Lesson 5 - Relativistic Wave Equations
Unit 5.2 Pauli Equation and the Spin

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Dirac equation with electromagnetic field (I)

Now we analyze the non-relativistic limit of the Dirac equation. Let us suppose that the relativistic particle has the electric charge q. In presence of an electromagnetic field, by using the Gauge-invariant substitution

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - q\,\phi(\mathbf{r},t) \quad (1)$$

$$-i\hbar\boldsymbol{\nabla} \to -i\hbar\boldsymbol{\nabla} - q\mathbf{A}(\mathbf{r},t) \quad (2)$$

in the Dirac equation, we obtain

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \Big(c\,\hat{\boldsymbol{\alpha}}\cdot(\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{r},t)) + \hat{\beta}\,mc^2 + q\,\phi(\mathbf{r},t)\Big)\,\Psi(\mathbf{r},t)\ , \quad (3)$$

where $\hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}$, $\phi(\mathbf{r},t)$ is the scalar potential and $\mathbf{A}(\mathbf{r},t)$ the vector potential.

Non-relativistic limit (I)

To workout the non-relativistic limit of Eq. (3) it is useful to set

$$\Psi(\mathbf{r},t) = e^{-imc^2t/\hbar}\begin{pmatrix}\psi_1(\mathbf{r},t)\\ \psi_2(\mathbf{r},t)\\ \chi_1(\mathbf{r},t)\\ \chi_2(\mathbf{r},t)\end{pmatrix} = e^{-imc^2t/\hbar}\begin{pmatrix}\psi(\mathbf{r},t)\\ \chi(\mathbf{r},t)\end{pmatrix}, \tag{4}$$

where $\psi(\mathbf{r},t)$ and $\chi(\mathbf{r},t)$ are two-component spinors, for which we obtain

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi\\ \chi\end{pmatrix} = \begin{pmatrix} q\,\phi & c\,\hat{\boldsymbol{\sigma}}\cdot(\hat{\mathbf{p}}-q\mathbf{A})\\ c\,\hat{\boldsymbol{\sigma}}\cdot(\hat{\mathbf{p}}-q\mathbf{A}) & q\,\phi-2mc^2\end{pmatrix}\begin{pmatrix}\psi\\ \chi\end{pmatrix} \tag{5}$$

where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_1,\hat{\sigma}_2,\hat{\sigma}_3)$.

Non-relativistic limit (II)

Remarkably, only in the lower equation of the previous system it appears the mass term mc^2, which is dominant in the non-relativistic limit. Indeed, under the approximation $\left(i\hbar\frac{\partial}{\partial t} - q\,\phi + 2mc^2\right)\chi \simeq 2mc^2\,\chi$, the previous equations become

$$\begin{pmatrix} i\hbar\frac{\partial\psi}{\partial t} \\ 0 \end{pmatrix} = \begin{pmatrix} q\,\phi & c\,\hat{\boldsymbol{\sigma}}\cdot(\hat{\mathbf{p}} - q\mathbf{A}) \\ c\,\hat{\boldsymbol{\sigma}}\cdot(\hat{\mathbf{p}} - q\mathbf{A}) & -2mc^2 \end{pmatrix} \begin{pmatrix} \psi \\ \chi \end{pmatrix}, \tag{6}$$

from which

$$\chi = \frac{\hat{\boldsymbol{\sigma}}\cdot(\hat{\mathbf{p}} - q\mathbf{A})}{2mc}\,\psi\,. \tag{7}$$

Inserting this expression in the upper equation of the system (6) we find

$$i\hbar\frac{\partial}{\partial t}\psi = \left(\frac{\left[\hat{\boldsymbol{\sigma}}\cdot(\hat{\mathbf{p}} - q\mathbf{A})\right]^2}{2m} + q\,\phi\right)\psi\,. \tag{8}$$

This is a non-relativistic Schordinger-like equation, derived from the relativistic Dirac equation.

Pauli equation and the spin (I)

From the identity

$$[\hat{\boldsymbol{\sigma}} \cdot (\hat{\mathbf{p}} - q\mathbf{A})]^2 = (\hat{\mathbf{p}} - q\mathbf{A})^2 - i\ q\ (\hat{\mathbf{p}} \wedge \mathbf{A}) \cdot \hat{\boldsymbol{\sigma}} \tag{9}$$

where $\hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}$, and using the relation $\mathbf{B} = \boldsymbol{\nabla} \wedge \mathbf{A}$ which introduces the magnetic field we finally get

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = \left(\frac{(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}(\mathbf{r}, t))^2}{2m} - \frac{q}{m}\mathbf{B}(\mathbf{r}, t) \cdot \hat{\mathbf{S}} + q\,\phi(\mathbf{r}, t) \right) \psi(\mathbf{r}, t)\ , \tag{10}$$

that is the so-called Pauli equation with

$$\hat{\mathbf{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}\ . \tag{11}$$

the spin operator. This equation was introduced in 1927 (a year before the Dirac equation) by Wolfgang Pauli as an extension of the Schrödinger equation with the phenomenological inclusion of the spin operator.

Pauli equation and the spin (II)

If the magnetic field $\mathbf{B}$ is constant, the vector potential can be written as

$$\mathbf{A} = \frac{1}{2}\mathbf{B} \wedge \mathbf{r} \tag{12}$$

and then

$$(\hat{\mathbf{p}} - q\mathbf{A})^2 = \hat{\mathbf{p}}^2 - 2q\mathbf{A} \cdot \hat{\mathbf{p}} + q^2\mathbf{A}^2 = \hat{\mathbf{p}}^2 - q\mathbf{B} \cdot \hat{\mathbf{L}} + q^2(\mathbf{B} \wedge \mathbf{r})^2 \ , \tag{13}$$

with $\hat{\mathbf{L}} = \mathbf{r} \wedge \hat{\mathbf{p}}$ the orbital angular momentum operator. Thus, the Pauli equation for a particle of charge q in a constant magnetic field reads

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = \left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} - \frac{q}{2m}\mathbf{B} \cdot \left(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}\right) + \frac{q^2}{2m}\,(\mathbf{B} \wedge \mathbf{r})^2 + q\,\phi(\mathbf{r}, t)\right)\psi(\mathbf{r}, t) \tag{14}$$

Pauli equation and the spin (III)

Thus, we have shown that the spin $\hat{\mathbf{S}}$ naturally emerges from the Dirac equation.
Moreover, the Dirac equation predicts very accurately the magnetic moment $\boldsymbol{\mu}_S$ of the electron ($q = -e$, $m = m_e$) which appears in the spin energy $E_s = -\hat{\boldsymbol{\mu}}_S \cdot \mathbf{B}$ of the Pauli equation. In particular, we have found

$$\boldsymbol{\mu}_S = -g_e \frac{\mu_B}{\hbar} \hat{\mathbf{S}} \tag{15}$$

where

$$g_e = 2 \tag{16}$$

is the gyromagnetic ratio and

$$\mu_B = \frac{e\hbar}{2m} \simeq 5.79 \cdot 10^{-5} \text{ eV/T} \tag{17}$$

is the Bohr magneton.