7.8

$$R_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

So

$$\bar{V} = \int_0^\infty V(r) \; R^2 \cdot 4\pi r^2 \, dr$$

$$\bar{V} = \int_0^\infty \frac{-e^2}{4\pi\varepsilon_0 r} \frac{1}{\pi a_0^3} e^{-2r/a_0} \; 4\pi r^2 \, dr$$

$$\bar{V} = \frac{-e^2}{4\pi\varepsilon_0 a_0} \int_0^\infty e^{-2r/a_0} \; \frac{4\pi r^{\cancel{2}} dr}{\pi a_0^2 \cancel{\pi}}$$

let $u = 2r/a_0$

$$\bar{V} = \frac{-e^2}{4\pi\varepsilon_0 a_0} \int_0^\infty e^{-u} \; u \, du \qquad \int_0^\infty x^n e^{-x} = n!$$

$$\bar{V} = \frac{-e^2}{4\pi\varepsilon_0 a_0} \cdot (1!)$$

b)

For the ground sate

$$E_1 = -\frac{\hbar^2}{2ma_0^2} = \frac{1}{2} \frac{-e^2}{4\pi\varepsilon_0 a_0} = -13.6\,\mathrm{eV}$$

So

$$E = \frac{+}{2} V$$

c) $E = \overline{K} + \overline{V}$

Proof

$$\int dx\ \psi^* E \psi = \int \psi^* \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right] \psi \, dx$$

$$E = \overline{KE} + \overline{V}$$

So

$$\overline{E} = \overline{K} + \overline{V}$$

$$+V/2 = \overline{K} + V \Rightarrow \boxed{\overline{K} = -V/2}$$

7.5 The time indep-schrodinger reads

$$\left[\frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + V(r) \right] R(r) = E \cdot R \qquad (*)$$

whith $R(r) = C e^{-r/a_0}$ we have

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial R}{\partial r} = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 C e^{-r/a_0}\left(\frac{-1}{a_0}\right)$$

$$= \frac{-C}{a_0}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 e^{-r/a_0} = \frac{-C}{a_0}\frac{1}{r^2}\left(2re^{-r/a_0} + r^2 e^{-r/a_0} \cdot \frac{-1}{a_0}\right)$$

$$= \frac{-C}{a_0^2}\left(\frac{2a_0 e^{-r/a_0}}{r} - e^{-r/a_0}\right)$$

Substituting into the Schrödinger Eq (*) we have

$$-\frac{\hbar^2}{2m}\overbrace{\left(\frac{-\cancel{C}}{a_0^2}\frac{2a_0 e^{-r/a}}{r} + \frac{\cancel{C}}{a_0^2} e^{-r/a_0}\right)}^{\text{from above}} + \frac{-e^2}{4\pi\varepsilon_0}\frac{1}{r}\cancel{C}e^{-r/a_0} = E\cancel{C}Re^{-r/a}$$

Organizing we have

$$-\frac{\hbar^2}{2ma_0^2}e^{-r/a_0} + \frac{2a_0}{r}\underbrace{\left(\frac{\hbar^2}{2ma_0^2} - \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 a_0}\right)}_{=0}e^{-r/a_0} = E e^{-r/a_0}$$

$= 0$ rember the bohr model

So

$$-\frac{\hbar^2}{2ma_0^2}e^{-r/a_0} = E e^{-r/a_0}$$

This is true provided $E = -\hbar^2/2ma_0^2$

7.7) For $n=2$ $l=1$ we have

$$R_{21}(r) = \frac{1}{\sqrt{96\pi a_0^3}}\left(\frac{r}{a_0}\right) e^{-r/2a_0}$$

So the probability density is

$$P(r)\,dr = |R|^2\, 4\pi r^2\, dr$$

$$P(r)\,dr = \frac{1}{96\pi a_0^3}\left(\frac{r}{a_0}\right)^2 e^{-r/a_0} \cdot 4\pi r^2\, dr = C\left(\frac{r}{a_0}\right)^4 e^{-r/a_0}\, d$$

