LECTURE 28 9-10-09

QUALITATIVE FIRST

SOLVE TISE FOR HYDROGEN

FIND ev's $\longrightarrow$ EIGEN ENERGIES

FIND $e\vec{v}$'s $\longrightarrow$ ENERGY EIGENFCNS

STATIONARY STATES

$$|n\,\ell\,m\rangle \longrightarrow \psi_{n\ell m}(\vec{r})$$

$$E_{n\ell m} \longrightarrow E_n$$

TWO POV:

(1) $\nabla^2 \longrightarrow$ RADIAL ∇^2 + ANGULAR ∇^2

SOLN'S $Y_{\ell m}$'S

SEPARATE $\Rightarrow$ RADIAL EQN

(2) $$H = \frac{\vec{p}^{\,2}}{2m} + V(r)$$

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r)$$

SPHERICAL SYMMETRY $V(\vec{r}) = V(x,y,z) = V(r)$

$$H = \frac{\vec{p}^{\,2}}{2m} + V(r)$$

$$\frac{\vec{p}^{\,2}}{2m} = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2}$$

PRODUCT ANSATZ $\psi = R_{nl}\, Y_{lm}$

$$\left[\frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r)\right] R_{nl} Y_{lm} = E_n R_{nl} Y_{lm}$$

$$\left[\frac{p_r^2}{2m} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right] R_{nl} = E_n R_{nl}$$

ANGULAR MOMENTUM BARRIER REPULSIVE

ATTRACTIVE COULOMB POTENTIAL

SOLUTIONS TO THE RADIAL EQUATION

$$R_{nl}(r) \sim \left(\begin{matrix}\text{ASYMPTOTIC}\\ \text{FORM}\end{matrix}\right)\left(\begin{matrix}\text{LAGUERRE}\\ \text{POLYNOMIALS}\end{matrix}\right)$$

$\exp(-r/na_0)$
HYDROGEN

HYDROGEN-LIKE
$\exp(-Zr/na_0)$

SOLVE RADIAL EQN

TWO METHODS:

