Schrödinger Equation → for non-relativistic particles

$\psi = N e^{i(kx - wt)}$ → EMW solution

$\psi = N e^{i(px - Et)/\hbar}$ where $k = \frac{p}{\hbar}$, $w = \frac{E}{\hbar}$

Non-relativistic relation btw E and p

$$E = \underbrace{\frac{p^2}{2m}}_{E_k} + \underbrace{V}_{E_p}$$

$\Downarrow$

$$\boxed{E\psi = \frac{p^2}{2m}\psi + V\psi}$$

Schrödinger Equation for a non-rel part, no-spin

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi}$$

$$\frac{\partial \psi}{\partial x} = N(ik)\, e^{i(kx - wt)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = N(ik)^2 e^{i(kx - wt)} = -k^2 \psi = -\frac{p^2}{\hbar^2}\psi$$

$$\boxed{p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2}}$$

$$\frac{\partial \psi}{\partial t} = N(-iw)\, e^{i(kx - wt)} = -i\frac{E}{\hbar}\psi \Rightarrow \boxed{E\psi = i\hbar \frac{\partial \psi}{\partial t}}$$

Contunuity Equation

$$\underbrace{-\frac{\partial \rho}{\partial t}}_{\text{Decrease of \# of particles in Vol.}} = \underbrace{\nabla \cdot \vec{j}}_{\text{\# of particles leaving Vol.}}$$

ρ: charge density

$\vec{j}$: current, flux of ρ

What's the relation with quantum mechanics?

Schrödinger Eqn. for a free particle $(V=0)$

$$i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi = 0$$

→ Multiply with ψ^*

$$\psi^* \left(i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi \right) = 0$$

→ Multiply with ψ

$$\psi \left(i\hbar \frac{\partial \psi^*}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi^* \right) = 0$$

→ Substract

$$\psi^* \left(i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi \right) - \psi \left(i\hbar \frac{\partial \psi^*}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi^* \right) = 0$$

$$\frac{i\hbar}{i\hbar}\left(\psi^*\frac{\partial\psi}{\partial t}+\psi\frac{\partial\psi^*}{\partial t}\right)+\frac{\hbar^2}{i\hbar\,2m}\left(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*\right)=0$$

$$\frac{\partial\overbrace{(\psi\psi^*)}^{\rho}}{\partial t}+\underbrace{\nabla\cdot\left(\frac{-i\hbar}{2m}\right)\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)}_{j}=0$$

$$\rho=\psi\psi^*=|\psi|^2$$

$$j=\left(\frac{-i\hbar}{2m}\right)\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)=0$$

The Klein-Gordon Equation → to describe relativistic electron

$$\boxed{E^2=p^2+m^2}$$ → relativistic relation

$$(\hat{E})^2\psi=(\hat{p})^2\psi+m^2\psi$$

$$\boxed{\hbar=1}$$

$$\hat{E}\Rightarrow i\frac{\partial}{\partial t}$$

$$\left(i\frac{\partial}{\partial t}\right)^2\psi=(-i\nabla)^2\psi+m^2\psi$$

$$\hat{p}_x\Rightarrow -i\frac{\partial}{\partial x}$$

$$\boxed{\frac{\partial^2\psi}{\partial t^2}=\nabla^2\psi-m^2\psi}$$

$$\hat{p}_y=-i\frac{\partial}{\partial y}$$

$$\hat{p}_z=-i\frac{\partial}{\partial z}$$

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \qquad \mu = 0, 1, 2, 3$$

$$\partial^\mu \partial_\mu = \left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \right)$$

$$\boxed{(\partial^\mu \partial_\mu + m^2)\,\psi = 0}$$

Problems with the Klein-Gordon Equation:

→ Negative Energy Solutions → $E = \pm\sqrt{|p|^2 + m^2}$

implies ↳ No ground state in atoms

→ Transitions to lower energy states always possible.

→ Negative particle densities associated with these solutions

For a plane wave $\psi = N e^{i(p.r - Et)}$

$$\rho = 2E|N|^2$$

Schrödinger Equation: $-\frac{1}{2m}\nabla^2\psi = i\frac{\partial\psi}{\partial t}$ $\nearrow$ 1st order in $\partial/\partial t$ $\searrow$ 2nd order in $\partial/\partial x$, $\partial/\partial y$, $\partial/\partial z$

Klein-Gordon Equation: $(\partial^\mu\partial_\mu + m^2)\psi = 0 \rightarrow$ 2nd order

