot\vec{l}$

There are eight degrees of freedom:

2 for pseudospin, 2 for $\vec{K}_\pm$, 2 for usual spin.

Velocity of light is replaced by $\frac{3t}{2} = v_F \approx 10^6 \frac{m}{s} \approx \frac{c}{300}$.



Linear dispersion relation makes quasiparticles behave differently than in case of metals.

Charge conjugation (electron-hole) symmetry is exact.

The effective fine structure constant is

$$\alpha_{eff} = \frac{e^2}{\hbar v_F \epsilon} \sim 1 \quad \text{with } \epsilon \approx 2.5.$$

Its large value makes the dynamics non-perturbative, compared to standard QED.

(1) Klein paradox : Barrier created by doping.
Massless fermions are easily pair-produced (no need for $\Delta V \sim 2mc^2$). Chirality is conserved.
There is a perfect transmission through barrier, and no backward scattering (pseudospin cannot flip).

(2) Zitterbewegung : Absence of complete localisation.
Percolation of states produces finite conductivity. (Mean free path $\gtrsim$ electron wavelength)
Even for $\mu = 0$ and $T = 0$ (no free charge carriers), there is minimal $\sigma \approx \frac{e^2}{h}$.

(3) Quantum Hall effect : The Landau level spectrum is given by $E_n = \sqrt{2|e|B\hbar v_F^2 (n+\frac{1}{2}\pm\frac{1}{2})}$,
with pseudospin contributing $\pm\frac{1}{2}$.
There is an $E=0$ level, with half the degeneracy compared to $E_n \neq 0$ levels.
Normal quantum Hall effect ; The conductance plateaus correspond to integer filling of the levels.
Here, they are shifted to half-integer plateaus.
(The ordinary spin is frozen by large $\vec{B}$.)
The properties of $E=0$ level are topological (as per the index theorem), and so robust in presence of perturbations.
The wavefunctions are localised on the scale of magnetic length, as usual in Landau levels.

(4) Vacuum polarisation: Charge impurities are screened by virtual pairs. The potential $V_0(r) = \frac{Ze^2}{\epsilon r}$ is screened to $V_0(r)\,F(r)$.
With large α_{eff}, Thomas-Fermi theory works reasonably well, giving $F(r) \approx \frac{1}{1+ZQ\ln(r/a)}$; for $r >> a$ and $Q \approx 2$. This is formally similar to QED. Impurity scattering is weakened, and charge carrier mobility is enhanced compared to perturbative estimates.
(5) Scattering: For short-range potentials, in two dimensions, the scattering cross-section is finite for Dirac equation ($\propto R^2$), but is log-divergent for Schrödinger equation ($\propto \ln^2(k_F R)$).

(6) Phonons: Long range order cannot exist in two dimensions. (No perfect crystals) Graphene gets crumpled by long wavelength phonons. The effect of lattice distortions near $\vec{K}_\pm$ is equivalent to an Abelian gauge field (random magnetic field). That suppresses weak localisation effects.