The radial eqn

The radial part of the Schrödinger Eqn is

(1) $$\left[\frac{-\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)+\frac{l(l+1)\hbar^2}{2\mu r^2}-\frac{Ze^2}{r}\right]R(r)=E\,R(r)$$

Before we get to solving it, lets clean up.

(1.1) Let $u(r) \equiv r\,R(r)$

(1.2) $$\rho \equiv \sqrt{\frac{8\mu|E|}{\hbar^2}}\; r$$

(1.3) $$\lambda \equiv \frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2E}}$$

With these definitions, (1) becomes

(2) $$\frac{d^2u}{d\rho^2}-\frac{l(l+1)}{\rho^2}u+\left(\frac{\lambda}{\rho}-\frac{1}{4}\right)u=0$$

You can check it later

As we did w/ the SHO, we'll try to develop a series sol'n. The first step in that game the last time was to pull of the asymptotic behavior.

First consider the $\rho \to \infty$ limit of (2). Only 2 terms remain.

Q1 (3) $$\frac{d^2u}{d\rho^2}-\frac{}{\_\_\_\_}=0$$ Fill in the blank.

The sol'n to (3) is

(4) $$u = Ae^{-\rho/2}+Be^{\rho/2}$$

Q2 Check that (4) solves (3).

Q3 We must have $B=0$ because ________

Consider now the small ρ behavior. In this limit we have

$$\frac{d^2u}{d\rho^2}-\frac{l(l+1)}{\rho^2}u=0$$

The sol'n here is $u(\rho) = C\rho^{\ell+1} + D\rho^{-\ell}$.

Q4 Check it!

We must have $D=0$ since it blows up as $\rho \to 0$

Having identified the asymptotic behavior at both large and small ρ, we'll try a full sol'n of the form

(5) $u(\rho) = \rho^{\ell+1} e^{-\rho/2} F(\rho)$

Plugging this guess into (2) we get

(6) $$\frac{d^2F}{d\rho^2} + \left(\frac{2\ell+2}{\rho} - 1\right)\frac{dF}{d\rho} + \left(\frac{\lambda}{\rho} - \frac{\ell+1}{\rho}\right)F = 0$$

Check it, maybe with Mathematica, later

Now we'll try a series sol'n for F. This will result in a recursion relation, that will need to terminate resulting in quantized energy. Hopefully that's familiar from the SHO. So into (6) plug

(7) $$F(\rho) = \sum_{k=0}^{\infty} C_k \rho^k$$

(8) $$\sum_{k=2}^{\infty} k(k-1)C_k\rho^{k-2} + \sum_{k=1}^{\infty}(2\ell+2)kC_k\rho^{k-2}$$
$$+ \sum_{k=0}^{\infty}\left[-k+\lambda-(\ell+1)\right]C_k\rho^{k-1} = 0$$

Q5 Pick at least one term in (8) and check it.

We want to factor the ρ's out of (8). Then we'll have something of the form

$$\sum_k \{ \text{No } \rho \text{ here} \} \rho^{\text{some power involving } k} = 0$$

Then we can conclude that the thing in $\{\ \}$

is zero, and that will give the recursion relation, and that will give the quantization. Remember the SHO?
If we use $k = k'+1$ in the first 2 sums of 8, then rename back to k, we'll have

$$\sum_{k=0}^{\infty} \left\{ \left[k(k+1) + (2\ell+2)(k+1) \right] c_{k+1} + \left[-k + \lambda - (\ell+1) \right] c_k \right\} \rho^{k-1} = 0$$

Q6 Show that this means:

(9) $$c_{k+1} = \frac{k+\ell+1-\lambda}{(k+1)(k+2\ell+2)} c_k$$

As with the SHO, this series will be unnormalizable if it does not end at finite k.
The way to make it end is if

(10) $\lambda = 1 + \ell + n_r$ with $n_r = 0, 1, 2, \ldots$

Q7 Convince yourself that (10) makes 9 end.

The quantization condition (10) with definition (1.3) gives

$$E = \frac{\mu Z^2 e^4}{2\hbar^2 \underbrace{(1+\ell+n_r)}_{\equiv n}{}^2} \Rightarrow E_n = \frac{\mu Z^2 e^4}{2\hbar^2 n^2} \quad n = 1, 2, 3 \ldots$$

The quantized energies of Hydrogen-like atoms. Woohoo!

