7.8

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

So

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

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

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

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

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

So

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

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

Proof

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

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

So

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

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

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

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

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

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

Substituting into the Schrödinger Eq (*) we have

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

Organizing we have

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

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

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

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

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)

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

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

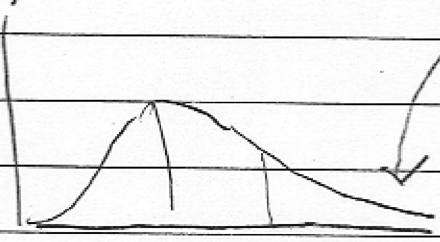
$$\bar{r} = a_0 \left(\frac{4\pi}{96\pi} \right) \int_0^\infty \frac{r^4\, dr}{a_0^5}\, e^{-r/a_0} \times \frac{r}{a_0}$$

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

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

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

Separation of Vars in Radial Eqn

The Schrödinger Eqn is

$$\frac{1}{\psi}\left[\frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{\mathbb{L}^2}{2mr^2}+V(r)\right]\psi = E$$

Where

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

Now substitute

$$\psi = R(r)\,Y(\theta,\varphi)$$

Using

$$\frac{1}{RY}\left(\frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right)RY = \frac{1}{R}\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r}\right)$$

and

$$\frac{1}{RY}\frac{\mathbb{L}^2}{2mr^2}RY = \frac{1}{2mr^2}\frac{1}{Y}\mathbb{L}^2 Y$$

and $\quad \frac{1}{\psi} V(r)\psi = V(r)$

We have

$$\overset{\checkmark}{\frac{1}{R}\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial R}{\partial r}\right)} + \overset{\checkmark}{\left(\frac{1}{2mr^2}\right)}\left(\frac{1}{Y}\mathbb{L}^2 Y\right) + \overset{\checkmark}{V(r)} = \overset{\checkmark}{E}$$

Now leave r <u>fixed</u> but change θ, φ

Since r is fixed the "checked" terms in are constant. Since the "$\checkmark$" terms are constant we must have .

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

const

indep of θ, φ

So we find

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

as claimed

From R to u

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

Write;

constant usually $\sqrt{4\pi}$ but sometimes one

$$u = C\,r\,R$$

So

$$R = \frac{u}{rC}$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\left(\frac{u}{Cr}\right) = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\left(\frac{u'}{r} - \frac{u}{r^2}\right)\times\frac{1}{C}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}(ru' - u)\times\frac{1}{C}$$

$$= \frac{1}{r^2}\,ru'' + u' - u'\times\frac{1}{C}$$

$$= \frac{u''}{r}\times\frac{1}{C}$$

Thus $(*)$ becomes

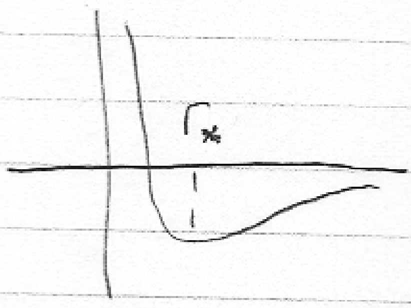
$$\frac{-\hbar^2}{2m}\left(\frac{u''}{Cr}\right) + \frac{l(l+1)\hbar^2}{2mr^2}\,\frac{u}{rC} + V(r)\,\frac{u}{rC} = E\,\frac{u}{rC}$$

So multiplying by rC we have

$$\boxed{\frac{-\hbar^2}{2m}u'' + \left(\frac{l(l+1)}{2mr^2} + V(r)\right)u = E\,u}$$

The minimum of Veff

$$V_{eff}(r) = \frac{-e^2}{4\pi\varepsilon_0}\frac{1}{r} + \frac{l(l+1)\hbar^2}{2mr^2}$$



δ_0

$$\left.\frac{\partial V}{\partial r}\right|_{r_*} = 0$$

$$\frac{+e^2}{4\pi\varepsilon_0}\frac{1}{r^2} - \frac{2(l(l+1)\hbar^2)}{2mr^3} = 0$$

Define $\bar{r} = \frac{r}{a_0}$ so this equn becomes

$$\frac{e^2}{4\pi\varepsilon_0}\frac{1}{a_0^2}\frac{1}{\bar{r}^2} = \frac{2(l(l+1)\hbar^2)}{2ma_0^3\bar{r}^3}$$

using

$$\underbrace{\frac{e^2}{4\pi\varepsilon_0}\frac{1}{a_0}}_{27.2eV} = \underbrace{\frac{\hbar^2}{2ma_0^2}}_{13.6eV}\cdot 2$$

