Lesson 5 - Relativistic Wave Equations
Unit 5.1 Klein-Gordon and Dirac equations

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Klein-Gordon equation (I)

The classical energy of a nonrelativistic free particle is given by

$$E = \frac{\mathbf{p}^2}{2m} , \tag{1}$$

where $\mathbf{p}$ is the linear momentum and m the mass of the particle. The Schrödinger equation of the corresponding quantum particle with wavefunction $\psi(\mathbf{r}, t)$ is easily obtained by imposing the quantization prescription

$$E \to i\hbar\frac{\partial}{\partial t} , \qquad \mathbf{p} \to -i\hbar\boldsymbol{\nabla} . \tag{2}$$

In this way one gets the time-dependent Schrödinger equation of the free particle, namely

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t) , \tag{3}$$

obtained for the first time in 1926 by Erwin Schrödinger.

Klein-Gordon equation (II)

The classical energy of a relativistic free particle is instead given by

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

where c is the speed of light in the vacuum. By applying directly the quantization prescription (2) one finds

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} \, \psi(\mathbf{r}, t) \ . \tag{5}$$

This equation is quite suggestive but the square-root operator on the right side is a very difficult mathematical object.
For this reason in 1927 Oskar Klein and Walter Gordon suggested to start with

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4 \tag{6}$$

and then to apply the quantization prescription (2). In this way one obtains

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right) \psi(\mathbf{r}, t) = 0 \ , \tag{7}$$

i.e. a generalization of Maxwell's wave equation for massive particles.

Klein-Gordon equation (III)

The Klein-Gordon equation has two problems:
i) it admits solutions with negative energy;
ii) the space integral over the entire space of the non negative probability density $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \geq 0$ is generally not time-independent, namely

$$\frac{d}{dt} \int_{\mathbb{R}^3} \rho(\mathbf{r}, t) \; d^3\mathbf{r} \neq 0 \; . \tag{8}$$

Nowadays we know that to solve completely these two problems it is necessary to promote $\psi(\mathbf{r}, t)$ to a quantum field operator. Within this second-quantization (quantum field theory) approach the Klein-Gordon equation is now used to describe relativistic particles with spin zero, like the pions or the Higgs boson.

Dirac equation (I)

In 1928 Paul Dirac proposed a different approach to the quantization of the relativistic particle. To solve the problem of Eq. (8) he considered a wave equation with only first derivatives with respect to time and space and introduced the classical energy

$$E = c\,\hat{\boldsymbol{\alpha}} \cdot \mathbf{p} + \hat{\beta}\, mc^2 \;, \tag{9}$$

such that squaring it one recovers the Klein-Gordon equation. This condition is fulfilled only if $\hat{\boldsymbol{\alpha}} = (\hat{\alpha}_1, \hat{\alpha}_2, \hat{\alpha}_3)$ and $\hat{\beta}$ satisfy the following algebra of matrices

$$\hat{\alpha}_1^2 = \hat{\alpha}_2^2 = \hat{\alpha}_3^2 = \hat{\beta}^{\,2} = \hat{I} \;, \tag{10}$$

$$\hat{\alpha}_i \hat{\alpha}_j + \hat{\alpha}_j \hat{\alpha}_i = \hat{0} \;, \qquad i \neq j \tag{11}$$

$$\hat{\alpha}_i \hat{\beta} + \hat{\beta}\, \hat{\alpha}_i = \hat{0} \;, \qquad \forall i \tag{12}$$

where $\hat{1}$ is the identity matrix and $\hat{0}$ is the zero matrix.

Dirac equation (II)

The smallest dimension in which the so-called Dirac matrices $\hat{\alpha}_i$ and $\hat{\beta}$ can be realized is four. In particular, one can write

$$\hat{\alpha}_i = \begin{pmatrix} \hat{0}_2 & \hat{\sigma}_i \\ \hat{\sigma}_i & \hat{0}_2 \end{pmatrix} , \qquad \hat{\beta} = \begin{pmatrix} \hat{I}_2 & \hat{0}_2 \\ \hat{0}_2 & -\hat{I}_2 \end{pmatrix} , \tag{13}$$

where $\hat{I}_2$ is the 2×2 identity matrix, $\hat{0}_2$ is the 2×2 zero matrix, and

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{14}$$

are the Pauli matrices. Eq. (9) with the quantization prescription (2) gives

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left(-i\hbar c \, \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\nabla} + \hat{\beta} \, mc^2 \right) \Psi(\mathbf{r}, t) , \tag{15}$$

which is the Dirac equation for a free particle.

Dirac equation (III)

The wavefunction $\Psi(\mathbf{r},t)$ of the Dirac equation has four components in the abstract space of Dirac matrices, i.e. this spinor field can be written

$$\Psi(\mathbf{r},t) = \begin{pmatrix} \psi_1(\mathbf{r},t) \\ \psi_2(\mathbf{r},t) \\ \psi_3(\mathbf{r},t) \\ \psi_4(\mathbf{r},t) \end{pmatrix} . \tag{16}$$

In explicit matrix form the Dirac equation is thus given by

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \psi_1(\mathbf{r},t) \\ \psi_2(\mathbf{r},t) \\ \psi_3(\mathbf{r},t) \\ \psi_4(\mathbf{r},t) \end{pmatrix} = \hat{H} \begin{pmatrix} \psi_1(\mathbf{r},t) \\ \psi_2(\mathbf{r},t) \\ \psi_3(\mathbf{r},t) \\ \psi_4(\mathbf{r},t) \end{pmatrix} \tag{17}$$

where the matrix operator $\hat{H}$ is given by

$$\begin{pmatrix} mc^2 & 0 & -i\hbar c\frac{\partial}{\partial z} & -i\hbar c(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}) \\ 0 & mc^2 & -i\hbar c(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}) & i\hbar c\frac{\partial}{\partial z} \\ -i\hbar c\frac{\partial}{\partial z} & -i\hbar c(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}) & -mc^2 & 0 \\ -i\hbar c(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}) & i\hbar c\frac{\partial}{\partial z} & 0 & -mc^2 \end{pmatrix} .$$

Dirac equation (IV)

It is easy to show that the Dirac equation satisfies the differential law of current conservation, given by

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) + \boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r},t) = 0 \ , \tag{19}$$

where

$$\rho(\mathbf{r},t) = \Psi^{+}(\mathbf{r},t)\Psi(\mathbf{r},\mathbf{t}) = \sum_{i=1}^{4}|\psi_i(\mathbf{r},t)|^2 \tag{20}$$

is the probability density, and $\mathbf{j}(\mathbf{r},t)$ is the probability current with three components

$$j_k(\mathbf{r},t) = c\,\Psi^{+}(\mathbf{r},t)\hat{\alpha}_k\Psi(\mathbf{r},t) \ . \tag{21}$$

Finally, we observe that from the continuity equation (19) one finds

$$\frac{d}{dt}\int_{\mathbb{R}^3}\rho(\mathbf{r},t)\ d^3\mathbf{r} = 0 \ , \tag{22}$$

by using the divergence theorem and imposing a vanishing current density on the border at infinity. Thus, contrary to the Klein-Gordon equation, the Dirac equation does not have the probability density problem.