Attempts to 'Relativize' Quantum Mechanics

Why Schrödinger equation is non-relativistic?

- The Schrödinger equation is
$$i\frac{\partial\psi(t,\mathbf{x})}{\partial t} = \hat{H}\psi(t,\mathbf{x}), \tag{1}$$
where $\psi(t,\mathbf{x})$ is the single-particle wave function which depends on time t and position $\mathbf{x} \in \mathbb{R}^3$ and $\hat{H}$ is the Hamilton operator given as
$$\hat{H} \equiv \frac{\hat{\mathbf{p}}^2}{2m} + V(t,\mathbf{x}), \tag{2}$$
m is the particle's mass, $\hat{\mathbf{p}}$ is the momentum operator and $V(t,\mathbf{x})$ is the particle's potential energy.

- The hats denote the operators which act in the space of states and there are used the natural units with $\hbar = c = 1$.

- The kinetic energy operator is expressed through the momentum operator in the same way as the classical non-relativistic kinetic energy is expressed through the momentum. This is the first kinematic reason why the Schrödinger equation is non-relativistic.

- The second reason is that the potential energy, which enters the Hamiltonian, assumes an instantaneous interaction.

Klein-Gordon equation

- Keeping in mind that in quantum mechanics the classical energy and momentum are replaced by the operators
$$\mathbf{p} \to -i\nabla, \qquad E \to i\frac{\partial}{\partial t}, \tag{3}$$
the free Schrödinger equation can be 'relativized' referring to the relativistic dispersion relation
$$E^2 = \mathbf{p}^2 + m^2 \to -\frac{\partial^2}{\partial t^2} = -\nabla^2 + m^2. \tag{4}$$
Then, we get the Klein-Gordon equation
$$-\frac{\partial^2}{\partial t^2}\,\phi(x) = \Big(-\nabla^2 + m^2\Big)\,\phi(x), \tag{5}$$
which is usually written as
$$\Big(\Box + m^2\Big)\,\phi(x) = 0, \tag{6}$$
where x is the position four-vector $x^\mu \equiv (t,\mathbf{x})$ with $\mu = 0,1,2,3$, $\Box \equiv \frac{\partial^2}{\partial t^2} - \nabla^2$ and $\phi(x)$ is supposed to be the relativistic wave function.

- Let us repeat the reasoning using the four-vectors
$$p^\mu = (E, p_x, p_y, p_z) \to \hat{p}^\mu = i\partial^\mu = i\Big(\frac{\partial}{\partial t}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}\Big). \tag{7}$$

One should remember that

$$p_\mu = (E, -p_x, -p_y, -p_z) \to \hat{p}_\mu = i\partial_\mu = i\Big(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\Big). \tag{8}$$

We write down the relation (4) as

$$p_\mu p^\mu = m^2 \to -\partial_\mu \partial^\mu = m^2, \tag{9}$$

and obviously we again get the Klein-Gordon equation (6) as $\partial_\mu \partial^\mu = \Box$.

- In relativistic classical mechanics the interaction of a particle of charge e with electromagnetic field is included replacing four-momentum p^μ by $p^\mu - eA^\mu(x)$ with $A^\mu(x)$ being the electromagnetic four-potential. Proceeding analogously, the Klein-Gordon becomes

$$\Big(\big(\partial^\mu + ieA^\mu(x)\big)\big(\partial_\mu + ieA_\mu(x)\big) + m^2\Big)\,\phi(x) = 0. \tag{10}$$

Conserved current

- The norm of wave function, which obeys the Schrödinger equation (1), is time independent that is

$$\frac{d}{dt}\int d^3x\,|\psi(t,\mathbf{x})|^2 = 0, \tag{11}$$

provided the Hamiltonian (2) is hermitian which requires $V(t,\mathbf{x}) \in \mathbb{R}$.

