Chapter 2

University of Delaware
Electrical and Computer Engineering Department
ELEG/PHYS667 Magnetism & Spintronics
Prof. Ian Appelbaum

Now that we have established the empirical fact that the electron has an intrinsic magnetic moment (which is called spin), let's take a look at the theory which predicts its existence *a priori*. Since electron spin is fundamentally a consequence of relativistic quantum mechanics, we need to study the relativistic version of the Schrödinger equation, called the Dirac Equation.

1 Schrödinger Equation

1.1 Classical background

Without assuming too much, let's first construct the *nonrelativistic* Schrödinger equation. This is a wave equation, so let's look at how the classical wave equation can be constructed from the general form of a 1-dimensional plane wave

$$\Psi(x,t) = e^{i(kx-\omega t)}. \tag{1}$$

The wavenumber $k = 2\pi/\lambda$ is related to the angular frequency $\omega = 2\pi\nu$ by the *dispersion relation*. For classical waves such as electromagnetic waves, we have $\lambda\nu = c$, so the dispersion relation is

$$\omega = kc \tag{2}$$

and, therefore,

$$\Psi(x,t) = e^{i(kx-kct)} \tag{3}$$

where c is the speed of light. The wave equation is a partial differential equation in x an t, so let's look at a few derivatives. First, with respect to x:

$$\frac{d}{dx}\Psi = ik\Psi \tag{4}$$

$$\frac{d^2}{dx^2}\Psi = -k^2\Psi \tag{5}$$

and with respect to t:

$$\frac{d}{dt}\Psi = ikc\Psi \tag{6}$$

$$\frac{d^2}{dt^2}\Psi = -k^2c^2\Psi. \tag{7}$$

Now, notice that

$$\frac{d^2}{dx^2}\Psi = \frac{1}{c^2}\frac{d^2}{dt^2}\Psi \tag{8}$$

This is the classical wave equation.

1.2 Matter Waves

For matter waves, we have a different dispersion relation since we have the deBroglie hypothesis

$$p = \hbar k \tag{9}$$

and the Einstein law

$$E = \hbar\omega \tag{10}$$

We know from classical mechanics that

$$E = \frac{1}{2}mv^2 = \frac{1}{2m}p^2 \tag{11}$$

(since p=mv). Applying DeBroglie's and Einstein's insight gives us

$$\hbar\omega = \frac{1}{2m}\hbar^2 k^2 \tag{12}$$

$$\omega = \frac{1}{2m}\hbar k^2. \tag{13}$$

which is the dispersion relation for matter waves we are looking for.
Now, this gives a plane wave

$$\Psi(x,t) = e^{i(kx - \frac{\hbar k^2}{2m}t)} \tag{14}$$

which has a second derivative with respect to x

$$\frac{d^2}{dx^2}\Psi(x,t) = -k^2\Psi \tag{15}$$

as before. However, unlike the classical case in which we need two derivatives in t to recover the k^2 term, this time the *first* derivative with respect to t gives it to us:

$$\frac{d}{dt}\Psi(x,t) = -i\frac{\hbar k^2}{2m}\Psi \tag{16}$$

Now, we can construct our matter wave equation by equating:

$$-\frac{1}{k^2}\frac{d^2}{dx^2}\Psi(x,t) = i\frac{2m}{\hbar k^2}\frac{d}{dt}\Psi(x,t) \tag{17}$$

which is re-arranged into its well known form:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x,t) = i\hbar\frac{d}{dt}\Psi(x,t) \tag{18}$$

the time-dependent Schrödinger Equation for a free particle (no potential energy). We can interpret this equation as the quantum analogue of

$$E = \frac{p^2}{2m} \tag{19}$$

If we make the identifications

$$E \rightarrow i\hbar\frac{d}{dt} \tag{20}$$

and

$$p \rightarrow \frac{\hbar}{i}\frac{d}{dx}. \tag{21}$$

This is justified because if these differential operators act on our wavefunction, we get *eigenvalues*

