Quantum Mechanics of a Charged Particle in an Electromagnetic Field

These notes present the Schrodinger equation for a charged particle in an external electromagnetic field. In order to obtain the relevant equation, we first examine the classical Hamiltonian of a charged particle in an electromagnetic field. We then use this result to obtain the Schrodinger equation using the principle of minimal substitution. We examine a special case of a uniform magnetic field. Finally, we demonstrate the origin of the coupling of the spin operator to the external magnetic field in the case of a charged spin-1/2 particle.

I. Classical Hamiltonian of a charged particle in an electromagnetic field

We begin by examining the classical theory of a charged spinless particle in and external electric field $\vec{\boldsymbol{E}}$ and magnetic field $\vec{\boldsymbol{B}}$. Gaussian (or cgs) units are employed for electromagnetic quantities. It is convenient to introduce the vector potential $\vec{\boldsymbol{A}}$ and the scalar potential ϕ:

$$\vec{\boldsymbol{B}} = \vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}\,, \qquad \vec{\boldsymbol{E}} = -\vec{\boldsymbol{\nabla}}\phi - \frac{1}{c}\frac{\partial \vec{\boldsymbol{A}}}{\partial t}\,. \tag{1}$$

These equations encode two of the four Maxwell equations,

$$\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{B}} = 0\,, \qquad \vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{E}} = -\frac{1}{c}\frac{\partial \vec{\boldsymbol{B}}}{\partial t}\,, \tag{2}$$

due to the vector identities

$$\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}(\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}) = 0\,, \qquad \vec{\boldsymbol{\nabla}} \times (\vec{\boldsymbol{\nabla}}\phi) = 0\,,$$

which are valid for any non-singular vector field $\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}}, t)$ and scalar field $\phi(\vec{\boldsymbol{r}}, t)$.

However, the fields $\vec{\boldsymbol{A}}$ and ϕ are not unique. Namely, the following transformations:

$$\vec{\boldsymbol{A}} \longrightarrow \vec{\boldsymbol{A}} + \vec{\boldsymbol{\nabla}}\chi(\vec{\boldsymbol{r}}, t)\,, \qquad \phi \longrightarrow \phi - \frac{1}{c}\frac{\partial \chi(\vec{\boldsymbol{r}}, t)}{\partial t}\,, \tag{3}$$

called *gauge transformations* leave the physical electromagnetic fields, $\vec{\boldsymbol{E}}$ and $\vec{\boldsymbol{B}}$, unchanged.

We wish to write down a classical Hamiltonian H that describes the motion of a charged particle q in an external electromagnetic field. Given H, we can use Hamilton's equations to derive the equations of motion for the charged particle. The correct Hamiltonian will yield the Lorentz force law:

$$\vec{\boldsymbol{F}} = \frac{d}{dt}(m\vec{\boldsymbol{v}}) = q\left(\vec{\boldsymbol{E}} + \frac{\vec{\boldsymbol{v}}}{c} \times \vec{\boldsymbol{B}}\right)\,. \tag{4}$$

The Hamiltonian for a charged particle in an electromagnetic field is given by:

$$\boxed{H = \frac{1}{2m}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) \boldsymbol{\cdot} \left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) + q\phi\,.} \tag{5}$$

We shall verify this result by using Hamilton's equations to compute the equations of motion and demonstrate that these coincide with eq. (4). For a Hamiltonian of the form $H = H(p_i, x_i)$, Hamilton's equations are given by:

$$\frac{\partial H}{\partial p_i} = \frac{dx_i}{dt}\,, \qquad\qquad -\frac{\partial H}{\partial x_i} = \frac{dp_i}{dt}\,,$$

where i runs over the three directions of space. In particular, the partial derivative with respect to p_i is computed at fixed x_i and the partial derivative with respect to x_i is computed at fixed p_i. Inserting eq. (5) into Hamilton's equations yields:

$$v_i \equiv \frac{dx_i}{dt} = \frac{p_i}{m} - \frac{q}{mc}A_i\,, \tag{6}$$

$$F_i \equiv \frac{dp_i}{dt} = \frac{q}{mc}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) \boldsymbol{\cdot} \frac{\partial \vec{\boldsymbol{A}}}{\partial x_i} - q\frac{\partial\phi}{\partial x_i}\,. \tag{7}$$