- The differential form of the condition (11) is

$$\frac{\partial}{\partial t}P(t,\mathbf{x}) + \nabla\cdot\mathbf{S}(t,\mathbf{x}) = 0, \tag{12}$$

where $P(t,\mathbf{x})$ and $\mathbf{S}(t,\mathbf{x})$ are the probability density and current

$$P(t,\mathbf{x}) \equiv |\psi(t,\mathbf{x})|^2, \tag{13}$$

$$\mathbf{S}(t,\mathbf{x}) \equiv \frac{i}{2m}\Big(\psi(t,\mathbf{x})\nabla\psi^*(t,\mathbf{x}) - \big(\nabla\psi(t,\mathbf{x})\big)\psi^*(t,\mathbf{x})\Big). \tag{14}$$

- One finds the equation (12) in the following way. We write down the pair of Schrödinger equations

$$i\frac{\partial\psi(t,\mathbf{x})}{\partial t} = \Big[-\frac{\nabla^2}{2m} + V(t,\mathbf{x})\Big]\psi(t,\mathbf{x}),$$
$$-i\frac{\partial\psi^*(t,\mathbf{x})}{\partial t} = \Big[-\frac{\nabla^2}{2m} + V(t,\mathbf{x})\Big]\psi^*(t,\mathbf{x}),$$

where $V(t,\mathbf{x}) \in \mathbb{R}$. Multiplying the first equation by $-i\psi^*(t,\mathbf{x})$, the second one by $i\psi(t,\mathbf{x})$ and summing up the equations, we get

$$\psi^*(t,\mathbf{x})\frac{\partial\psi(t,\mathbf{x})}{\partial t} + \psi(t,\mathbf{x})\frac{\partial\psi^*(t,\mathbf{x})}{\partial t} = i\psi^*(t,\mathbf{x})\frac{\nabla^2}{2m}\psi(t,\mathbf{x}) - i\psi(t,\mathbf{x})\frac{\nabla^2}{2m}\psi^*(t,\mathbf{x}), \tag{15}$$

which is manipulated to

$$\frac{\partial}{\partial t}\Big(\psi^*(t,\mathbf{x})\,\psi(t,\mathbf{x})\Big) - \nabla\Big(i\psi^*(t,\mathbf{x})\frac{\nabla}{2m}\psi(t,\mathbf{x}) - i\psi(t,\mathbf{x})\frac{\nabla}{2m}\psi^*(t,\mathbf{x})\Big) = 0, \tag{16}$$

and finally gives Eq. (12).

- Let us proceed analogously with the Klein-Gordon equation.

$$\Big(\big(\partial^\mu + ieA^\mu(x)\big)\big(\partial_\mu + ieA_\mu(x)\big) + m^2\Big)\,\phi(x) = 0, \tag{17}$$

$$\Big(\big(\partial^\mu - ieA^\mu(x)\big)\big(\partial_\mu - ieA_\mu(x)\big) + m^2\Big)\,\phi^*(x) = 0. \tag{18}$$

where $A^\mu(x) \in \mathbb{R}$ and $m \in \mathbb{R}$. Multiplying the first equation by $\phi^*(x)$, the second one by $-\phi(x)$ and summing up the equations, we get

$$\phi^*(x)\,\big(\partial^\mu + ieA^\mu(x)\big)\big(\partial_\mu + ieA_\mu(x)\big)\,\phi(x) - \phi(x)\big(\partial^\mu - ieA^\mu(x)\big)\big(\partial_\mu - ieA_\mu(x)\big)\,\phi^*(x) = 0,$$

which gives

$$\partial_\mu\Big[\phi^*(x)\,\big(\partial^\mu + ieA^\mu(x)\big)\,\phi(x) - \Big(\big(\partial^\mu - ieA^\mu(x)\big)\phi^*(x)\Big)\,\phi(x)\Big] = 0.$$

The four-current thus reads

$$j^\mu(x) \equiv i\phi^*(x)\,\big(\partial^\mu + ieA^\mu(x)\big)\,\phi(x) - i\Big(\big(\partial^\mu - ieA^\mu(x)\big)\phi^*(x)\Big)\,\phi(x). \tag{19}$$

Because of the extra i the current $j^\mu = (j^0, \mathbf{j})$ is real. The current obeys the continuity equation

$$\partial_\mu j^\mu(x) = 0, \tag{20}$$

but j^0 can be both positive and negative. So, j^0 cannot be interpreted as a probability density.

- j^μ can be interpreted as an electric four-current.