(1) DIFF EQN METHOD

FIND ASYMPTOTIC FORM

SEPARATE IT

DIFFERENTIAL EQN for each value of l

MAKE DIMENSIONLESS

ORDER ~~no.~~ HIGHEST DERIVATIVE FIRST

COEFF OF HIGHEST DERIVATIVE TERM = 1

FUTZ AROUND

DISCOVER RADIAL EQN IS EQUIVALENT TO

THE ASSOCIATED LAGUERRE EQN

DECLARE VICTORY

NORMALIZE WAVEFCNS

(2) USE LADDER OPERATORS

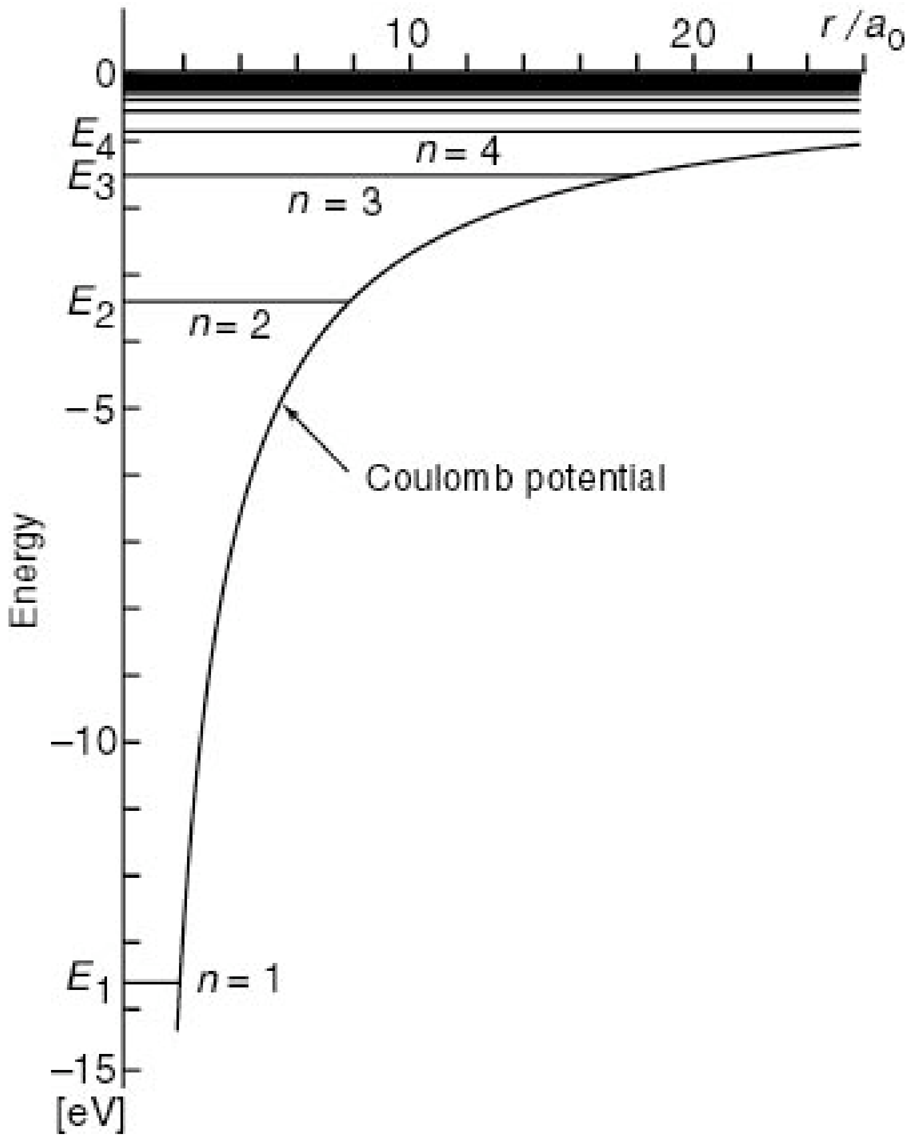
EIGENFCNS ⇒ ENERGY EIGEN FCNS

EIGENVALUES ⇒ EIGEN ENERGIES

$$E_n = \frac{-Ry}{n^2} = \frac{-13.6\ eV}{n^2} \qquad \text{HYDROGEN}$$

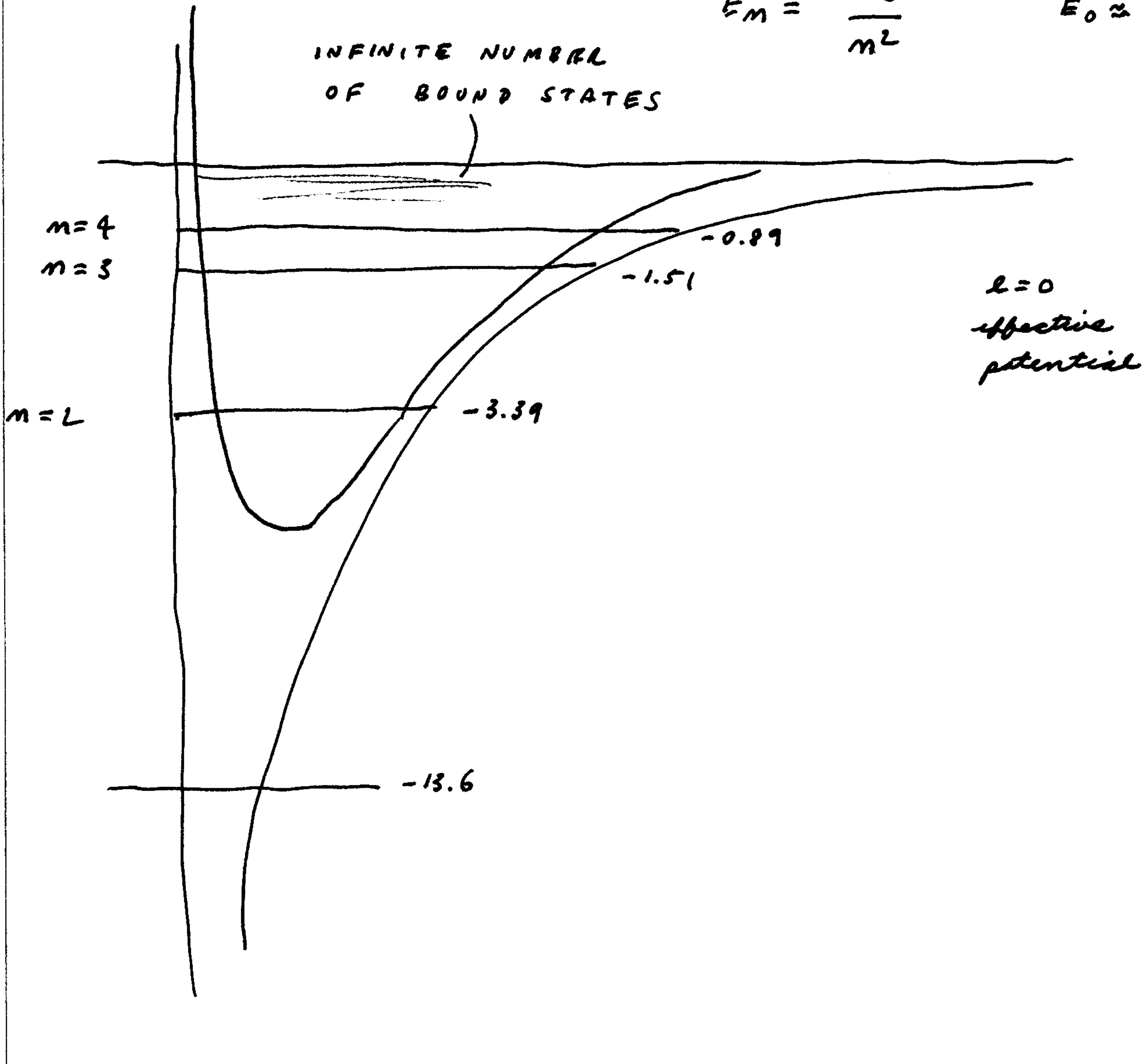
$$E_n' = -\frac{Z^2 Ry}{n^2} \qquad \text{HYDROGEN-LIKE}$$

