

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):

$$(0.1) \quad \psi_{nlm}(r, \theta, \phi) = \frac{U_{El}(r)}{r} Y_l^m(\theta, \phi)$$

Here, we have

$$(0.2) \quad U_{El} = e^{-\rho} v_{El}$$

$$(0.3) \quad v_{El} = \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k$$

$$(0.4) \quad \rho = \sqrt{\frac{-2mE}{\hbar^2}} r$$

The energy levels of the hydrogen atom are

$$(0.5) \quad E = -\frac{me^4}{2\hbar^2 n^2}$$

where $n = 1, 2, 3, \dots$. The coefficients C_k in 0.3 are given by a recursion relation

$$(0.6) \quad C_{k+1} = \frac{-e^2 \lambda + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)} C_k$$

$$(0.7) \quad \lambda = \sqrt{-\frac{2mE}{\hbar^2}}$$

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

$$(0.8) \quad \psi_{210} = \frac{1}{r} \rho^2 e^{-\rho} C_0 Y_1^0$$

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

$$(0.9) \quad E_2 = -\frac{me^4}{8\hbar^2}$$

This gives

$$(0.10) \quad \rho = \sqrt{\frac{2m^2 e^4}{8\hbar^4}} r = \frac{me^2}{2\hbar^2} r = \frac{r}{2a_0}$$

where a_0 is the Bohr radius

$$(0.11) \quad a_0 \equiv \frac{\hbar^2}{me^2}$$

Plugging everything into 0.8, using $Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$, we have

$$(0.12) \quad \psi_{210} = \sqrt{\frac{3}{4\pi}} \frac{C_0}{4a_0^2} r e^{-r/2a_0} \cos \theta$$

Normalizing gives the condition

$$(0.13) \quad \int_0^{2\pi} \int_0^\pi \int_0^\infty \psi_{210}^2 r^2 \sin \theta dr d\theta d\phi = 1$$

Working out the integral (using software or tables) gives

$$(0.14) \quad \frac{3}{2} a_0 C_0^2 = 1$$

$$(0.15) \quad C_0 = \sqrt{\frac{2}{3a_0}}$$

So the final wave function is

$$(0.16) \quad \psi_{210} = \frac{1}{\sqrt{32\pi a_0^3}} \frac{r}{a_0} e^{-r/2a_0} \cos \theta$$

which agrees with Shankar's equation 13.1.27.