Relativistic Quantum Mechanics

The Klein-Gordon equation
Interpretation of the Klein-Gordon equation
The Dirac equation
Dirac representation for the matrices α and β
Covariant form of the Dirac equation

Why Relativistic Quantum Mechanics?

The Schrödinger equation: correctly describes the phenomena only if particle velocities are $v \ll c$.

It is not invariant under a Lorentz change of the reference frame (required by the principle of relativity).

Need: a relativistic generalization!

Free particle of spin zero

The Klein-Gordon equation

So, how to come up with such an equation?

For the relativistic particle with rest mass m and momentum $\mathbf{p}$,

$$E = \sqrt{m^2c^4 + \mathbf{p}^2c^2}.$$

Using the correspondence rule

$$E \to E_{op} = i\hbar\frac{\partial}{\partial t}; \qquad \mathbf{p} \to \mathbf{p}_{op} = -i\hbar\nabla$$

one can write: $i\hbar\frac{\partial}{\partial t}\Psi = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)^{1/2}\Psi.$

Problems: 1. It is not clear how to interpret the operator on right-hand side. If expanded in power series it lead to differential operator of infinite order.

2. The time and space coordinates do not appear in a symmetric way (no relativistic invariance ?).

Free particle of spin zero

The Klein-Gordon equation

So we remove the square root and try again (there will be consequences of removing this square root!)

$$E^2 = m^2c^4 + \mathbf{p}^2c^2$$

$$E \to E_{op} = i\hbar\frac{\partial}{\partial t}; \qquad \mathbf{p} \to \mathbf{p}_{op} = -i\hbar\nabla$$

$$\boxed{-\hbar^2\frac{\partial^2\Psi}{\partial t^2} = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)\Psi.} \Longleftarrow \text{The Klein-Gordon equation}$$

Notes: it is second-order differential equation with respect to the time unlike the Schrödinger equation.

Probabilistic interpretation of non-relativistic quantum mechanics

$P(\mathbf{r},t) = \left|\Psi(\mathbf{r},t)\right|^2 = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t) \longleftarrow$ Position probability density

Probability is conserved: $\frac{\partial}{\partial t}\int P(\mathbf{r},t)d\mathbf{r} = 0$

Using the Schrödinger equation $i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right)\Psi(\mathbf{r},t)$

we obtain $\frac{\partial P(\mathbf{r},t)}{\partial t} + \nabla\mathbf{j}(\mathbf{r},t) = 0$, where **j** can be interpreted as probability current density

$$\mathbf{j}(\mathbf{r},t) = \frac{\hbar}{2mi}\left[\Psi^*(\nabla\Psi) - \left(\nabla\Psi^*\right)\Psi\right].$$

Interpretation of the Klein-Gordon equation: Problem 1

We try to construct a position probability density P(**r**,t) and probability current density **j**(**r**,t) which satisfy the continuity equation:

$$\frac{\partial P(\mathbf{r},t)}{\partial t} + \nabla\mathbf{j}(\mathbf{r},t) = 0.$$

multiply by Ψ^* $\left[-\hbar^2\frac{\partial^2\Psi}{\partial t^2} = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)\Psi\right]$

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multiply by Ψ $\left[-\hbar^2\frac{\partial^2\Psi^*}{\partial t^2} = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)\Psi^*\right]$

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

Interpretation of the Klein-Gordon equation: Problem 1

If we require that the expressions from **j**(**r**,t) and P(**r**,t) had correct non-relativistic limits we define

$$\mathbf{j}(\mathbf{r},t) = \frac{\hbar}{2mi}\left[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\right].$$

Then, we obtain the equation $\dfrac{\partial P(\mathbf{r},t)}{\partial t} + \nabla\mathbf{j}(\mathbf{r},t) = 0.$

with $P(\mathbf{r},t) = \dfrac{i\hbar}{2mc^2}\left[\Psi^*\dfrac{\partial\Psi}{\partial t} - \Psi\dfrac{\partial\Psi^*}{\partial t}\right].$

P(**r**,t) is not positive-definite and can not be interpreted as position probability density.

Interpretation of the Klein-Gordon equation: Problem 2

Free particle Klein-Gordon equation: $-\hbar^2\dfrac{\partial^2\Psi}{\partial t^2} = \left(m^2c^4 - \hbar^2c^2\nabla^2\right)\Psi.$

Plane wave solutions: $\Psi(\mathbf{r},t) = Ae^{i(\mathbf{kr}-\omega t)}.$

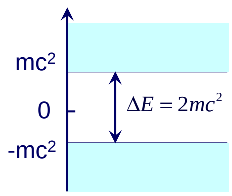
$$E = \hbar\omega$$

$$\mathbf{p} = \hbar\mathbf{k}$$

$$\hbar^2\omega^2 = m^2c^4 + \hbar^2c^2k^2$$

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

We get additional "negative-energy" solutions and energy spectrum is not bound from below. Then, arbitrary large energy can be extracted from the system if external perturbation leads to transition between positive and negative energy states.



