DIRAC EQUATION: DERIVATION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 20, Exercise 20.1.1.

The Dirac equation arose out of the need for a quantum mechanical wave equation that treats position and time on an equal basis. The first attempt at such an equation resulted in the Klein-Gordon equation, in which both time and position occur as second derivatives. However, the wave function in this equation is a scalar, meaning that it does not incorporate spin, which requires the wave function to have at least two components (in the case of spin-$\frac{1}{2}$; more components for higher spin).

Dirac began with the relativistic equation for the energy of a particle, which is

$$E=\sqrt{p^2c^2+m^2c^4} \tag{1}$$

where p is the momentum and m is the rest mass. The usual quantum mechanical prescription for converting the energy to an operator therefore requires replacing the numerical momentum p by its operator equivalent P, and doing this results in a square root containing an operator. It's not obvious how this can be handled.

Dirac's solution was essentially to turn the problem on its head. Rather than trying to find the square root of an existing quantity, he postulated that the quantity inside the square root is the perfect square of an expression that is linear in the momentum. That is, he proposed

$$P^2c^2+m^2c^4 = \left(c\alpha_xP_x+c\alpha_yP_y+c\alpha_zP_z+\beta mc^2\right)^2 \tag{2}$$

$$= \left(c\alpha\cdot\mathbf{P}+\beta mc^2\right)^2 \tag{3}$$

The problem is then to find the quantities α_i and β. We can do this by substituting

$$\mathbf{P}=P_x\hat{\mathbf{x}}+P_y\hat{\mathbf{y}}+P_z\hat{\mathbf{z}} \tag{4}$$

on the LHS of 3 and then matching terms. The LHS becomes

$$LHS = P^2c^2 + m^2c^4 = \mathbf{P}\cdot\mathbf{P}c^2 + m^2c^4 \tag{5}$$
$$= \left(P_x^2 + P_y^2 + P_z^2\right)c^2 + m^2c^4 \tag{6}$$

The RHS becomes

$$RHS = c^2\sum_{i=x,y,z}\alpha_i^2P_i^2 + c^2\left[\left(\alpha_x\alpha_y + \alpha_y\alpha_x\right)P_xP_y + \right. \tag{7}$$
$$\left.\left(\alpha_x\alpha_z + \alpha_z\alpha_x\right)P_xP_z + \left(\alpha_y\alpha_z + \alpha_z\alpha_y\right)P_yP_z\right] + \tag{8}$$
$$mc^3\sum_{i=x,y,z}\left(\alpha_i\beta + \beta\alpha_i\right)P_i + \beta^2m^2c^4 \tag{9}$$

Notice that this expansion assumes that α and β commute with $\mathbf{P}$, since we've factored out the terms involving P_i. This is equivalent to assuming that α and β do not depend on position, since the $\mathbf{P}$ operator contains derivatives with respect to position. For a free particle, this is reasonable, since such a particle is not localized anywhere in space. Note also that we do *not* assume that the α_is and β commute with each other, which is why we've written out the terms with these objects in a particular order.

In fact, if we require the LHS equal the RHS above, the α_is and β *cannot* commute. This is so because all the terms on the RHS except for the first and last terms must be zero. That is

$$\left[\alpha_i,\alpha_j\right]_+ = \alpha_i\alpha_j + \alpha_j\alpha_i = 0 \text{ if } i \neq j \tag{10}$$
$$\left[\alpha_i,\beta\right]_+ = \alpha_i\beta + \beta\alpha_i = 0 \tag{11}$$
$$\alpha_i^2 = \beta^2 = 1 \tag{12}$$

where $[]_+$ denotes an anticommutator.

Thus the α_is and β cannot be just numbers (real or complex), as all numbers commute. We *can* find α and β if we take them to be matrices. Since $c\alpha\cdot\mathbf{P} + \beta mc^2$ is to represent the Hamiltonian, it must be hermitian and, since $\mathbf{P}$ is hermitian (it's the momentum, which is observable), then α and β must also be hermitian.

To find them, we recall some properties of hermitian matrices. For hermitian matrices that satisfy

$$M^iM^j + M^jM^i = 2\delta^{ij}I \tag{13}$$

we found that their eigenvalues are ±1, they have zero trace and must be even-dimensional.

Our first thought is that the α_is and β are 2×2 matrices. This would be especially nice since it would then imply that the wave function ψ has two components which is just what we need to describe particles such as the electron with spin-$\frac{1}{2}$. However, we know that any 2×2 matrix can be written as a linear combination of the Pauli matrices and the 2×2 unit matrix and that there is no non-zero matrix that commutes with all three Pauli matrices. Thus there is no way to satisfy both 10 and 11 with 2×2 matrices. We are therefore forced to try the next simplest type of even-dimensional matrices, which are 4×4.

