HYDROGEN ATOM: A SAMPLE WAVE FUNCTION

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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

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

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

$$\rho=\sqrt{\frac{2m^{2}e^{4}}{8\hbar^{4}}}r=\frac{me^{2}}{2\hbar^{2}}r=\frac{r}{2a_{0}} \tag{10}$$

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

$$\psi_{210}=\sqrt{\frac{3}{4\pi}}\frac{C_{0}}{4a_{0}^{2}}re^{-r/2a_{0}}\cos\theta \tag{12}$$

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.