Computing hydrogen ground state wavefunction on a sunny day

Abstract

Computing hydrogen wave function with little information to remember.

Index Terms

hydrogen atom, transitions

Contents

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:

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

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Find the interactive HTML-document here.

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

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

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 [1] "Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States"

[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