We have

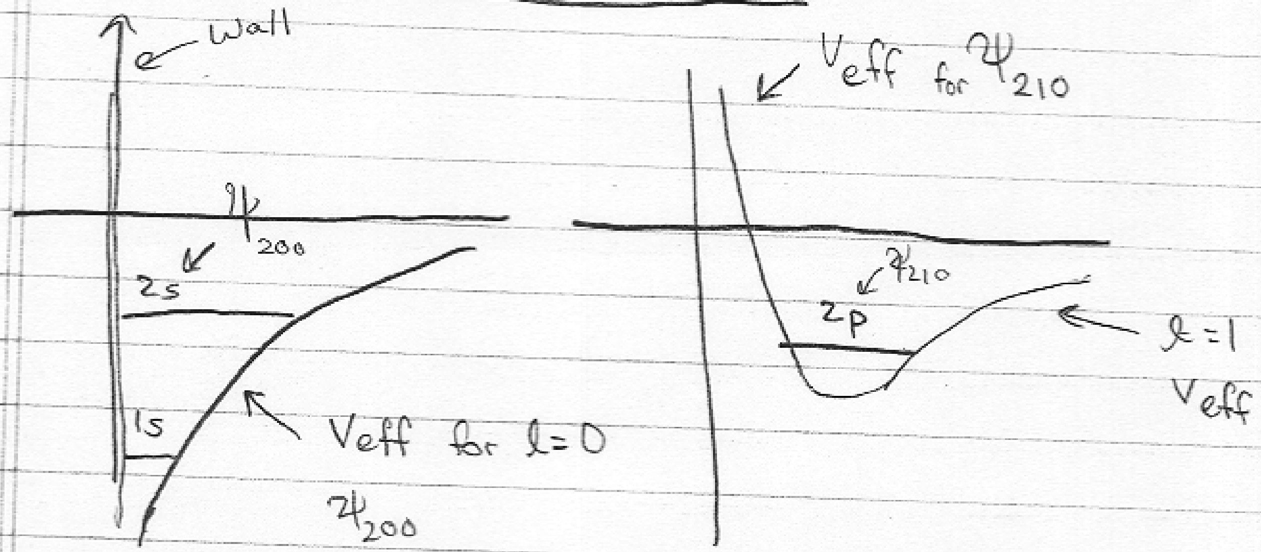
$$\frac{1}{a_0}\frac{1}{\bar{r}^2} = \frac{l(l+1)}{a_0\bar{r}^3}$$

$$\bar{r} = l(l+1)$$

$$r = l(l+1)a_0$$

Differences between ψ_{210} + ψ_{200}

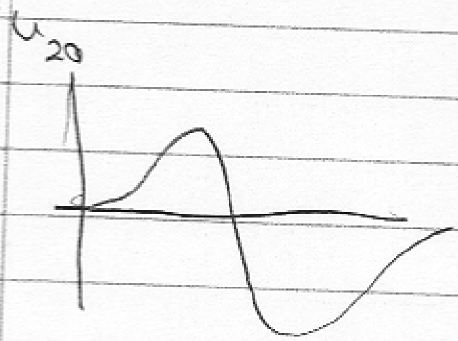
a)

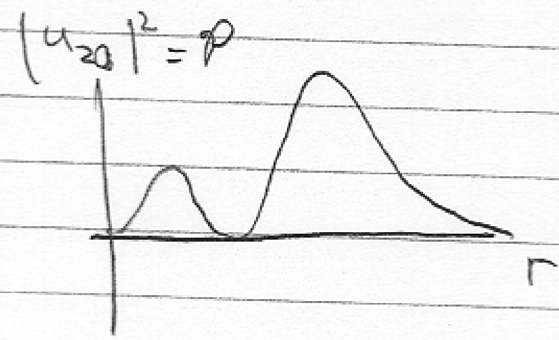


b) Now ψ_{200} is the first excited state of the $l=0$ eff pot. $(n-1)-l$ = # of rad excitation

