The Klein-Gordon Equation

Conservation of probability in "classical" quantum mechanics

A quantum state $|\psi\rangle$ evolves in time according to the Schrodinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

according to one of the postulates of quantum mechanics. The Schrodinger equation in the position representation is

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V\psi, \tag{1}$$

and the complex conjugate of the Schrodinger equation is

$$-i\hbar\frac{\partial}{\partial t}\psi^* = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi^* + V\psi^*. \tag{2}$$

Multiplying Eq. (1) by ψ^* and Eq. (2) by ψ we obtain

$$i\hbar\psi^*\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\psi^*\boldsymbol{\nabla}^2\psi + V\psi^*\psi \tag{3}$$

and

$$-i\hbar\psi\frac{\partial}{\partial t}\psi^* = -\frac{\hbar^2}{2m}\psi\boldsymbol{\nabla}^2\psi^* + V\psi^*\psi. \tag{4}$$

Subtracting Eq. (4) from Eq. (3) leads to

$$i\hbar\psi^*\frac{\partial}{\partial t}\psi + i\hbar\psi\frac{\partial}{\partial t}\psi^* = -\frac{\hbar^2}{2m}\psi^*\boldsymbol{\nabla}^2\psi + \frac{\hbar^2}{2m}\psi\boldsymbol{\nabla}^2\psi^*,$$

$$i\hbar\frac{\partial}{\partial t}\big(\psi^*\psi\big) = -\frac{\hbar^2}{2m}\big(\psi^*\boldsymbol{\nabla}^2\psi - \psi\boldsymbol{\nabla}^2\psi^*\big). \tag{5}$$

The right side of Eq. (5) can be simplified using that

$$\boldsymbol{\nabla}\cdot\big(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\big) = \boldsymbol{\nabla}\cdot\big(\psi^*\boldsymbol{\nabla}\psi\big) - \boldsymbol{\nabla}\cdot\big(\psi\boldsymbol{\nabla}\psi^*\big)$$

$$= \boldsymbol{\nabla}\psi^*\cdot\boldsymbol{\nabla}\psi + \psi^*\boldsymbol{\nabla}^2\psi - \boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\psi^* - \psi\boldsymbol{\nabla}^2\psi^* = \psi^*\boldsymbol{\nabla}^2\psi - \psi\boldsymbol{\nabla}^2\psi^*,$$

which allows us to write

$$i\hbar\frac{\partial}{\partial t}\big(\psi^*\psi\big) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}\cdot\big(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\big),$$

$$\frac{\partial}{\partial t}\big(\psi^*\psi\big) = \frac{i\hbar}{2m}\boldsymbol{\nabla}\cdot\big(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\big),$$

$$\frac{\partial}{\partial t}\big(\psi^*\psi\big) - \boldsymbol{\nabla}\cdot\left[\frac{i\hbar}{2m}\big(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\big)\right] = 0,$$

$$\frac{\partial}{\partial t}\big(\psi^*\psi\big) + \boldsymbol{\nabla}\cdot\left[\frac{i\hbar}{2m}\big(\psi\boldsymbol{\nabla}\psi^* - \psi^*\boldsymbol{\nabla}\psi\big)\right] = 0. \tag{6}$$

Eq. (6) has the form of a continuity equation

$$\frac{\partial}{\partial t}\rho + \boldsymbol{\nabla}\cdot\mathbf{j} = 0,$$

where

$$\rho \equiv \psi^*\psi$$

is the probability density to find the particle in a particular position according to the Born rule, and thus

$$\mathbf{j} \equiv \frac{i\hbar}{2m}\big(\psi\boldsymbol{\nabla}\psi^* - \psi^*\boldsymbol{\nabla}\psi\big)$$

is interpreted as the probability current density.

