Intermediate Quantum Mechanics
Lecture 5 Notes (2/4/15)

Electron Spin in a General Direction

Spin in three dimensions

- Two parameters are needed, the zenith angle, θ, and the azimuthal angle, ϕ, in order to specify the direction of an arrow in 3-dimensional physical space.

- We can specify the spin state of an electron in three physical dimensions by a 2-dimensional complex vector. A real vector is not sufficient since once the $|\alpha|^2 + |\beta|^2 = 1$ condition is imposed there is only one degree of freedom left.

- A two dimensional complex vector has four degrees of freedom: the real and imaginary parts of α and the real and imaginary parts of β. The condition that $|\alpha|^2 + |\beta|^2 = 1$ removes one of these. Once the magnitude or modulus of α is set, this fixes the magnitude or modulus of β. That leaves three degrees of freedom, one too many.

- One of the remaining three degrees of freedom is superfluous. If we multiply $|\psi\rangle$ by a complex number of unit modulus, $e^{-i\theta}$, the resulting state $|\psi'\rangle = e^{i\theta}\,|\psi\rangle$ is indistinguishable from $|\psi\rangle$.

- The only physical connection to a state is through determining the probability of observing the various possible values of the observables. If $|a\rangle$ is an eigenstate of the Hermitian operator corresponding to observable A and if the eigenvalue associated with $|a\rangle$ is λ_a, then the probability of measuring λ_a for a system in the state $|\psi\rangle$ is:

  $$\text{Prob}_\psi(\lambda_a) \;=\; \langle \psi \,|\, a \,\rangle \, \langle a \,|\, \psi \,\rangle$$

  If the system is in state $|\psi'\rangle = e^{i\theta}\,|\psi\rangle$, we have:

  $$\text{Prob}_{\psi'}(\lambda_a) \;=\; \langle \psi' \,|\, a \,\rangle \, \langle a \,|\, \psi' \,\rangle \;=\; e^{-i\theta}e^{i\theta}\,\langle \psi \,|\, a \,\rangle \, \langle a \,|\, \psi \,\rangle \;=\; \langle \psi \,|\, a \,\rangle \, \langle a \,|\, \psi \,\rangle \;=\; \text{Prob}_\psi(\lambda_a)$$

  We can't tell the difference between $|\psi\rangle$ and $|\psi'\rangle$. They, therefore, represent the same physical state.

- Since we can multiply the state by any complex phase (complex number with unit norm) without affecting the physics. We can, if we like, choose the phase to be such that α is real. Then besides the magnitude of α the only other degree of freedom is the phase of β.

- Two parameters are needed to specify the direction of an arrow in 3-dimensional physical space and 2-dimensional complex vector states have two degrees of freedom. It's a perfect match. There is a one-to-one correspondence between the direction of the spin arrow in 3-dimensional physical space and a vector of unit norm in a n-dimensional complex vector space that represents the state of the spin. I don't know whether this is profound or not. Decide for yourself.

Spin in an arbitrary direction

- There is nothing special about the x, y and z directions. We could measure the spin of the electron in any direction.
- A general direction in 3-dimensional physical space is give by the unit vector $\hat{n}$ with:
$$n_x = \sin\theta\cos\phi \qquad n_y = \sin\theta\sin\phi \qquad n_z = \cos\theta$$
- The operator corresponding to measuring spin in the $\hat{n}$ direction is given by:
$$\hat{\sigma}_n = \hat{\sigma}_x n_x + \hat{\sigma}_y n_y + \hat{\sigma}_z n_z \implies \begin{pmatrix} 0 & n_x \\ n_x & 0 \end{pmatrix} + \begin{pmatrix} 0 & -in_y \\ in_y & 0 \end{pmatrix} + \begin{pmatrix} n_z & 0 \\ 0 & -n_z \end{pmatrix}$$
$$= \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}$$
- In a homework problem, you showed that the solution to the equation for the eigenvector of $\hat{\sigma}_n$ with eigenvalue $+1$, $\hat{\sigma}_n |n\!\uparrow\rangle = |n\!\uparrow\rangle$ is:
$$|n\!\uparrow\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$$
Using the freedom to choose the overall phase, we could also write this as:
$$|n\!\uparrow\rangle = \begin{pmatrix} e^{-i\phi/2}\cos\frac{\theta}{2} \\ e^{i\phi/2}\sin\frac{\theta}{2} \end{pmatrix}$$

