Quantum Physics 2006/07

Lecture 16: The Dirac Equation

Dirac tried to avoid the twin difficulties of negative energy and negative probability by proposing a relativistic equation which, like the Schödinger equation, is *linear* in $\frac{\partial}{\partial t}$, hoping to avoid the sign ambiguity in the square-root of E^2, and also the presence of time derivatives in the 'probability density'. Relativity then dictates that the equation should also be linear in the spatial derivatives in order to treat space and time on an equal footing.

Following Dirac, we start with a Hamiltonian equation of the form

$$i\hbar \frac{\partial}{\partial t}\,\psi(\underline{r},t) \;=\; \hat{H}\,\psi(\underline{r},t)$$

and write

$$i\hbar \frac{\partial}{\partial t}\,\psi(\underline{r},t) \;=\; -i\hbar c\left\{\alpha^1\frac{\partial}{\partial x^1} \;+\; \alpha^2\frac{\partial}{\partial x^2} \;+\; \alpha^3\frac{\partial}{\partial x^3}\right\}\psi(\underline{r},\,t) \;+\; \beta\, mc^2\,\psi(\underline{r},\,t) \quad (1)$$

$$= \left\{c\,\underline{\alpha}\cdot\underline{\hat{p}} \;+\; \beta\, mc^2\right\}\psi(\underline{r},\,t) \;=\; \hat{H}\psi(\underline{r},\,t) \quad (2)$$

$$\text{where}\qquad \underline{\alpha}\cdot\underline{\hat{p}} \;\equiv\; \alpha^i\,\hat{p}^i \;=\; -\,i\hbar\alpha^i\frac{\partial}{\partial x^i} \qquad \left(\text{with}\quad \alpha^i\,\hat{p}^i \;\equiv\; \sum_{i=1}^{3}\alpha^i\,\hat{p}^i \text{ etc.}\right)$$

Initially, we attempt to construct an equation for a *free particle*, so no terms in the Hamiltonian $\hat{H}$ should depend on $\underline{r}$ or t as these would describe forces. By assumption the α^i and β are independent of derivatives, therefore $\underline{\alpha}$ and β commute with $\underline{r}$, t, $\underline{\hat{p}}$ and E but not necessarily with each other.

Since relativistic invariance must be maintained, *ie* $E^2 \;=\; |\underline{p}|^2c^2 \;+\; m^2c^4$, Dirac demanded that

$$\hat{H}^2\,\psi(\underline{r},t) \;=\; \left(c^2\,|\underline{\hat{p}}|^2 \;+\; m^2c^4\right)\,\psi(\underline{r},t) \quad (3)$$

From equation (2) we have

$$\hat{H}^2\,\psi(\underline{r},\,t) \;=\; \left\{c\,\underline{\alpha}\cdot\underline{\hat{p}} \;+\; \beta\, mc^2\right\}\left\{c\,\underline{\alpha}\cdot\underline{\hat{p}} \;+\; \beta\, mc^2\right\}\;\psi(\underline{r},\,t)$$

Expand the RHS of this equation, being very careful about the ordering of the, as yet undetermined, quantities α^i and β

$$\begin{aligned}
&\hat{H}^2\,\Psi(\underline{r},\,t)\\
&= \left\{c^2\left[(\alpha^1)^2\,(\hat{p}^1)^2 \;+\; (\alpha^2)^2\,(\hat{p}^2)^2 \;+\; (\alpha^3)^2\,(\hat{p}^3)^2\right] \;+\; m^2c^4\,\beta^2\right\}\psi(\underline{r},t)\\
&\quad +\; c^2\left\{\left(\alpha^1\alpha^2 \;+\; \alpha^2\alpha^1\right)\hat{p}^1\hat{p}^2 \;+\; \left(\alpha^2\alpha^3 \;+\; \alpha^3\alpha^2\right)\hat{p}^2\hat{p}^3 \;+\; \left(\alpha^3\alpha^1 \;+\; \alpha^1\alpha^3\right)\hat{p}^1\hat{p}^3\right\}\psi(\underline{r},t)\\
&\quad +\; mc^3\left\{\left(\alpha^1\beta \;+\; \beta\alpha^1\right)\hat{p}^1 \;+\; \left(\alpha^2\beta \;+\; \beta\alpha^2\right)\hat{p}^2 \;+\; \left(\alpha^3\beta \;+\; \beta\alpha^3\right)\hat{p}^3\right\}\psi(\underline{r},t)
\end{aligned}$$