Maximizig we find r such that

$$\frac{dP}{dr} = \left[\frac{4r^3}{a_0^4} e^{-r/a_0} + \left(\frac{r}{a_0}\right)^4 e^{-r/a_0}\,\frac{-1}{a_0}\right] \times \text{const} = 0$$

So need to find where

$$e^{-r/2a_0} \times \left[\frac{4r^3}{a_0^4} - \left(\frac{r}{a_0}\right)^4 \frac{1}{a_0}\right] = 0$$

$$\frac{4r^3}{a_0^4} - \frac{r^4}{a_0^4}\,\frac{1}{a_0} = 0$$

or $r = 4a_0$

agrees w Bohr model

b)

$$\bar{r} = \int_0^\infty \mathcal{P}(r)\, r\, dr$$

$$\bar{r} = \int_0^\infty \underbrace{\left(\frac{1}{96\pi a_0^3} \frac{r^2}{a_0^2} e^{-r/a_0}\, 4\pi r^2\, dr \right)}_{\mathcal{P}(r)dr} \times \underbrace{r}_{r}$$

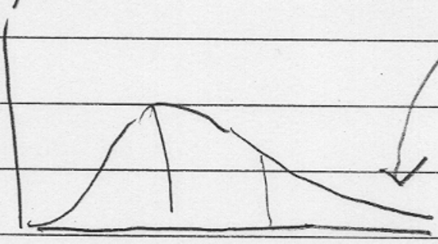
$$\bar{r} = a_0 \left(\frac{4\pi}{96\pi} \right) \int_0^\infty \frac{r^4\, dr}{a_0^5}\, e^{-r/a_0} \times \frac{r}{a_0}$$

$$\bar{r} = a_0 \cdot \frac{4\pi}{96\pi} \int_0^\infty u^5\, du\, e^{-u}$$

$$\bar{r} = a_0 \cdot \left(\frac{4\pi}{96\pi}\, 5! \right) = 5a_0$$

c)

$\mathcal{P}(r)$



$r_{mp} = 4a_0 \quad 5a_0 = \bar{r}$

The lengthy tail of the probability distribution pushes the average out farther than the most probable radius

7.13

o $\psi_{432} \Rightarrow$ a) $E = \frac{-13.6\,eV}{4^2} =$

b) $R_{43} =$ Hmm I. don't know how you could have known this

c) $\overline{L^2} = \ell(\ell+1)\hbar^2$

$\sqrt{\overline{L^2}} = \sqrt{\ell(\ell+1)}\,\hbar = \sqrt{3 \cdot 4}\,\hbar$

d) $\overline{L_z} = 3\hbar$

7.14

It Suffice to work piece by piece: look at Table 7-2

$|\psi_{300}|^2$ = sperically symmetric since ψ_{300} indep of angle

$|\psi_{310}|^2 + |\psi_{311}|^2 + |\psi_{31-1}|^2 \propto 2\cos^2\theta + \sin^2\theta\,|e^{+i\varphi}|^2$

$+ \sin^2\theta\,|e^{-i\varphi}|^2$

$\propto 2(\cos^2\theta + \sin^2\theta)$ ~~spec~~ ~~sperically~~

Thus:

$$|\psi_{300}|^2 + |\psi_{311}|^2 + |\psi_{31-1}|^2 \propto 2$$ sperical symmetric

$$|\psi_{322}|^2 + |\psi_{32-2}|^2 + |\psi_{321}|^2 + |\psi_{32-1}|^2 + |\psi_{320}|^2 =$$

$$\frac{1}{4}\sin^4\theta + \frac{1}{4}\sin^4\theta + \sin^2\theta\cos^2\theta + \sin^2\theta\cos^2\theta + \frac{1}{6}(3\cos^2\theta - 1)^2$$

$$= \text{———————} \| \text{———————} + \frac{1}{6}(9\cos^4\theta - 6\cos^2\theta + 1$$

