HYDROGEN ATOM: COMBINED POSITION AND SPIN STATE

So far, we’ve considered only states that depend either on position or spin, but not both. Here’s an example in which both are combined into a single state.

Suppose an electron in a hydrogen atom is in a state given by

\[
\psi = R_{21} \left( \sqrt{\frac{1}{3}} Y^0_1 \chi_+ + \sqrt{\frac{2}{3}} Y^1_1 \chi_- \right)
\]

(1)

The key to analyzing states like this is to remember that the position and spin states are completely separate, so a position operator will operate only on the spatial parts (the \( R_{21} \) and the spherical harmonics) and a spin operator will operate only on the spinors (the \( \chi \) matrices).

Look first at the orbital angular momentum. Since both terms contain spherical harmonics with \( l = 1 \), there is only one possible value for \( L^2 \):

\[
l(l+1)\hbar^2 = 2\hbar^2.
\]

For the \( z \) component, we would measure \( L_z = 0 \) with probability \( 1/3 \) and

\[
L_z = \hbar \text{ with probability } 2/3.
\]

For the spin (remember we’re looking only at the electron), both spinors are for spin \( 1/2 \) so \( S^2 = 3\hbar^2/4 \). \( S_z = +1/2 \) with probability \( 1/3 \) and \(-1/2 \) with probability \( 2/3 \).

For the total angular momentum \( J \equiv L + S \), one ‘spin’ is really a spin (spin \( 1/2 \)) while the other is the orbital angular momentum \( l = 1 \). The possible total angular momentum values are therefore \( j = \frac{1}{2}, \frac{3}{2} \). From Clebsch-Gordan tables, we have

\[
|1 \ 0 \rangle |1 \ 1 \rangle = \sqrt{\frac{2}{3}} |3 \ 1 \rangle - \sqrt{\frac{1}{3}} |1 \ 1 \rangle.
\]

(2)

\[
|1 \ 1 \rangle |\frac{1}{2} \ - \frac{1}{2} \rangle = \sqrt{\frac{1}{3}} |3 \ 1 \rangle + \sqrt{\frac{2}{3}} |1 \ 1 \rangle.
\]

(3)

This expresses the two states making up \( \psi \) as combinations of eigenfunctions of \( J^2 \). Making the substitution, we get
\[
\psi = \frac{\sqrt{2}}{3} \begin{pmatrix} 3 & 1 \\ 2 & 2 \end{pmatrix} - \frac{1}{3} \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix} + \frac{\sqrt{2}}{3} \begin{pmatrix} 3 & 1 \\ 2 & 2 \end{pmatrix} + 2 \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix} \\
= \frac{2\sqrt{2}}{3} \begin{pmatrix} 3 & 1 \\ 2 & 2 \end{pmatrix} + \frac{1}{3} \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix}
\]

(4)

The probability of getting \( j = \frac{3}{2} \) is therefore \( \left( \frac{2\sqrt{2}}{3} \right)^2 = \frac{8}{9} \) and the probability of getting \( j = \frac{1}{2} \) is \( \frac{1}{9} \).

The \( z \) components are simply additive, so \( J_z = L_z + S_z = +\hbar/2 \) for both terms, thus this is the only possible value of \( J_z \).

The probability density for finding the electron at a given location in spherical coordinates is the square modulus of the wave function, so, since the \( \chi \) spinors are orthonormal, we can use results for the radial functions and spherical harmonics to get

\[
\rho(r,\theta,\phi) = R_{21}^2 \left( \sqrt{\frac{1}{3}} Y_{1}^{0} \chi_{+} + \sqrt{\frac{2}{3}} Y_{1}^{1} \chi_{-} \right)^\dagger \left( \sqrt{\frac{1}{3}} Y_{1}^{0} \chi_{+} + \sqrt{\frac{2}{3}} Y_{1}^{1} \chi_{-} \right)
\]

(6)

\[
= \frac{1}{24} \frac{r^2}{a^5} e^{-r/a} \left( \frac{1}{4\pi} \cos^2 \theta + \frac{1}{4\pi} \sin^2 \theta \right)
\]

(8)

That is, this density depends only on \( r \) so is spherically symmetric. As a check, we note that \( \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \rho(r,\theta,\phi) r^2 \sin \theta \, dr \, d\theta \, d\phi = 1 \).

Now suppose we want the probability of finding the electron at radius \( r \) and with spin up, that is, in state \( \chi_{+} \). The probability density for finding the electron at a given point in this spin state is found by considering only the term in [1] that includes spin up, and is

\[
\rho_{+} = R_{21}^2 \left( \sqrt{\frac{1}{3}} Y_{1}^{0} \chi_{+} \right)^\dagger \left( \sqrt{\frac{1}{3}} Y_{1}^{0} \chi_{+} \right)
\]

(10)

\[
= \frac{1}{24} \frac{r^2}{a^5} e^{-r/a} \frac{1}{4\pi} \cos^2 \theta
\]

(11)
To find the probability of finding the electron at a given radius, we need to integrate over the angular coordinates, so we have

\[
P(r, +) = \frac{1}{24} \frac{r^2}{a^5} e^{-r/a} \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \cos^2 \theta \sin \theta d\phi d\theta
\]

\[
= \frac{1}{72} \frac{r^2}{a^5} e^{-r/a}
\]