1 Readings

Liboff, Introductory Quantum Mechanics, Ch. 11

2 The Hamiltonian with spin

Previously we discussed the Hamiltonian in position representation. For a single particle, e.g., an electron, this is $H_0\psi(x) = E\psi(x)$, with

$$H_0(x) = \frac{\hat{p}^2}{2m} + V(x).$$

Now we expand the wave function to include spin, by considering it to be a function with two components, one for each of the S_z basis states in the $\mathscr{C}^2$ spin state space.

$$\begin{bmatrix} \psi(x,+1/2) \\ \psi(x,-1/2) \end{bmatrix}$$

Note that the spatial part of the wave function is the same in both spin components.

Now we can act on the spin-space wave function with either spin operators σ_i (or equivalently, S_i) or spatial operators such as H_0. Each of these acts only on the spin and space degrees of freedom, respectively. Does the spin variable (S_z) ever interact with the space variable (x)? Yes, of course, this is how we detected spin originally - via the interaction of the spin angular momentum $\vec{S}$ with a spatially varying magnetic field. For an electron in an atom there is also another interaction, the spin-orbit interaction. The full Hamiltonian for an electron with spin is of the form

$$\left[H_0 + H_1 + H_2 + \frac{\hbar}{i}\frac{\partial}{\partial t}\right]\psi(z, S_z) = 0$$

where

$$\begin{aligned} H_1 &= \frac{e\hbar}{2m}\vec{B}\cdot\left(\vec{l} + g\vec{S}\right) \\ H_2 &= (g-1)\frac{e\hbar}{2m}\vec{B}_{int}\cdot\vec{S} \\ &= 2(g-1)Z\left(\frac{e\hbar}{2m}\right)^2\frac{1}{r^3}\left(\vec{l}\cdot\vec{S}\right). \end{aligned}$$

H_1 is the interaction of the spin angular momentum with an external magnetic field $\vec{B}$. We have added the spin angular momentum to the orbital angular momentum $\vec{l}$, which is a function of real space variables (recall $\vec{l} = \vec{r}\times\vec{p}$. H_2 is the interaction of the spin angular momentum with the internal magnetic field. This is the magnetic field in the rest frame of the electron that appears when the electron moves in the electric field of the nucleus, through a Lorentz transformation:

$$\vec{B}_{int} = \frac{1}{c}\frac{\vec{E}\times\vec{v}}{\sqrt{1-v^2/c^2}}.$$

It is therefore a relativistic effect. Substitution of the electric field $\vec{E} = Ze\vec{r}/r^3$ and hence the orbital angular momentum as $\vec{r}\times\vec{p}$ leads to the expression of spin-orbit coupling, i.e., an interaction between the spin angular momentum $\vec{S}$ and the orbital angular momentum $\vec{l}$.

3 Two spins: addition of angular momenta

Consider two angular momenta $\vec{L}_1$ and $\vec{L}_2$. Our treatment is general, and does not distinguish orbital from spin angular momentum. We can make a composite state $\left|L_1,L_2,m_1,m_2\right\rangle$ since the four operators L_1^2, L_2^2, L_{1z} and L_{2z} are mutually commuting. We refer to this as the 'uncoupled representation'. But we can also measure the total angular momentum and its z-projection, $\vec{L}^2 = (\vec{L}_1+\vec{L}_2)^2$ and $L_z = L_{z1}+L_{z2}$. Furthermore, these two operators commute with L_1 and L_2 (check). So we can also form the state $\left|L,m,L_1,L_2\right\rangle$ where $m = L_z$. We refer to this as the 'coupled representation.

Now the question is, what are the allowed values of L and m? Well, the maximum value of m must be $m_{max} = m_{1max}+m_{2max} = L_1+L_2$. Hence the maximum allowed value of L is also equal to L_1+L_2. This L value will have $2L+1$ possible m values associated with it.

What other states of L are possible? We can use a state counting argument to find them, together with the requirement that L change by integral values only. In the uncoupled representation we have a total of $(2L_1+1)(2L_2+1)$ states. On changing to the coupled representation we are just relabeling states and must preserve the dimensionality of the space. So we must have

$$\sum_{L_{min}}^{L_1+L_2}(2L+1) = (2L_1+1)(2L_2+1).$$

This is satisfied if $L_{min} = |L_1-L_2|$. Hence our allowed values of total angular momentum are given by

$$\begin{aligned} L &= |L_1-L_2|, |L_1-L_2|+1, ..., L_1+L_2 \\ m &= -L, -L+1, ..., +L. \end{aligned}$$

Now lets evaluate this for 2 spins, e.g., 2 electrons. $S_1 = S_2 = 1/2$. Hence the allowed values of total spin are $S = 1, S = 0$. The $S = 1$ state has three values of $m = -1, 0, +1$ associated with it and is called a spin triplet. The $S = 0$ state has one value of $m = 0$ associated with it and is called a spin singlet.