$$E \rightarrow i\hbar\frac{d}{dt}\Psi = \hbar\omega\Psi \tag{22}$$

(Einstein's Law) and

$$p \rightarrow \frac{\hbar}{i}\frac{d}{dx}\Psi = \hbar k \Psi. \tag{23}$$

(DeBroglie's Hypothesis). When a potential is present, the Schrödinger Equation becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi(x,t) = i\hbar\frac{d}{dt}\Psi(x,t) \tag{24}$$

which is equivalent to quantum-mechanically saying

$$E_{total} = \frac{p^2}{2m} + V(x) = E_{kinetic} + E_{potential}. \tag{25}$$

1.3 Separation of Variables

The variables x and t in the time-dependent equation can be decoupled by using the method of separation of variables. This assumes the wavefunction for arbitrary (time-independent) potential is the product of two time-dependent and spatially dependent functions:

$$\Psi(x,t) = \psi(x)\phi(t). \tag{26}$$

Then our Schödinger equation is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x)\phi(t) = i\hbar\frac{d}{dt}\psi(x)\phi(t). \tag{27}$$

Since the derivatives act on only one of the variables, we can divide by $\psi(x)\phi(t)$ to find

$$-\frac{\hbar^2}{2m}\frac{\psi(x)''}{\psi(x)} + V(x) = i\hbar\frac{\dot{\phi}(t)}{\phi(t)}. \tag{28}$$

where primes denote spatial derivatives and the dot is a time derivative.

Now, since the LHS depends only on x and the RHS depends only on t, they each must be equal to the same constant, which we can immediately identify as E, the eigenvalue of energy. This gives us two decoupled equations

$$i\hbar\dot{\phi}(t) = E\phi(t). \tag{29}$$

and

$$-\frac{\hbar^2}{2m}\psi(x)'' + V(x)\psi(x) = E\psi(x) \tag{30}$$

The first one can be immediately solved:

$$\phi(t) = e^{-\frac{iEt}{\hbar}} \tag{31}$$

which is not surprising since $E/\hbar = \omega$.

The second equation is the time-independent Schrdinger equation and can be written explicitly as an *eigenvalue equation*

$$H\psi = E\psi \tag{32}$$

where H, the differential operator in the Schrödinger equation, is known for historical reasons as the Hamiltonian.

2 Dirac Equation

As we saw, the non-relativistic Schödinger Equation starts with $E = \frac{p^2}{2m}$ and ends with:

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\Psi = i\hbar\frac{d}{dt}\Psi \tag{33}$$

This is not consistent with relativity which says

$$E = \sqrt{(mc^2)^2 + p^2c^2} \tag{34}$$

(Although this looks completely different, this expression is consistent with the non-relativistic limit:

$$E = mc^2\sqrt{1 + \frac{p^2c^2}{m^2c^4}} = mc^2(1 + \frac{p^2c^2}{2m^2c^4} + \ldots) \approx mc^2 + \frac{p^2}{2m} \tag{35}$$

In the non-relativistic limit, the kinetic energy is much smaller than the rest mass energy mc^2 and the dynamics are determined by the former.)

The problem with starting with this relativistic form of the energy is that it results in a relativistic Schrödinger Equation which does not treat space (the spatial derivative contained in p) and time (on the right hand side) equivalently, breaking the major axiom of relativity saying these dimensions should be treated on equal footing:

$$\sqrt{(mc^2)^2 + p^2c^2}\Psi = i\hbar\frac{d}{dt}\Psi \tag{36}$$

If, somehow, the term in the squareroot was a perfect square, space and time *would* be treated equally. Dirac first showed how this was done:

$$m^2c^4 + p^2c^2 = (\alpha_0 mc^2 + \sum_{j=1}^{3}\alpha_j p_j c)^2 \tag{37}$$

where j indexes each spatial x,y,z dimension. The only way for this to occur is if the α_j's obey the following rules:

$$\alpha_i^2 = 1, i = 0, 1, 2, 3 \tag{38}$$

and

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 0, i \neq j \tag{39}$$

This is known as a "Clifford Algebra", and obviously cannot be satisfied by scalar quantities. However, it can be satisfied by four matrices, and the simplest representation is 4×4:

$$\alpha_0 = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \tag{40}$$

(I is the 2×2 identity) and

$$\alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix} \tag{41}$$

where the σ_j's are the 2×2 "Pauli matrices". This results in a 4×4 Dirac Hamiltonian operator (matrix)

$$\alpha_0 mc^2 + \sum_{j=1}^{3}\alpha_j p_j c \tag{42}$$

and the wavefunction ψ is likewise a 4-component spinor (a spinor is like a vector, only its rotational transormation properties are different).