Q8 In a sentence, conceptually, what caused quantization?
Using (1.1) (5) (7) and (9), we can construct the radial wave f'n

$$R(r) = \frac{u(r)}{r} = \rho^{\ell+1} e^{-\rho/2} F(\rho) = \rho^{\ell+1} e^{-\rho/2} \sum_{k=0}^{\infty} c_k \rho^k$$

lets do the ground state, $\lambda = 1 \Rightarrow k = 0$ is the max
$\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad + \ell = 0$

So $n=1$, we lable w/ $n + \ell$

$$R_{10} = C_0 \rho e^{-\rho/2}$$

The normalization is

$$\int_0^\infty |R_{n\ell}(r)|^2 r^2 dr = 1$$

(probability to find particle at some r must be 1)

With the definition of ρ at (1.2) and the normalization, we find

$$R_{1,0} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}.$$

Other radial wave f'ns are listed on pages 355 + 356 of Townsend, and they are plotted on the next page.

Q9 Jeporde : I am an electron most likely to be found at about $4a_0$. I will not be caught dead in the $\theta = \pi/2$ plane. Who is the e^- with $E =$ _____, $n =$ _____, $\ell =$ _____, $m =$ _____?

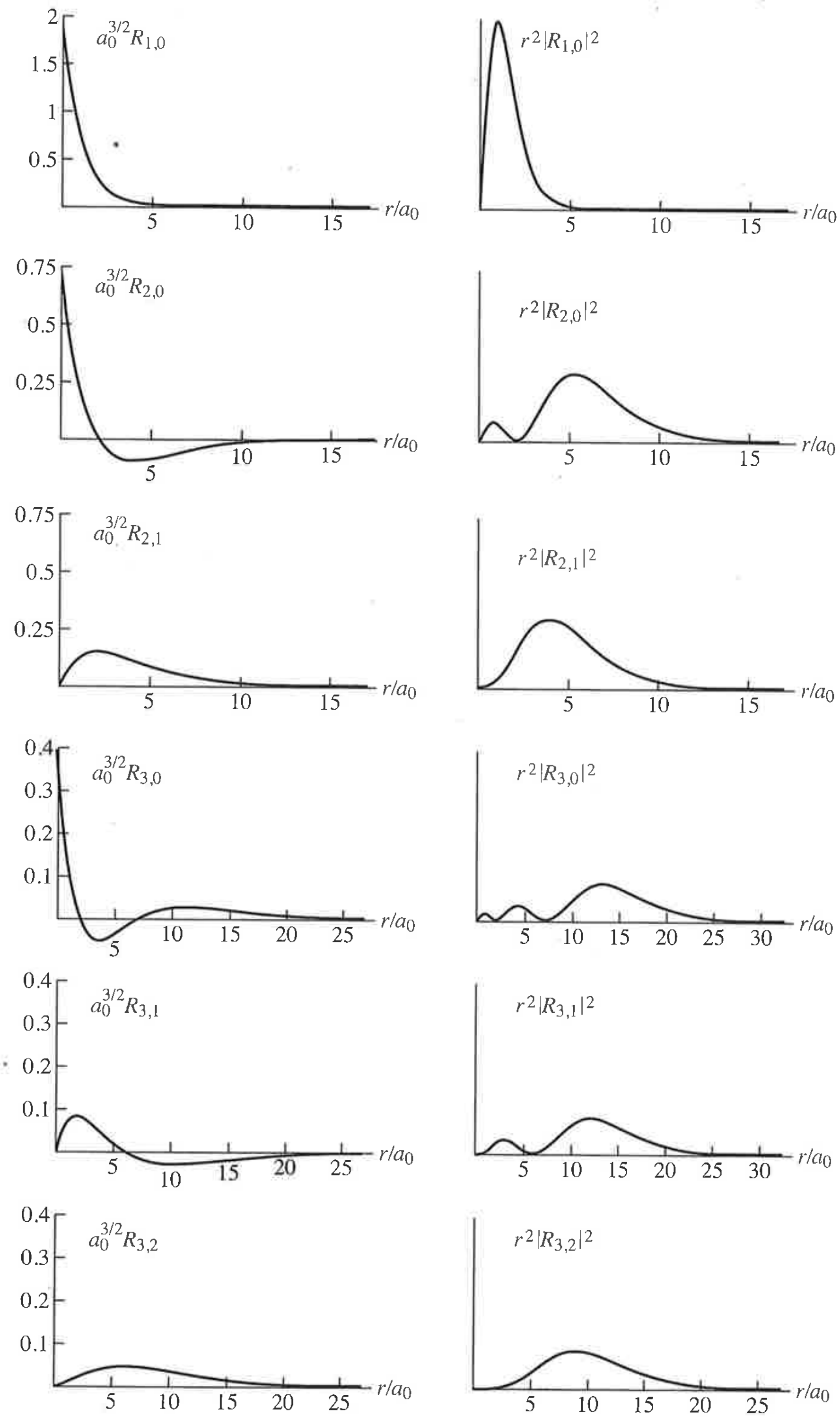

Figure 10.5 Plots of the radial wave function $R_{n,l}(r)$ and the radial probability density $r^2|R_{n,l}(r)|^2$ for the wave functions in (10.43), (10.44), and (10.45).