(22) More on Spin

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- Perturbations
- Intro to Spin

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- Adding spin to Hydrogen
- Multi-particle states

3   Spin and Angular Momentum

Last time we spoke, I left you with a somewhat fuzzy notion of spin as a property of the electron which had something to do with angular momentum, but I didn't do anything mathematically rigorous with that notion. Vladan took things further by talking about spin decomposition and procession in a magnetic field. This time we'll connect spin to orbital angular momentum, and then move on to entanglement.

For a spin 1/2 particle, like the electron,

$$S_z = \pm\tfrac{1}{2}\hbar, \quad |S|^2 = \tfrac{1}{2}(\tfrac{1}{2}+1)\hbar^2 = \tfrac{3}{4}\hbar^2$$

The evidence that spin is related to angular momentum comes from the fact that orbital angular momentum, L, is *not* conserved in atomic experiments, but rather the sum of orbital and spin angular momentum is conserved.

Total Angular Momentum
$$\vec{J} = \vec{L} + \vec{S}$$

It is also true that spin obeys all of the commutation relations which apply to the orbital angular momentum operators.

Spin Commutators

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z, \quad \left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y, \quad \left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x$$

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y \quad \left[\hat{S}^2, \hat{S}_z\right] = 0 \quad \left[\hat{S}^2, \hat{S}_\pm\right] = 0$$

For notational convenience, let's define up and down spin states as eigenstates of $\hat{S}_z$

Spin along Z

$$\hat{S}_z|\uparrow\rangle = \tfrac{1}{2}\hbar|\uparrow\rangle, \quad \hat{S}_z|\downarrow\rangle = -\tfrac{1}{2}\hbar|\downarrow\rangle$$

From the up and down along Z states we can also easily see that superpositions of states with fixed S_z can be used to make states with spin in the x or y directions.

Spin along X and Y

$$\begin{aligned}
\hat{S}_x|\tfrac{1}{\sqrt{2}}(\uparrow + \downarrow)\rangle &= \tfrac{1}{2}\left(\hat{S}_+ + \hat{S}_-\right)|\tfrac{1}{\sqrt{2}}(\uparrow + \downarrow)\rangle \\
&= \tfrac{1}{2}\hbar|\tfrac{1}{\sqrt{2}}(\downarrow + \uparrow)\rangle \\
&= \tfrac{1}{2}\hbar|\uparrow_x\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{S}_y|\tfrac{1}{\sqrt{2}}(\uparrow +i \downarrow)\rangle &= \tfrac{1}{2i}\left(\hat{S}_+ - \hat{S}_-\right)|\tfrac{1}{\sqrt{2}}(\uparrow +i \downarrow)\rangle \\
&= \tfrac{1}{2i}\hbar|\tfrac{1}{\sqrt{2}}(- \downarrow +i \uparrow)\rangle \\
&= \tfrac{1}{2}\hbar|\tfrac{1}{\sqrt{2}}(i \downarrow + \uparrow)\rangle \\
&= \tfrac{1}{2}\hbar|\uparrow_y\rangle
\end{aligned}$$

Similarly...

$$|\downarrow_x\rangle = |\tfrac{1}{\sqrt{2}}(\uparrow - \downarrow)\rangle$$
$$|\downarrow_y\rangle = |\tfrac{1}{\sqrt{2}}(\uparrow - i\downarrow)\rangle$$

Which is just to say that there is nothing fundamentally special about the z-axis.

Note that these superposition states have the same magnitude of angular moment as the individual Z-axis states. The superposition is a sum of *states*, not a sum of angular momenta.

Spin Magnitude

$$\hat{S}^2|\tfrac{1}{\sqrt{2}}(\uparrow + \downarrow)\rangle = \tfrac{3}{4}\hbar^2|\tfrac{1}{\sqrt{2}}(\uparrow + \downarrow)\rangle$$

This state is not an eigenstate of $\hat{S}_z$ and does not have definite m_s.