Eq. (6) is equivalent to:

$$\boxed{\vec{\boldsymbol{p}} = m\vec{\boldsymbol{v}} + \frac{q}{c}\vec{\boldsymbol{A}}\,.}$$

The quantity $m\vec{\boldsymbol{v}}$ is called the *mechanical momentum*, which is *not* equal to $\vec{\boldsymbol{p}}$, which is called the *canonical momentum*. The reason for this nomenclature will be addressed later. If we now substitute the equation for $\vec{\boldsymbol{p}}$ in eq. (7), we obtain:

$$\frac{d}{dt}\left(mv_i + \frac{q}{c}A_i\right) = \frac{q}{c}\,\vec{\boldsymbol{v}}\boldsymbol{\cdot}\frac{\partial \vec{\boldsymbol{A}}}{\partial x_i} - q\frac{\partial\phi}{\partial x_i}\,. \tag{8}$$

As noted above, the partial derivative with respect to x_i is computed while holding p_i (or equivalently holding v_i) fixed. Hence,

$$\vec{\boldsymbol{v}}\boldsymbol{\cdot}\frac{\partial \vec{\boldsymbol{A}}}{\partial x_i} = \frac{\partial}{\partial x_i}(\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{A}})\,.$$

Thus, we can rewrite eq. (8) as:

$$\frac{d}{dt}(mv_i) = \frac{q}{c}\left[\frac{\partial}{\partial x_i}(\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}) - \frac{dA_i}{dt}\right] - q\frac{\partial\phi}{\partial x_i}\,,$$

or equivalently in vector form as,

$$\frac{d}{dt}(m\vec{\boldsymbol{v}}) = \frac{q}{c}\left[\vec{\boldsymbol{\nabla}}(\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}) - \frac{d\vec{\boldsymbol{A}}}{dt}\right] - q\vec{\boldsymbol{\nabla}}\phi\,. \tag{9}$$

To make further progress, note that $d\vec{\boldsymbol{A}}/dt$ is a *full* time-derivative of $\vec{\boldsymbol{A}}$. By the chain rule,

$$\frac{d\vec{\boldsymbol{A}}}{dt} = \frac{\partial \vec{\boldsymbol{A}}}{\partial t} + \sum_{i=1}^{3} \frac{\partial \vec{\boldsymbol{A}}}{\partial x_i}\,\frac{dx_i}{dt}\,.$$

The chain rule reflects the physical fact that the full time-derivative of $\vec{\boldsymbol{A}}$ has two sources: (i) explicit time-dependence of $\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}}, t)$, and (ii) implicit time-dependence by virtue of the fact that the charged particle moves on a trajectory $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}(t)$. Noting that $v_i \equiv dx_i/dt$ [where $\vec{\boldsymbol{r}} \equiv (x_1\,,\,x_2\,,\,x_3)$], we can rewrite the chain rule above as:

$$\frac{d\vec{\boldsymbol{A}}}{dt} = \frac{\partial A}{\partial t} + (\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}})\vec{\boldsymbol{A}}\,.$$

Inserting this result in eq. (9) yields:

$$\frac{d}{dt}(m\vec{\boldsymbol{v}}) = \frac{q}{c}\left[\vec{\boldsymbol{\nabla}}(\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}) - (\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}})\vec{\boldsymbol{A}} - \frac{\partial \vec{\boldsymbol{A}}}{\partial t}\right] - q\vec{\boldsymbol{\nabla}}\phi\,. \tag{10}$$

Finally, we make use of the vector identity:

$$\vec{\boldsymbol{v}} \times (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}) = \vec{\boldsymbol{\nabla}}(\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}) - (\vec{\boldsymbol{v}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}})\vec{\boldsymbol{A}}\,.$$

This should remind you of the famous BAC-CAB rule for computing the triple cross-product: $\vec{\boldsymbol{A}} \times (\vec{\boldsymbol{B}} \times \vec{\boldsymbol{C}}) = \vec{\boldsymbol{B}}(\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{C}}) - \vec{\boldsymbol{C}}(\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{B}})$. In the case of the identity above, you have to be a little careful since one of the vectors is a differential operator. So, the more correct version is $\vec{\boldsymbol{A}} \times (\vec{\boldsymbol{B}} \times \vec{\boldsymbol{C}}) = \vec{\boldsymbol{B}}(\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{C}}) - (\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{B}})\vec{\boldsymbol{C}}$. The easiest way to prove the identity above is to write both sides in component form and simplify the left hand side until it takes the form of the right hand side. I leave this as an exercise for the reader. Applying the above identity to eq. (10) yields:

$$\frac{d}{dt}(m\vec{\boldsymbol{v}}) = \frac{q}{c}\vec{\boldsymbol{v}} \times (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}) - q\left(\vec{\boldsymbol{\nabla}}\phi + \frac{1}{c}\frac{\partial \vec{\boldsymbol{A}}}{\partial t}\right)\,.$$