Solutions of Klein-Gordon equation

- We are going to solve the Klein-Gordon equation using the Fourier transformation

$$\phi(p) = \int d^4x\, e^{ipx}\phi(x), \tag{21}$$

and its inverse

$$\phi(x) = \int \frac{d^4p}{(2\pi)^4}\, e^{-ipx}\phi(p). \tag{22}$$

- Substituting the field $\phi(x)$ in the form (22) to Eq. (6), one obtains

$$\int \frac{d^4p}{(2\pi)^4}\, e^{-ipx}[-p^2 + m^2]\phi(p) = 0. \tag{23}$$

Since the equality holds for any x, we get the equation

$$[-p^2 + m^2]\phi(p) = 0, \tag{24}$$

which is solved by

$$\phi(p) = \delta(p^2 - m^2)\, f(p), \tag{25}$$

where $f(p)$ is an arbitrary function of p.

- Using the identity
$$\delta(p^2 - m^2) = \frac{1}{2\omega_{\mathbf{p}}}\Big[\delta(p_0 - \omega_{\mathbf{p}}) + \delta(p_0 + \omega_{\mathbf{p}})\Big], \tag{26}$$
where $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2}$, the solution (25) can be written as
$$\phi(p) = \frac{1}{2\omega_{\mathbf{p}}}\Big[\delta(p_0 - \omega_{\mathbf{p}})f_+(\mathbf{p}) + \delta(p_0 + \omega_{\mathbf{p}})f_-(-\mathbf{p})\Big], \tag{27}$$
where $f_\pm(\pm\mathbf{p}) \equiv f(\pm\omega_{\mathbf{p}}, \mathbf{p})$.

Exercise: Prove the formula (26).

- Computing the inverse Fourier transform of the solution (27), we get the desired solution
$$\begin{aligned}\phi(x) &= \int \frac{d^3p}{(2\pi)^4 2\omega_{\mathbf{p}}}\Big[e^{-i(\omega_{\mathbf{p}}t - \mathbf{p}\cdot\mathbf{x})}f_+(\mathbf{p}) + e^{-i(-\omega_{\mathbf{p}}t - \mathbf{p}\cdot\mathbf{x})}f_-(-\mathbf{p})\Big] \\ &= \int \frac{d^3p}{(2\pi)^4 2\omega_{\mathbf{p}}}\Big[e^{-ipx}f_+(\mathbf{p}) + e^{ipx}f_-(\mathbf{p})\Big],\end{aligned} \tag{28}$$
where the trivial integration over p_0 has been taken and $\mathbf{p}$ has been replaced by $-\mathbf{p}$ in the second term.
- We note that the four-momentum $p^\mu = (\omega_{\mathbf{p}}, \mathbf{p})$, which enters Eq. (28), obeys the mass-shell constraint $p^2 = m^2$.
- The analogous solution of the Schrödinger equation is
$$\psi(t, \mathbf{x}) = \int \frac{d^3p}{(2\pi)^3}\, e^{-i(E_{\mathbf{p}}t - \mathbf{p}\cdot\mathbf{x})}f(\mathbf{p}), \tag{29}$$
where $E_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m}$.
- Comparing the solutions (28) and (29), we see that there are negative energy solutions of the Klein-Gordon equation. Consequently, the energy spectrum is not bounded below.
- The negative energy solutions correspond to antiparticles.

Dirac equation

- One suspects that the negative energy solutions of the Klein-Gordon equation occur because the Hamiltonian is squared in the equation. The Dirac equation is an attempt to resolve the problem constructing the equation linear in $\hat{H}$, as the Schrödinger equation
$$i\frac{\partial\psi(x)}{\partial t} = \hat{H}\psi(x), \tag{30}$$
with the Hamiltonian $\hat{H}$ given as
$$\hat{H} = \boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + \beta m = \alpha^i\hat{p}^i + \beta m, \tag{31}$$
where the indices $i, j = 1, 2, 3$ label components of three-vectors and α^1, α^2, α^3 and β are matrices which are hermitian to guarantee that $\hat{H}$ is hermitian.

- Since α^i and β are matrices, $\psi(x)$ is a multi-component function.
- To satisfy the relativistic dispersion relation we demand that

$$\hat{H}^2 = (\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta m)^2 = \hat{\mathbf{p}}^2 + m^2, \tag{32}$$

which gives

$$\alpha^i \alpha^j + \alpha^j \alpha^i = 2\delta^{ij}, \tag{33}$$
$$\alpha^i \beta + \beta \alpha^i = 0, \tag{34}$$
$$\beta^2 = 1. \tag{35}$$

- According to the first equation α^i and β satisfy $(\alpha^i)^2 = \mathbb{1}$. Consequently the eigenvalues of the matrices α^i and β are ± 1. Further on, due to the conditions (33, 34, 35), the matrices α^i and β are traceless.