Commutation of operators and (in)compatible observables

- Two operators $\hat{A}$ and $\hat{B}$ commute if $\hat{A}\hat{B} = \hat{B}\hat{A}$. [More correctly, we should say $\hat{A}\hat{B}|\psi\rangle = \hat{B}\hat{A}|\psi\rangle$.] We define $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$. Two operators commute if $[\hat{A},\hat{B}] = 0$.
- Theorem: If two Hermitian operators have common eigenvectors, they commute. [Note that since the eigenvectors of a Hermitian operator are mutually orthogonal, if two Hermitian operators share one eigenvector, then they share all of their eigenvectors.]

  Proof: Assume that $|\psi\rangle$ is an eigenvector of both $\hat{A}$ and $\hat{B}$.
$$\hat{A}\hat{B}|\psi\rangle = \hat{A}\lambda_b|\psi\rangle = \lambda_b\hat{A}|\psi\rangle = \lambda_b\lambda_a|\psi\rangle$$
$$= \lambda_a\lambda_b|\psi\rangle = \lambda_a\hat{B}|\psi\rangle = \hat{B}\lambda_a|\psi\rangle = \hat{B}\hat{A}|\psi\rangle$$
- Theorem: If two Hermitian operators commute, they have common eigenvectors.

  Proof: Assume that $\hat{A}$ and $\hat{B}$ commute and that $|\psi\rangle$ is an eigenvector of $\hat{A}$.

$$\hat{A}\hat{B}\,|\psi\rangle \;=\; \hat{B}\hat{A}\,|\psi\rangle \;=\; \hat{B}\lambda_a\,|\psi\rangle \;=\; \lambda_a\hat{B}\,|\psi\rangle$$

So, we have:

$$\hat{A}\left(\hat{B}\,|\psi\rangle\right) \;=\; \lambda_a\left(\hat{B}\,|\psi\rangle\right) \qquad \Rightarrow \qquad \hat{B}\,|\psi\rangle \;\text{ is an eigenvector of } \hat{A}$$

$$\Rightarrow \qquad \hat{B}\,|\psi\rangle \;\text{ is a multiple of }\; |\psi\rangle \qquad \Rightarrow \qquad |\psi\rangle \text{ is an eigenvector of } \hat{B}$$

- It follows from these two theorems that, if two Hermitian operators do not commute, they do not have any common eigenvectors. This means that there is no state for which the observables of both operators have definite values. The observables are said to be **incompatible**.

- Here is an example involving spin. We can run an electron in the spin state $|\psi\rangle$ through a z-oriented Stern-Gerlach device. This will measure the spin in the z-direction. We will either measure either spin-up or spin-down. Let's assume we measure spin-up. Then, the electron is in a state of spin-up along z. Now run this electron through an x-oriented Stern-Gerlach device to measure its spin in the x-direction. We will measure either spin-up or spin-down along x. Let's assume we measure spin-up. Does that mean that we have now determined that the spin of the electron is both up along z and up along x. No, because if we now run the electron through the z-oriented Stern-Gerlach device again to check the spin in z, we will measure spin-up with a 50% probability and spin-down with a 50% probability. After we measured the spin in x we destroyed the information that we had about the spin in the z-direction. Spin in the x-direction and spin in the z-direction are incompatible, $\hat{\sigma}_x$ and $\hat{\sigma}_y$ do not commute.

Properties of the σ operators

- The σ operators have several important properties.

- Because their eigenvalues are ± 1, their square must be the identity operator. This means that $\lambda_{\pm 1}^2 \;=\; 1$. Alsotheir trace must be zero. This means that $\lambda_+ + \lambda_- \;=\; 0$. The trace of an operator is the sum of the diagonal elements of the corresponding matrix. The trace of a matrix is independent of representation. In the representation in which the matrix is diagonal (has only diagonal elements), the trace is the sum of the eigenvalues.

$$\hat{\sigma}_i^2 \;=\; \hat{I} \qquad\qquad\qquad \mathrm{Tr}(\hat{\sigma}_i) \;=\; 0$$

- As you showed in homework, the sigma operators do not commute.