Fig. (B)


10
20
r / a_0
0
E_4
$n = 4$
E_3
$n = 3$
E_2
$n = 2$
−5
Coulomb potential
Energy
−10
E_1
$n = 1$
−15
[eV]

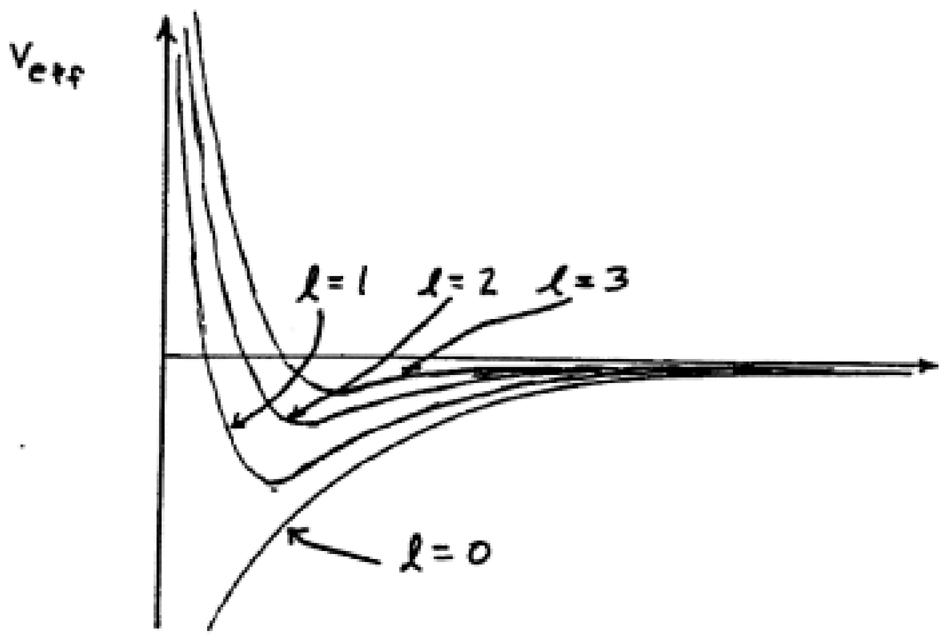
ENERGY DEGENERACY only n

$$E_n = \frac{E_0}{n^2} \qquad E_0 \approx -13.$$

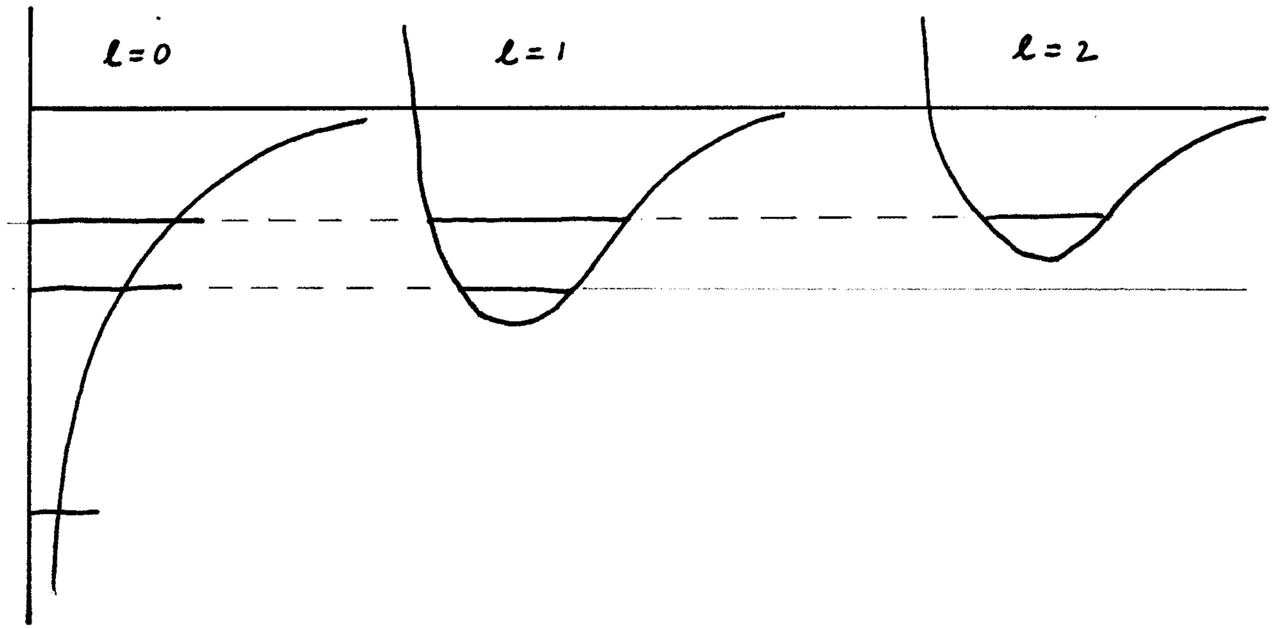


The Effective Potential Depends on the Angular Momentum

=> Series of Nested Wells



