

HYDROGEN ATOM: COMBINED POSITION AND SPIN STATE

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.55.

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

$$(0.1) \quad \psi = R_{21} \left(\sqrt{\frac{1}{3}} Y_1^0 \chi_+ + \sqrt{\frac{2}{3}} Y_1^1 \chi_- \right)$$

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 χ 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 $L_z = \hbar$ 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 $\mathbf{J} \equiv \mathbf{L} + \mathbf{S}$, 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

$$(0.2) \quad |1\ 0\rangle \left| \frac{1}{2} \ \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} \left| \frac{3}{2} \ \frac{1}{2} \right\rangle - \sqrt{\frac{1}{3}} \left| \frac{1}{2} \ \frac{1}{2} \right\rangle$$

$$(0.3) \quad |1\ 1\rangle \left| \frac{1}{2} \ -\frac{1}{2} \right\rangle = \sqrt{\frac{1}{3}} \left| \frac{3}{2} \ \frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} \left| \frac{1}{2} \ \frac{1}{2} \right\rangle$$

This expresses the two states making up 0.1 as combinations of eigenfunctions of J^2 . Making the substitution, we get

$$(0.4) \quad \psi = \frac{\sqrt{2}}{3} \left| \begin{matrix} 3 & 1 \\ 2 & 2 \end{matrix} \right\rangle - \frac{1}{3} \left| \begin{matrix} 1 & 1 \\ 2 & 2 \end{matrix} \right\rangle + \frac{\sqrt{2}}{3} \left| \begin{matrix} 3 & 1 \\ 2 & 2 \end{matrix} \right\rangle + \frac{2}{3} \left| \begin{matrix} 1 & 1 \\ 2 & 2 \end{matrix} \right\rangle$$

$$(0.5) \quad = \frac{2\sqrt{2}}{3} \left| \begin{matrix} 3 & 1 \\ 2 & 2 \end{matrix} \right\rangle + \frac{1}{3} \left| \begin{matrix} 1 & 1 \\ 2 & 2 \end{matrix} \right\rangle$$

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 χ spinors are orthonormal, we can use results for the radial functions and spherical harmonics to get

$$(0.6)$$

$$\rho(r, \theta, \phi) = R_{21}^2 \left(\sqrt{\frac{1}{3}} Y_1^0 \chi_+ + \sqrt{\frac{2}{3}} Y_1^1 \chi_- \right)^\dagger \left(\sqrt{\frac{1}{3}} Y_1^0 \chi_+ + \sqrt{\frac{2}{3}} Y_1^1 \chi_- \right)$$

$$(0.7) \quad R_{21}^2 \left(\frac{(Y_1^0)^2}{3} + \frac{2(Y_1^1)^2}{3} \right)$$

$$(0.8) \quad = \frac{1}{24} \frac{r^2}{a^5} e^{-r/a} \left(\frac{1}{4\pi} \cos^2 \theta + \frac{1}{4\pi} \sin^2 \theta \right)$$

$$(0.9) \quad = \frac{1}{96\pi} \frac{r^2}{a^5} e^{-r/a}$$

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 χ_+ . The probability density for finding the electron at a given point in this spin state is found by considering only the term in 0.1 that includes spin up, and is

$$(0.10) \quad \rho_+ = R_{21}^2 \left(\sqrt{\frac{1}{3}} Y_1^0 \chi_+ \right)^\dagger \left(\sqrt{\frac{1}{3}} Y_1^0 \chi_+ \right)$$

$$(0.11) \quad = \frac{1}{24} \frac{r^2}{a^5} e^{-r/a} \frac{1}{4\pi} \cos^2 \theta$$

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

$$(0.12) \quad P(r, +) = \frac{1}{24} \frac{r^2}{a^5} e^{-r/a} \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \cos^2 \theta \sin \theta d\phi d\theta$$

$$(0.13) \quad = \frac{1}{72} \frac{r^2}{a^5} e^{-r/a}$$