The most commonly used such matrices are given by

$$\alpha = \left[\begin{array}{cc} 0 & \sigma \\ \sigma & 0 \end{array}\right] \tag{14}$$

$$\beta = \left[\begin{array}{cc} I & 0 \\ 0 & -I \end{array}\right] \tag{15}$$

where σ represents the vector of 3 Pauli matrices, 0 represents a 2×2 zero matrix and I is the 2×2 unit matrix.

These aren't the only matrices that satisfy the conditions, since we can apply a unitary transformation with a unitary operator S. For example if we transform as follows:

$$\alpha_i' = S^\dagger \alpha_i S \tag{16}$$

$$\beta' = S^\dagger \beta S \tag{17}$$

then we have, since $S^\dagger = S^{-1}$:

$$\begin{aligned}
\left[\alpha_i',\alpha_j'\right]_+ &= \alpha_i'\alpha_j' + \alpha_j'\alpha_i' && (18)\\
&= S^\dagger\alpha_i S S^\dagger \alpha_j S + S^\dagger \alpha_j S S^\dagger \alpha_i S && (19)\\
&= S^\dagger \alpha_i \alpha_j S + S^\dagger \alpha_j \alpha_i S && (20)\\
&= S^\dagger \left[\alpha_i,\alpha_j\right]_+ S && (21)\\
&= 0 && (22)
\end{aligned}$$

Putting everything together, we get the Dirac equation

$$\boxed{i\hbar\frac{\partial\left|\psi\right\rangle}{\partial t} = \left(c\alpha\cdot\mathbf{P} + \beta mc^2\right)\left|\psi\right\rangle} \tag{23}$$

In this equation, since α and β are 4×4 matrices, the wave function $\left|\psi\right\rangle$ must be a 4-component vector. We'll see later how to make this consistent with a wave function describing a 2-component object such as an electron.

Finally, we can show that the Dirac equation still allows us to interpret $\psi^\dagger\psi$ as a probability density, provided we define the probability current appropriately. Conservation of probability requires the probability density ρ satisfies the continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0 \tag{24}$$

where $\mathbf{j}$ is the probability current. Starting with

$$\rho=\psi^{\dagger}\psi \tag{25}$$

we have (note that since ψ is now a vector, we need to maintain the correct order of terms):

$$\frac{\partial\rho}{\partial t}=\frac{\partial\psi^{\dagger}}{\partial t}\psi+\psi^{\dagger}\frac{\partial\psi}{\partial t} \tag{26}$$

$$=\frac{1}{-i\hbar}\left[\left(c\alpha^{\dagger}\cdot\mathbf{P}^{\dagger}+\beta^{\dagger}mc^{2}\right)\right]\psi^{\dagger}+\psi^{\dagger}\frac{1}{i\hbar}\left[\left(c\alpha\cdot\mathbf{P}+\beta mc^{2}\right)\right]\psi \tag{27}$$

Since α and β are hermitian, we have, using $\mathbf{P}=-i\hbar\nabla$ and $\mathbf{P}^{\dagger}=i\hbar\nabla$:

$$\frac{\partial\rho}{\partial t}=\frac{1}{-i\hbar}\left[\left(i\hbar c\alpha\cdot\nabla+\beta mc^{2}\right)\psi^{\dagger}\right]\psi+\psi^{\dagger}\frac{1}{i\hbar}\left[\left(-i\hbar c\alpha\cdot\nabla+\beta mc^{2}\right)\psi\right] \tag{28}$$

$$=-c\left(\alpha\cdot\nabla\psi^{\dagger}\right)\psi-\psi^{\dagger}c\left(\alpha\cdot\nabla\psi\right)-\frac{1}{i\hbar}\beta mc^{2}\psi^{\dagger}\psi+\frac{1}{i\hbar}\beta mc^{2}\psi^{\dagger}\psi \tag{29}$$

$$=-c\left(\alpha\cdot\nabla\psi^{\dagger}\right)\psi-\psi^{\dagger}c\left(\alpha\cdot\nabla\psi\right) \tag{30}$$

$$=-c\nabla\left(\psi^{\dagger}\alpha\psi\right) \tag{31}$$

We can therefore identify as the probability current

$$\mathbf{j}=c\psi^{\dagger}\alpha\psi \tag{32}$$