Series of States in each Well
Ground, 1st, 2nd, 3rd, ... excited



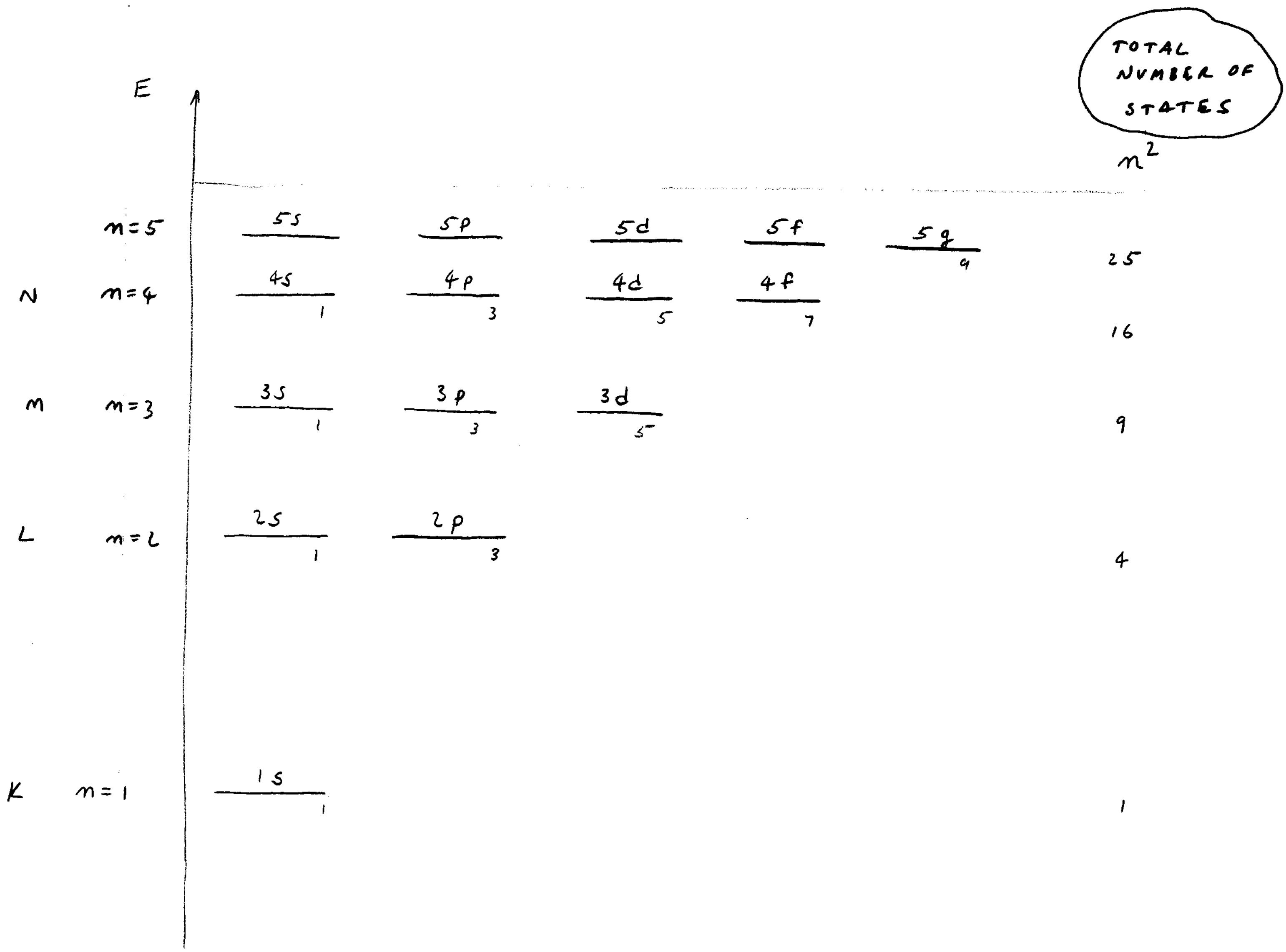
l=0
l=1
l=2

Energy
Degeneracy

for each n: $\ell = 0, 1, \ldots, n$

$$E_n = - Z^2 \frac{E_0}{n^2}$$

for each ℓ: $m = -\ell, \ldots, +\ell$



	$\ell=0$	$\ell=1$	$\ell=2$	$\ell=3$	$\ell=4$	
	s	p	d	f	g	h i j k
$(2\ell+1)$	1	3	5	7	9	

