2 Current conservation for Schrödinger equation

Schrödinger wave equation (for one particle):

$$\left(-\frac{\hbar^2}{2m}\Delta + V(x)\right) = i\hbar\frac{\partial\psi}{\partial t} \qquad (2.1)$$

$$H\psi(\vec{x},t) = i\hbar\frac{\partial\psi}{\partial t} \qquad (2.2)$$

From Eq.(2.1) and its complex conjugate (∗), we get

$$(H\psi) = i\hbar\frac{\partial\psi}{\partial t} \Rightarrow \psi^*(H\psi) = i\hbar\psi^*\frac{\partial\psi}{\partial t}$$

$$(H\psi^*) = -i\hbar\frac{\partial\psi^*}{\partial t} \Rightarrow \psi(H\psi^*) = -i\hbar\psi\frac{\partial\psi^*}{\partial t}$$

Taking the difference of these two equations, we get

$$\psi^*(H\psi) - \psi(H\psi^*) = i\hbar\frac{\partial}{\partial t}(\psi^*\psi)$$

$$-\frac{\hbar^2}{2m}(\psi^*\Delta\psi - \psi\Delta\psi^*) = i\hbar\frac{\partial}{\partial t}(\psi^*\psi)$$

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

This gives the "current conservation" (continuity equation):

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0 \qquad (2.3)$$

where ρ is the probability density

$$\rho = \psi^*\psi$$

and $\vec{j}$ is the probability current

$$\vec{j} = \frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)$$

From Eq.(2.3) we get the "conservation of probability"

$$\frac{\partial}{\partial t}\int \mathrm{d}^3x\,\rho(\vec{x},t) = 0$$

Important point: Schrödinger equation (2.1) is of first order in time!

Plane wave solutions of (2.1) for free particles:

$$\psi(\vec{x},t) = e^{-i(Et-\vec{p}\cdot\vec{x})/\hbar} \qquad (2.4)$$

where $\vec{p}$ are the eigenvalues of the momentum operator $-i\hbar\vec{\nabla}$, and $E = \vec{p}^2/(2m)$ is the energy.

3 Dirac equation

Wave equation of Schrödinger form (first order in $\partial/\partial t$):

$$H\psi(\vec{x},t) = i\hbar\frac{\partial\psi}{\partial t} \tag{3.1}$$

What is the relativistic Hamiltonian H for a free particle ? - In theory of relativity, space and time enter very symmetrically (see, for example, Lorentz transformation).

$\Rightarrow$ H should be of first order in $\vec{\nabla}$ (or: first order in momentum operator $\vec{p} = -i\hbar\vec{\nabla}$), and have dimension of energy. Try

$$H = (\alpha_1\, p_1)\, c + (\alpha_2\, p_2)\, c + (\alpha_3\, p_3)\, c + \beta\,(mc^2) \equiv (\vec{\alpha}\cdot\vec{p})\, c + \beta\,(mc^2) \tag{3.2}$$

where $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are dimensionless constants (independent of $\vec{x}$ and t.)

But: If $\alpha_1, \alpha_2, \alpha_3; \beta$ are just numbers, then H is not invariant under rotations !

Later, we will see that this problem can be solved if $\alpha_1, \alpha_2, \alpha_3; \beta$ are not constant numbers, but constant matrices ! In this case, ψ is a vector!

Take $i\hbar(\partial/\partial t)$ of wave equation (3.1):

$$\begin{aligned} -\hbar^2\frac{\partial^2\psi}{\partial t^2} &= \left((\vec{\alpha}\cdot\vec{p})c + \beta(mc^2)\right)^2\psi \\ &= \left[c^2\,(\vec{\alpha}\cdot\vec{p})\,(\vec{\alpha}\cdot\vec{p}) + mc^3\,((\vec{\alpha}\cdot\vec{p})\,\beta + \beta\,(\vec{\alpha}\cdot\vec{p})) + (mc^2)^2\,\beta^2\right]\psi \end{aligned} \tag{3.3}$$

Here $\vec{p} = -i\hbar\vec{\nabla}$ is the momentum operator.

The solution for a free particle (momentum $\vec{p}$) *must* be of the form

$$\psi(\vec{x},t) = w(\vec{p})\, e^{-i(Et-\vec{p}\cdot\vec{x})/\hbar} \tag{3.4}$$

where $w(\vec{p})$ ist a vector, independent of $(\vec{x},t)$.

