

Physics 195a
Problem set number 7 – Solution to Problem 40
Due 2 PM, Thursday, November 21, 2002

READING: Read sections 1-5 of the “Solving the Schrödinger Equation: Resolvents” course note.

PROBLEMS:

35. Harmonic oscillator in three dimensions: Exercise 2 of the Harmonic Oscillator course note.
36. Resolvent mathematics: Exercise 1 of the Resolvent course note.
37. More resolvent mathematics: Exercise 2 of the Resolvent course note.
38. Still more resolvent mathematics: Exercise 3 of the Resolvent course note.
39. Green’s function solution of the infinite square well: Exercise 4 of the Resolvent course note.
40. The one-electron atom (review?): We have had a couple of examples of looking at the qualitative features of wave functions. Now apply the same reasoning to the one-electron atom. Thus, sketch the effective potential and the lowest three radial wave functions (do both $R(r)$ and $u(r) = rR(r)$) for the 1-electron atom for $\ell = 0$. Now do the same for the qualitative solutions for $\ell = 1$. Pay attention to the turning points, and to the dependence at $r = 0$. Since you have already computed the actual wave functions, you may produce graphs of the functions you obtained. If you do this, however, you should look carefully at your graphs and make sure you understand at a physically intuitive level the qualitative features.

Solution: Since we have solved for the wave functions, we’ll plot them. The effective equivalent one-dimensional potential is:

$$V_{\text{eff}}(r) = -\frac{Ze^2}{r} + \frac{\ell(\ell + 1)}{2mr^2}. \quad (12)$$

We found the solutions:

$$R_{n_p \ell}(r) = - \left(\frac{2Z}{n_p a_0} \right)^{3/2} \sqrt{\frac{(n_p - \ell - 1)!}{2n_p [(n_p + \ell)!]^3}} (\rho/n_p)^\ell e^{-\rho/2n_p} L_{n_p + \ell}^{2\ell+1}(\rho/n_p), \quad (13)$$

where

$$\rho = \frac{2Z}{a_0} r, \quad (14)$$

$$a_0 = \frac{1}{m e^2} = \frac{1}{m \alpha}, \quad \text{is the **Bohr radius**,} \quad (15)$$

$$n_p = n_r + \ell + 1. \quad (16)$$

The Associated Laguerre polynomials are given by:

$$L_{n+\ell}^{2\ell+1}(x) = \sum_{k=0}^{n-\ell-1} \frac{(-)^{k+1} [(n+\ell)!]^2}{(n-\ell-1-k)!(2\ell+1+k)!k!} x^k. \quad (17)$$

The first few of these polynomials are:

$$L_1^1(x) = -1 \quad (18)$$

$$L_2^1(x) = 2(-2+x) \quad (19)$$

$$L_3^1(x) = 6(-3+3x-\frac{1}{2}x^2) \quad (20)$$

$$L_3^3(x) = -6 \quad (21)$$

$$L_4^3(x) = 24(-4+x) \quad (22)$$

$$L_5^3(x) = 120(-10+5x-\frac{1}{2}x^2). \quad (23)$$

Hence, the first few radial wave functions are:

$$R_{10}(\rho) = 2 \left(\frac{Z}{a_0} \right)^{3/2} e^{-\rho/2} \quad (24)$$

$$R_{20}(\rho) = \frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0} \right)^{3/2} (2-\rho/2)e^{-\rho/4} \quad (25)$$

$$R_{30}(\rho) = \frac{2}{9\sqrt{3}} \left(\frac{Z}{a_0} \right)^{3/2} (3-\rho+\rho^2/18)e^{-\rho/6} \quad (26)$$

$$R_{21}(\rho) = \frac{1}{4\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} \rho e^{-\rho/4} \quad (27)$$

$$R_{31}(\rho) = \frac{1}{27\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} \rho(4 - \rho/3)e^{-\rho/6} \quad (28)$$

$$R_{41}(\rho) = \frac{1}{64\sqrt{15}} \left(\frac{Z}{a_0}\right)^{3/2} \rho \left(10 - \frac{5}{4}\rho + \frac{\rho^2}{32}\right) e^{-\rho/8}. \quad (29)$$

In terms of ρ , we may express the effective potential as:

$$U_{\text{eff}}(\rho) \equiv \frac{a_0 V_{\text{eff}}(r(\rho))}{2Z^2 e^2} = -\frac{1}{\rho} + \frac{\ell(\ell+1)}{\rho^2}. \quad (30)$$

The bond state energies are:

$$E_{n_p} = -\frac{Z^2 e^4 m}{2} \frac{1}{n_p^2}. \quad (31)$$

In terms of our scaled $U_{\text{eff}}(\rho)$ potential, they appear at:

$$E_{n_p} = -\frac{1}{4n_p^2}. \quad (32)$$

We'll make graphs of $U_{\text{eff}}(\rho)$ and of $R_{n_p \ell}(\rho)(a_0/Z)^{3/2}$ (as well as u).