FIRST FEW RADIAL WAVEFUNCTIONS $\quad z = Z/a_0$

$n=1$

$$R_{10}(r) = 2\, z^{3/2}\, e^{-zr}$$

$n=2$

$$R_{20}(r) = \frac{1}{\sqrt{2}}\, z^{3/2} \left(1 - \tfrac{1}{2} z r\right) e^{-zr/2}$$

$$R_{21}(r) = \frac{1}{2\sqrt{6}}\, z^{5/2}\, (r)\, e^{-zr/2}$$

$n=3$

$$R_{30}(r) = \frac{2}{3\sqrt{3}}\, z^{3/2} \left(1 - \tfrac{2}{3} z r + \tfrac{2}{27} z^2 r^2\right) e^{-zr/3}$$

$$R_{31}(r) = \frac{8}{27\sqrt{6}}\, z^{5/2} \left(z r - \tfrac{1}{6} z^2 r^2\right) e^{-zr/3}$$

$$R_{32}(r) = \frac{4}{81\sqrt{30}}\, z^{7/2}\, (r^2)\, e^{-zr/3}$$

general form $\qquad$ $(\text{NORM})\,(\text{POLYNOMIAL})\, e^{-Zr/na_0}$

WHAT DO THE RADIAL WAVEFCNS LOOK LIKE?

" " " RADIAL PROB DISTS " " ?

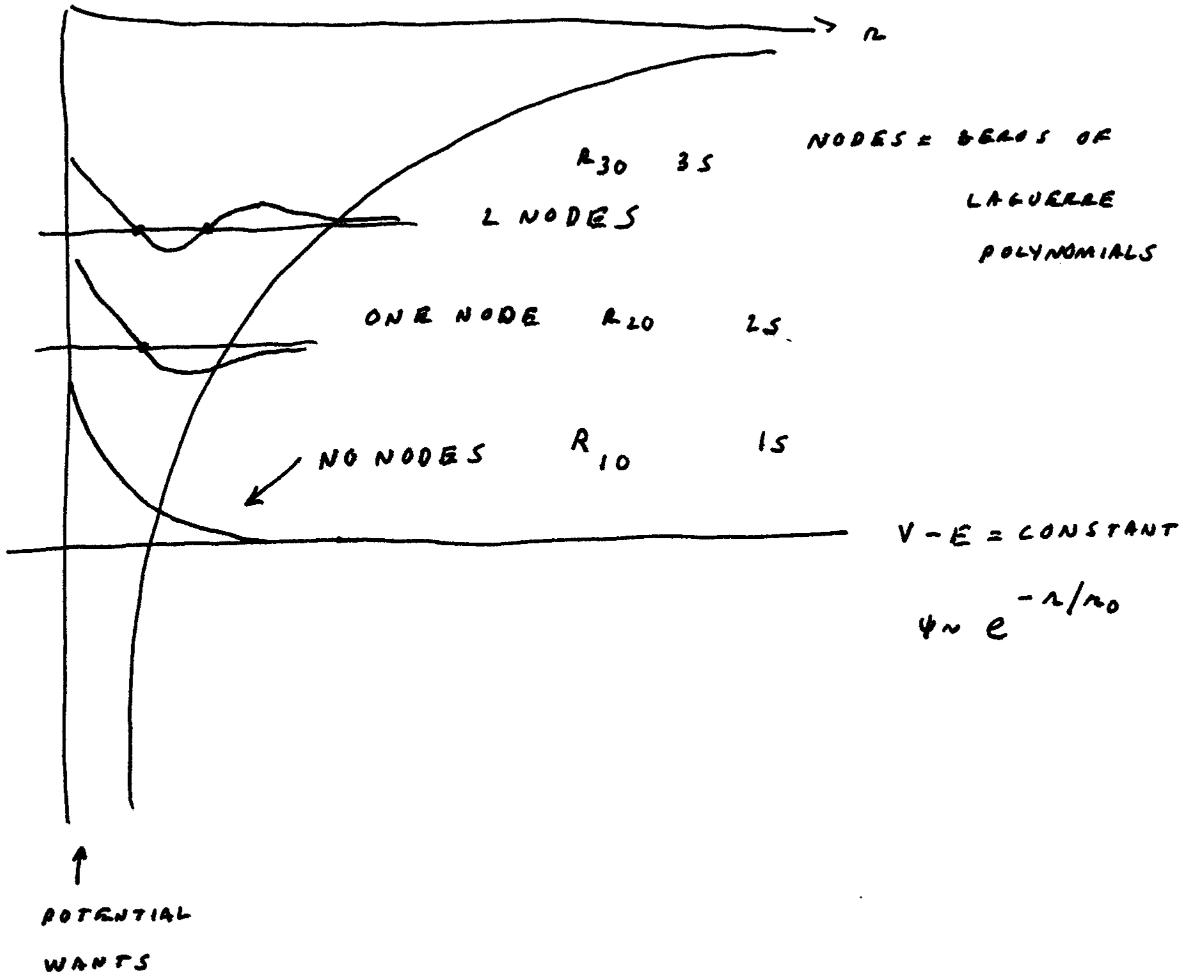
" " " 3d " " " " ?

1S 2S 3S 4S...