Dirac interpreted this result as being twofold: in addition to the relativistic wave equation for the electron (2 components), we get another equation for a particle which was not discovered at the time, which was first called a "hole" and later a positron. The 2 components for the electron were interpreted as the amplitude of the wavefunction in the spin up and down directions. Carl Anderson discovered this particle in 1932 and received the Nobel Prize four years later. Paul Dirac received the Nobel prize earlier in 1933, along with Erwin Schrödinger.

3 Pauli Matrices

If we are interested only in the electron, we can use only the 2 components corresponding to those states. But we need to derive the elements of the Pauli matrices.

Consider a general Hamiltonian

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \tag{43}$$

and corresponding Schrödinger equation $H\psi = E\psi$:

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \cdot \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = E \cdot \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \tag{44}$$

This equation has a non-trivial solution only if the following is true:

$$det \begin{bmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{bmatrix} = 0 \tag{45}$$

we can expand this equation as:

$$(H_{11} - E)(H_{22} - E) - H_{21}H_{12} = 0 \tag{46}$$

$$E^2 - (H_{11} + H_{22})E + (H_{11}H_{22} - H_{21}H_{12}) = 0 \tag{47}$$

This quadratic equation can be solved easily with the quadratic equation:

$$E = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{(H_{11} + H_{22}) \pm \sqrt{(H_{11} + H_{22})^2 - 4(H_{11}H_{22} - H_{21}H_{12})}}{2} \tag{48}$$

$$E = \frac{H_{11} + H_{22}}{2} \pm \sqrt{\frac{(H_{11} + H_{22})^2}{4} - (H_{11}H_{22} - H_{21}H_{12})} \tag{49}$$

$$E = \frac{H_{11} + H_{22}}{2} \pm \sqrt{\frac{H_{11}^2 + 2H_{11}H_{22} + H_{22}^2}{4} - H_{11}H_{22} + H_{21}H_{12}} \tag{50}$$

$$E = \frac{H_{11} + H_{22}}{2} \pm \sqrt{\frac{H_{11}^2 - 2H_{11}H_{22} + H_{22}^2}{4} + H_{21}H_{12}} \tag{51}$$

$$E = \frac{H_{11} + H_{22}}{2} \pm \sqrt{\frac{(H_{11} - H_{22})^2}{4} + H_{21}H_{12}} \tag{52}$$

3.1 Pause

Now let's imagine we have a spin 1/2 electron in a DC B field. We know from our earlier studies

$$E = \pm g_S \frac{\mu_B}{2} B = \pm \mu_B B. \tag{53}$$

Let's define two orthogonal wavefunctions with projections $+1/2\hbar$ and $-1/2\hbar$ with B along $\hat{z}$:

$$\psi_{up} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \psi_{down} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{54}$$

with associated Energy eigenvalues $-\mu_B B$ and $\mu_B B$. This means that

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = -\mu_B B \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{55}$$

and

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \mu_B B \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{56}$$

This can only be true if $H_{11} = -\mu_B B$ and $H_{22} = \mu_B B$.

3.2 back to the grind

The results of the above section mean that the first term in Eq. 52 is zero.

Therefore,

$$E^2 = \frac{(H_{11} - H_{22})^2}{4} + H_{21}H_{12}. \tag{57}$$

Now, if we have an arbitrary field such that $B = B_x\hat{x} + B_y\hat{y} + B_z\hat{z}$, we know that

$$E^2 = \mu_B^2 \left(B_x^2 + B_y^2 + B_z^2\right). \tag{58}$$

giving

$$\frac{(H_{11} - H_{22})^2}{4} + H_{21}H_{12} = \mu_B^2(B_x^2 + B_y^2 + B_z^2) \tag{59}$$