Finally, using eq. (1), we end up with

$$\frac{d}{dt}(m\vec{\boldsymbol{v}}) = q\vec{\boldsymbol{E}} + \frac{q}{c}\,\vec{\boldsymbol{v}} \times \vec{\boldsymbol{B}}\,,$$

which coincides with eq. (4), as required.

So far, we have described the motion of a charged particle in an external electromagnetic field. If the particle also feels an external potential $V(\vec{\boldsymbol{r}}, t)$ that is unrelated to the external electromagnetic field, then we should use the more general Hamiltonian,

$$\boxed{H = \frac{1}{2m}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) + q\phi + V(\vec{\boldsymbol{r}}, t)\,.} \tag{11}$$

Eq. (11) suggests *the principle of minimal substitution*, which states that the Hamiltonian for a charged particle (of charge q) in an external electromagnetic field can be obtained from the corresponding Hamiltonian for an uncharged particle by making the following substitutions:

$$\vec{\boldsymbol{p}} \longrightarrow \vec{\boldsymbol{p}} - \frac{q}{c}\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}}, t)\,, \qquad V(\vec{\boldsymbol{r}}, t) \longrightarrow V(\vec{\boldsymbol{r}}, t) + q\phi(\vec{\boldsymbol{r}}, t)\,.$$

II. Schrodinger equation for a charged particle in an external electromagnetic field

We first write down the time-dependent Schrodinger equation,

$$H\,|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle\ ,$$

where

$$H = \frac{1}{2m}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) + q\phi + V(\vec{\boldsymbol{r}}, t)\,.$$

For simplicity, we will set the external potential $V(\vec{\boldsymbol{r}}, t)$ to zero, and assume that the electromagnetic potentials are time-independent. Then, the time-independent Schrodinger equation for stationary state solutions $|\psi\rangle$ is given by:

$$\frac{1}{2m}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)^2|\psi\rangle = (E - q\phi)\,|\psi\rangle\ .$$

Comparing this with the time-independent Schrodinger equation for a free particle, one can introduce the *principle of minimal substitution* at this point by noting that the time-independent Schrodinger equation for a charged particle of charge q is obtained by the substitution:

$$\vec{\boldsymbol{p}} \longrightarrow \vec{\boldsymbol{p}} - \frac{a}{c}\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}}, t)\,, \qquad E \longrightarrow E - q\phi(\vec{\boldsymbol{r}}, t)\,.$$

In the coordinate representation, we identify $\vec{\boldsymbol{p}}$ with the differential operator $-i\hbar\vec{\boldsymbol{\nabla}}$. Hence, the time-independent Schrodinger equation is given by:

$$\boxed{\frac{1}{2m}\left[i\hbar\vec{\boldsymbol{\nabla}} + \frac{q}{c}\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}})\right]^2\psi(\vec{\boldsymbol{r}}) + q\phi(\vec{\boldsymbol{r}})\psi(\vec{\boldsymbol{r}}) = E\psi(\vec{\boldsymbol{r}})\,.}$$

In obtaining the above result, we implicitly assumed that we should identify the canonical momentum $\vec{\boldsymbol{p}}$ [and *not* the mechanical momentum $m\vec{\boldsymbol{v}}$] with the operator $-i\hbar\vec{\boldsymbol{\nabla}}$. The momentum operator $\vec{\boldsymbol{p}}$ is called the *canonical* momentum because it satisfies the canonical commutation relations,

$$[x_i\,,\,p_j] = i\hbar\delta_{ij}\,.$$

This is one of the essential postulates of quantum mechanics. Had we tried to identify $m\vec{\boldsymbol{v}}$ with $-i\hbar\vec{\boldsymbol{\nabla}}$, we would have found that the resulting theory does not reduce to the classical limit as $\hbar \to 0$.

