10 Dirac equation in external electromagnetic field

Gauge principle: Any wave equation should be invariant under local (space-time dependent) "gauge transformations" of the wave function:

$$\psi(x) \to \psi'(x) = e^{i\frac{q}{\hbar c}\chi(x)}\,\psi(x) \tag{10.1}$$

where q is a constant, and $\chi(x)$ is an arbitrary "gauge function". This $\psi'(x)$ should satisfy the same wave equation as $\psi(x)$.

If χ is a constant ("global gauge transformation"), any wave equation is invariant under $\psi \to \psi'$. But if χ depends on x ("local gauge transformation"), the free wave equations are not gauge invariant, because of derivative terms. For example, because of the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ in the free Dirac equation

$$\left[\left(\vec{\alpha}\cdot\hat{\vec{p}}\right)\,c + \beta\,mc^2\right]\psi(x) = i\hbar\dot{\psi}(x) \tag{10.2}$$

there is no invariance under the local gauge transformation (10.1).
In order to have invariance under (10.1), one has to introduce four "gauge fields" $A^\mu(x) = \left(\phi(x), \vec{A}(x)\right)$, which also transform under gauge transformations such that the wave equation is invariant. Physically, $\phi(x)$ is the "scalar potential", and $\vec{A}(x)$ the "vector potential". The new wave equation is

$$\left[\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}(x)\right)\,c + \beta\,mc^2 + q\phi(x)\right]\psi(x) = i\hbar\dot{\psi}(x) \tag{10.3}$$

Here we show that (10.3) is invariant under (10.1) and, at the same time

$$\phi(x) \to \phi'(x) = \phi(x) - \frac{1}{c}\dot{\chi}(x)\,, \qquad \vec{A}(x) \to \vec{A}'(x) = \vec{A}(x) + \vec{\nabla}\,\chi(x) \tag{10.4}$$

We show that, *if* the Dirac equation (10.3) is satisfied, then also

$$\left[\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}'(x)\right)\,c + \beta\,mc^2 + q\phi'(x)\right]\psi'(x) = i\hbar\dot{\psi}'(x) \tag{10.5}$$

is satisfied.

- Using (10.1) and (10.4) we have

$$\begin{aligned}\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}'(x)\right)\psi'(x) &= \vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}(x) - \frac{q}{c}\vec{\nabla}\chi\right)\,e^{i\frac{q}{\hbar c}\chi(x)}\,\psi(x)\\ &= e^{i\frac{q}{\hbar c}\chi(x)}\,\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}(x)\right)\,\psi(x)\end{aligned}$$

  where we used $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ in the last step.

- In the same way we obtain

$$\left(i\hbar\frac{\partial}{\partial t} - q\,\phi'(x)\right)\,\psi'(x) \;=\; \left(i\hbar\frac{\partial}{\partial t} - q\,\phi(x) + \frac{q}{c}\dot{\chi}(x)\right)\,e^{i\frac{q}{\hbar c}\chi(x)}\,\psi(x)$$
$$= e^{i\frac{q}{\hbar c}\chi(x)}\left(i\hbar\frac{\partial}{\partial t} - q\,\phi(x)\right)\,\psi(x)$$

Therefore, by cancelling an overall phase factor $e^{i\frac{q}{\hbar c}\chi(x)}$, Eq.(10.5) becomes the same as (10.3). This completes the proof of gauge invariance of Eq.(10.3).

Physically, the invariance under (10.4) means that the electric and magnetic fields $\vec{E}(x)$ and $\vec{B}(x)$ do not change under the gauge transformation. This follows from

$$\vec{E} = -\vec{\nabla}\,\phi - \frac{1}{c}\,\dot{\vec{A}}, \qquad \vec{B} = \vec{\nabla}\times\vec{A} \tag{10.6}$$

The "electromagnetic current" $j^\mu(x) = q\overline{\psi}(x)\gamma^\mu\psi(x)$ is conserved ($\partial_\mu j^\mu = 0$), and is gauge invariant. The Dirac equation (10.3) can be obtained from the free Dirac equation $\left[\vec{\alpha}\cdot\hat{\vec{p}}c + \beta\,mc^2\right] = i\hbar\dot{\psi}$ by the "minimal substitutions" $i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - q\,\phi$ and $\hat{\vec{p}} \to \hat{\vec{p}} - \frac{q}{c}\vec{A}$, or: [1]

$$\hat{p}^\mu \to \hat{p}^\mu - \frac{q}{c}\,A^\mu \tag{10.7}$$

The r.h.s. of (10.7) is called the <u>covariant derivative</u>. In covariant form, the free Dirac equation is then changed by the presence of an external electromagnetic field according to

$$\left(\hat{\not{p}} - mc\right)\psi = 0 \Rightarrow \left(\hat{\not{p}} - \frac{q}{c}\not{A} - m\,c\right)\psi = 0$$