Spin along Z

$$\hat{S}_z|\tfrac{1}{\sqrt{2}}(\uparrow + \downarrow)\rangle = \tfrac{1}{2}\hbar|\tfrac{1}{\sqrt{2}}(\uparrow - \downarrow)\rangle$$
$$\hat{S}_z|\uparrow_x\rangle = \tfrac{1}{2}\hbar|\downarrow_x\rangle$$

4 Adding Spin to Hydrogen

- Li 9.4 and 12.1, Ga 10.5, Sc. 8.3

Last time we went off on a tangent about spin which started with the anomalous Zeeman effect. Let's wrap that up by talking about how to include spin in our description of an electron in hydrogen. This is an additional degree of freedom in the state of an electron, which we can tack on to its energy eigenstates (by separation of variables since the Coulomb potential does not depend on spin). This means that an orbiting electron in a hydrogen atom, is completely described by the state:

State with Spin

$$|\phi_{nlm_lm_s}\rangle = |R_{nl}(r)Y_{lm_l}(\theta,\phi)\rangle \; |\uparrow \;\; \text{or} \;\; \downarrow\rangle \;\;\; \text{where} \;\; m_s = \pm\tfrac{1}{2}$$

At least in the unperturbed Coulomb potential, we have

Recall: Separation of Variables

$$\text{given} \;\; V(r,\theta,\phi,m_s) \;\; = \;\; V(r) + \underbrace{V(\theta) + V(\phi) + V(m_s)}_{=0}$$

$$\Rightarrow \phi(r,\theta,\phi,m_s) \;\; = \;\; f(r)\, g(\theta)\, h(\phi)\, p(m_s)$$

The total angular momentum of such a state is a sum of orbital and spin angular momentum, and the math is not totally trivial, so let's explore this briefly.

Total Angular Momentum

$$\vec{J} = \vec{L} + \vec{S}$$

Eigenstates of total angular momentum follow all of the rules we have already seen for orbital and spin angular momentum separately.

Eigenstates of J

$$\hat{J}^2|j\,m_j\rangle \;\; = \;\; \hbar^2\, j(j+1)\, |j\,m_j\rangle$$

$$\hat{J}_z|j\,m_j\rangle \;\; = \;\; \hbar\, m_j\, |j\,m_j\rangle \;\; \text{with} \;\; m_j \in \{-j,\cdots,j\}$$

And, for the Z component of angular momentum, things continue to be easy.

Eigenstates of J_z

$$\hat{J}_z \;\; = \;\; \hat{L}_z + \hat{S}_z$$

$$\Rightarrow \hat{J}_z\,|\phi_{nlm_lm_s}\rangle \;\; = \;\; (\hat{L}_z + \hat{S}_z)\,|\phi_{nlm_lm_s}\rangle$$

$$= \;\; \hbar(m_l + m_s)\,|\phi_{nlm_lm_s}\rangle$$

$$\Rightarrow m_j \;\; = \;\; m_l + m_s$$

However, the magnitude of the total angular momentum depends on the relative orientation of $\vec{L}$ and $\vec{S}$.

Total Angular Momentum

$$J^2 = L^2 + 2\vec{L} \cdot \vec{S} + S^2 \neq L^2 + S^2$$

$$\left[\hat{\vec{L}} \cdot \hat{\vec{S}}, \hat{L}_z\right] \neq 0 \qquad \text{since} \quad \left[\hat{L}_z, \hat{L}_{x,y}\right] \neq 0$$

$$\left[\hat{\vec{L}} \cdot \hat{\vec{S}}, \hat{S}_z\right] \neq 0 \qquad \text{since} \quad \left[\hat{S}_z, \hat{S}_{x,y}\right] \neq 0$$

Of course, I would like to give you a nice translation from a state with known l, s, m_l and m_s to something with known j, but that *isn't possible*. We cannot have such a state because it would need to be an eigenstate of $\hat{J}^2$, $\hat{L}_z$ and $\hat{S}_z$, but these operators do not commute in general (since $\left[\hat{\vec{L}} \cdot \hat{\vec{S}}, \hat{L}_z\right] \neq 0$ unless $l = 0$ or $s = 0$). The best I can do is this range of j values!