Now, we know that H_{11} and H_{22} are $\pm\mu_B B$:

$$\frac{(H_{11} - H_{22})^2}{4} + H_{21}H_{12} = \frac{(-\mu_B B - (+\mu_B B))^2}{4} + H_{21}H_{12} \tag{60}$$

$$\mu_B^2 B_z^2 + H_{21}H_{12} = \mu_B^2(B_z^2 + B_x^2 + B_y^2). \tag{61}$$

$$H_{21}H_{12} = \mu_B^2(B_x^2 + B_y^2). \tag{62}$$

Because H must be Hermitian to restrict its eigenvalues E to real values, this has a solution

$$H_{12} = \mu_B B_x \mp iB_y \tag{63}$$

$$H_{21} = H_{12}^\dagger = \mu_B B_x \pm iB_y \tag{64}$$

Therefore,

$$H = -\mu_B \begin{bmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{bmatrix} \tag{65}$$

$$= -\mu_B \left[B_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + B_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + B_y \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \right] \tag{66}$$

$$= -\mu_B(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z) = -\mu_B \vec{\sigma} \cdot \vec{B} \tag{67}$$

The σs are the 2×2 Pauli matrices we are after, and they tell us how a quantized spin couples to a field in the x, y, or z directions.

4 Time-Dependent Spin Mechanics

Now lets use the Pauli matrices to determine the mechanics of a spin in a magnetic field consisting of a DC component in the ẑ direction and an AC component in the x̂ direction. As seen previously, our Hamiltonian is

$$-\mu\vec{\sigma} \cdot \vec{B} \tag{68}$$

With a field in the x and z directions $B = B\hat{z} + A\cos\omega t\hat{x}$, the dot product with the vector of matrices $\hat{\sigma}$ gives

$$H = -\mu \left[\begin{bmatrix} B & 0 \\ 0 & -B \end{bmatrix} + \begin{bmatrix} 0 & A\cos\omega t \\ A\cos\omega t & 0 \end{bmatrix} \right] = -\mu \begin{bmatrix} B & A\cos\omega t \\ A\cos\omega t & -B \end{bmatrix} \tag{69}$$

Now we need to use this Hamiltonian in the Schrödinger equation to solve for the spin wavefunction which will tell us about the mechanics of state evolution in time given this field configuration:

$$H\Psi = i\hbar \frac{d}{dt}\Psi \tag{70}$$

To solve this equation, we make a guess or *ansatz* that the solution will look generally like:

$$\Psi = \begin{bmatrix} C_1(t)e^{-i\omega_1 t} \\ C_2(t)e^{-i\omega_2 t} \end{bmatrix} \tag{71}$$

Therefore, if $\gamma = -\mu A$ and $E_{1,2} = \pm\mu_B B$,

$$\begin{bmatrix} E_1 & \gamma\cos\omega t \\ \gamma\cos\omega t & E_2 \end{bmatrix} \cdot \begin{bmatrix} C_1(t)e^{-i\omega_1 t} \\ C_2(t)e^{-i\omega_2 t} \end{bmatrix} = i\hbar\frac{d}{dt}\begin{bmatrix} C_1(t)e^{-i\omega_1 t} \\ C_2(t)e^{-i\omega_2 t} \end{bmatrix} \tag{72}$$

This matrix equation represents two coupled differential equations:

$$\gamma\cos\omega t C_2 e^{-i\omega_2 t} + E_1 C_1 e^{-i\omega_1 t} = i\hbar\left[C_1' e^{-i\omega_1 t} - iC_1\omega_1 e^{-i\omega_1 t}\right] \tag{73}$$

and

$$\gamma\cos\omega t C_1 e^{-i\omega_1 t} + E_2 C_2 e^{-i\omega_2 t} = i\hbar\left[C_2' e^{-i\omega_2 t} - iC_2\omega_2 e^{-i\omega_2 t}\right] \tag{74}$$

where the prime denotes time derivative and the explicit time dependence in the Cs is assumed.