The Schrodinger equation written above can be expanded out:

$$\frac{-\hbar^2}{2m}\vec{\boldsymbol{\nabla}}^2\psi + \frac{iq\hbar}{mc}\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\psi + \frac{iq\hbar}{2mc}\psi(\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}) + \frac{q^2}{2mc^2}\vec{\boldsymbol{A}}^2\psi + q\phi\psi = E\psi\,,$$

where we have suppressed the coordinate arguments of the electromagnetic vector and scalar potentials and the wave function ψ. At this point, the equation can be simplified by *choosing a gauge*. I claim that given any $\vec{\boldsymbol{A}}$ and ϕ, I can perform a gauge transformation [cf. eq. (3)] such that the resulting $\vec{\boldsymbol{A}}$ and ϕ satisfy:

$$\boxed{\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{A}} = 0\,, \qquad \phi = 0\,, \qquad \text{Coulomb gauge conditions}}$$

Suppose $(\vec{\boldsymbol{A}}\,,\,\phi)$ are the initial vector and scalar potential. Making a gauge transformation,

$$\vec{\boldsymbol{A}}' = \vec{\boldsymbol{A}} + \vec{\boldsymbol{\nabla}}\chi(\vec{\boldsymbol{r}},t)\,, \qquad \phi' = \phi - \frac{1}{c}\frac{\partial\chi(\vec{\boldsymbol{r}},t)}{\partial t}\,.$$

To ensure that the Coulomb gauge conditions are satisfied, we require that:

$$\vec{\boldsymbol{\nabla}}^2\chi(\vec{\boldsymbol{r}},t) = -\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}},t)\,, \qquad \frac{\partial\chi(\vec{\boldsymbol{r}},t)}{\partial t} = c\phi(\vec{\boldsymbol{r}},t)\,.$$

One can always find a $\chi(\vec{\boldsymbol{r}},t)$ such that the above conditions are satisfied! By choosing such a $\chi(\vec{\boldsymbol{r}},t)$, it then follows that $\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}' = \phi' = 0$ as desired. Thus, the Schrodinger equation in the Coulomb gauge is given by:

$$\boxed{\frac{-\hbar^2}{2m}\vec{\boldsymbol{\nabla}}^2\psi + \frac{iq\hbar}{mc}\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\psi + \frac{q^2}{2mc^2}\vec{\boldsymbol{A}}^2\psi + q\phi\psi = E\psi\,.}$$

III. Schrodinger equation for a charged particle in a uniform electromagnetic field

We can use the results obtained Section II to examine two cases.

1. A uniform electric field

In this case, it is *not* convenient to use the Coulomb gauge. Instead, we choose $\vec{\boldsymbol{A}} = 0$ and $\vec{E} = -\vec{\boldsymbol{\nabla}}\phi$. The Schrodinger equation becomes:

$$\frac{-\hbar^2}{2m}\vec{\boldsymbol{\nabla}}^2\psi + q\phi\psi = E\psi\,,$$

which has the same form as the usual Schrodinger equation for a particle in a potential.

2. A uniform magnetic field

In this case, we will choose the Coulomb gauge. If $\vec{\boldsymbol{B}}$ is uniform in space and time-independent, then, one may choose:

$$\vec{\boldsymbol{A}} = -\tfrac{1}{2}\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}}\,, \qquad\qquad \phi = 0\,.$$

To check that this is correct, we use eq. (1) to compute $\vec{\boldsymbol{E}}$ and $\vec{\boldsymbol{B}}$. Since $\vec{\boldsymbol{A}}$ is time-independent and $\phi = 0$, it follows that $\vec{\boldsymbol{E}} = 0$. Next, we compute $\vec{\boldsymbol{B}} = \vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}$. Noting that:

$$A_x = -\tfrac{1}{2}(yB_z - zB_y)\,, \qquad A_y = -\tfrac{1}{2}(zB_x - xB_z)\,, \qquad A_z = -\tfrac{1}{2}(xB_y - yB_x)\,,$$

one easily evaluates:

$$\begin{aligned}\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}} &= \hat{\boldsymbol{x}}\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) + \hat{\boldsymbol{y}}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right) + \hat{\boldsymbol{z}}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) \\ &= \hat{\boldsymbol{x}}B_x + \hat{\boldsymbol{y}}B_y + \hat{\boldsymbol{z}}B_z = \vec{\boldsymbol{B}}\,.\end{aligned}$$