$$[\hat{\sigma}_i, \hat{\sigma}_j] \;\equiv\; \hat{\sigma}_i\hat{\sigma}_j \;-\; \hat{\sigma}_j\hat{\sigma}_i \;=\; 2i\epsilon_{ijk}\hat{\sigma}_k$$

  They do anticommute.

$$\hat{\sigma}_i, \hat{\sigma}_j \;\equiv\; \hat{\sigma}_i\hat{\sigma}_j \;+\; \hat{\sigma}_j\hat{\sigma}_i \;=\; 2\delta_{ij} \qquad \Rightarrow \qquad \hat{\sigma}_i\hat{\sigma}_j = -\hat{\sigma}_j\hat{\sigma}_i \qquad \text{if } i \neq j$$

  Together these give: $\quad \hat{\sigma}_i\hat{\sigma}_j \;=\; i\epsilon_{ijk}\hat{\sigma}_k$

- In a few weeks, we will discuss the rotation by an angle θ of a state with spin-up in a given direction. We'll find that the σ operators play a fundamental and unexpected role in rotational transformations related to their commutation property given above.

Expectation Values

- The quantity $\langle\psi|\hat{A}\,|\psi\rangle$ gives the average value of the observable corresponding to the operator $\hat{A}$ that we would get if we made measurements of the observable corresponding to $\hat{A}$ on an ensemble of identical systems all in the same state $|\psi\rangle$.

  Proof: Let: $\quad |\psi\rangle \;=\; \alpha_1\,|a_1\rangle \;+\; \alpha_2\,|a_2\rangle \;+\; \cdots \;+\; \alpha_n\,|a_n\rangle$

  where the states $|a_i\rangle$ are the set of eigenvectors of the operator $\hat{A}$. Then:

$$\hat{A}\,|\psi\rangle \;=\; \lambda_1\alpha_1\,|a_1\rangle \;+\; \lambda_2\alpha_2\,|a_2\rangle \;+\; \cdots \;+\; \lambda_n\alpha_n\,|a_n\rangle$$

  where λ_i is the eigenvalue corresponding to the eigenvector $|a_i\rangle$. Now take the inner product of this with $\langle a|$.

$$\langle\psi|\hat{A}\,|\psi\rangle \;=\; \Big(\langle a_1|\alpha_1^* + \langle a_2|\alpha_2^* + \cdots + \langle a_n|\alpha_n^*\Big)\Big(\lambda_1\alpha_1\,|a_1\rangle + \lambda_2\alpha_2\,|a_2\rangle + \cdots + \lambda_n\alpha_n\,|a_n\rangle\Big)$$

  Using the orthonormality of the eigenvectors, $\langle a_i\,|\,a_j\,\rangle \;=\; \delta_{ij}$, we have

$$\langle\psi|\hat{A}\,|\psi\rangle \;=\; \lambda_1\alpha_1^*\alpha_1 \;+\; \lambda_2\alpha_2^*\alpha_2 \;+\; \cdots \;+\; \lambda_n\alpha_n^*\alpha_n \;=\; \sum_i \lambda_i \mathrm{Prob}(\lambda_i) \;=\; \overline{\lambda}$$

  where $\overline{\lambda}$ is the average value of the observable.

Summary of spin

- We have now covered essentially everything related to spin of a single electron. I'll summarize it here. There is one more thing to discuss about spin that has to do with the operation that transforms a spin state by rotating it through an angle. We'll discuss this a few lectures from now.

- We can observe (measure) the spin of an electron in the x, y or z directions. By Postulate 2, there must be Hermitian operators associated with each of these observables. These operators are: $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$.

- When the spin is observed along any direction, only two values are obtained, either spin-up (+1) or spin-down (-1) along that direction. That means that $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ have only two eigenvectors and that, therefore the spin of the electron is specified by a vector in a two-dimensional vector space.

