5.1: The Difference Between Relativistic and Non-Relativistic Quantum Mechanics

One of the key points in particles physics is that special relativity plays a key role. As you all know, in ordinary quantum mechanics we ignore relativity. Of course people attempted to generate equations for relativistic theories soon after Schrödinger wrote down his equation. There are two such equations, one called the Klein-Gordon and the other one called the Dirac equation.

The structure of the ordinary Schrödinger equation of a free particle (no potential) suggests what to do. We can write this equation as

\[ \hat{H}\psi = \frac{1}{2m}\vec{p}^2 \psi = i\hbar \frac{\partial}{\partial t}\psi.\]

This is clearly a statement of the non-relativistic energy-momentum relation, \( E = \frac{1}{2} m v^2 \), since a time derivative on a plane wave brings down a factor energy. Remember, however, that \( \vec{p} \) as an operator also contains derivatives, \( \vec{p} = \frac{\hbar}{i} \vec{\nabla} \). A natural extension would to use the relativistic energy expression,

\[ \hat{H}\psi = \sqrt{m^2c^4+\vec{p}^2c^2}\; \psi = i\hbar \frac{\partial}{\partial t}\psi. \label{EQ3} \]

This is a nonsensical equation, unless we specify how to take the square root of the operator. The first attempt to circumvent this problem, by Klein and Gordon, was to take the square of Equation \ref{EQ3} to generate the Klein-Gordon Equation (Equation \ref{KG}):

Klein-Gordon Equation

\[ \left( m^2c^4+\vec{p}^2c^2 \right) \psi = -\hbar^2 \frac{\partial^2}{\partial t^2}\psi. \label{KG} \]

\[ \left( m^2c^4+\vec{p}^2c^2 \right) \psi = -\hbar^2 \frac{\partial^2}{\partial t^2}\psi. \label{KG} \]
This is an excellent equation for spin-less particles or spin one particles (bosons), but not to describe fermions (half-integer spin), since there is no information about spin is in this equation. This needs careful consideration, since spin must be an intrinsic part of a relativistic equation!

Dirac realized that there was a way to define the square root of the operator. The trick he used was to define four matrices \(\alpha\), \(\beta\) that each have the property that their square is one, and that they anticommute,

\[
\begin{aligned}
2 \alpha_i \alpha_i &= I, & \beta \beta &= I, \\
\alpha_i \beta + \beta \alpha_i &= 0, & \alpha_i \alpha_j + \alpha_j \alpha_i &= 0 \quad (i \neq j).
\end{aligned}
\]

This then leads to an equation that is linear in the momenta – and very well behaved:

Dirac Equation

\[
(\beta mc^2 + c \vec{\alpha} \cdot \vec{p}) \Psi = i \hbar \frac{\partial}{\partial t} \Psi
\]

Note that the minimum dimension for the matrices in which we can satisfy all conditions is \(4\), and thus \(\Psi\) is a four-vector! This is closely related to the fact that these particles have spin.

Let us investigate this equation a bit further. One of the possible forms of \(\alpha_i\) and \(\beta\) is

\[
\alpha_i = \begin{pmatrix} 0 & \sigma_i \\
\sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\
0 & -I \end{pmatrix},
\]

where \(\sigma_i\) are the two-by-two Pauli spin matrices

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

(These matrices satisfy some very interesting relations. For instance

\[
\sigma_1 \sigma_2 = i \sigma_3, \quad \sigma_2 \sigma_1 = -i \sigma_3, \quad \sigma_2 \sigma_3 = i \sigma_1,
\]

etc. Furthermore \(\sigma_i^2 = 1\).)

Once we know the matrices, we can try to study a plane-wave solution (i.e., free particle):

\[
\Psi(\vec{x}, t) = u(\vec{p}) e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar}.
\]

(Note that the exponent is a “Lorentz scalar”, it is independent of the Lorentz frame!).

If substitute this solution we find that \(u(\vec{p})\) satisfies the eigenvalue equation

\[
\begin{pmatrix} mc^2 & 0 & p_3c & p_1c-i p_2c \\\n0 & mc^2 & p_1c+ip_2c & -p_3c \\\np_3c & p_1c -ip_2c & -mc^2 & 0 \\\np_1c+ip_2c & -p_3c & 0 & -mc^2 \end{pmatrix} \begin{pmatrix} u_1 \\
u_2 \\
u_3 \\
u_4 \end{pmatrix} = E \begin{pmatrix} u_1 \\
u_2 \\
u_3 \\
u_4 \end{pmatrix}.
\]
The eigenvalue problem can be solved easily, and we find the eigenvalue equation

\[(m^2c^4 + p^2 c^2 - E^2)^2 = 0\]

which has the solutions \((E = \pm \sqrt{m^2c^4 + p^2 c^2})\). The eigenvectors for the positive eigenvalues are

\[
\begin{pmatrix}
1 \\
0 \\
p_3c/(E+mc^2) \\
(p_1c-ip_2c)/(E+mc^2)
\end{pmatrix}
\text{, and }
\begin{pmatrix}
0 \\
1 \\
(p_1c+ip_2c)/(E+mc^2) \\
-p_3c/(E+mc^2)
\end{pmatrix},
\]

with similar expressions for the two eigenvectors for the negative energy solutions. In the limit of small momentum the positive-energy eigenvectors become

\[
\begin{pmatrix}
1 \\
0 \\
0 \\
0
\end{pmatrix}
\text{, and }
\begin{pmatrix}
0 \\
1 \\
0 \\
0
\end{pmatrix},
\]

and seem to denote a particle with spin up and down. We shall show that the other two solutions are related to the occurrence of anti-particles (positrons).

Just as photons are the best way to analyze (decompose) the electro-magnetic field, electrons and positrons are the natural way to decompose the Dirac field that is the general solution of the Dirac equation. This analysis of a solution in terms of the particles it contains is called (incorrectly, for historical reasons) “second quantisation”, and just means that there is a natural basis in which we can say there is a state at energy \((E)\), which is either full or empty. This could more correctly be referred to as the “occupation number representation” which should be familiar from condensed matter physics. This helps us to see how a particle can be described by these wave equations. There is a remaining problem, however!