4 Exchange (permutation) symmetry

Consider two electrons. Their total spin satisfies

$$\begin{aligned} |S_1+S_2|^2 &= S_1^2+S_2^2+2S_1\cdot S_2 \\ &= \frac{3}{2}\hbar^2+2S_1\cdot S_2. \end{aligned}$$

Now evaluate $S_1 \cdot S_2$ in terms of the Pauli spin matrices, and act on the column vector $\psi(S_{1z}, S_{2z}) = \begin{bmatrix} \psi(+1/2,+1/2) \\ \psi(+1/2,-1/2) \\ \psi(-1/2,+1/2) \\ \psi(-1/2,-1/2) \end{bmatrix}$. Adding the constant $\frac{3}{2}\hbar^2$ allows one to obtain the action of the total angular momentum on the two spin wavefunction:

$$|S_1 + S_2|^2 \psi = \hbar^2 \begin{bmatrix} 2\psi(+1/2,+1/2) \\ \psi(+1/2,-1/2) + \psi(-1/2,1/2) \\ \psi(-1/2,1/2) + \psi(1/2,-1/2) \\ 2\psi(-1/2,-1/2) \end{bmatrix}.$$

Comparing the form of this wave function with that of ψ above, we find that

- for $S = 1$, we need $\psi(+1/2,-1/2) = \psi(-1/2,1/2)$, i.e., $\psi(S_{1z}, S_{2z}) = \psi(S_{2z}, S_{1z})$, the triplet spin wave function is symmetric with respect to particle interchange
- for $S = 0$, we need $\psi(+1/2,-1/2) = \psi(-1/2,1/2) = 0$ and $\psi(+1/2,+1/2) = \psi(-1/2,-1/2) = 0$. These conditions are only satisfied if$\psi(S_{1z}, S_{2z}) = -\psi(S_{2z}, S_{1z})$, i.e., the spin wave function is antisymmetric with respect to particle interchange.

There is a fundamental restriction that indistinguishable particles with half integer spin (fermions) have total wavefunctions that are antisymmetric with respect to particle interchange. Thus an $S = 1$ spin wave function must combine with an antisymmetric spatial wave function and an $S = 0$ spin wave function with a symmetric spatial wave function. This gives rise to the Pauli principle, two fermions cannot exist in the same quantum state. Since

$$\psi_A(r_1, S_1, r_2, S_2) = -\psi_A(r_2, S_2, r_1, S_1),$$

if we set $r_1 = r_2$ and S_1, S_2, then we arrive at

$$\psi_A(r_1, S_1, r_1, S_1) = -\psi_A(r_1, S_1, r_1, S_1),$$

which is only satisfied by $\psi_A(r_1, S_1, r_1, S_1) = 0$. So there is zero probability of finding the electrons at the same location in space and with the same spin.

Is this important for qubits? NO! Generally it is not, since we always assume we can address the qubits individually and they are then no longer indistinguishable. So we don't have to worry about the Pauli principle for qubits although it is very important for electrons in atoms.

5 Unitary spin manipulation I: Larmor Precession

Turning on a magnetic field $\vec{B}$, the qubit state rotates. There are two steps to understanding this process, essentially the same steps we make to understand any quantum process:

- Find $\hat{H}$
- Solve Schrödinger equation

For the second step, we first solve the "time-independent" Schrödinger equation; that is, we find energy eigenstates

$$\hat{H}\big|\psi_n\big\rangle = E_n\big|\psi_n\big\rangle \quad .$$

The "time-dependent" Schrödinger equation

$$i\hbar\tfrac{d}{dt}\big|\psi(t)\big\rangle = \hat{H}\big|\psi(t)\big\rangle$$

then has solution

$$\big|\psi(t)\big\rangle = e^{-i\frac{\hat{H}}{\hbar}t}\big|\psi(t=0)\big\rangle \quad .$$

Expanding $\big|\psi(t=0)\big\rangle = \sum_n c_n\big|\psi_n\big\rangle$, we get

$$\big|\psi(t)\big\rangle = \sum_n c_n e^{-iE_nt/\hbar}\big|\psi_n\big\rangle \quad .$$

(This assumes that $\hat{H}$ is time-independent. If the Hamiltonian is itself a function of t, $\hat{H} = \hat{H}(t)$, then we must directly solve the time-dependent Schrödinger equation.)

5.1 Find $\mathscr{H}$

for a spin in a B-field.

Assume there is only potential energy, not kinetic energy. Classically, $E = -\vec{\mu}\cdot\vec{B}$. Quantumly, the magnetic moment is in fact a vector *operator*, $\hat{\vec{\mu}} = \frac{gq}{2m}\hat{\vec{S}} = -\frac{e}{m}\hat{\vec{S}}$. Hence we set the quantum Hamiltonian to be

$$\hat{H} = \tfrac{e}{m}\hat{\vec{S}}\cdot\vec{B} \quad .$$

We may choose our coordinate system so $\vec{B} = B\hat{z}$; then

$$\hat{H} = \tfrac{eB}{m}\hat{S}_z \quad .$$

5.2 Solve Schrödinger Equation

Following the recipe we gave above, we start by finding the eigendecomposition of $\hat{H}$. The eigenstates of $\hat{H}$ are just those of $\hat{S}_z$: $\big|0\big\rangle$ (up, $m = +1/2$) and $\big|1\big\rangle$ (down, $m = -1/2$). The corresponding eigenenergies are $E_0 = \frac{eB}{2m}\hbar$, $E_1 = -\frac{eB}{2m}\hbar$, respectively.