- The eigenvectors of the σ operators are:

$$\begin{array}{lll}
\hat{\sigma}_x: & |\rightarrow\rangle \;=\; \dfrac{1}{\sqrt{2}}\left(|\uparrow\rangle \;+\; |\downarrow\rangle\right) & |\leftarrow\rangle \;=\; \dfrac{1}{\sqrt{2}}\left(|\uparrow\rangle \;-\; |\downarrow\rangle\right) \\
\hat{\sigma}_y: & |\otimes\rangle \;=\; \dfrac{1}{\sqrt{2}}\left(|\uparrow\rangle \;+\; i\,|\downarrow\rangle\right) & |\odot\rangle \;=\; \dfrac{1}{\sqrt{2}}\left(|\uparrow\rangle \;-\; i\,|\downarrow\rangle\right) \\
\hat{\sigma}_z: & |\uparrow\rangle & |\downarrow\rangle
\end{array}$$

$$\hat{\sigma}_x \,|\!\rightarrow\rangle \;=\; |\!\rightarrow\rangle \qquad\qquad \hat{\sigma}_x \,|\!\leftarrow\rangle \;=\; -\,|\!\leftarrow\rangle$$

$$\hat{\sigma}_y \,|\otimes\rangle \;=\; |\otimes\rangle \qquad\qquad \hat{\sigma}_y \,|\odot\rangle \;=\; -\,|\odot\rangle$$

$$\hat{\sigma}_z \,|\!\uparrow\rangle \;=\; |\!\uparrow\rangle \qquad\qquad \hat{\sigma}_z \,|\!\downarrow\rangle \;=\; -\,|\!\downarrow\rangle$$

- By Postulate 1, any vector with unit norm in this space is a possible state of the spin:
$$|\psi\rangle \;=\; \alpha\,|\!\uparrow\rangle + \beta\,|\!\downarrow\rangle \qquad \text{with} \qquad |\alpha|^2 + |\beta|^2 \;=\; 1$$
- By Postulate 4, if the electron is in the state $|\psi\rangle = \alpha\,|\!\uparrow\rangle + \beta\,|\!\downarrow\rangle$, then a measurement of the spin in the z direction will yield $|\!\uparrow\rangle$ with a probability of $|\alpha|^2$ and $|\!\downarrow\rangle$ with a probability of $|\beta|^2$.
- By Postulate 3, if an electron is in the state $|\!\uparrow\rangle$, an eigenstate of $\hat{\sigma}_z$, then a measurement of the spin in the z-direction will yield $|\!\uparrow\rangle$ with probability 1.
- By postulate 5, if the spin in the z-direction is measured to be spin-up, then after the measurement, the electron is in the $|\!\uparrow\rangle$ state.
- Usually we work in the representation:

$$|\!\uparrow\rangle \;\Longrightarrow\; \begin{pmatrix}1\\0\end{pmatrix} \qquad\qquad |\!\downarrow\rangle \;\Longrightarrow\; \begin{pmatrix}0\\1\end{pmatrix}$$

$$|\!\rightarrow\rangle \;\Longrightarrow\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad\qquad |\!\leftarrow\rangle \;\Longrightarrow\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

$$|\otimes\rangle \;\Longrightarrow\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \qquad\qquad |\odot\rangle \;\Longrightarrow\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

$$\hat{\sigma}_x \;\Longrightarrow\; \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \qquad \hat{\sigma}_y \;\Longrightarrow\; \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \qquad \hat{\sigma}_z \;\Longrightarrow\; \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

- For a general direction given by the unit arrow $\hat{n}$ with $n_x = \sin\theta\cos\phi$, $n_y = \sin\theta\sin\phi$, and $n_z = \cos\theta$, we have:

$$\hat{\sigma}_n \;=\; \hat{\sigma}_x n_x + \hat{\sigma}_y n_y + \hat{\sigma}_z n_z \;=\; \begin{pmatrix}\cos\theta & e^{-i\phi}\sin\theta\\ e^{i\phi}\sin\theta & -\cos\theta\end{pmatrix}$$

$$|n\!\uparrow\rangle \;=\; \begin{pmatrix}e^{-i\phi/2}\cos\frac{\theta}{2}\\ e^{i\phi/2}\sin\frac{\theta}{2}\end{pmatrix}$$

$$\langle n\!\uparrow|\hat{\sigma}_x\,|n\!\uparrow\rangle \;=\; \sin\theta\cos\phi \qquad \langle n\!\uparrow|\hat{\sigma}_y\,|n\!\uparrow\rangle \;=\; \sin\theta\sin\phi \qquad \langle n\!\uparrow|\hat{\sigma}_z\,|n\!\uparrow\rangle \;=\; \cos\theta$$