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

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

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 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

$$|1\;0\rangle\left|\frac{1}{2}\;\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|\frac{3}{2}\;\frac{1}{2}\right\rangle - \sqrt{\frac{1}{3}}\left|\frac{1}{2}\;\frac{1}{2}\right\rangle \tag{2}$$

$$|1\;1\rangle\left|\frac{1}{2}\;-\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|\frac{3}{2}\;\frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|\frac{1}{2}\;\frac{1}{2}\right\rangle \tag{3}$$

This expresses the two states making up 1 as combinations of eigenfunctions of J^2. Making the substitution, we get

$$\psi = \frac{\sqrt{2}}{3}\left|\frac{3}{2}\ \frac{1}{2}\right\rangle - \frac{1}{3}\left|\frac{1}{2}\ \frac{1}{2}\right\rangle + \frac{\sqrt{2}}{3}\left|\frac{3}{2}\ \frac{1}{2}\right\rangle + \frac{2}{3}\left|\frac{1}{2}\ \frac{1}{2}\right\rangle \tag{4}$$

$$= \frac{2\sqrt{2}}{3}\left|\frac{3}{2}\ \frac{1}{2}\right\rangle + \frac{1}{3}\left|\frac{1}{2}\ \frac{1}{2}\right\rangle \tag{5}$$

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

$$\rho(r,\theta\phi) = R_{21}^2\left(\sqrt{\frac{1}{3}}Y_1^0\chi_+ + \sqrt{\frac{2}{3}}Y_1^1\chi_-\right)^\dagger\left(\sqrt{\frac{1}{3}}Y_1^0\chi_+ + \sqrt{\frac{2}{3}}Y_1^1\chi_-\right) \tag{6}$$

$$R_{21}^2\left(\frac{(Y_1^0)^2}{3} + \frac{2(Y_1^1)^2}{3}\right) \tag{7}$$

$$= \frac{1}{24}\frac{r^2}{a^5}e^{-r/a}\left(\frac{1}{4\pi}\cos^2\theta + \frac{1}{4\pi}\sin^2\theta\right) \tag{8}$$

$$= \frac{1}{96\pi}\frac{r^2}{a^5}e^{-r/a} \tag{9}$$

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

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 1 that includes spin up, and is

$$\rho_+ = R_{21}^2\left(\sqrt{\frac{1}{3}}Y_1^0\chi_+\right)^\dagger\left(\sqrt{\frac{1}{3}}Y_1^0\chi_+\right) \tag{10}$$

$$= \frac{1}{24}\frac{r^2}{a^5}e^{-r/a}\frac{1}{4\pi}\cos^2\theta \tag{11}$$

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

$$P(r,+) = \frac{1}{24}\frac{r^2}{a^5}e^{-r/a}\frac{1}{4\pi}\int_0^{\pi}\int_0^{2\pi}\cos^2\theta\sin\theta d\phi d\theta \tag{12}$$

$$= \frac{1}{72}\frac{r^2}{a^5}e^{-r/a} \tag{13}$$