

Spin

We looked at the orbital angular momentum before but electrons have an "intrinsic" angular momentum.

This internal degree of freedom is referred to as spin.

For each electron, we define two commuting operators

\hat{S}^2 and \hat{S}_z for square of spin and z -component of spin.

For an electron the \hat{S}^2 always gives eigenvalue of $\frac{3\hbar^2}{4}$

The \hat{S}_z always gives eigenvalues of $\pm \frac{\hbar}{2}$

Note the \pm . In Dirac notation, we refer to the states that \downarrow as spin up $|\uparrow\rangle$ and spin down $|\downarrow\rangle$
give us these spins

Combining Spin and Wavefunction

The spin operator $\hat{\mathbf{S}}$ and the position operator $\hat{\mathbf{x}}$ commute
 $[\hat{\mathbf{S}}, \hat{\mathbf{x}}] = 0$ so it is possible to know both precisely.

Let's see if we can build a framework that will tell us position and spin simultaneously.

Let's say the electron definitely has spin up. So we can write:
 $\hat{S}_z |\uparrow\rangle = \frac{\hbar}{2} |\uparrow\rangle$

If the electron is definitely in some position x' :

$$\hat{x} |x'\rangle = x' |x'\rangle$$

From these statements, we can see that the wavefunction of this electron must be proportional to both states. i.e. it is of the form of the product state $|\uparrow\rangle |x'\rangle$

The position operator \hat{x} is the same as simply multiplying by x . So we need to find a function for $|x\rangle$ which satisfies the eigenvalue equation.

$$x \delta(x-x') = x' \delta(x-x')$$

so we have found $|x\rangle$

So for spin up, the wavefunction is proportional to $\delta(x-x')|\uparrow\rangle$

Similarly, for spin down, the wave fn. is proportional to $\delta(x-x')|\downarrow\rangle$

Using the expansion theorem: $\psi(x) = \sum_i a_i \psi_i(x)$

$$\text{where } a_i = \int \psi_i^* \psi dx$$

$$\rightarrow \psi \propto |x'\rangle|\uparrow\rangle \\ \text{or } \propto |x'\rangle|\downarrow\rangle$$

$$\psi(x) = \int \psi_{\uparrow}(x') |x'\rangle |\uparrow\rangle dx'$$

$$+ \int \psi_{\downarrow}(x') |x'\rangle |\downarrow\rangle dx'$$

$$= \int \psi_{\uparrow}(x') \delta(x-x') |\uparrow\rangle dx' + \int \psi_{\downarrow}(x') \delta(x-x') |\downarrow\rangle dx'$$

$$\psi(x) = \psi_{\uparrow}(x) |\uparrow\rangle + \psi_{\downarrow}(x) |\downarrow\rangle$$

We can write the spin in matrix form as $\begin{pmatrix} \psi_{\uparrow}(x) \\ \psi_{\downarrow}(x) \end{pmatrix}$

We can also express $\psi(x)$ as:

$$\psi = \sum_{n,s} a_{n,s} \psi_n(\underline{r}) |s\rangle$$

where s can be \uparrow or \downarrow , n selects the single electron orbital, $a_{n,s}$ is a coefficient amplitude to find the electron with spin s occupying the orbital ψ_n .