11 Nonrelativistic limit and g-factor of electron

Consider the Dirac equation(10.3) for time-independent (static) fields $\phi(\vec{x})$ and $\vec{A}(\vec{x})$. Then, as usual, $\psi(\vec{x},t) = e^{-iEt/\hbar}\,\psi(\vec{x})$, and (10.3) becomes

$$\left[\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right)\,c + \beta\,mc^2 + q\phi(x)\right]\,\psi = E\,\psi(x) \tag{11.1}$$

Denoting $\vec{\pi} \equiv \left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right)$, and writing ψ in the form $\psi = (\varphi,\,\chi)$, we obtain from (11.1)

$$c\,(\vec{\sigma}\cdot\vec{\pi})\;\chi(\vec{x}) \;=\; \left(E - mc^2 - q\phi\right)\;\varphi(\vec{x}) \tag{11.2}$$

$$c\,(\vec{\sigma}\cdot\vec{\pi})\;\varphi(\vec{x}) \;=\; \left(E + mc^2 - q\phi\right)\;\chi(\vec{x}) \tag{11.3}$$

[1]Remember: $\hat{p}^\mu = i\hbar\partial^\mu = i\hbar\left(\frac{1}{c}\frac{\partial}{\partial t}, -\vec{\nabla}\right)$.

From (11.3) we obtain

$$\chi(\vec{x}) = \frac{c\,(\vec{\sigma}\cdot\vec{\pi})}{E + mc^2 - q\phi(\vec{x})}\,\varphi(\vec{x}) \tag{11.4}$$

Define the "binding energy" (ε) by $E \equiv mc^2 + \varepsilon$. (Note: This ε is the energy eigenvalue which appears in the Schrödinger equation.) Then we consider the <u>nonrelativistic limit</u>: All energies (like ε, $q\phi(\vec{x})$) are small compared to the rest energy mc^2. Then, from (11.4),

$$\chi(\vec{x}) \simeq \frac{(\vec{\sigma}\cdot\vec{\pi})}{2mc}\,\varphi(\vec{x})$$

and from (11.2) we obtain the Schrödinger-like equation for $\varphi(\vec{x})$ as

$$\left(\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} + q\phi(\vec{x})\right)\,\varphi(\vec{x}) = \varepsilon\,\varphi(\vec{x}) \tag{11.5}$$

What is $(\vec{\sigma}\cdot\vec{\pi})^2$? Using the identity $(\vec{\sigma}\cdot\vec{a})\left(\vec{\sigma}\cdot\vec{b}\right) = \left(\vec{a}\cdot\vec{b}\right) + i\vec{\sigma}\cdot\left(\vec{a}\times\vec{b}\right)$, we obtain

$$(\vec{\sigma}\cdot\vec{\pi})^2 = \vec{\pi}^2 + i\vec{\sigma}\cdot(\vec{\pi}\times\vec{\pi})$$

where $(\vec{\pi}\times\vec{\pi})$ is given by [2]

$$\begin{aligned}
(\vec{\pi}\times\vec{\pi}) &= \left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right)\times\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right) \\
&= -\frac{q}{c}\left(\hat{\vec{p}}\times\vec{A} + \vec{A}\times\hat{\vec{p}}\right) = -\frac{q}{c}\left(\hat{\vec{p}}\times\vec{A}\right) \\
&= \frac{i\hbar q}{c}\left(\vec{\nabla}\times\vec{A}\right) = \frac{i\hbar q}{c}\,\vec{B}
\end{aligned}$$

where $\vec{B}$ is the magnetic field. Then the Schrödinger-type equation (11.5) becomes

$$\left[\frac{\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right)^2}{2m} - \frac{q\hbar}{2mc}\,\vec{\sigma}\cdot\vec{B} + q\phi\right]\,\varphi(\vec{x}) = \varepsilon\,\varphi(\vec{x}) \tag{11.6}$$