Inserting (3.4) into (3.3) we get

$$E^2 = c^2\,(\vec{\alpha}\cdot\vec{p})\,(\vec{\alpha}\cdot\vec{p}) + mc^3\,((\vec{\alpha}\cdot\vec{p})\,\beta + \beta\,(\vec{\alpha}\cdot\vec{p})) + (mc^2)^2\,\beta^2) \tag{3.5}$$

This *must* be the energy squared of a free particle with momentum $\vec{p}$, i.e., $E^2 = (pc)^2 + (mc^2)^2$. Therefore

$$(\vec{\alpha}\cdot\vec{p})\,(\vec{\alpha}\cdot\vec{p}) = \vec{p}^2 \tag{3.6}$$

$$(\vec{\alpha}\cdot\vec{p})\,\beta + \beta\,(\vec{\alpha}\cdot\vec{p}) = 0 \tag{3.7}$$

$$\beta^2 = 1 \tag{3.8}$$

This must hold for *any* vector $\vec{p}$, therefore

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij} \qquad (i,j=1,2,3) \tag{3.9}$$

$$\alpha_i\beta + \beta\alpha_i = 0 \qquad (i=1,2,3) \tag{3.10}$$

$$\alpha_i^2 = 1 \quad (i=1,2,3)\,, \qquad \beta^2 = 1 \tag{3.11}$$

Conditions for matrices $\alpha_1, \alpha_2, \alpha_3, \beta$:

- Hermite (because Hamiltonian H must be hermite).
- Eigenvalues are ± 1 (because of Eq.(3.11)).
- Trace is zero: For example, from Eq.(3.10), $\mathrm{Tr}(\alpha_i) = -\mathrm{Tr}(\beta\alpha_i\beta) = -\mathrm{Tr}(\beta^2\alpha_i) = -\mathrm{Tr}(\alpha_i) = 0$.

Therefore, sum of eigenvalues must be zero $\Rightarrow$ dimension of matrices must be even ($N = 2, 4, 6, \dots$).
But $N = 2$ is not possible: The four independent hermite 2×2 matrices are the Pauli matrices $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ and the unit matrix 1. But then (3.10) is not satisfied.
Lowest dimension is $N = 4$. For example, the following matrices satisfy all conditions (3.9) - (3.11):

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.12}$$

Home work: Show that these matrices satisfy the conditions (3.9) - (3.11).

Current conservation for Dirac equation:
Dirac equation (3.1) and its hermite conjugate (†):

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\,\vec{\alpha}\cdot\left(\vec{\nabla}\psi\right) + \beta\,mc^2\,\psi \tag{3.13}$$

$$-i\hbar\frac{\partial\psi^\dagger}{\partial t} = i\hbar c\left(\vec{\nabla}\psi^\dagger\right)\cdot\vec{\alpha} + \psi^\dagger\,\beta\,mc^2 \tag{3.14}$$

Multiply (3.13) from left by $\psi^\dagger$, and (3.14) from right by ψ, and take the difference of these equations:

$$i\hbar\frac{\partial}{\partial t}\left(\psi^\dagger\psi\right) = -i\hbar c\,\vec{\nabla}\cdot\left(\psi^\dagger\vec{\alpha}\psi\right)$$

This has the form of current conservation:

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0 \tag{3.15}$$

with the probability density

$$\rho = \psi^\dagger \psi \tag{3.16}$$

and the probability current

$$\vec{j} = c\psi^\dagger \vec{\alpha} \psi \tag{3.17}$$

Relation to the spin:

- There must be four independent solutions to the Dirac equation (3.1).
- The are two different energy eigenvalues: From (3.5), $E = \pm\sqrt{(pc)^2 + (mc^2)^2}$.
- Therefore, two solutions have energy $E = +\sqrt{(pc)^2 + (mc^2)^2}$, and two solutions have energy $E = -\sqrt{(pc)^2 + (mc^2)^2}$.
  This 2-fold degeneracy means spin 1/2: For a free particle, spin up (↑) and spin down (↓) have the same energy.

The angular momentum operator for the Dirac equation is given by

$$\vec{J} = \vec{L} + \vec{S} = \vec{r} \times \vec{p} + \frac{\hbar}{2}\vec{\Sigma} \tag{3.18}$$

where the 4×4 matrices $\vec{\Sigma} = (\Sigma_1, \Sigma_2, \Sigma_3)$ are given by

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \tag{3.19}$$

The commutation relations of $\vec{L}$ and $\vec{S}$ with the Hamiltonian $H = c(\vec{\alpha} \cdot \vec{p}) + \beta\, mc^2$ are as follows:

$$\begin{aligned} [H, L_i] &= -i\hbar c\, (\vec{\alpha} \times \vec{p})_i \\ [H, S_i] &= i\hbar c\, (\vec{\alpha} \times \vec{p})_i \end{aligned}$$

Try to check these relations!
Therefore $\left[H, \vec{J}\right] = 0$, and the total angular momentum $\vec{J}$ (sum of orbital and spin angular momentum) is conserved !