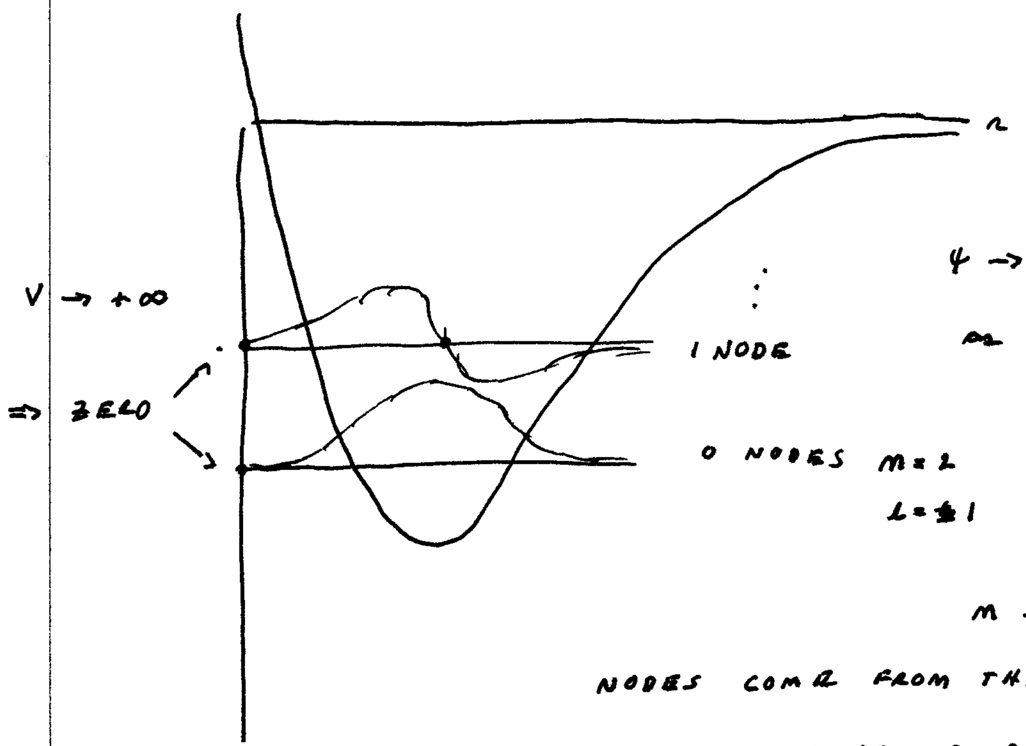
energy

$\ell = 0$ WAVE FCNS $\qquad R_{n\ell} \Rightarrow R_{n0}$'s $= nS$

$\ell = 0$
WELL



$\ell = 1$ WAVE FCNS



$\psi \to e^{-r/r_0}$

as $x \to \infty$

$n = 2$ R_{21}

$\ell = \cancel{2}\,1$

2p

3p

$n \to$ 4p $\leftarrow \ell$

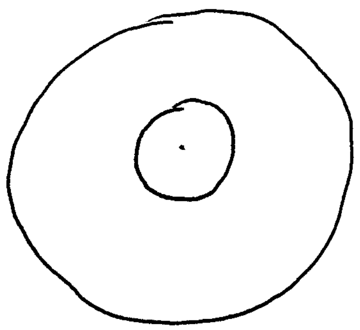
NODES COME FROM THE ZEROS OF THE LAGUERRE POLYNOMIALS

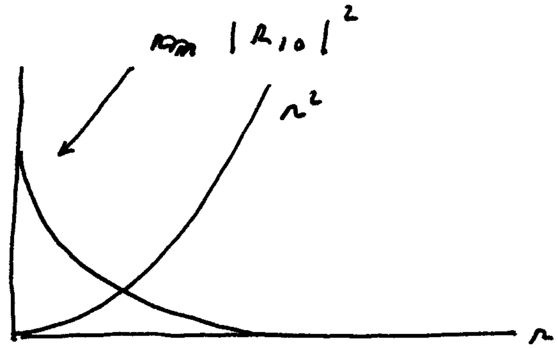
KNOW $R_{n\ell}$'s

FIND $P_{n\ell}$'s

$$P(x)\,dx = |\Psi(x)|^2\,dx$$

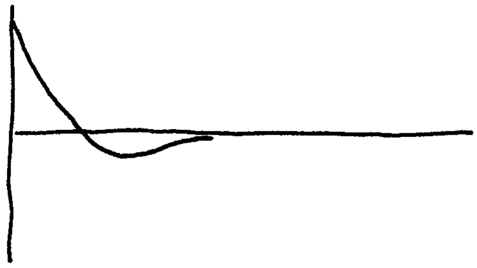
$$P_{n\ell}(r) = |R_{n\ell}(r)|^2\, r^2\, dr$$





