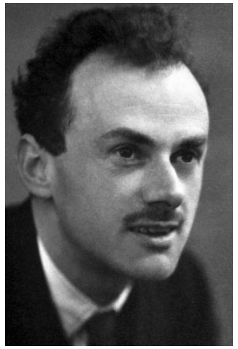
PC3130

Quantum Mechanics II

Dirac Equation
(for information only)

Dirac Equation for a relativistic free particle (1928)



Paul Dirac
Nobel Prize in Physics (1933) (awarded at 31 years of age)

https://www.youtube.com/watch?v=t7OVtGyQCIw&t=122s

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left(c\alpha\cdot p + \beta mc^2\right)\Psi(\mathbf{r},t),$$

where c is the speed of light, m is the electron mass and α and β are 4×4 matrices.

$$\beta^2 = I \qquad \{\alpha_k, \beta\} = 0 \qquad \{\alpha_k, \alpha_j\} = 2\delta_{kj}$$

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

σ_i turns out to obey the same algebraic relations as the Pauli matrices.

This is how the spin-half angular momentum arises naturally in the context of Dirac's equation for a relativistic free particle.

Dirac Equation (1928)

The solutions of the Dirac equation are four-component spinors:

$$\Psi(\mathbf{r},t) = \begin{pmatrix} \Psi_1(\mathbf{r},t) \\ \Psi_2(\mathbf{r},t) \\ \Psi_3(\mathbf{r},t) \\ \Psi_4(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} \Psi_A(\mathbf{r},t) \\ \\ \Psi_B(\mathbf{r},t) \end{pmatrix},$$

where $\Psi_A(\mathbf{r},t)$ and $\Psi_B(\mathbf{r},t)$ are two-component spinors.

Dirac Equation – Interaction with an electromagnetic field

$$i\hbar\frac{\partial\Psi_A(\mathbf{r},t)}{\partial t} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\Psi_B(\mathbf{r},t) + \left(mc^2 + q\phi(\mathbf{r})\right)\Psi_A(\mathbf{r},t),$$
$$i\hbar\frac{\partial\Psi_B(\mathbf{r},t)}{\partial t} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\Psi_A(\mathbf{r},t) - \left(mc^2 - q\phi(\mathbf{r})\right)\Psi_B(\mathbf{r},t),$$

where $\boldsymbol{\pi} = \mathbf{p} - q\mathbf{A}(\mathbf{r})$, and q is the electron charge (a negative number).

Consider the limit of small $\frac{v}{c}$.

Ignoring terms of order $\left(\frac{v}{c}\right)^2$ will give

$$\left[\frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) + q\phi(\mathbf{r}) - E'\right]\Psi_A(\mathbf{r}) = 0.$$

This is known as Pauli's equation, and its solutions are two-component spinors.

Pauli's Equation – small v/c limit of Dirac's equation

Using the relationship:

$$(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})(\boldsymbol{\sigma} \cdot \boldsymbol{\pi}) = \boldsymbol{\pi}^2 - \hbar q \boldsymbol{\sigma} \cdot \nabla \times \mathbf{A}(\mathbf{r}),$$

we can rewrite the Pauli equation as:

$$\left[\frac{\boldsymbol{\pi}^2}{2m} - \frac{\hbar q}{2m}\boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{r}) + q\phi(\mathbf{r}) - E'\right]\Psi_A(\mathbf{r}) = 0.$$

Dirac Equation – relativistic corrections

Pauli equation

$$\left[\frac{\pi^2}{2m} - \frac{\hbar q}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}(\mathbf{r}) + q\phi(\mathbf{r}) - E'\right]\Psi_A(\mathbf{r}) = 0.$$

Keeping terms in the Dirac equation up to order $\left(\frac{v}{c}\right)^2$ gives

$$\begin{aligned} H &= H_{Pauli} \\ &- \frac{p^4}{8m^3c^2} && \text{mass} - \text{velocity} \\ &+ \frac{\hbar^2 q}{8m^2c^2}\nabla\cdot\nabla\phi(\mathbf{r}) && \text{Darwin} \\ &- \frac{\hbar q}{4m^2c^2}\boldsymbol{\sigma}\cdot\left[\boldsymbol{\pi}\times\nabla\phi(\mathbf{r})\right]. && \text{spin} - \text{orbit} \end{aligned}$$

Without external magnetic field,
this is ***p***, which is proportional to ***v***

$$\boldsymbol{B} = -\frac{1}{2c^2}(\boldsymbol{v}\times\boldsymbol{E})$$

Dirac Hamiltonian: Existence of Spin

The Pauli Hamiltonian contains the interaction of spin with an external magnetic field. For a particle in an external potential, or interacting with other particles, a spin-dependence can also be present via the exchange term. But the spin up and spin down Hamiltonians can be separated and solved independently.

$$
\begin{aligned}
H &= \boxed{H_{Pauli}} \\
&- \frac{p^4}{8m^3c^2} \qquad \text{mass} - \text{velocity} \\
&+ \frac{\hbar^2 q}{8m^2c^2}\nabla\cdot\nabla\phi(\mathbf{r}) \qquad \text{Darwin} \\
&- \frac{\hbar q}{4m^2c^2}\boldsymbol{\sigma}\cdot\left[\boldsymbol{\pi}\times\nabla\phi(\mathbf{r})\right]. \qquad \text{spin} - \text{orbit}
\end{aligned}
$$

these terms are independent of spin

Only the spin-orbit term couples the spin up and spin down Hamiltonians, and also relates the spin to the lattice degrees of freedom. Without the spin-orbit term, we do not need two-component spinors.

Solutions are two-component spinors

Dirac Hamiltonian: Prediction of Antiparticle

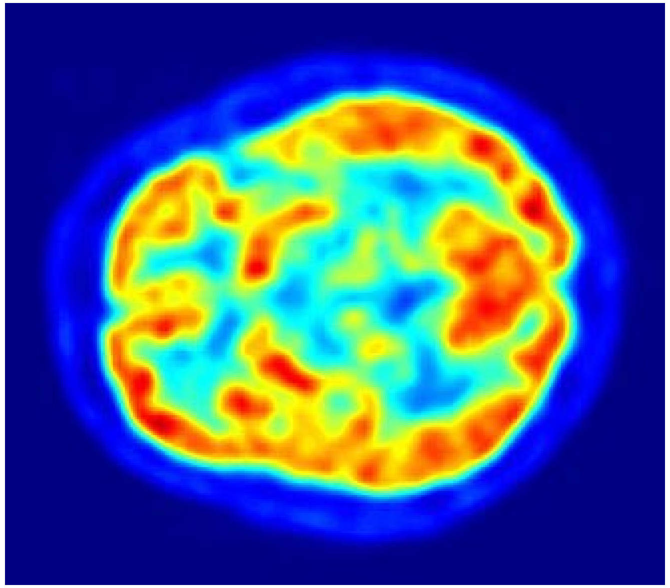
$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left(c\alpha \cdot p + \beta mc^2\right)\Psi(\mathbf{r},t),$$

where c is the speed of light, m is the electron mass and α and β are 4×4 matrices. The form of α and β is not unique. In

Solutions are <u>four</u>-component spinors

- The other two-components of the spinor represent an antiparticle, the positron (similar to an electron, except with positive charge).
- Discovered by Carl David Anderson in 1932 during the study of cosmic radiation.

Applications of Positrons in Imaging



PET image of the human brain (used for diagnosis of Alzheimer’s disease, for example)