If we neglect the term $\propto \vec{A}^2$ (weak magnetic field), we have

$$\begin{aligned}
\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right)^2 &\simeq \hat{\vec{p}}^2 - \frac{q}{c}\left(\hat{\vec{p}}\cdot\vec{A} + \vec{A}\cdot\hat{\vec{p}}\right) \\
&= \hat{\vec{p}}^2 - \frac{q}{c}\left(\hat{\vec{p}}\cdot\vec{A}\right) - \frac{2q}{c}\vec{A}\cdot\hat{\vec{p}}
\end{aligned} \tag{11.7}$$

[2] Note that $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ acts on all functions to the right, not only on $\vec{A}$ but also on the wave function φ. Therefore, $\hat{\vec{p}}\times\vec{A} = \left(\hat{\vec{p}}\times\vec{A}\right) - \vec{A}\times\hat{\vec{p}}$, where in the first term $\left(\hat{\vec{p}}\times\vec{A}\right)$ the momentum operator acts *only* on $\vec{A}$.

For a uniform magnetic field $\vec{B}$ we can choose the vector potential as follows [3]:

$$\vec{A} = \frac{1}{2}\left(\vec{B} \times \vec{x}\right) \tag{11.8}$$

In this gauge, $\left(\hat{\vec{p}} \cdot \vec{A}\right) = 0$, and Eq.(11.7) becomes

$$\begin{aligned}\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}\right)^2 &\simeq \hat{\vec{p}}^2 - \frac{q}{c}\left(\vec{B} \times \vec{x}\right) \cdot \hat{\vec{p}} \\ &= \hat{\vec{p}}^2 - \frac{q}{c}\vec{B} \cdot \left(\vec{x} \times \hat{\vec{p}}\right) = \hat{\vec{p}}^2 - \frac{q}{c}\vec{B} \cdot \vec{L}\end{aligned}$$

where $\vec{L} = \vec{x} \times \hat{\vec{p}}$ is the orbital angular momentum operator. Using also the spin operator $\vec{S} = (\hbar/2)\,\vec{\sigma}$, we finally obtain for (11.6):

$$\left[\frac{\hat{\vec{p}}^2}{2m} - \mu_B\,\vec{B} \cdot \left(\vec{L} + 2\vec{S}\right)\frac{1}{\hbar} + q\phi\right]\varphi(\vec{x}) = \varepsilon\,\varphi(\vec{x}) \tag{11.9}$$

Here $\mu_B = q\hbar/(2mc)$ is the Bohr magneton. The interaction with the magnetic field in (11.9) can be expressed as $-\mu_B\left(\vec{\mu} \cdot \vec{B}\right)$, where $\vec{\mu}$ is the magnetic moment operator given by

$$\vec{\mu} = \frac{1}{\hbar}\left(\vec{L} + 2\vec{S}\right) \equiv \frac{1}{\hbar}\left(g_\ell\,\vec{L} + g_s\,\vec{S}\right) \tag{11.10}$$

Here the orbital g-factor $g_\ell = 1$, and the spin g-factor $g_s = 2$. The prediction that $g_s = 2$ for the electron (and also the muon) was the first success of the Dirac equation. Eq.(11.10) was known before the Dirac equation, and is called the "Pauli equation".

Homework: One can "derive" the Pauli equation Eq.(11.9) also from the nonrelativistic free Schrödinger wave equation

$$\frac{\hat{\vec{p}}^2}{2m}\,\varphi(\vec{x}, t) = i\hbar\frac{\partial}{\partial t}\varphi(\vec{x}, t) \tag{11.11}$$

by the following trick: Use the identity for the Pauli spin matrices $(\vec{\sigma} \cdot \vec{a}) = \vec{a}^2$ for the case where the vector $\vec{a}$ is the momentum operator: $\vec{a} = \hat{\vec{p}}$. Use this trick in Eq.(11.11), and perform the minimal substitutions given above Eq.(10.7). Assume that the external electromagnetic fields are static to write $\varphi(\vec{x}, t) = e^{-i\varepsilon t/\hbar}\,\varphi(\vec{x})$, and show that $\varphi(\vec{x}, t)$ satisfies the Pauli equation (11.9). - Of course, this is not a very convincing proof, but it shows that $g_s = 2$ can be understood intuitively also without the Dirac equation.

[3] We can confirm that (11.8) satisfies $\vec{B} = \vec{\nabla} \times \vec{A}$. Eq.(11.8) is a special gauge, where $\left(\hat{\vec{p}} \cdot \vec{A}\right) = 0$, and is called the "transverse gauge".