First, we note that since $\hbar\omega_1 = E_1$ and $\hbar\omega_2 = E_2$, the second terms on each side are equal and cancel out. Thus, substituting $\cos\omega t = \frac{1}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)$, we are left with

$$\frac{\gamma C_2}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)e^{-i\omega_2 t} = i\hbar C_1' e^{-i\omega_1 t} \tag{75}$$

and

$$\frac{\gamma C_1}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)e^{-i\omega_1 t} = i\hbar C_2' e^{-i\omega_2 t} \tag{76}$$

Writing $\omega_0 = \omega_2 - \omega_1$, we have

$$\frac{\gamma C_2}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)e^{-i\omega_0 t} = i\hbar C_1' \tag{77}$$

and

$$\frac{\gamma C_1}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)e^{i\omega_0 t} = i\hbar C_2' \tag{78}$$

Distributing,

$$\frac{\gamma C_2}{2}\left(e^{i(\omega-\omega_0)t} + e^{-i(\omega+\omega_0)t}\right) = i\hbar C_1' \tag{79}$$

and

$$\frac{\gamma C_1}{2}\left(e^{i(\omega+\omega_0)t} + e^{-i(\omega-\omega_0)t}\right) = i\hbar C_2' \tag{80}$$

Since we are interested in behavior near resonance, i.e. when $\omega \approx \omega_0$, the terms like $e^{\pm i(\omega-\omega_0)t}$ will be close to one but the other term like $e^{\pm i(\omega+\omega_0)t}$ will be oscillating very fast and average out to zero. Therefore, we discard these terms and are left with

$$\frac{\gamma C_2}{2}e^{i(\omega-\omega_0)t} = i\hbar C_1' \tag{81}$$

and

$$\frac{\gamma C_1}{2}e^{-i(\omega-\omega_0)t} = i\hbar C_2' \tag{82}$$

Solving the Equation 81 for C_2:

$$C_2 = \frac{2i\hbar}{\gamma}e^{-i(\omega-\omega_0)t}C_1' \tag{83}$$

and substituting into Equation 82 gives

$$\frac{\gamma C_1}{2}e^{-i(\omega-\omega_0)t} = i\hbar\frac{2i\hbar}{\gamma}\left[C_1'' e^{-i(\omega-\omega_0)t} - i(\omega-\omega_0)C_1' e^{-i(\omega-\omega_0)t}\right] \tag{84}$$

which simplifies to

$$C_1 = -\frac{4\hbar^2}{\gamma^2}\left(C_1'' - i(\omega-\omega_0)C_1'\right) \tag{85}$$

Rearranging gives

$$C_1'' - i(\omega - \omega_0)C_1' + \frac{\gamma^2}{4\hbar^2}C_1 = 0 \tag{86}$$

This is a linear, second-order differential equation in C_1. The form of this equation comes up many times in physics and elecronics. Take for example the LRC circuit with characteristic equation

$$I'' + \frac{R}{L}I' + \frac{1}{LC}I = 0 \tag{87}$$

or "mass on a damped spring" F=ma:

$$X'' + \frac{\eta}{m}X' + \frac{k}{m}X = 0 \tag{88}$$

4.1 Resonance

When we are at resonance, $\omega = \omega_0$. The damping term disappears and we have

$$C_1'' + \frac{\gamma^2}{4\hbar^2}C_1 = 0 \tag{89}$$

This has solution

$$C_1 = \cos\frac{\gamma}{2\hbar}t \tag{90}$$

which we substitute into Equation 81 to get

$$i\hbar C_2' = \frac{\gamma}{2}\cos\frac{\gamma}{2\hbar}t \tag{91}$$

This can be easily integrated to find

$$C_2 = -i\int \frac{\gamma}{2\hbar}\cos\frac{\gamma}{2\hbar}t\,dt = -i\sin\frac{\gamma}{2\hbar}t \tag{92}$$

The probability of finding the spin in the "up" state $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is

$$C_1^* C_1 = \cos^2\frac{\gamma}{2\hbar}t \tag{93}$$

whereas the probability of finding the spin in the down state $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ is

$$C_2^* C_2 = \sin^2\frac{\gamma}{2\hbar}t \tag{94}$$

Under resonant excitation, the spin apparently flip-flops back and forth between up and down states at a rate determined by the intensity of the excitation (A in $\gamma = -\mu A$).