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Solving the Dirac Equation: Using Fourier Transform

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Abstract

When looking at the spin of a particle, the Dirac Equation is used to explain the significance of the spin. Here we solve Dirac Equation using the Fourier Transform, as well as explain and define the terms of the Dirac Equation. In addition, the Dirac Hamiltonian changes in Quantum Mechanics are examined. There will be a discussion of what the alpha matrices and beta matrix are made up of. The end result is defining the Dirac Equation for a particle in an electromagnetic field and solving this equation.

Introduction

The Dirac Equation is a relativistic quantum wave equation which was formulated by Paul Adrien Maurice Dirac in 1928. The Dirac Equation is used for the description of elementary spin – ½ particles, for example electrons. The equation demands the existence of antiparticles and actually predated their experimental discovery. This made the discovery of the positron, the antiparticle of the electron, one of the greatest triumphs of modern theoretical physics. The Dirac Equation looks as follows:

\[ H_D \Psi = E\Psi \]  

(1)

Where the \( H_D \) is Dirac’s Hamiltonian. This Hamiltonian is given by:

\[ H_D = c\alpha_k \cdot \vec{P} + \beta mc^2 \]  

(2)

Where the alpha matrix, \( \alpha_k \), and the beta matrix, \( \beta \), are 4 x 4 matrices. The \( \alpha_k \) consists of the Pauli Matrices. Pauli Matrices will be discussed later. The momentum, \( \vec{p} \), is a 3-D vector in the X, Y, Z direction, normally seen in the Cartesian coordinate system. The momentum is given by:

\[ \vec{P} = [p_x, p_y, p_z] \]  

(3)

The momentum in quantum mechanics is represented as operator and then becomes:
\[ \vec{P} \rightarrow -i\hbar \vec{V} \]  

(4)

where \( \vec{V} = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right] \)

And where \( \hbar \) is Dirac’s constant, which is Planck’s constant divided by \( 2\pi \). For relativistic effects to occur the particle has to be travelling close to or a fraction of the speed of light, which is designated by \( c \). And, \( m \) is the mass of the particle. The momentum is a vector and the dot product is being done between the momentum and \( \hat{\alpha}_\alpha \). Also \( \hat{\alpha}_\alpha \) is in 3 dimensions just like the momentum. Now Dirac’s Hamiltonian takes the form of:

\[ H_D = -i\hbar c \hat{\alpha}_\alpha \cdot \vec{V} + \beta mc^2 \]  

(5)

\[ H_D = -i\hbar \left( \hat{\alpha}_1 \frac{\partial}{\partial x} + \hat{\alpha}_2 \frac{\partial}{\partial y} + \hat{\alpha}_3 \frac{\partial}{\partial z} \right) + \beta mc^2 \]  

(6)

Now the steady state Dirac Equation is denoted by:

\[ \left[ -i\hbar c \left( \hat{\alpha}_1 \frac{\partial}{\partial x} + \hat{\alpha}_2 \frac{\partial}{\partial y} + \hat{\alpha}_3 \frac{\partial}{\partial z} \right) + \beta mc^2 \right] \Psi = E\Psi \]  

(7)

The above equation is also known as time independent Dirac Equation. But the time dependent Dirac Equation, the total energy, \( E \), becomes an operator in quantum mechanics. The operator looks as follows:

\[ E \rightarrow i\hbar \frac{\partial}{\partial t} \]  

(8)

From using equations 7 and 8, the time dependent Dirac Equation becomes:

\[ \left[ -i\hbar c \left( \hat{\alpha}_1 \frac{\partial}{\partial x} + \hat{\alpha}_2 \frac{\partial}{\partial y} + \hat{\alpha}_3 \frac{\partial}{\partial z} \right) + \beta mc^2 \right] \Psi = i\hbar \frac{\partial \Psi}{\partial t} \]  

(9)

**Pauli Matrices and Beta Matrix**

Since \( \hat{\alpha}_\alpha \) consist of Pauli Matrices, the Pauli Matrices are:

\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]  