Dirac looked for an alternative which was first order throughout

$$\hat{H}\psi = (\alpha.p + \beta m)\psi = i\frac{\partial\psi}{\partial t}$$

Hamiltonian operator $\qquad -i\nabla$

$$\left(-i\alpha_x\frac{\partial}{\partial x} - i\alpha_y\frac{\partial}{\partial y} - i\alpha_z\frac{\partial}{\partial z} + \beta m\right)^2\psi = \left(i\frac{\partial}{\partial t}\right)^2\psi \qquad (1)$$

$$\Big(-\alpha_x^2\frac{\partial^2\psi}{\partial x^2} - \alpha_y^2\frac{\partial^2\psi}{\partial y^2} - \alpha_z^2\frac{\partial^2\psi}{\partial z^2} + \beta^2m^2\psi$$

$$-(\alpha_x\alpha_y + \alpha_y\alpha_x)\frac{\partial^2\psi}{\partial x\partial y} - (\alpha_y\alpha_z + \alpha_z\alpha_y)\frac{\partial^2\psi}{\partial y\partial z} - (\alpha_z\alpha_x + \alpha_x\alpha_z)\frac{\partial^2\psi}{\partial z\partial x}$$

$$-(\alpha_x\beta + \beta\alpha_x)m\frac{\partial\psi}{\partial x} - (\alpha_y\beta + \beta\alpha_y)m\frac{\partial\psi}{\partial y} - (\alpha_z\beta + \beta\alpha_z)m\frac{\partial\psi}{\partial z}$$

It must obey $E^2 = p^2 + m^2$ (Klein Gordon)

$$-\frac{\partial^2\psi}{\partial t^2} = -\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi}{\partial y^2} - \frac{\partial^2\psi}{\partial z^2} + m^2\psi$$

$\Big\downarrow$ Thus

$$\boxed{\begin{aligned} &\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1 \\ &\alpha_j \beta + \beta \alpha_j = 0 \\ &\alpha_j \alpha_k + \alpha_k \alpha_j = 0 \quad (j = k) \end{aligned}}$$

α_i and β can not be numbers!

4 mutually anti-commuting matrices

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \rightarrow \text{Dirac spinor}$$

For the Hamiltonian $\hat{H}$ to be Hermitian

$$\alpha_x = \alpha_x^\dagger \; ; \; \alpha_y = \alpha_y^\dagger \; ; \; \alpha_z = \alpha_z^\dagger \; ; \; \beta = \beta^\dagger$$

Let's choose

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}_{4\times4} \qquad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$$

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Dirac Equation : Probability density and current

$$\nabla \cdot (\underbrace{\psi^{+} \alpha \psi}_{\vec{j}}) + \frac{\partial (\overbrace{\psi^{+}\psi}^{\rho})}{\partial t} = 0$$

$$\psi^{+} = (\psi_1^{+}, \psi_2^{+}, \psi_3^{+}, \psi_4^{+})$$

$$\rho = \psi^{+}\psi = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2 > 0$$

Unlike the KG equation, Dirac Equation has prob. densities which are always positive.

Dirac gamma matrices

$$\gamma^0 = \beta \;, \quad \gamma^1 \equiv \beta \alpha_x \;, \quad \gamma^2 = \beta \alpha_y \;, \quad \gamma^3 \equiv \beta \alpha_z$$

Multiply Eq(1) with $-\beta$

$$\left(i\beta\alpha_x \frac{\partial}{\partial x} + i\beta\alpha_y \frac{\partial}{\partial y} + i\beta\alpha_z \frac{\partial}{\partial z} - \underbrace{\beta^2}_{(\gamma^0)^2 = 1} m \right)\psi = -\left(i\beta \frac{\partial}{\partial t} \right)\psi$$

$$i\gamma^1 \frac{\partial \psi}{\partial x} + i\gamma^2 \frac{\partial \psi}{\partial y} + i\gamma^3 \frac{\partial}{\partial z} - m\psi = -i\gamma^0 \frac{\partial \psi}{\partial t}$$

where $\partial_\mu = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$

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

Gamma matrices are not four-vectors → they're constant matrices which remain invariant under a Lorentz transformation

Examples: Particle at rest where $p = 0$

$$\left(i\gamma^0 \frac{\partial}{\partial t} - m\right)\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix} \quad \text{where} \quad \gamma^0 = \begin{pmatrix} I & 0 \\ 0 & I\end{pmatrix}$$

$$i\begin{pmatrix} I & 0 \\ 0 & -I\end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix} = m\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix} \qquad (2)$$

Spinor ψ naturally splits into 2-component bi-spinors : $\psi = \begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}$

$$i\frac{\partial \psi_A}{\partial t} = m\psi_A \quad , \quad i\frac{\partial}{\partial t}\psi_B = -m\psi_B$$

$$\psi_A = v_A e^{-imt} \qquad \psi_B = u_B e^{imt}$$

$E > 0$ (positive energy sol) $\qquad E < 0$ (negative energy sol)

$$\begin{pmatrix} mI & 0 \\ 0 & -mI \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = m \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$i \frac{\partial \psi_A}{\partial t} = i u_A (-im) e^{-iMt}$$
$$= M u_A e^{-iMt}$$