Exercise: Prove that $\mathrm{Tr}\beta = 0 = \mathrm{Tr}\alpha^i$ using Eqs. (33, 34, 35).

- Knowing that the matrices α^i and β are hermitian, traceless and their eigenvalues are ± 1, we see that the matrix dimension is even number with ± 1 on the diagonal.
- The matrices α^i and β cannot be 2×2 as there are only three such matrices which are hermitian, traceless and their eigenvalues are ± 1.
- The minimal dimension of α^i and β is 4×4 and they can be chosen in *e.g.* the so-called *Pauli-Dirac representation* as

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{36}$$

where σ^i the 2×2 Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{37}$$

- Since the matrices α^i i β are 4×4, the function $\psi(x)$ is the four-component object known as the *bispinor* or *Dirac spinor*

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \\ \psi_4(x) \end{pmatrix}. \tag{38}$$

Conserved current

- The Dirac equations of $\psi(x)$ and $\psi^\dagger(x)$ are

$$i\frac{\partial \psi(x)}{\partial t} = (-i\boldsymbol{\alpha} \cdot \nabla + \beta m)\, \psi(x), \tag{39}$$
$$-i\frac{\partial \psi^\dagger(x)}{\partial t} = \psi^\dagger(x)\, (i\boldsymbol{\alpha} \cdot \overleftarrow{\nabla} + \beta m). \tag{40}$$

- Multiplying the first equation by $-i\psi^\dagger(x)$ from the left, the second one by $i\psi(x)$ from the right and summing up the equations we get the continuity equation

$$\frac{\partial}{\partial t}\Big(\psi^\dagger(x)\,\psi(x)\Big) + \nabla\Big(\psi^\dagger(x)\boldsymbol{\alpha}\psi(x)\Big) = 0. \tag{41}$$

- The quantity $\psi^\dagger(x)\psi(x) = \psi^*_\alpha(x)\psi_\alpha(x)$ with $\alpha = 1, 2, 3, 4$ being the spinor index is non-negative. So, it seems the probabilistic interpretation is possible. However, it is not the case.

Solutions of Dirac equation

- For simplicity we consider the Dirac equation of vanishing momentum which is

$$\Big[i\frac{\partial}{\partial t} - \beta m\Big]\psi(x) = 0. \tag{42}$$

In the Pauli-Dirac representation (36) the equation (42) is

$$\Big[i\frac{\partial}{\partial t} - m\Big]\psi_\alpha(x) \;=\; 0 \qquad \text{for} \qquad \alpha = 1, 2, \tag{43}$$

$$\Big[i\frac{\partial}{\partial t} + m\Big]\psi_\alpha(x) \;=\; 0 \qquad \text{for} \qquad \alpha = 3, 4. \tag{44}$$

- The solutions are

$$\psi_\alpha(x) = e^{\mp imt} w_\alpha, \tag{45}$$

where the sign minus is for $\alpha = 1, 2$ and plus for $\alpha = 3, 4$; w_α is any bispinor independent of x.

- The solutions with $\alpha = 1, 2$ are of positive energy and those with $\alpha = 3, 4$ of negative energy. Therefore, the Dirac equation which is linear in the Hamiltonian still has negative energy solutions.

- Four linearly independent solutions of Eq. (42) can be written as

$$\psi^1(x) = e^{-imt}\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \qquad \psi^2(x) = e^{-imt}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \tag{46}$$

$$\psi^3(x) = e^{imt}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \qquad \psi^4(x) = e^{imt}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{47}$$

- The Diraca spinor $\psi(x)$ describes particles and antiparticles of spin 1/2. The solutions $\psi^1(x)$, $\psi^2(x)$ correspond to particles with two spin orientations and the solutions $\psi^3(x)$, $\psi^4(x)$ to antiparticles.

- Difficulties with probabilistic interpretation reflect that fact that in relativistic theory the particle number is not conserved as the particle-antiparticle pairs can be generated from vacuum.

- A relativistic quantum theory needs to be formulated differently then the non-relativistic quantum mechanics.