Physics 308 Introduction to Quantum Mechanics Spring 2005

Homework 12: Solutions 3 and 4

Background

The ground state wave function of the hydrogen atom was found in class by solving the Schrödinger equation. Let's review that. First, it's intuitively obvious that the lowest energy wave function should have no dependence on angle, because such dependence only increases kinetic energy. Thus we just need a radial dependence of the wave function. The equation is

$$-(\psi''(r) + 2\psi'(r)/r) - 2\psi(r)/ar = 2mE\psi(r)/\hbar^2 \quad ,$$

where $a = \hbar^2/me^2 = .53 \times 10^{-10}$ m $= .53$ Å is the Bohr radius. Trying a wave function of the form $\psi = e^{-\kappa r}$, we get for the terms in the Schrödinger equation $(-\kappa^2 + 2\kappa/r - 2/ar)\psi = (2mE_1/\hbar^2)\psi$, which is solved by $\kappa = 1/a$ and therefore $E_1 = -\hbar^2/2ma^2 = -e^2/2a = -13.6eV$.

3. Find the wave function corresponding to the first radial excitation of the ground state, meaning a wave function depending only on r, but with a factor $(1 - br)$ multiplying a declining exponential. Because the binding energy must be smaller than for the ground state, the exponential factor must decline more slowly, so you have to find both the new κ and the value of b. Check that this wave function is orthogonal to the ground state wave function $e^{-r/a}$.

Solution: Because this wave function depends only on r, we may use the same Schrödinger equation described above, just substituting in the form $\psi = (1 - br)e^{-\kappa' r}$. In the previous solution, we had terms of the form $e^{-\kappa r}$ and of the form $e^{-\kappa r}/r$, and the coefficients of both types of term, when put all on one side of the equation, had to add to zero. This time, we have also terms of the form $re^{-\kappa r}$, except now each κ become κ'. Plugging into the equation, we get for the coefficient of terms going as r^1

$$[-(\kappa')^2 - 2mE/\hbar^2]b \quad ,$$

for the coefficient of terms going as r^0

$$-(\kappa')^2 - 2mE/\hbar^2 - b[2\kappa' + 2\kappa' - 2/a] \quad ,$$

and for the coefficient of terms going as r^{-1}

$$2b + 2\kappa' - 2/a \quad .$$

Setting all these expressions to zero, we get $\kappa' = 1/2a$, $b = 1/2a$, and $E_2 = -e^2/8a = E_1/4$.

Orthogonality: Is $0 = \int_0^\infty r^2 dr e^{-3r/2a}(1 - r/2a)$? Note that the angular integration is trivial because no function depends on angles, so that is omitted from the integral. This can be converted to an integral of a dimensionless coordinate $\int y^2 dy (1 - y/3) e^{-y}$. Remembering $\int y^n e^{-y} = n!$, we see the result is $2! - 3!/3$, which indeed vanishes.

4. Find the lowest hydrogen wave function corresponding to $\ell = 1$. Now the Schrödinger equation has an extra term (the "centrifugal potential" term) $(\hbar^2 \ell(\ell+1)/2mr^2)\psi$. This time the radial dependence of the wave function is $f(r) = re^{-\kappa r}$, where again the value of κ must be smaller than for the ground state.

Solution: This time the wave function is supposed to be $\psi = re^{-\bar{\kappa}}$. Because we have $\ell = 1$, there is an extra term in the radial Schrödinger equation $\ell(\ell+1)/r^2$. Once again we have terms going as r^1, r^0, and r^{-1}. There is no term r^{-2} because of the explicit factor r in the wave function. We now get for the first term

$$-\bar{\kappa}^2 - 2mE/\hbar^2$$

, for the second

$$4\bar{\kappa} - 2/a$$

, and for the third

$$2 - \ell(\ell+1)$$

The last confirms we needed a factor r in the wave function, the second gives $\bar{\kappa} = 1/2a = \kappa'$, and so the first gives $E = -e^2/8a = E_2$.

This time orthogonality with the ground state wave function and with the first radial excitation is automatic, because the angular wave functions for $\ell = 1$ are orthogonal to the constant angular wave function for $\ell = 0$.