An attempt at relativistic quantum mechanics

The relativistic energy-momentum relation (for a free particle) is

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

Applying the operator $H = i\hbar\dfrac{d}{dt}$ twice on the state $|\psi\rangle$ and equating H with the relativistic energy (with $\mathbf{p}$ now interpreted as an operator) leads to

$$-\hbar^2\frac{d^2}{dt^2}|\psi\rangle = \big(\mathbf{p}^2c^2 + m^2c^4\big)|\psi\rangle,$$

which in the position representation is

$$-\hbar^2\frac{\partial^2}{\partial t^2}\psi = \big(-\hbar^2c^2\boldsymbol{\nabla}^2 + m^2c^4\big)\psi,$$

or using natural units $\hbar = c = 1$,

$$-\frac{\partial^2}{\partial t^2}\psi = \big(-\boldsymbol{\nabla}^2 + m^2\big)\psi,$$

$$\left(\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2 + m^2\right)\psi = 0. \tag{7}$$

The space-time gradient is given by

$$\partial_\mu = \left(\frac{\partial}{\partial t},\ \boldsymbol{\nabla}\right).$$

So we can write Eq. (7) as

$$\left(\partial^\mu \partial_\mu + m^2\right)\psi = 0. \tag{8}$$

which is the Klein-Gordon equation. The solutions of the free-particle Schrodinger equation are $\psi \propto e^{-i(Et - \mathbf{p}\cdot\mathbf{x})}$. We can try a solution of the Klein-Gordon equation on the same form. Since

$$\frac{\partial^2}{\partial t^2} e^{-i(Et-\mathbf{p}\cdot\mathbf{x})} = (-iE)^2 e^{-i(Et-\mathbf{p}\cdot\mathbf{x})}$$

$$\boldsymbol{\nabla}^2 e^{-i(Et-\mathbf{p}\cdot\mathbf{x})} = (i\mathbf{p})^2 e^{-i(Et-\mathbf{p}\cdot\mathbf{x})},$$

we have from Eq. (7) that

$$\left[(-iE)^2 - (i\mathbf{p})^2 + m^2\right] e^{-i(Et-\mathbf{p}\cdot\mathbf{x})} = 0,$$

$$-E^2 + \mathbf{p}^2 + m^2 = 0,$$

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

which is the relativistic energy-momentum relation. Note however that both positive and negative energies in the plane-wave solution $e^{-i(Et-\mathbf{p}\cdot\mathbf{x})}$ will satisfy the Klein-Gordon equation, wheras only positive energies $E = \mathbf{p}^2 / 2m$ satisfy the Schrodinger equation.

We can try to find a continuity equation corresponding to the Klein-Gordon equation by following the same procedure as with the Schrodinger equation. Then we end up with

$$\psi^* \partial_t^2 \psi - \psi^* \boldsymbol{\nabla}^2 \psi + m^2 \psi^* \psi - \psi \partial_t^2 \psi^* + \psi \boldsymbol{\nabla}^2 \psi^* - m^2 \psi^* \psi = 0,$$

$$\psi^* \partial_t^2 \psi - \psi \partial_t^2 \psi^* + \psi \boldsymbol{\nabla}^2 \psi^* - \psi^* \boldsymbol{\nabla}^2 \psi = 0,$$

$$\frac{\partial}{\partial t}\left(\psi^*\partial_t\psi - \psi\partial_t\psi^*\right) - \nabla\cdot\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) = 0.$$

Multiplying both sides by $-i\,/\,2m$ results in

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

where we recover the familiar probability current density from classical quantum mechanics. However, the term that is supposed to contain the probability density looks completely different. Substituting the plain-wave solutions of the Klein-Gordon equation into the "probability density" reveals that there is possibly a problem with the probability interpretation. Since

$$\partial_t\psi \propto \partial_t e^{-i(Et-\mathbf{p}\cdot\mathbf{x})} = -iEe^{-i(Et-\mathbf{p}\cdot\mathbf{x})},$$

we have that

$$\rho = \frac{i}{2m}\left(\psi\partial_t\psi^* - \psi^*\partial_t\psi\right)$$

$$\propto \frac{i}{2m}\left\{e^{-i(Et-\mathbf{p}\cdot\mathbf{x})}\cdot\left[iEe^{i(Et-\mathbf{p}\cdot\mathbf{x})}\right] - e^{i(Et-\mathbf{p}\cdot\mathbf{x})}\cdot\left[-iEe^{-i(Et-\mathbf{p}\cdot\mathbf{x})}\right]\right\}$$

$$= \frac{i}{2m}(iE+iE) = -\frac{E}{m},$$

where positive energies lead to a negative probability density.