With $\vec{L}$ and $\vec{S}$ aligned and anti-aligned, we can set limits on J^2.

Total Angular Momentum

$$\max(J^2) = L^2 + 2\,|L|\,|S| + S^2 = (|L| + |S|)^2$$

$$\min(J^2) = L^2 - 2\,|L|\,|S| + S^2 = (|L| - |S|)^2$$

$$\Rightarrow |l - s| \leq j \leq l + s$$

This is not to say that we can't make states with definite j, they just won't have definite m_s and m_l.

It turns out that the Zeeman effect becomes quite complicated when you include spin, and thus the "anomalous Zeeman" effect was the source of much discontent. Ignoring other perturbations, the Zeeman effect in "hydrogen" with spin causes energy level splitting as

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Zeeman (Strong Field)

$$E_{n\,m_l\,m_s} = -\frac{E_{Ry}}{n^2} + \mu_B(m_l + g_s m_s), \qquad g_s \simeq 2$$

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5 Multiple Particle Systems

- Gr. 5.1, Li 8.5, Ga 13.1, Sc. 13.1

During the last lecture we will talk about an experiment which touches on one of the must unnerving aspects of QM: the instantaneous nature of wave-function collapse over any distance, in the form of the Einstein-Podolsky-Rosen paradox (a.k.a., EPR). In order to understand the EPR experiment, we will need to have an understanding of how to represent multiple particles in QM.

In classical mechanics, where all is easy and intuitive, there isn't much need to talk about how to handle multiple particles; you just add more position and momentum vectors. But how does this work in QM? How do we combine the wave functions of 2 particles into one description of the state of our system? (I'll focus here on non-interacting particles to keep things easy.)

2-particles

$\qquad$ Classically $\qquad x_A, p_A, x_B, p_B$

$$E = E_A + E_B = \frac{p_A^2}{2m_A} + \frac{p_B^2}{2m_B} + V_A(x_A) + V_B(x_B)$$

$\qquad$ Quantum $\qquad \psi_A(x_A), \psi_B(x_B) \xrightarrow{??} \psi(x_A, x_B)$

$$\hat{E} = \hat{E}_A + \hat{E}_B = \frac{\hat{p}_A^2}{2m_A} + \frac{\hat{p}_B^2}{2m_B} + V_A(x_A) + V_B(x_B)$$

Much like adding a degree of freedom (e.g., spin) to a state, the separability of the energy operator suggests that we can use the product of our single particle wave functions to make a combine wave function.

Separable States

$$\hat{E}\,\psi(x_A, x_B) = \hat{E}\,\psi_A(x_A)\,\psi_B(x_B)$$
$$= \left(\hat{E}_A + \hat{E}_B\right)\psi_A(x_A)\,\psi_B(x_B)$$
$$= \psi_B(x_B)\,\hat{E}_A\,\psi_A(x_A) + \psi_A(x_A)\,\hat{E}_B\,\psi_B(x_B)$$

for energy eigenstates...

$$= (E_A + E_B)\,\psi_A(x_A)\,\psi_B(x_B)$$
$$= (E_A + E_B)\,\psi(x_A, x_B)$$

As an example, we'll consider 2 equal mass particles in an infinite square well. (In case you are worried, these are distinguishable, non-interacting particles). The energy eigenstates of such a system are the product of the single particle energy eigenstates.