Now one needs some methodoloy

write $\sin^2\theta = 1 - \cos^2\theta$

$\sin^4\theta = (1 - \cos^2\theta)^2$ and chug away

Straight forward algebra gives $c \equiv \cos\theta$

$$= \frac{1}{2}(1-c^2)^2 + 2(1-c^2)c^2 + \frac{1}{6}(3c^2-1)^2$$

$$= \frac{1}{2}(1-c^2)^2 + 2(1-c^2)c^2 + \frac{1}{6}(3c^2 - 1)^2 = 2/3$$

$$= \frac{1}{2}(1 - 2c^2 + c^4) + 2c^2 - 2c^4 + \frac{9}{6}c^4 - \frac{6}{6}c^2 + \frac{1}{6} = 2/3$$

So

$$|\psi_{322}|^2 + |\psi_{32-2}|^2 + |\psi_{321}|^2 + |\psi_{32-1}|^2 + |\psi_{320}|^2 \propto 2/3$$

which is indep of angle

↑

This last part got a little involved

Problems

① Schrödinger Equation $\frac{u}{r} = R$

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} R = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\left(\frac{u}{r}\right)$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \left[-\frac{1}{r^2}u + \frac{1}{r}\frac{\partial u}{\partial r}\right]$$

$$= -\frac{1}{r^2}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)$$

$$= -\frac{1}{r^2}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial u}{\partial r} + \frac{1}{r}\frac{\partial^2 u}{\partial r^2} = \frac{1}{r}\frac{\partial^2 u}{\partial r^2}$$

as claimed!

Problem 2

The Schrödinger Eq;

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\mathbb{L}^2}{2mr^2} + V(r)\right] RY = E\,RY$$

Then

$$\frac{1}{RY}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}RY + \frac{1}{R\,2mr^2}\frac{1}{Y}\mathbb{L}^2 RY + V(r) = E$$

This

Now Y goes through and R goes through this

where $\mathbb{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

So

$$\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R \checkmark + \overbrace{\frac{1}{2mr^2}}^{\checkmark}\frac{1}{Y}\mathbb{L}^2 Y + \overbrace{V(r)}^{\checkmark} = \overbrace{E}^{\checkmark}$$

So if I leave r fixed and change θ and φ then the checked terms are constant so

$$\frac{1}{Y}\mathbb{L}^2 Y = C \Rightarrow \mathbb{L}^2 Y = CY$$

Then

$$\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} R + \frac{1}{2mr^2} \cdot C + V(r) = E$$

or

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{C}{2mr^2} + V(r)\right] R = E R$$

<u>Problem 3</u>

Let $u = \sqrt{4\pi}\, r R$

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} R = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \frac{u}{r\sqrt{4\pi}}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \left(\frac{u'}{r} - \frac{u}{r^2}\right) \frac{1}{\sqrt{4\pi}}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r} (r u' - u) \frac{1}{\sqrt{4\pi}}$$

$$= \left(\frac{1}{r^2} r u'' + \frac{u'}{r^2} - \frac{u'}{r^2}\right) \frac{1}{\sqrt{4\pi}}$$

$$= \frac{u''}{r} \frac{1}{\sqrt{4\pi}}$$

So the Schrödinger Eq

$$-\frac{\hbar^2}{2m}\frac{u''}{r}\frac{1}{\sqrt{4\pi}} + \frac{l(l+1)\hbar^2}{2mr^2}\frac{u}{\sqrt{4\pi}\,r} + V(r)\frac{u}{\sqrt{4\pi}\,r} = E\frac{u}{\sqrt{4\pi}\,r}$$

Multiplying by

$\sqrt{4\pi}\,r$ gives

$$\left[-\frac{\hbar^2}{2m}u'' + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]u = Eu$$

Problem 4

3s, 3p, 3d

	n l m	E	$\overline{L^2}$	$\overline{L_z}$
3s	3 0 0	$-13.6/3^2$	0	0
3p	3 1 0	$-13.6/3^2$	$2\hbar^2$	0
	3 1 1	$-13.6/3^2$	$2\hbar^2$	$\hbar$
	3 1 -1	$-13.6/3^2$	$2\hbar^2$	$-\hbar$
3d	3 2 0	$-13.6/3^2$	$6\hbar^2$	0
	3 2 ±1	$-13.6/3^2$	$6\hbar^2$	$\pm\hbar$
	3 2 ±2	$-13.6/3^6$	$6\hbar^2$	$\pm 2\hbar$