Computing hydrogen ground state wavefunction on a sunny day

2020-10-27

A practical approach to computing the hydrogen ground state wavefunction using minimal information. This post demonstrates how to derive the wavefunction from basic principles of normalization and the Schrödinger equation, then applies this knowledge to calculate transition probabilities in beta decay processes. The analysis covers the transition from tritium to helium-3, showing how quantum mechanics governs nuclear decay processes and atomic state transitions.

blog: https://tetraquark.vercel.app/posts/hydrogen_ground_state/?src=pdf

email: quarktetra@gmail.com

Consider yourself sitting on a sunny beach, minding your own business... And all of a sudden you realize you can't write down the ground state wavefunction of a hydrogen-like atom (e.g., He+, Li++) from memory. What a shame! The only thing you remember is that it was of this form:

$$\psi(r) = A\exp(-\beta r) \tag{1}$$

where A and β are constants. However, you know that ψ has to be normalized:

$$\begin{aligned}
\int d^3x|\psi(r)|^2 &= 1 = A^2\int 4\pi dr r^2 e^{-2\beta r} = 4\pi A^2\frac{1}{(2\beta)^3}\int_0^\infty du u^2 e^{-u} \\
&= \frac{\pi A^2}{\beta^3} \\
&\Rightarrow A^2 = \frac{\beta^3}{\pi}.
\end{aligned} \tag{2}$$

Furthermore, ψ satisfies the Schrodinger equation:

$$\begin{aligned} E\psi(r) &= -\frac{1}{2m}\nabla^2\psi(r) - \frac{Ze^2}{r}\psi(r) \\ &= -\frac{1}{2mr^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}\psi(r)) - \frac{Ze^2}{r}\psi(r) \\ &= \left(\frac{-\beta^2}{2m} + \frac{\beta}{mr} - \frac{Ze^2}{r}\right)\psi(r), \end{aligned} \tag{3}$$

where Ze is the nuclear charge. You match the powers of r to get

$$\beta = me^2 Z = \frac{Z}{a_0}, \quad E = -\frac{\beta^2}{2m} = -\frac{me^4}{2}Z^2, \tag{4}$$

which yields all the unknown coefficients.

Now imagine that the atom you started with is tritium (an isotope of hydrogen) and it suddenly decays into a helium nucleus with the emission of a fast electron that leaves the atom without perturbing the atomic electron outside the nucleus. What is the probability that the resulting He+ ion will be left in the $1s$ state? This is a beta-decay:

$$n \longrightarrow p \quad + e \quad + \bar{\nu}_e \tag{5}$$

The initial wave function is $1s$ state of a hydrogen-like atom, tritium ($Z = 1$), and the final one is the $1s$ state of ^{3}He ($Z = 2$). The wave functions for these state can be found using Eqs. 1 and 4:

$$\psi_{tr}(r) = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/a_0}, \quad \psi_{He}(r) = \sqrt{\frac{8}{\pi a_0^3}}e^{-2r/a_0} \tag{6}$$

The transition probability can be calculated as

$$\begin{aligned} Prob(1s \to 2s) &= |\langle\psi_{tr}|\psi_{He}\rangle|^2 \\ &= \left|\frac{2\sqrt{2}}{\pi a_0^3}\int_0^\infty dr 4\pi r^2 e^{-3r/a_0}\right|^2 \\ &= \left|\frac{2\sqrt{2}}{a_0^3}\frac{a_0^3}{27}\int_0^\infty du u^2 e^{-u}\right|^2 = \left|\frac{16\sqrt{2}}{27}\right|^2 = 0.70 \end{aligned} \tag{7}$$

The only possible value for l is 0, because of the orthogonality of the spherical harmonics. If you are concerned about the missing probability, 0.3, you are welcome to calculate probabilities for transitions to $2s$, $3s$, $4s$... Here are some of the results, 0.25, 0.013 and 0, 004. The probability builds up to 1 slowly, which also says that there is no room for new values of l.

The image in the thumbnail is taken from "Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States"[1]

---

[1] [1]

[1] A. S. Stodolna *et al.*, “Hydrogen atoms under magnification: Direct observation of the nodal structure of stark states,” *Phys. Rev. Lett.*, vol. 110, p. 213001, May 2013, doi: 10.1103/PhysRevLett.110.213001. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.110.213001