Furthermore, note that

$$\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{A}} = -\tfrac{1}{2}\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}}) = 0\,,$$

which confirms that we have indeed chosen the Coulomb gauge. Thus, the time-independent Schrodinger equation reads:

$$\frac{-\hbar^2}{2m}\vec{\boldsymbol{\nabla}}^2\psi - \frac{iq\hbar}{2mc}(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}})\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\psi + \frac{q^2}{8mc^2}(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}})^2\psi = E\psi\,.$$

This equation can be simplified by noting the vector identity:

$$(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}})\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\psi = -\vec{\boldsymbol{B}}\boldsymbol{\cdot}(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{\nabla}}\psi)\,.$$

Hence,

$$-\frac{iq\hbar}{2mc}(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}})\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\psi = -\frac{q}{2mc}\vec{\boldsymbol{B}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{r}} \times \frac{\hbar}{i}\vec{\boldsymbol{\nabla}}\psi\right)\,.$$

We identify the *canonical angular momentum operator*,

$$\vec{\boldsymbol{L}} \equiv \vec{\boldsymbol{r}} \times \frac{\hbar}{i}\vec{\boldsymbol{\nabla}}\,. \tag{12}$$

This is to be distinguished from the mechanical angular momentum $\vec{\boldsymbol{r}} \times (m\vec{\boldsymbol{v}})$. You can check that the canonical angular momentum operators of eq. (12) satisfy the usual angular momentum commutation relations,

$$[L_i\,,\,L_j] = i\hbar\sum_{k=1}^{3}\epsilon_{ijk}L_k\,.$$

Hence, we can write:

$$-\frac{iq\hbar}{2mc}(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}})\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\psi = -\frac{q}{2mc}\vec{\boldsymbol{B}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}\psi\,.$$

Finally, if we use the vector identity,

$$(\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}})^2 = r^2 \vec{\boldsymbol{B}}^2 - (\vec{\boldsymbol{r}} \boldsymbol{\cdot} \vec{\boldsymbol{B}})^2 ,$$

then the time-independent Schrodinger equation for a charged particle of charge q in an external uniform magnetic field $\vec{\boldsymbol{B}}$ is given by:

$$\boxed{\frac{-\hbar^2}{2m}\vec{\boldsymbol{\nabla}}^2\psi - \frac{q}{2mc}\vec{\boldsymbol{B}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}\,\psi + \frac{q^2}{8mc^2}\left[r^2\vec{\boldsymbol{B}}^2 - (\vec{\boldsymbol{r}}\boldsymbol{\cdot}\vec{\boldsymbol{B}})^2\right]\psi = E\psi\,.} \tag{13}$$

IV. Schrodinger equation for a charged spin-1/2 particle in an electromagnetic field

So far, we have neglected spin. For a spin-1/2 particle, the wave function is a spinor of the form

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} .$$

Likewise, the Hamiltonian operator must be a 2×2 matrix.

To determine the correct Hamiltonian for a charged spin-1/2 particle in an electromagnetic field, we choose the Hamiltonian for a free uncharged spin-1/2 particle to be:

$$H = \frac{(\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\vec{\boldsymbol{p}})^2}{2m} . \tag{14}$$

Noting that $(\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\vec{\boldsymbol{p}})^2 = \vec{\boldsymbol{p}}^{\,2}\mathbf{I}$, where $\mathbf{I}$ is the 2×2 identity matrix, we recover the expected free particle Hamiltonian. In order to obtain the Hamiltonian for a charged spin-1/2 particle, we apply the principle of minimal substitution to eq. (14).[1] Thus, we choose

$$H = \frac{1}{2m}\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) + q\phi\mathbf{I}\,.$$

We can simplify the first term above by writing:

$$\begin{aligned}
\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) &= \sum_{ij}\sigma_i\sigma_j\left(p_i - \frac{qA_i}{c}\right)\left(p_j - \frac{qA_j}{c}\right) \\
&= \sum_{ijk}(\delta_{ij}\mathbf{I} + i\epsilon_{ijk}\sigma_k)\left(p_i - \frac{qA_i}{c}\right)\left(p_j - \frac{qA_j}{c}\right) \\
&= \left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)^2\mathbf{I} - \frac{iq}{c}\sum_{ijk}\epsilon_{ijk}(p_iA_j + A_ip_j)\sigma_k\,,
\end{aligned} \tag{15}$$