Interpretation of the Klein-Gordon equation

In 1934 W. Pauli and V. Weisskopf reinterpreted Klein-Gordon equation as a field equation and quantized it using the formalism of quantum field theory.

Klein-Gordon equation

$\Downarrow$

Relativistic wave equation for spinless particles in the framework of many-particle theory; negative energy states are interpreted in terms of antiparticles.

Still, is it possible to define positive-definite position probability density within the framework of the relativistic theory? $\longrightarrow$ Dirac equation

Note: we will still get negative-energy states…

Dirac equation

P.A. Dirac (1928)

We start from the wave equation in the form $i\hbar\frac{\partial}{\partial t}\Psi = H\Psi.$

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{pmatrix}$$

Spatial coordinates (x_1=x, x_2=y, x_3=z) of a space-time point (event) and the time coordinate (x_4=ict) have to enter on the same footing. Therefore, the hamiltonian H must be linear in space derivatives as well.

Free particle

Simplest Hamiltonian:

1) Must be independent of **r** and t
2) Must be linear in **p** and m

$$\boxed{H = c\,\boldsymbol{\alpha}\cdot\mathbf{p}_{op} + \beta mc^2} \qquad \mathbf{p}_{op} = -i\hbar\nabla$$

$\alpha_1, \alpha_2, \alpha_3$ and β
1) are independent of **r**, t, **p**, and E
2) do not have to commute with each other

How to determine α and β?

$$i\hbar\frac{\partial}{\partial t}\Psi = -i\hbar c\,\boldsymbol{\alpha}\cdot\nabla\Psi + \beta mc^2\Psi \quad \text{or} \quad \left[E_{op} - c\,\boldsymbol{\alpha}\cdot\mathbf{p}_{op} - \beta mc^2\right]\Psi = 0$$

The solution of the Dirac equation also must be a solution of the Klein-Gordon equation

$$\left[E_{op}^2 - c^2\mathbf{p}_{op}^2 - m^2c^4\right]\Psi = 0.$$

We use it to determine the restrictions on the values of α and β by matching the coefficients in

$$\left[E_{op} - c\,\boldsymbol{\alpha}\cdot\mathbf{p}_{op} - \beta mc^2\right]\left[E_{op} - c\,\boldsymbol{\alpha}\cdot\mathbf{p}_{op} - \beta mc^2\right]\Psi = 0$$

and

$$\left[E_{op}^2 - c^2\mathbf{p}_{op}^2 - m^2c^4\right]\Psi = 0.$$

Note: we drop the index $_{op}$ in the derivation below.

How to determine α and β? Some transformations

$$\left[E - c\,\boldsymbol{\alpha}\cdot\mathbf{p} - \beta mc^2\right]\left[E - c\,\boldsymbol{\alpha}\cdot\mathbf{p} - \beta mc^2\right]\Psi = 0$$

$$\left[E^2 - Ec(\boldsymbol{\alpha}\cdot\mathbf{p}) - E\beta mc^2 - c(\boldsymbol{\alpha}\cdot\mathbf{p})E + c^2(\boldsymbol{\alpha}\cdot\mathbf{p})(\boldsymbol{\alpha}\cdot\mathbf{p}) + c(\boldsymbol{\alpha}\cdot\mathbf{p})\beta mc^2\right.$$
$$\left. -\beta mc^2 E + \beta mc^3(\boldsymbol{\alpha}\cdot\mathbf{p}) + \beta^2 m^2c^4\right]\Psi = 0$$

$$\left[E^2 - 2E\left(c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2\right) + c^2(\boldsymbol{\alpha}\cdot\mathbf{p})(\boldsymbol{\alpha}\cdot\mathbf{p}) + mc^3\left[(\boldsymbol{\alpha}\cdot\mathbf{p})\beta + \beta(\boldsymbol{\alpha}\cdot\mathbf{p})\right] + \beta^2m^2c^4\right]\Psi = 0$$

$$\left[E^2 - c^2(\boldsymbol{\alpha}\cdot\mathbf{p})(\boldsymbol{\alpha}\cdot\mathbf{p}) - mc^3\left[(\boldsymbol{\alpha}\cdot\mathbf{p})\beta + \beta(\boldsymbol{\alpha}\cdot\mathbf{p})\right] - \beta^2m^2c^4\right]\Psi = 0$$

$$\left[E^2 - c^2\sum_{i=1}^{3}\alpha_i^2 p_i^2 - c^2\sum_{i<j}\left(\alpha_i\alpha_j + \alpha_j\alpha_i\right)p_i\,p_j - mc^3\sum_{i=1}^{3}\left(\alpha_i\beta + \beta\alpha_i\right)p_i - \beta^2m^2c^4\right]\Psi = 0$$

How to determine α and β?