(10)
The $\hat{\alpha}_k$ has 3 parts, as shown in equation 2, and is constructed from the Pauli Matrices. So, the 3 $\alpha$-matrices are as follows:

$$
\hat{\alpha}_1 = \begin{pmatrix} O & \sigma_1 \\ \sigma_1 & O \end{pmatrix} \quad \hat{\alpha}_2 = \begin{pmatrix} O & \sigma_2 \\ \sigma_2 & O \end{pmatrix} \\
\hat{\alpha}_3 = \begin{pmatrix} O & \sigma_3 \\ \sigma_3 & O \end{pmatrix}
$$

Where $O$ represents the null matrix that consists of a 2 x 2 matrix with all zeros. This makes the alpha matrices a 4 x 4 matrix, which is governed by:

$$
\hat{\alpha}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \hat{\alpha}_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \\
\hat{\alpha}_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}
$$

Similarly to the 3 $\alpha$-matrices, beta matrix, $\beta$, consists of the identity matrix.

$$
\beta = \begin{pmatrix} I & O \\ O & -I \end{pmatrix}
$$

Since the alpha matrices and beta matrix are both 4 x 4 matrices, therefore the wave function, $\Psi$, has to be a 4-component spinor. This is because the wave function consists of the particle spin – $\frac{1}{2}$ up and down, made up of two components. But the other two components are made up of the anti-particle spin, – $\frac{1}{2}$ up and down. The 4-component spinor is:

$$
\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}
$$

**Electromagnetic Field Dirac Equation**

When a particle is in an electromagnetic field, there are terms that must be accounted for. Due to the interaction of the electromagnetic fields, the energy and
momentum are changed slightly. The generalized Dirac Equation is obtained by making the following substitution:

\[ E \rightarrow i\hbar \frac{\partial}{\partial t} - q\phi \]  
(16)

\[ P \rightarrow -i\hbar \vec{\nabla} - q\vec{A} \]  
(17)

Where \( q \) is the charge of the particle, \( \phi \) is the electric scalar potential, and \( \vec{A} \) is the magnetic vector potential. This vector has X, Y, and Z components. The dot product of the \( \vec{A} \) and the alpha matrices is just like the dot product of momentum and the alpha matrices as explained before. This is so that the first alpha matrix goes with the X components of the momentum and the X component of the magnetic vector potential. The magnetic vector potential, \( \vec{A} \), is known as:

\[ \vec{A} = [A_x, A_y, A_z] \]  
(18)

With this change the Dirac Equation for a particle in an electromagnetic field becomes:

\[ \left[ -i\hbar c \hat{\alpha}_K \cdot \vec{\nabla} - cq\hat{\alpha}_K \cdot \vec{A} + \beta mc^2 \right] \Psi \]  
(19)

\[ = i\hbar \frac{\partial \Psi}{\partial t} - q\phi \Psi \]

Equation 19 can be changed to where the Dirac Equation becomes:

\[ \left[ -i\hbar c \hat{\alpha}_K \cdot \vec{\nabla} + \beta mc^2 \right] \Psi + V \Psi = i\hbar \frac{\partial \Psi}{\partial t} \]  
(20)

\[ V = q\left( \phi - c \hat{\alpha}_K \cdot \vec{A} \right) \]  
(21)

### Solution Using Fourier Transform

From looking at the steady state (time independent) Dirac Equation for a particle in an electromagnetic field, you can use Fourier transform to get the solution. Starting with:

\[ V \Psi = \left[ E + i\hbar c \hat{\alpha}_K \cdot \vec{\nabla} - \beta mc^2 \right] \Psi \]  
(22)

The 3-D Fourier transform then becomes:

\[ \chi_{j(\vec{k})} = \frac{1}{(2\pi)^{3/2}} \int \int \int \psi_j e^{-i\vec{k} \cdot \vec{x}} d^3 x \]  
(23)

where \( j = 1,2,3,4 \)
Next the gradient of the 3-D Fourier transform is developed into:

\[ \vec{\nabla} \cdot \chi_{j(\vec{s})} = (-i)^3 s^j \bar{\chi}_{j(\vec{s})} = i\vec{s} \chi_{j(\vec{s})} \]  \hspace{1cm} (24)