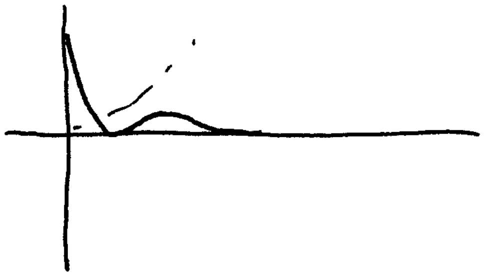
R_{nl}

R_{20}



$|R_{nl}|^2$

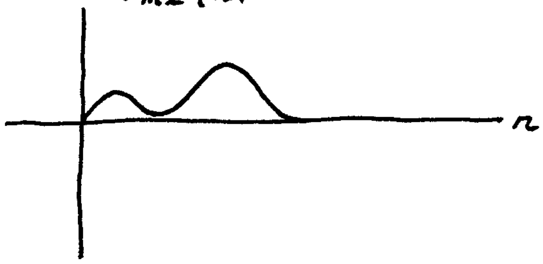
$|R_{20}|^2$



$r^2 |R_{20}|$

RADIAL PROB DIST

$P_{nl}(r)$



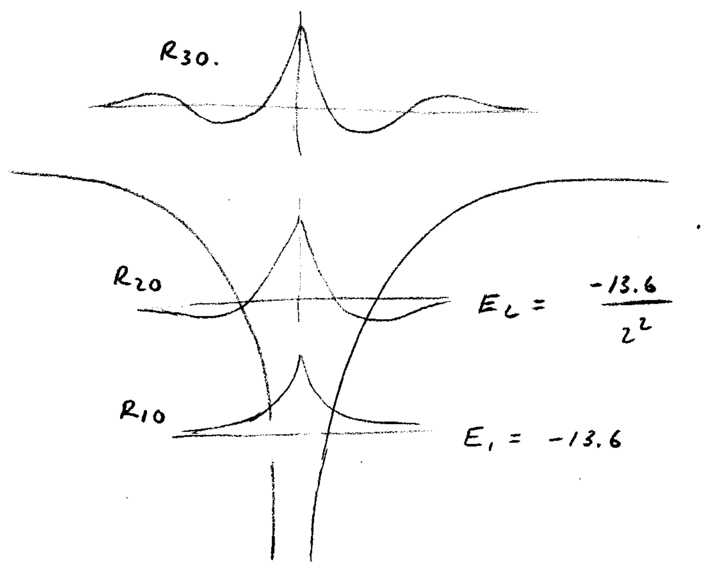
Probability distributions

$$P(\vec{r}) = |\psi_{n\ell m}(\vec{r})|^2 \, d^3r.$$

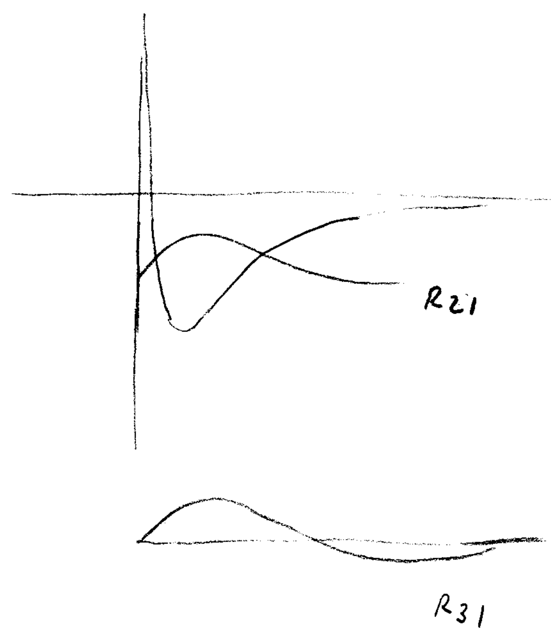
$$|R_{n\ell}(r)|^2 \, r^2 \, dr$$

$$|Y_{\ell m}(\theta, \varphi)|^2 \, d\Omega$$

$\ell = 0$



$\ell = 1$



p 142 pauling

p 266 Eisberg.

Angular dependence

$$|Y_{lm}(\theta,\varphi)|^2 = \Theta(\theta)\, e^{im\varphi}\, \Theta^*(\theta)\, e^{-im\varphi}$$

phase changes as you go around z axis but the prob does not change

$$|\Theta(\theta)|^2$$

Polar plot

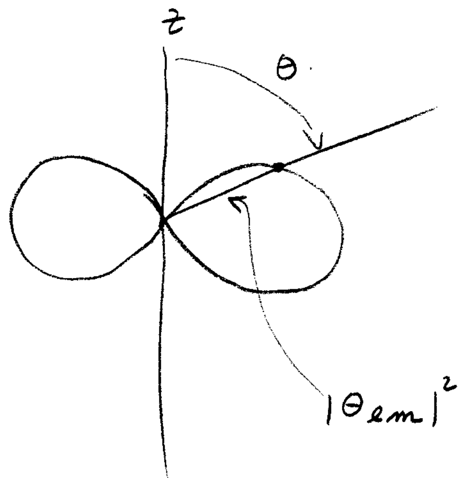
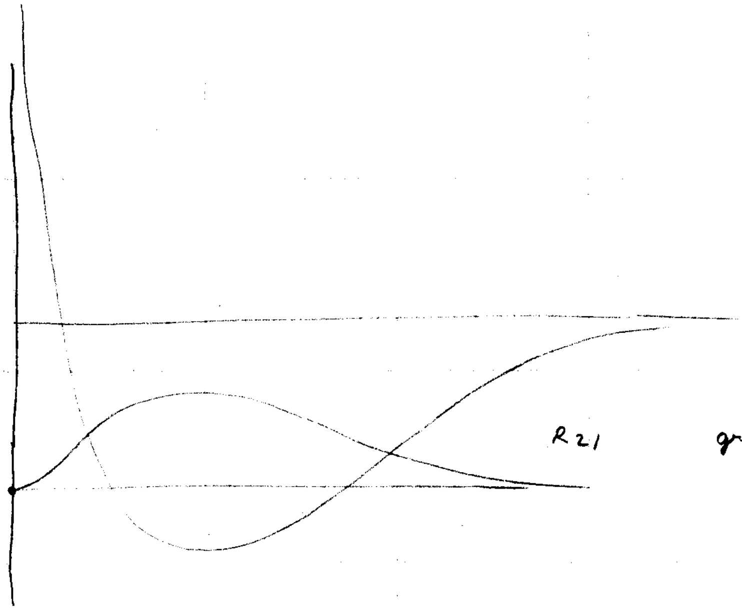