Next we solve the time-dependent Schrödinger equation. Consider

$$\big|\psi(t=0)\big\rangle = \alpha\big|0\big\rangle + \beta\big|1\big\rangle \quad .$$

Then

$$\begin{aligned}\big|\psi(t)\big\rangle &= \alpha e^{-i\frac{eB}{2m}t}\big|0\big\rangle + \beta e^{i\frac{eB}{2m}t}\big|1\big\rangle \\ &\propto \alpha\big|0\big\rangle + \beta e^{i\frac{eB}{m}t}\big|1\big\rangle \quad ,\end{aligned}$$

where the proportionality is up to a global phase (a convenient representation for the Bloch Sphere. On the Bloch sphere,

$$\big|\psi(t=0)\big\rangle = \cos\tfrac{\theta}{2}\big|0\big\rangle + \sin\tfrac{\theta}{2}e^{i\varphi}\big|1\big\rangle$$

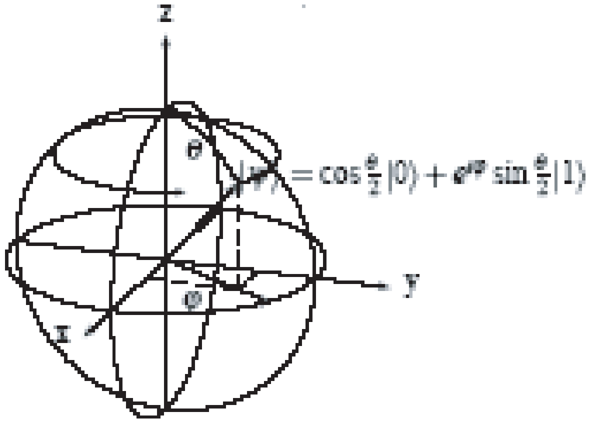

Figure 1:

thus evolves to

$$\left|\psi(t)\right\rangle = \cos\tfrac{\theta}{2}\left|0\right\rangle + \sin\tfrac{\theta}{2}e^{i(\varphi+\frac{eB}{m}t)}\left|1\right\rangle \quad .$$

Thus the state rotates counterclockwise around the z axis (counterclockwise when viewed from above), at frequency $\omega_0 \equiv \frac{eB}{m}$ (ω_0 is known as the cyclotron frequency, since it is the same frequency with which a classical e^- cycles in a magnetic field, due to the Lorentz force). See Figure 1. In time t, the azimuth has changed by an amount $\Delta\phi = (eB/m)t$.

5.3 Rotations around z-axis

This provides us with a "quantum gate", $\hat{R}_z$, for rotating around the Bloch sphere at a given latitude determined by θ. $\hat{R}_z(\Delta\varphi) = e^{-i\frac{\hat{S}_z}{\hbar}\Delta\varphi}$ is a unitary operation which rotates by $\Delta\varphi$ about the z axis. (Proof: $\hat{R}_z(\Delta\varphi)$ is exactly $e^{-i\frac{\hat{H}}{\hbar}t}$ for $t = \Delta\varphi/\omega_0$.) Being unitary means $\hat{R}_z(\Delta\varphi)^\dagger = \hat{R}_z(\Delta\varphi)^{-1} = \hat{R}_z(-\Delta\varphi)$.

So aligning $\vec{B}$ with the z axis results in rotation of the spin about the z axis. Each state is restricted to the line of latitude it starts on, as illustrated above. For a more general rotation about a different axis, simply point the $\vec{B}$ field in a different direction. For example, the unitary operator

$$\hat{R}_n(\Delta\gamma) = e^{-i\frac{\hat{\vec{S}}\cdot\hat{n}}{\hbar}\Delta\gamma}$$

rotates by $\Delta\gamma$ about the axis $\hat{n}$. To achieve this unitary transformation, set $\vec{B} = B\hat{n}$ for exactly time $t = \Delta\gamma/\omega_0$.

5.4 Rotations around arbitrary axis

Any unitary transformation on a single qubit, up to a global phase, is a rotation on the Bloch sphere about some axis; mathematically, this is the well-known isomorphism $SU(2)/\pm 1 \cong SO(3)$ between 2×2 unitary matrices up to phase and 3×3 real rotation matrices. Hence Larmor precession, or spin rotation, allows us to achieve any single qubit unitary gate. While theoretically simple, Larmor precession can unfortunately be inconvenient in real life, mostly because of the high frequencies involved and the susceptibility to noise. A more practical method for achieving rotations on the Bloch sphere is spin resonance, which we will describe in the next lecture.