2-particle Infinite Square Well

$$\phi_{nm}(x_A, x_B) = \phi_n(x_A)\,\phi_m(x_B)$$
$$= \frac{2}{L}\sin(k_n x_A)\sin(k_m x_B)$$

$$k_n = \frac{(n+1)\pi}{L} \qquad E_n = \frac{\hbar^2 k_n^2}{2m_A}$$

same for k_m and E_m

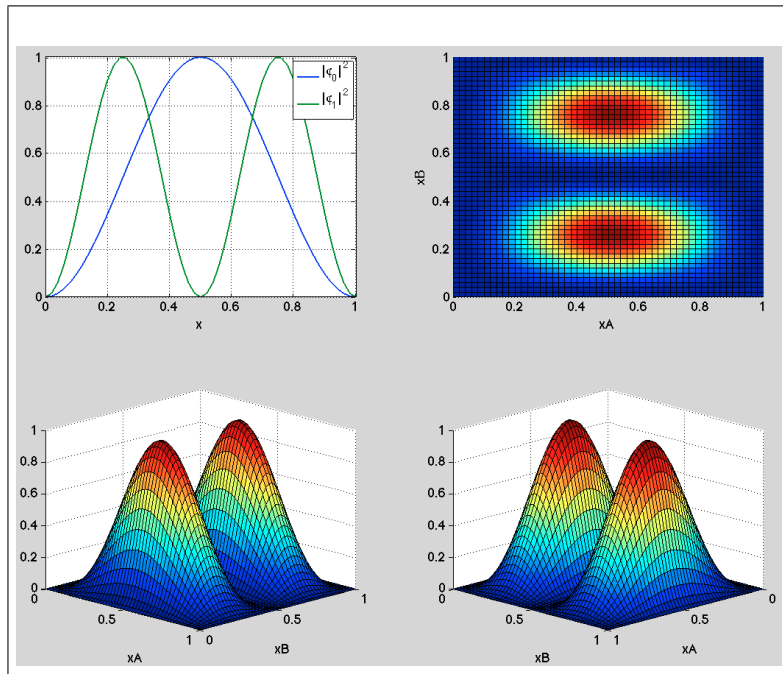The $n = 0, m = 1$ state $\phi_{01}(x_A, x_B)$, for instance, looks like this:
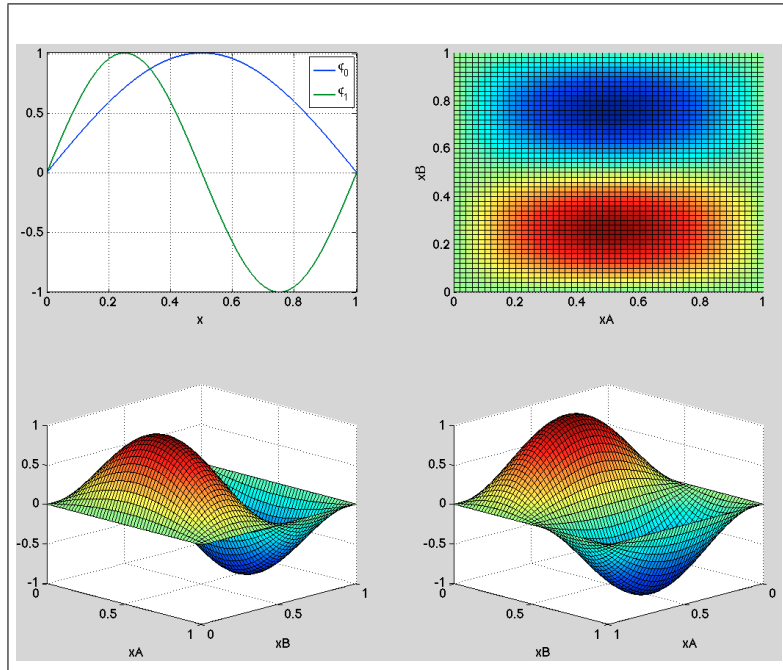
(You will note that this is exactly the same as what I would draw if we were talking about a single particle in a 2-D well.)

The probability density associated with finding the A at x_A *and* B at x_B is

Probability Density

$$\mathbb{P}(x_A, x_B) = |\psi(x_A, x_B)|^2 = \frac{4}{L^2} \sin^2(k_n x_A) \sin^2(k_m x_B)$$

which for $n = 0$, $m = 1$ looks like this:

This tells me about the probability of getting a particular result if I measure the positions of *both* particles at the same time. But what happens if I measure the position of A in such a way as to leave B undisturbed?