Condition (3) is satisfied if

$$\begin{aligned}
(\alpha^1)^2 \;=\; (\alpha^2)^2 \;=\; (\alpha^3)^2 \;=\; \beta^2 \;&=\; 1\\
\alpha^i\,\alpha^j \;+\; \alpha^j\,\alpha^i \;&=\; 0 \qquad (i \neq j)\\
\alpha^i\,\beta \;+\; \beta\,\alpha^i \;&=\; 0
\end{aligned}$$

or, more compactly, as

$$\left\{\alpha^i,\, \alpha^j\right\} \;=\; 2\,\delta^{ij} \qquad \text{the } \textbf{anticommutator} \text{ of } \alpha^i \text{ and } \alpha^j$$

$$\left\{\alpha^i,\, \beta\right\} \;=\; 0 \quad , \qquad \beta^2 \;=\; 1$$

1. From these relations it is clear that the α^i and β cannot be just numbers. Let's assume they are *matrices*. Since $\hat{H}$ is hermitian, they must be *square* $(n \times n)$ matrices.

2. The square of each matrix α^i, β is the unit matrix. Since they are hermitian, their eigenvalues are real, therefore all eigenvalues must be ± 1.

3. $\mathrm{Tr}\;(\alpha^i) \;=\; \mathrm{Tr}\;(\beta) \;=\; 0.$

   Proof:
   $$\begin{aligned} \mathrm{Tr}\;(\alpha^i) &= \mathrm{Tr}\;(\beta^2\,\alpha^i) \;=\; \mathrm{Tr}\;(\beta\,\alpha^i\,\beta) \qquad (\text{using } \mathrm{Tr}\;(AB) \;=\; \mathrm{Tr}\;(BA)\;) \\ &= -\mathrm{Tr}\;(\alpha^i\,\beta^2) \qquad (\text{using } \alpha^i\,\beta \;=\; -\,\beta\alpha^i) \\ &= -\mathrm{Tr}\;(\alpha^i) \;=\; 0 \end{aligned}$$

   Therefore, since the eigenvalues are ± 1, n must be *even.* It is not possible to find a set of traceless hermitian 2×2 matrices which satisfy the anti-commutation relations – the 3 Pauli matrices σ^i are good start, but there is no 4th matrix. The simplest representation is 4×4. The *standard representation* has β diagonal:

$$\beta \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\alpha^1 \;=\; \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \alpha^2 \;=\; \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \alpha^3 \;=\; \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

We usually write these in block 2×2 form as:

$$\beta \;=\; \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \alpha^i \;=\; \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \qquad \text{or} \qquad \underline{\alpha} \;=\; \begin{pmatrix} 0 & \underline{\sigma} \\ \underline{\sigma} & 0 \end{pmatrix}$$

with each element a 2×2 submatrix, and where the σ^i are the usual Pauli matrices.
Exercise: Check that these matrices satisfy the correct anti-commutation relations.

Since the Hamiltonian is a 4×4 matrix, the wave-function $\psi(\underline{r}, t)$ it acts on must be a 4-*component column vector*:

$$\psi(\underline{r}, t) \;=\; \begin{pmatrix} \psi_1(\underline{r}, t) \\ \psi_2(\underline{r}, t) \\ \psi_3(\underline{r}, t) \\ \psi_4(\underline{r}, t) \end{pmatrix}$$

Probability Density

The Dirac equation for a free particle is

$$i\hbar \frac{\partial}{\partial t}\,\psi(\underline{r},t) \;=\; \left(-i\hbar c\,\underline{\alpha}\cdot\underline{\nabla} \;+\; \beta\, mc^2\right)\psi(\underline{r},t) \tag{4}$$

Construction of the probability density is straightforward. Take the Hermitian conjugate of equation (4) (ie complex conjugate and transpose)

$$-i\hbar \frac{\partial}{\partial t}\,\psi^\dagger(\underline{r},t) \;=\; \psi^\dagger(\underline{r},t)\left(i\hbar c\,\underline{\alpha}\cdot\overleftarrow{\underline{\nabla}} \;+\; \beta\, mc^2\right) \tag{5}$$

