HYDROGEN ATOM: A SAMPLE WAVE FUNCTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercise 13.1.3.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The wave function for the hydrogen atom can be obtained by a series solution of the differential equation, leading to the result (which I've rewritten in Shankar's notation, although my original post used Griffiths's notation):

$$\psi_{nlm}(r,\theta,\phi)=\frac{U_{El}(r)}{r}Y_l^m(\theta,\phi) \tag{1}$$

Here, we have

$$U_{El} = e^{-\rho}v_{El} \tag{2}$$

$$v_{El} = \rho^{l+1}\sum_{k=0}^{\infty}C_k\rho^k \tag{3}$$

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}}r \tag{4}$$

The energy levels of the hydrogen atom are

$$E=-\frac{me^4}{2\hbar^2n^2} \tag{5}$$

where $n=1,2,3,\ldots$. The coefficients C_k in 3 are given by a recursion relation

$$C_{k+1}=\frac{-e^2\lambda+2(k+l+1)}{(k+l+2)(k+l+1)-l(l+1)}C_k \tag{6}$$

$$\lambda=\sqrt{-\frac{2m}{\hbar^2E}} \tag{7}$$

Combining λ and E, the formula becomes, for a given n

$$C_{k+1}=\frac{2(k+l+1)-2n}{(k+l+2)(k+l+1)-l(l+1)}C_k$$

The coefficient C_0 which starts everything off is determined by normalization.

As an example, we can find the wave function ψ_{210}. In this case $n=2$ and $l=1$ so the first term in the recursion, with $k=0$ gives $k+l+1=2$ and $C_1=0$. The full wave function is then

$$\psi_{210} = \frac{1}{r}\rho^2 e^{-\rho} C_0 Y_1^0 \tag{8}$$

To evaluate ρ we use the energy for $n=2$:

$$E_2 = -\frac{me^4}{8\hbar^2} \tag{9}$$

This gives

$$\rho = \sqrt{\frac{2m^2e^4}{8\hbar^4}}r = \frac{me^2}{2\hbar^2}r = \frac{r}{2a_0} \tag{10}$$

where a_0 is the Bohr radius

$$a_0 \equiv \frac{\hbar^2}{me^2} \tag{11}$$

Plugging everything into 8, using $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, we have

$$\psi_{210} = \sqrt{\frac{3}{4\pi}}\frac{C_0}{4a_0^2} r e^{-r/2a_0}\cos\theta \tag{12}$$

Normalizing gives the condition

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\psi_{210}^2 r^2 \sin\theta dr\, d\theta\, d\phi = 1 \tag{13}$$

Working out the integral (using software or tables) gives

$$\frac{3}{2}a_0 C_0^2 = 1 \tag{14}$$

$$C_0 = \sqrt{\frac{2}{3a_0}} \tag{15}$$

So the final wave function is

$$\psi_{210} = \frac{1}{\sqrt{32\pi a_0^3}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta \tag{16}$$

which agrees with Shankar's equation 13.1.27.