[1]If one applies the principle of minimal substitution to $H = (\vec{\boldsymbol{p}}^2/(2m))\mathbf{I}$, one obtains a spin-independent Hamiltonian, which is in conflict with experiment. Remarkably, applying the principle of minimal substitution to eq. (14) yields a spin-dependent Hamiltonian, which is in very good agreement with experiment.

where we have used the sigma matrix identity,

$$\sigma_i\sigma_j = \mathbf{I}\,\delta_{ij} + i\sum_{k=1}^{3}\epsilon_{ijk}\sigma_k\,.$$

Note that

$$\sum_{ij}\epsilon_{ijk}p_ip_j = \sum_{ij}\epsilon_{ijk}A_iA_j = 0\,,$$

since $\epsilon_{ijk} = -\epsilon_{jik}$ is a totally antisymmetric tensor.

To evaluate the second term in eq. (15) above, we use

$$\sum_{ijk}\epsilon_{ijk}(p_iA_j + A_ip_j)\sigma_k = \sum_{ijk}\epsilon_{ijk}(p_iA_j - A_jp_i)\sigma_k\,,$$

where we have used the antisymmetry of ϵ_{ijk} followed by an appropriate relabeling of indices. Employing the operator identity (which is most easily checked in the coordinate representation),

$$p_iA_j - A_jp_i = [p_i, A_j] = -i\hbar\frac{\partial A_j}{\partial x_i}\,,$$

it follows that

$$\sum_{ij}\epsilon_{ijk}(p_iA_j + A_ip_j) = \sum_{ij}\epsilon_{ijk}[p_i, A_j] = -i\hbar\sum_{ij}\epsilon_{ijk}\frac{\partial A_j}{\partial x_i} = -i\hbar B_k\,,$$

after recognizing that $\vec{\boldsymbol{B}} = \vec{\boldsymbol{\nabla}}\times\vec{\boldsymbol{A}}$ implies that:

$$B_k = \sum_{ij}\epsilon_{ijk}\frac{\partial A_j}{\partial x_i}\,.$$

Consequently,

$$\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right) = \left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)^2\mathbf{I} - \frac{\hbar q}{c}\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\vec{\boldsymbol{B}}\,.$$

Thus, the Hamiltonian for a charged spin-1/2 particle in an external electromagnetic field is:

$$\boxed{H = \frac{1}{2m}\left(\vec{\boldsymbol{p}} - \frac{q\vec{\boldsymbol{A}}}{c}\right)^2\mathbf{I} - \frac{\hbar q}{2mc}\vec{\boldsymbol{\sigma}}\boldsymbol{\cdot}\vec{\boldsymbol{B}} + q\phi\,\mathbf{I}\,.}$$

That is, if H_0 is the spin-independent part of the Hamiltonian, then

$$H = H_0 - \frac{q}{mc}\vec{\boldsymbol{S}}\boldsymbol{\cdot}\vec{\boldsymbol{B}}\,, \tag{16}$$

where we have identified the spin-1/2 operator, $\vec{\boldsymbol{S}} = \frac{1}{2}\hbar\vec{\boldsymbol{\sigma}}$.

Let us apply the above results to obtain the time-independent Schrodinger equation for a charged spin-1/2 particle in a uniform magnetic field. Using eqs. (13) and (16), it follows that:

$$\boxed{\frac{-\hbar^2}{2m}\vec{\boldsymbol{\nabla}}^2\psi - \frac{q}{2mc}\vec{\boldsymbol{B}}\boldsymbol{\cdot}(\vec{\boldsymbol{L}}+2\vec{\boldsymbol{S}})\,\psi + \frac{q^2}{8mc^2}\left[r^2\vec{\boldsymbol{B}}^2 - (\vec{\boldsymbol{r}}\boldsymbol{\cdot}\vec{\boldsymbol{B}})^2\right]\psi = E\psi\,.}$$

Note especially the relative factor of 2 in $\vec{\boldsymbol{L}}+2\vec{\boldsymbol{S}}$ above. This means that we have predicted that an elementary charged spin-1/2 particle has a g-factor equal to 2. In more general circumstances, we will replace $\vec{\boldsymbol{L}}+2\vec{\boldsymbol{S}}$ in the above equation with $\vec{\boldsymbol{L}}+g\vec{\boldsymbol{S}}$, where g is determined from experiment.