From plugging equation 24 into equation 22, the Dirac Equation then can be converted into:

\[ [E - \hbar c (\hat{\alpha}_\gamma \cdot \vec{s}) - \beta mc^2] \chi_{j(\vec{s})} = F(s) \] \hspace{1cm} (25)

\[ F(s) = \frac{1}{(2\pi)^{3/2}} \int \int \int_{-\infty}^{\infty} e^{-\vec{s} \cdot \vec{\chi}} d^3x \] \hspace{1cm} (26)

Since the wave function is the 4 component spinor, then \( \chi_{j(\vec{s})} \) and \( F(s) \) also have to be 4 components. There then is a lot of algebra that ultimately leads to:

\[
\begin{bmatrix}
(E-mc^2) \chi_1 \\
(E-mc^2) \chi_2 \\
(E+mc^2) \chi_3 \\
(E+mc^2) \chi_4
\end{bmatrix} - i\hbar \left( \sum_{k=1}^{3} O \sigma_k \right) \cdot \vec{s}_k \begin{bmatrix}
\chi_1 \\
\chi_2 \\
\chi_3 \\
\chi_4
\end{bmatrix} = \begin{bmatrix}
F_{1(\gamma)} \\
F_{2(\gamma)} \\
F_{3(\gamma)} \\
F_{4(\gamma)}
\end{bmatrix} \hspace{1cm} (27)
\]

This system can be simplified down to a \( \tilde{D} \) matrix times \( \chi_{j(\vec{s})} \), which looks as follows:

\[
\begin{bmatrix}
\chi_1 \\
\chi_2 \\
\chi_3 \\
\chi_4
\end{bmatrix} = \begin{bmatrix}
F_{1(\gamma)} \\
F_{2(\gamma)} \\
F_{3(\gamma)} \\
F_{4(\gamma)}
\end{bmatrix} \hspace{1cm} (28)
\]

\[
\begin{bmatrix}
(E-mc^2) \\
(E-mc^2) \\
(E+mc^2) \\
(E+mc^2)
\end{bmatrix} - i\hbar \left( \sum_{k=1}^{3} O \sigma_k \right) \cdot \vec{s}_k = \tilde{D} \hspace{1cm} (29)
\]

From taking the inverse \( \tilde{D} \) matrix, equation 28 becomes:
For \( \tilde{D} \) to have an inverse, the determinant of \( \tilde{D} \) must exist. If not then this solution does not work. Using the inverse 3-D Fourier transform, the solution can be turned into:

\[
\begin{bmatrix}
\psi_1 \\
\psi_2 \\
\psi_3 \\
\psi_4
\end{bmatrix} = \left(2\pi\right)^{3/2} \iiint_{-\infty}^{\infty} e^{i\tilde{\mathbf{x}} \cdot \tilde{\mathbf{r}}} \tilde{D}^{-1} d^3\tilde{s}
\]

\[
\begin{bmatrix}
F_{1,0} \\
F_{2,0} \\
F_{3,0} \\
F_{4,0}
\end{bmatrix}
\]

(31)

**Conclusion**

The Dirac Equation for a particle in an electromagnetic field shows us how the particle is affected by the electric field and the magnetic field. Also the Dirac equation tells how the field affects the spin and the polarity of the particle itself. From this solution, one can model the particle and place different potential energies into the equation. There are models that are currently being built to model how the particle would react in Gaussian potential energy.

A reminder is that the \( \tilde{D} \) matrix has to have a determinant for the Fourier solution to work at all. If \( \tilde{D} \) does not have a determinant, then the solution would have to be found another way. But \( \tilde{D} \) should always be able to have a determinant; therefore, a solution will always be able to be obtained.

A Couple of things that are next are to look at some of the numerical solutions of, first, the 1-D Fourier solution, then 2-D and 3-D numerical solutions, as well as looking at the Dirac Equation in spherical coordinates instead of Cartesian coordinates, as looked at here.

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