Homework 11

PHYSICS 450
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1. Study Chapter 4.2.
2. Starting from (4.60),

$$\begin{aligned}
u(\rho) &= \rho^{\ell+1}e^{-\rho}v(\rho) \\
u'(\rho) &= (\ell+1)\rho^{\ell}e^{-\rho}v(\rho) - \rho^{\ell+1}e^{-\rho}v(\rho) + \rho^{\ell+1}e^{-\rho}v'(\rho) \\
&= \rho^{\ell}e^{-\rho}\left[(\ell+1-\rho)v(\rho) + \rho v'(\rho)\right] \\
u''(\rho) &= \ell\rho^{\ell-1}e^{-\rho}\left[(\ell+1-\rho)v(\rho) + \rho v'(\rho)\right] - \rho^{\ell}e^{-\rho}\left[(\ell+1-\rho)v(\rho) + \rho v'(\rho)\right] \\
&\quad + \rho^{\ell}e^{-\rho}\left[(\ell+1)v'(\rho) - v(\rho) - \rho v'(\rho) + \rho v''(\rho) + v'(\rho)\right] \\
&= \dots
\end{aligned}$$

3. Using (4.76), for R_{30}, the coefficients are given by

$$\begin{aligned}
c_1 &= \frac{2(0+0+1-3)}{1(0+0+2)}c_0 = -2c_0 \\
c_2 &= \frac{2(1+0+1-3)}{2(1+0+2)}(-2c_0) = c_0 \\
c_3 &= \frac{2(2+0+1-3)}{(\dots)} = 0.
\end{aligned}$$

So, $v(\rho)$ becomes

$$\begin{aligned}
v(\rho) &= \left(1 - 2\rho + \rho^2\right)c_0 \\
R_{30} &= \frac{1}{r}\rho\left(1 - \frac{2}{3a}r + \frac{1}{9a^2}r^2\right)e^{-r/3a}.
\end{aligned}$$

Similarly for R_{31},

$$\begin{aligned}
c_1 &= \frac{2(0+1+1-3)}{2+2}c_0 = -\frac{1}{2}c_0 \\
c_2 &= \frac{2(1+1+1-3)}{2(1+2+2)}(-1/2)c_0 = 0. \\
v(\rho) &= (1 - \frac{1}{2}\rho)c_0 \\
R_{31} &= \frac{r}{9a^2}\left(1 - \frac{1}{6a}r\right)e^{-r/3a}.
\end{aligned}$$

Lastly, for R_{32},

$$\begin{aligned}
c_1 &= \frac{2(2+1-3)}{(\dots)} = 0. \\
v(\rho) &= c_0 \\
R_{32} &= \frac{r^2}{9a^3}e^{-r/3a}
\end{aligned}$$

4. (a) The ground state of hydrogen has wavefunction

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}. \tag{4.80}$$

For $\langle r \rangle$,

$$\begin{aligned}\langle r \rangle &= \frac{1}{\pi a^3} \int_0^\pi \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \int_0^\infty r^3 e^{-2r/a} \, \mathrm{d}r \\ &= \frac{4}{a^3} \frac{3a^4}{8} \\ &= \frac{3a}{2}.\end{aligned}$$

Similarly, for $\langle r^2 \rangle$,

$$\begin{aligned}\langle r^2 \rangle &= \frac{1}{\pi a^3} \int_0^\pi \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \int_0^\infty r^4 e^{-2r/a} \, \mathrm{d}r \\ &= \frac{4}{a^3} \frac{3a^5}{4} \\ &= 3a^2.\end{aligned}$$

(b) As $r^2 = x^2 + y^2 + z^2$, the electron will be in the x direction $1/\sqrt{3}$ of the time and in the "x^2" direction $1/3$rd the time, so

$$\begin{aligned}\langle x \rangle &= \frac{3a}{2\sqrt{3}} \\ \langle x^2 \rangle &= a^2.\end{aligned}$$

(c) From (4.89), for that state, the wavefunction is

$$\begin{aligned}\psi_{211}(r,\theta,\phi) &= \sqrt{\left(\frac{1}{a}\right)^3 \frac{1}{4(3!)}} e^{-r/2a} \left(\frac{r}{a}\right) L_0^3(2r/na) Y_1^1(\theta,\phi) \\ &= -\sqrt{\frac{3}{192a^5}} r e^{-r/2a} \sin\theta e^{i\phi} \\ &= -\frac{1}{8a^{5/2}\sqrt{\pi}} r e^{-r/2a} \sin\theta e^{i\phi}.\end{aligned}$$

The expectation $\langle x^2 \rangle$ is then

$$\begin{aligned}\langle \psi_{211} | x^2 \psi_{211} \rangle &= \langle \psi | r^2 \sin^2\theta \cos^2\phi \psi \rangle \\ &= \frac{1}{64\pi a^5} \int_0^\pi \sin^5\theta \, \mathrm{d}\theta \int_0^{2\pi} \cos^2\phi \, \mathrm{d}\phi \int_0^\infty r^6 e^{-r/a} \, \mathrm{d}r \\ &= \frac{1}{64\pi a^5} \left(\frac{16}{15}\right) (\pi) \left(720 a^7\right) \\ &= 12a^2.\end{aligned}$$

5. The probability density is given by

$$\rho(r) = |\Psi|^2 = \frac{1}{\pi a^3} e^{-2r/a}.$$

The most probable point is where the probability is maximized, i.e. the r where

$$\begin{aligned} \frac{\mathrm{d}P}{\mathrm{d}r} &= \frac{\mathrm{d}4\pi r^2 \rho(r)}{\mathrm{d}r} = 0. \\ \implies \frac{\mathrm{d}}{\mathrm{d}r}\left[r^2 e^{-2r/a}\right] &= e^{-2r/a}\left(2r - 2r^2/a\right) = 0 \\ 2r - 2r^2/a &= 0. \\ \boxed{r = a.} \end{aligned}$$

6. The quantities are just scaled by Z or Z^2, so:

$$\begin{aligned} E_n(Z) &= (-13.6\,\mathrm{eV})\,\frac{Z^2}{n^2} \\ E_1(Z) &= (-13.6\,\mathrm{eV})\,Z^2 \\ a_0(Z) &= \left(0.529 \times 10^{-10}\,\mathrm{m}\right)\frac{1}{Z} \\ \mathcal{R}(Z) &= \left(1.097 \times 10^{7}\,\mathrm{m}^{-1}\right) Z^2. \end{aligned}$$

The Lyman series is roughly

$$\begin{aligned} &E_{2\to1}(2) = (13.6\,\mathrm{eV})\,\frac{4}{4-1} \approx 18\,\mathrm{eV} \quad \text{(visible or uv?)} \\ &E_{2\to1}(3) \approx 40\,\mathrm{eV}. \quad \text{(uv)} \end{aligned}$$