Figure of revolution around z axis

p 271 272 Eisberg

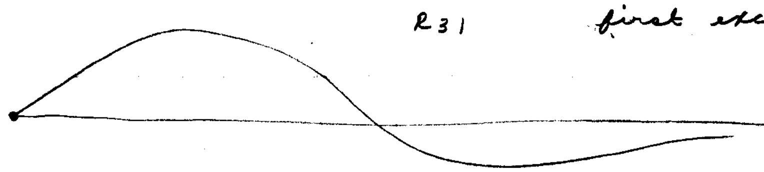
$l = 1$ well



ZERO AT ORIGIN

$V = \infty \Rightarrow$

R_{21} ground state of $l=1$ well

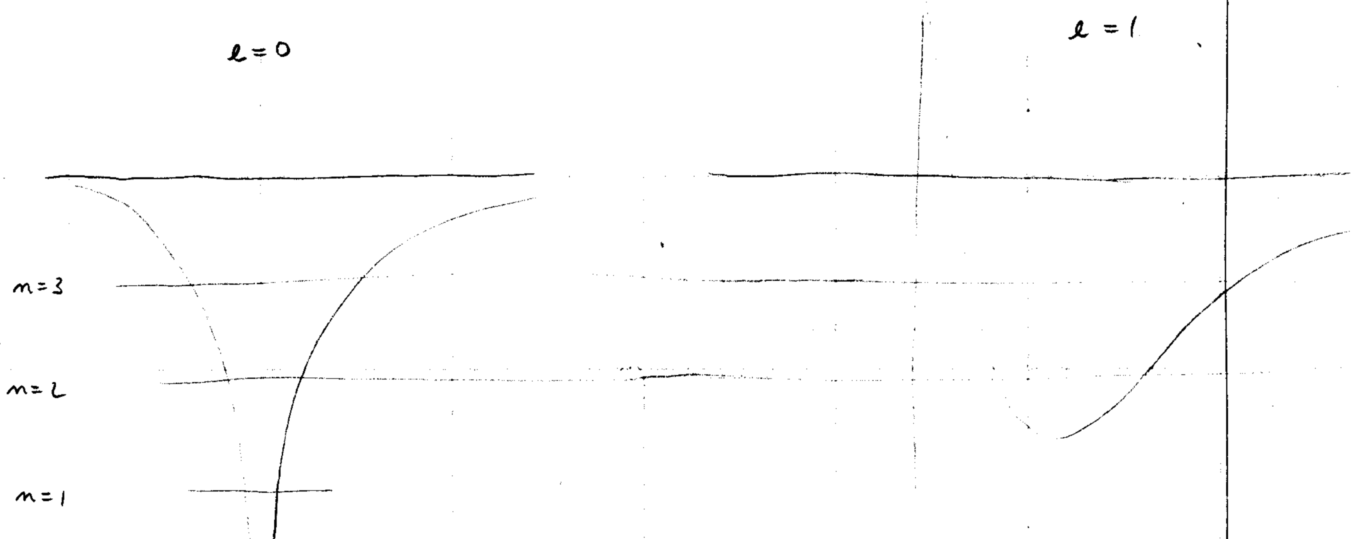


R_{31} first excited state of $l=1$ well.

degeneracy :

$l = 0$

$l = 1$



R_{20} has same energy as R_{21}

all R_{nl}'s have same energy.

$$R_{30} = \frac{2}{3\sqrt{3}} \, Z^{3/2} \left(1 - \tfrac{2}{3} Zr + \frac{2}{27} Z^2 r^2\right) e^{-Zr/3}$$

$$R_{31} = \frac{8}{27\sqrt{6}} \, Z^{3/2} \left(Zr - \frac{1}{6} Z^2 r^2\right) e^{-Zr/3}$$

$$R_{32} = \frac{4}{81\sqrt{30}} \, Z^{7/2} \, r^2 \, e^{-Zr/3}$$

$\vdots$

for each n: $\quad \ell = 0, \ldots, n-1$

$$e^{-Zr/n a_0}$$

$\ell = 1$