Found A at x_0

$$\begin{aligned} \psi(x_A, x_B) \;\; &\rightarrow \;\; \delta(x_A - x_0)\psi_B(x_B) \\ &= \;\; N\delta(x_A - x_0)\sin(k_m x_B) \end{aligned}$$

Since any $\psi_B(x_B)$ is an eigenfunction of $\hat{x}_A$, we can just collapse the wavefunction of A and leave B alone.

6 Superposition and Entanglement

This would all remain pretty uninteresting if it weren't for that little feature of QM which makes everything possible: superposition. What happens if we have a 2-particle wavefunction which is *not separable* into the product of 2 single-particle wavefunctions? We can easily make such a state by adding 2 of the separable wavefunctions.

Let's return to our infinite square well example and give this a shot.

> ## 2-particle Infinite Square Well
>
> $$\phi_{nm}(x_A, x_B) \;=\; \frac{1}{\sqrt{2}}\left(\phi_0(x_A)\phi_1(x_B) + \phi_1(x_A)\phi_0(x_B)\right)$$

> *show WF and PDF*

The PDF of this state tells us that if we find A at some positive value of x_A, for instance, well know that B is very likely to have a positive x_B. That is, the positions of the 2 particles are correlated (not independent), and so we know something about one by measuring the other.

> *show PDF of many different correlations*

Now, let's say we measure the energy of A. This will collapse its wavefunction to a single energy eigenstate, and as before B will come along for the ride.

> ## Measure $E_A = E_0$
>
> $$\phi_{nm}(x_A, x_B) \;\rightarrow\; \phi_0(x_A)\phi_1(x_B)$$

> *The odd bit is that while the energy of B was uncertain before the measurement of A's energy, we now know the energy of B.*

These 2 particles are said to be "entangled", which is just a neat way of saying that their combined state is not separable into 2 individual states, but it carries the implication that if you measure either of them you change the state of both of them.

A classic example of this kind of state is produced as follows: the decay of the neutral pi meson (spin 0) into a positron and an electron produces a state which has 2 spin $\frac{1}{2}$ particles, but no total angular momentum (c.f. Gr. 4.4.3, Sc. 8.7, Ga 10.4, Li 11.10).

Entangled Spins

$$\pi^0 \rightarrow e^- + e^+$$
$$\psi_\pm = \frac{1}{\sqrt{2}} (\uparrow_- \ \downarrow_+ \ - \ \downarrow_- \ \uparrow_+)$$
$$\hat{S}^2|\psi_\pm\rangle = \hat{S}_z|\psi_\pm\rangle = 0$$

This is an example of addition of angular momentum! (In this case, 2 spins instead of an orbital and a spin angular momentum.)

Adding Spins

$$\hat{S}^2|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle$$
$$\hat{S}_z|l, m\rangle = \hbar m|l, m\rangle$$
$$|1, 1\rangle = \uparrow\uparrow$$
$$|1, 0\rangle = \frac{1}{\sqrt{2}} (\uparrow\downarrow \ + \ \downarrow\uparrow)$$
$$|0, 0\rangle = \frac{1}{\sqrt{2}} (\uparrow\downarrow \ - \ \downarrow\uparrow)$$
$$|1, -1\rangle = \downarrow\downarrow$$

If the pion was at rest in the lab, the electron and positron are produced with considerable kinetic energy, and go flying off in opposite directions. Now, if we measure the electron to be spin up, we know that the positron, wherever it may be, is spin down. If, on the other hand, we measure the positron first we could get anything, but whatever we get we will then know for sure the state of the electron.

Take this a little further: imagine that we wait a while to make the measurement so that the electron and positron are very far apart... say 1 light-minute. If I measure the state of the electron, and you measure the state of the positron 1 second later, I know what you will get. But how does the positron know what to give you?

More on this next time!

7 Next Time

- EPR
- Review