Note that $\psi^\dagger$ is a row vector whose components are the complex conjugates of the components of ψ. Now multiply (4) by $\psi^\dagger$ from the left and (5) by ψ from the right and subtract:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\left(\psi^\dagger\,\psi\right) &= -i\hbar c\left(\psi^\dagger\underline{\alpha}\cdot\underline{\nabla}\psi \;+\; \psi^\dagger\underline{\alpha}\cdot\overleftarrow{\underline{\nabla}}\psi\right) \\ &= -i\hbar c\left(\psi^\dagger\underline{\alpha}\cdot\underline{\nabla}\psi \;+\; \left(\underline{\nabla}\psi^\dagger\right)\cdot\underline{\alpha}\,\psi\right) \\ &= -i\hbar c\,\underline{\nabla}\cdot\left(\psi^\dagger\,\underline{\alpha}\,\psi\right) \end{aligned}$$

which can be written as a continuity equation

$$\frac{1}{c}\frac{\partial\rho}{\partial t} \;+\; \underline{\nabla}\cdot\underline{j} \;=\; 0$$

where

$$\rho \;=\; \psi^\dagger\psi \qquad \text{and} \qquad \underline{j} \;=\; \psi^\dagger\,\underline{\alpha}\,\psi$$

Thus $\rho \;=\; \psi^\dagger\psi \;\equiv\; |\psi|^2$ is a positive definite quantity as is required of a probability density.

We can write the continuity equation in covariant form as

$$\partial_\mu\, j^\mu \;=\; 0 \qquad \text{with} \qquad j^\mu \;=\; (\rho,\,\underline{j})$$

This implies that $\psi^\dagger\psi$ transforms like the zero-component of a 4-vector, with $\psi^\dagger\,\underline{\alpha}\,\psi$ the corresponding space part which we identify as the probability current density.

Free Particle Solutions

Let us look for plane-wave solutions of the form

$$\begin{aligned} \psi(\underline{r},t) &= \exp(-ik^\mu\, x_\mu)\, w(p) \\ &= \exp(-ik\cdot x)\, w(p) \;=\; \exp(-ip\cdot x/\hbar)\, w(p) \\ &= \exp\left\{-\frac{i}{\hbar}\left(cp^0 t \;-\; \underline{p}\cdot\underline{r}\right)\right\} w(p) \end{aligned}$$

with $w(p)$ a 4-component column vector.

Substituting this into the Dirac equation (4) and dividing out by $c\exp(-ip\cdot x/\hbar)$, yields

$$p^0\, w(p) \;=\; \left(\underline{\alpha}\cdot\underline{p} \;+\; \beta mc\right)\, w(p) \tag{6}$$

The trial solution presumably represents a particle of energy cp^0 and momentum $\underline{p}$.

Writing out equation (6) by substituting the matrices β and α^i gives a set of 4-simultaneous linear equations which we write in matrix form as:

$$\begin{pmatrix} (-p^0 + mc) & 0 & p^3 & (p^1 - ip^2) \\ 0 & (-p^0 + mc) & (p^1 + ip^2) & -p^3 \\ p^3 & (p^1 - ip^2) & -(p^0 + mc) & 0 \\ (p^1 + ip^2) & -p^3 & 0 & -(p^0 + mc) \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} = 0$$

The condition for non-trivial solutions for w_i is that the determinant of the matrix vanishes. On multiplying out the determinant, we find (slightly laborious exercise!)

$$\left\{m^2c^2 + |\underline{p}|^2 - (p^0)^2\right\}^2 = 0 \tag{7}$$

which is the (square of the) required energy-momentum relation. Of course, this had to happen because we constructed the matrices α^i and β so that it would!

Taking the square-root of the energy-momentum relation, we have

$$p^0 = \pm\left\{(m^2c^2 + |\underline{p}|^2\right\}^{1/2}$$

so the negative energy solutions are still with us!

Viewed more formally, equation (6) is an eigenvalue problem which we wish to solve for the *eigenvalues* p_0 and *eigenvectors* w. The eigenvalue condition, equation (7), is a quartic equation whose four solutions are

$$p^0 = +\left\{(m^2c^2 + |\underline{p}|^2\right\}^{1/2} \quad \text{(twice)} \qquad \text{and} \qquad p^0 = -\left\{(m^2c^2 + |\underline{p}|^2\right\}^{1/2} \quad \text{(twice)}$$

ie, the four eigenvalues p^0 come in two degenerate pairs of equal magnitude but opposite sign.

Summary: The Dirac equation removes the problematic negative probabilities, but the negative energy solutions remain. We must also interpret the 4 components of the wave-function. We shall investigate these topics in the next lecture.