HYDROGEN PART ONE

So FAR, SINCLE PARTICLE WAVEFORS  

$$\begin{aligned}
\Psi(\vec{\lambda}, t) \\
\\
\text{HYOROGER ATOM HAS 2 PARTICLES} \\
\Psi(\vec{\lambda}, t) \\
\downarrow \\
\Psi($$

CAN DEMEABLIBE TO N PARTICLES  

$$\rightarrow 3N deque Af from this
Schrodinke de Regulation tose
$$H | \Psi \rangle = i \frac{1}{2} \frac{1}{4t} | \Psi \rangle$$

$$H = \frac{\vec{P}_{1}}{Lm} + \frac{\vec{P}_{1}}{2m} + \sqrt{(\vec{n}_{1},\vec{n}_{2})}$$

$$\left[ -\frac{\hbar^{L}}{2m} \frac{\vec{P}_{2}}{V_{1}} - \frac{\hbar^{L}}{2m} \frac{\vec{P}_{2}}{V_{2}} + \sqrt{(\vec{n}_{1},\vec{n}_{2})} \right] \Psi(\vec{n}_{1},\vec{n}_{2},t)$$

$$= i \frac{\hbar}{4t} \Psi(\vec{n}_{1},\vec{n}_{2},t)$$

$$= i \frac{\hbar}{4t} \Psi(\vec{n}_{1},\vec{n}_{2},t)$$

$$= 7 P DIMENSIONAL DIFF EQ$$

$$(3N+1) DIM$$

$$E DON'T WANT TO SECRE FOR 4d DIFF EQ!$$

$$BAEAK PROBLEM INTO PIECES...$$$$

$$\int_{a}^{a} \frac{d}{dt} \varphi(\vec{x}, \vec{z}, t) = f(\vec{z}, t) + g(\vec{z}, \vec{z}, t)$$

$$\begin{bmatrix} -\frac{\hbar^{2}}{2\mu} \quad \vec{\nabla}_{n}^{\perp} - \frac{\hbar^{2}}{2m} \quad \vec{\nabla}_{n}^{\perp} + v(\vec{z}) \end{bmatrix} \quad f \cdot g$$

$$= i \frac{\hbar}{dt} \quad (f \cdot g)$$

$$\frac{1}{f(\vec{x}, t)} \begin{bmatrix} -\frac{\hbar^{2}}{2\mu} \quad \vec{\nabla}_{n}^{\perp} + v(\vec{z}) - i \frac{\hbar}{dt} \quad \frac{d}{dt} \end{bmatrix} \quad g(\vec{z}, t)$$

$$\frac{1}{r \cdot g} \quad \vec{z}_{n}^{\perp} \quad (\vec{z}) \begin{bmatrix} \frac{\hbar^{2}}{2m} + i \frac{\hbar}{dt} \quad \frac{d}{dt} \end{bmatrix} \quad f(\vec{z}, t)$$

$$\frac{1}{r(\vec{z}, t)} \quad \begin{bmatrix} \frac{\hbar^{2}}{2m} + i \frac{\hbar}{dt} \quad \frac{d}{dt} \end{bmatrix} \quad f(\vec{z}, t)$$

$$\frac{1}{r(\vec{z}, t)} \quad \text{superstands only } \vec{z}_{n} t$$

$$\frac{1}{r(\vec{z}, t)} = p \text{ and supplified what can is at } \vec{z}$$

$$g(\vec{z}, t) = p \text{ and supplified what superstain is } \vec{z}$$

$$dt \quad \text{trive } t$$

$$servertag equations = td = \frac{3+1}{2+1} em \qquad gal$$

$$receal: \left[ -\frac{\hbar^{2}}{2m} -\frac{3}{2\mu^{2}} \right] f(\vec{z}_{1}t) = i \pm \frac{d}{4t} - f(\vec{z}_{1}t)$$

$$3d free particle$$

$$f(\vec{z}_{1}t) = e - i [\vec{p}^{2} \cdot \vec{z}^{2} - (r^{2}/2m) \cdot t)/\hbar$$

$$cm = i [\vec{p}^{2} \cdot \vec{z}^{2} - (r^{2}/2m) \cdot t)/\hbar$$

$$cm = i [\vec{p}^{2} \cdot \vec{z}^{2} - (r^{2}/2m) \cdot t)/\hbar$$

$$serve et = \frac{1}{2\mu} - \vec{\nabla}_{n} + v(\vec{n}) ] = i \pm \frac{d}{4t} = g(\vec{z}_{1}t)$$