Since left hand side is diagonal, one can find decoupled solutions for u_A and u_B and choose set of eigenvectors

$u_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $u_A = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ with $E = +M$

$u_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $u_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ with $E = -M$

Solutions:

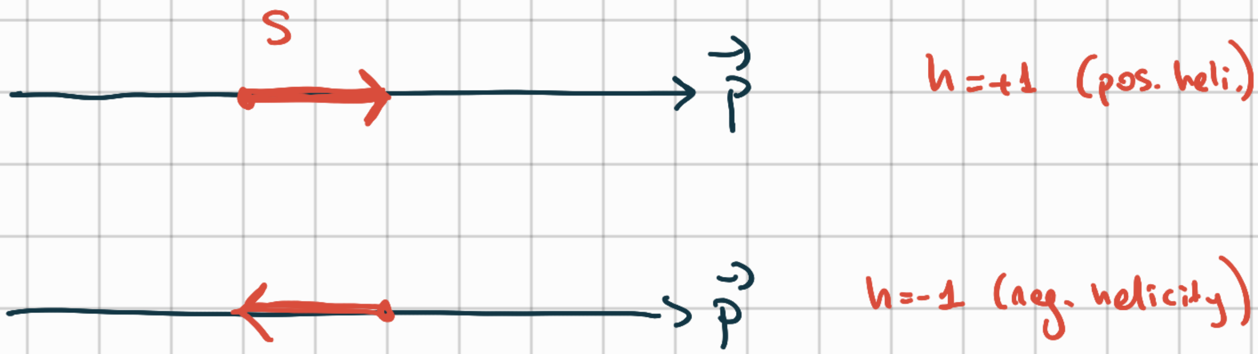
$\psi_0^{(1)} = N \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-iMt}$ $\quad \psi_0^{(2)} = N \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-iMt}$ with positive E

$\psi_0^{(3)} = N \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{+iMt}$ $\quad \psi_0^{(4)} = N \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{+iMt}$ with negative E

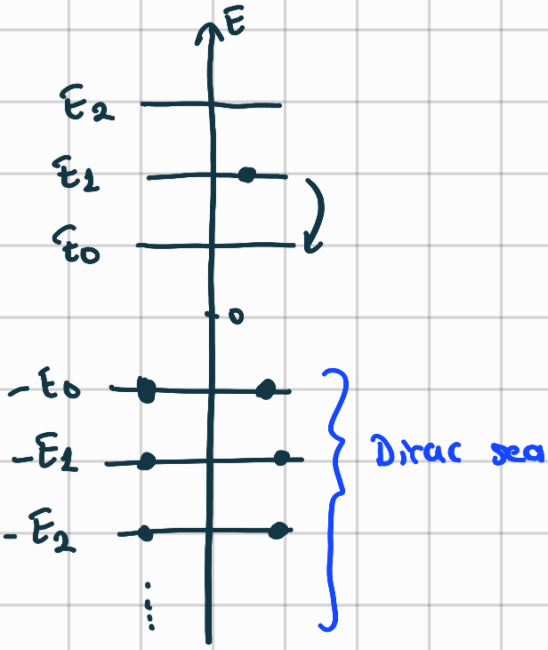
* The fact that there are two identical fermions with the same energy implies that there's another quantum number that allows to distinguish them

Helicity

The corresponding operator projects the spin on the direction of motion

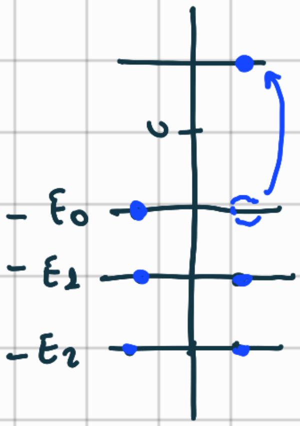


Dirac's explanation for negative energy solutions



Dirac hypothesized that all the states of negative energy are already occupied by 2 electrons, preventing another electron to reach these states.

If sufficient energy provided to an e^- of Dirac sea



Missing $\bar{e}$ appears like a hole in the sea

Missing $E<0$ $\Rightarrow$ Presence of $E>0$

Missing $q=-e$ $\Rightarrow$ Presence of $q=+e$

$\downarrow$

Positron :)

Discored by C. Anderson (1932)

Instead of Dirac sea $\rightarrow$ Feynman - Stückelberg Interpretation for $E<0$ (1940)

* Each particle of mass m and charge q corresponds an antiparticle of mass m and charge $-q$

$E<0$ $\quad -Et \rightarrow E(-t)$