Now we can match the coefficients of

$$\left[E^2 - c^2\sum_{i=1}^{3}\alpha_i^2 p_i^2 - c^2\sum_{i<j}\left(\alpha_i\alpha_j + \alpha_j\alpha_i\right)p_i\,p_j - mc^3\sum_{i=1}^{3}\left(\alpha_i\beta + \beta\alpha_i\right)p_i - \beta^2 m^2 c^4\right]\Psi = 0$$

and

$$\left[E^2 - c^2\mathbf{p}^2 - m^2c^4\right]\Psi = 0.$$

$$\boxed{\alpha_i^2 = 1}$$

$$\boxed{\beta^2 = 1}$$

$$\boxed{\alpha_i\beta + \beta\alpha_i = 0,\ i = 1, 2, 3}$$

$$\boxed{\begin{array}{c}\alpha_i\alpha_j + \alpha_j\alpha_i = 0 \\ i \neq j\end{array}}$$

Properties of α and β

$$\alpha_1^2 = 1 \qquad \{\alpha_1, \beta\} = 0 \qquad \{\alpha_1, \alpha_2\} = 0$$

$$\alpha_2^2 = 1 \qquad \{\alpha_2, \beta\} = 0 \qquad \{\alpha_2, \alpha_3\} = 0 \qquad \alpha_i = \alpha_i^\dagger$$

$$\alpha_3^2 = 1 \qquad \{\alpha_3, \beta\} = 0 \qquad \{\alpha_1, \alpha_3\} = 0 \qquad \beta = \beta^\dagger$$

$$\beta^2 = 1$$

Therefore, α_1, α_2, α_3,and β anticommute in pairs and their squares are equal to unity.

Clearly, they must be matrices.
The eigenvalues of α and β are ±1.

$$\beta\alpha_i = -\alpha_i\beta \qquad Tr\left(\alpha_i\right) = Tr\left(\beta\right) = 0$$

$$\alpha_i = -\beta\alpha_i\beta = \alpha_i\beta\beta = \alpha_i\beta^2$$

$$Tr\left(\alpha_i\right) = Tr(-\beta\alpha_i\beta) = Tr(\alpha_i\beta^2) = Tr(\beta\alpha_i\beta) = 0$$

What if the lowest rank of α and β? Dirac representation of α and β.

What is the lowest rank of the representation for α and β?

$Tr(\alpha_i) = Tr(\beta) = 0$ Therefore, rank N must be even.

For 2x2 matrices we can not find a representation of more than 3 anticommuting matrices.
Therefore, the lowest representation has N=4.

Dirac representation:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

where σ_i (i=1,2,3) are Pauli matrices

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

Dirac equation

For N=4, the wave function $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{pmatrix}$ is a four-component spinor

and describes spin ½ particles.

We note that this result may be foreseen as in non-relativistic quantum mechanics spin ½ particles are described by 2-component spinors and each spin ½ particle has an antiparticle with the same mass and spin, which lead to 4-component wave function.

Higher rank matrix representations correspond to particle with spin greater than ½.

Covariant form of the Dirac equation

$$i\hbar\frac{\partial}{\partial t}\Psi = -i\hbar c\,\boldsymbol{\alpha}\cdot\nabla\Psi + \beta mc^2\Psi \qquad x_\mu \equiv (\mathbf{x}, ict)$$

$$\beta\times\left[-\hbar\frac{\partial\Psi}{\partial x_4} + i\hbar\sum_{i=1}^{3}\alpha_i\frac{\partial}{\partial x_i}\Psi - \beta mc\Psi = 0\right]$$

$$\left[-i\beta\sum_{i=1}^{3}\alpha_i\frac{\partial}{\partial x_i} + \beta\frac{\partial}{\partial x_4} + \frac{mc}{\hbar}\right]\Psi = 0$$

$$\boxed{\left[\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right]\Psi = 0} \qquad \gamma_i = -i\beta\alpha_i \qquad \gamma_4 = \beta$$

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \quad \mu,\nu = 1,2,3,4$$

From the Dirac representation for the α and β

$$\gamma_i = i\begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$