$$serve et = rime = particle = \frac{1}{2\mu} - \vec{\nabla}_{n} + v(\vec{n}) = i \pm \frac{d}{4t} = g(\vec{z}_{1}t)$$

$$serve et = \frac{1}{2\mu} - \vec{\nabla}_{n} + v(\vec{n}) = rime = i \pm \frac{d}{4t} = g(\vec{z}_{1}t)$$

$$f(\vec{z}_{1}t) = -g(\vec{z}_{1}) + (t)$$

$$f(\vec{z}_{1}t) = -\frac{\pi^{2}}{2\mu} - \vec{\nabla}_{n} + v(\vec{n}) = i \pm \frac{d}{4t} = \frac{1}{2\mu} - \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} + \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} + \frac{\pi^{2}}{2\mu} + \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} + \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} + \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} + \frac{\pi^{2}}{2\mu} - \frac{\pi^{2}}{2\mu} -$$

SEPARATION CONSTANT En  
energy enjaceden = aparetic endent.  

$$\frac{1}{\Psi_{m}} \left[ -\frac{hL}{L_{m}} \vec{\nabla}_{n}^{L} + V(\vec{n}) \right] \Psi_{m}(\vec{n}) = E_{m}$$

$$E_{m} = \frac{1}{h(6)} \left[ i + \frac{dh}{dt} \right]$$

$$KPEPT \qquad \frac{dh}{dt} = -i - \frac{E_{m}}{\pi} + h$$

$$h(t) = e^{-iE_{m}t/\hbar}$$

$$\left[ -\frac{\hbar L}{L_{p}} \vec{\nabla}_{n}^{L} + V(\vec{n}) \right] \Psi_{m}(\vec{n}) = E_{m} \Psi_{m}(\vec{n})$$

$$3d \quad TISE \quad pn \quad relative \quad metrin$$

$$so, THE ANERGY \quad RIFANSTATES \quad ARE$$

$$\Psi_{m}(\vec{n}, \vec{k}, t) = -f(\vec{k}, t) = f(\vec{k}, t) = (F^{1}\cdot L^{-1}) - F^{1}\pi + F^{$$

Т

$$TISE = \left[ -\frac{\hbar^{2}}{2\mu} - \vec{\nabla}^{L} + v(\vec{x}) \right] \Psi_{m}(\vec{x}) = E_{m} \Psi_{m}(\vec{x})$$

$$SPECIAL CASE = 0 \quad V(\vec{x}) = V(x) = -\frac{cL}{n} + V PEOGRA = -\frac{bcL}{n} + V(x) = R(x) - L(0, 0)$$

$$\left[ -\frac{\hbar^{2}}{2\mu} - \vec{\nabla}^{L} + V(x) \right] R(x) - L(0, 0)$$

$$\left[ -\frac{\hbar^{2}}{2\mu} - \vec{\nabla}^{L} + V(x) \right] R(x) - L(0, 0)$$

$$= E_{m} R(x) - L(0, 0)$$

$$= -\frac{\hbar^{2}}{2\mu} \left[ -\frac{1}{n} - \frac{2L}{2\mu} - x + -\frac{L}{2\mu} \right] \left\{ -\frac{2L}{2\mu} + col(0, 0) + \frac{L}{2\mu} + \frac{L^{2}}{2\mu} \right\}$$

$$H = -\frac{\hbar^{2}}{2\mu^{n}} \frac{2L}{2\pi^{L}} + \frac{\tilde{L}^{2}}{2\mu^{nL}} + V(n)$$
  
roupled system of signequations  

$$H \mathcal{Q}_{m, \ell, m}(\vec{n}) = E_{m} \mathcal{Q}_{m, \ell, m}(\vec{n})$$

$$L^{L} \mathcal{Q}_{m, \ell, m}(\vec{n}) = \ell(\ell + i) \hbar^{L} \mathcal{Q}_{m, \ell, m}(\vec{n})$$

$$L^{L} \mathcal{Q}_{m, \ell, m}(\vec{n}) = m \hbar \mathcal{Q}_{m, \ell, m}(\vec{n})$$