$(2-1)-0$ = ——"——

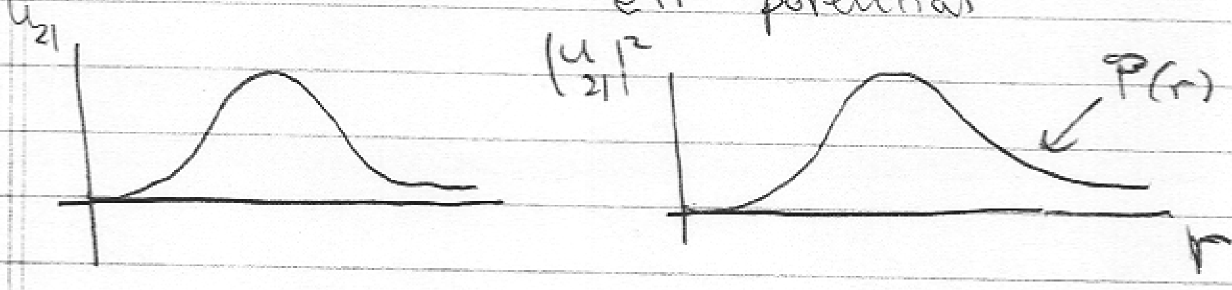
1 = rad exicitation





While ψ_{210} has $(n-1)-\ell = (2-1)-1 = 0$ rad excitat

So u_{21} is the ground state of the $\ell = 1$ eff potential



- These are qual diff because u_{21} is a radial ground state while u_{20} is a radial first excited state.

<u>Note</u>: We still call ψ_{210} a first excited state of Hydrogen because it is excited in the angular directions

For ψ_{200} find Most likely position:

const

$$u_{20} = C\, r\, R_{20}$$

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

a new const

$$u_{20} = C' \frac{r}{a_0}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$$

$$u_{20} = C\,\bar{r}\,(2-\bar{r})\,e^{-\bar{r}/2} \qquad \bar{r} = r/a_0$$

$$\mathcal{P}(r) = |u_{20}|^2 = \bar{r}^2(2-\bar{r})^2 e^{-\bar{r}}$$

To find where this is max we differentiate.

$$\frac{d\mathcal{P}}{dr} = e^{-r}\left(\bar{r}^2(2-\bar{r})^2(-)\right)$$

$$+ e^{-\bar{r}}\left(\bar{r}^2\, 2(2-\bar{r})(-)\right)$$

$$+ e^{-\bar{r}}\left(2\bar{r}\,(2-\bar{r})^2\right)$$

$$= e^{-\bar{r}}(2-r)\,\bar{r}\left(-\bar{r}(2-\bar{r}) - 2\bar{r} + 2(2-\bar{r})\right)$$

$$\frac{d\mathcal{P}}{dr} = e^{-\bar{r}}(2-\bar{r})\,\bar{r}\left(-\bar{r}^2 - 6\bar{r} + 4\right)$$

So

$\frac{dP}{dr} = 0$ at $\bar{r} = 2$ and

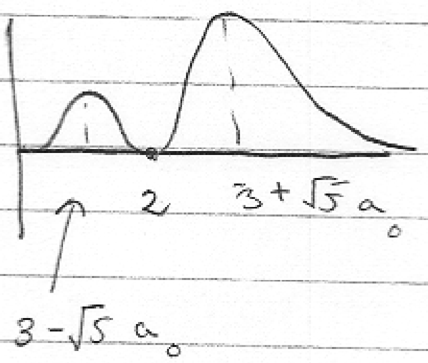
When

$$\bar{r}^2 + 6\bar{r} - 4 = 0$$

$$\bar{r} = 3 \pm \sqrt{5}$$

So the maxima and minima happen at

$$r = (3 \pm \sqrt{5}\, a_0),\ 2a_0$$



So the maximum is at

$$\boxed{r = 3 + \sqrt{5}\, a_0}$$

Second Excited States levels

name	n	l	m	L^2	E	L_z	
3s	3	0	0	0	$-13.6/3^2$	0	1 state
3p	3	1	0	$2\hbar^2$	$-13.6/3^2$	0	3stat
3p	3	1	$\pm$	$2\hbar^2$	"	$\pm\hbar$	
3d	3	2	0	$6\hbar^2$	"	0	5 sta
	3	2	± 1	$6\hbar^2$	"	$\pm\hbar$	
	3	2	± 2	"	"	$\pm 2\hbar$