$$We denote the L^{L}, L_{L} pullim$$

$$\mathcal{Q}_{m, \ell, m}(\vec{n}) = R_{m}(n) \mathcal{Y}_{\ell, m}(\theta, \varphi)$$

$$\left[ -\frac{\hbar L}{2\mu^{n}} \frac{2L}{2n^{L}} - \frac{e^{L}}{n} \right] R_{m} \mathcal{Y}_{\ell, m}$$

$$+ \left[ -\frac{L^{L}}{2\mu^{n}} \right] R_{m} \mathcal{Y}_{\ell, m} = E_{m} R_{m} \mathcal{Y}_{\ell, m}$$

$$\ell(\ell + 1) \hbar^{L}$$



Fig. (B)

ENERGY DEGENERACY only n



#### The Effective Potential Depends on the Angular Momentum

=> Series of Nested Wells



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

for each m: L=0,1,..., m

for each l; m=-l,...,+l

 $E_m = - z^2 \frac{E_0}{m^2}$ 

TOTAL NUMBER OF STATES

	E	1					NUMBER STATES m <sup>2</sup>	
Ν	m=5 m=4	<u>- 55</u> <u>- 45</u> 1	<u>5p</u> <u>4p</u> 3	<u>5d</u> <u>4d</u> 5	<u>5</u> f <u>4</u> f 7	<u>59</u> 9	2 5 <sup>-</sup> 1 6	
Μ	m = 3	3.5	<u>3 p</u> 3	<u>3d</u>			9	
L	m=L	25	<u>2p</u> 3				4	
K	m = 1	<u> </u>					I	
		L = 0	L = 1	<b>L=</b> 2	L= 3	<b>L =</b> 4		
		S	ρ	ø	f	۶	hijk	
	(2 L+1)	I	3	سى	7	9		

FEW 3= 2/an FIRST RADIAL WAVE FUNCTION S  $R_{10}(n) = 2 \frac{3}{2} e^{-3n}$ M = 1 $R_{20}(n) = \frac{1}{\sqrt{2}} \frac{3^{3/2}}{2} (1 - \frac{1}{2} \frac{3}{2} n) e^{-\frac{3}{2} n/2}$ M= 2  $R_{21}(n) = \frac{1}{2\sqrt{6}} \frac{3^{5/2}}{2}(n) e^{-\frac{3}{2}n/2}$  $R_{30}(n) = \frac{2}{3\sqrt{3}} \frac{3^{3}n}{2} \left(1 - \frac{2}{5} \frac{3}{7} n + \frac{2}{27} \frac{3^{2}n^{2}}{7} \right) e^{-\frac{3n}{3}}$ M=3 $R_{31}(n) = \frac{9}{27\sqrt{6}} \frac{3^{5}h}{3^{7}} \left(\frac{3n-\frac{1}{6}}{3^{2}n^{2}}\right) e^{-\frac{3n}{3}}$  $R_{32}(n) = \frac{4}{8!\sqrt{2n}} 3^{\frac{3}{2}} (n^2) e^{-\frac{3}{2}n/3}$ (NORM) (POLYNOMIAL) e Zr/mao general form RADIAL WAVEFONS LOOK LIKE? DO THE WHAT h 11 17 RADIAL PRUB DISTS " 12 7 /{ // 4/ 11 11 3d 4 7 11



Fig. 13.14. Radial eigenfunctions  $R_{n\ell}(\rho)$  for the electron in the hydrogen atom. Their zeros are the  $n - \ell - 1$  zeros of the Laguerre polynomials  $L_{n-\ell-1}^{2\ell+1}(2\rho/n)$ . Here the argument of the Laguerre polynomial is  $2\rho/n$  with n being the principal quantum number and  $\rho = r/a$  the distance between electron and nucleus divided by the Bohr radius a.

From The Picture Book of Quantum Mechanics, S. Brandt and H.D. Dahmen, 3<sup>rd</sup> ed., © 2001 by Springer-Verlag New York.

A hydrogen atom lost its electron and went to the police station to file a missing electron report. He was questioned by the police: "Haven't you just misplaced it somewhere? Are you sure that your electron is really lost?" *"I'm positive."* replied the atom.

### Probability Distribution for the 1s Wave Function



(a)

## Radial Probability Distribution



# **Probability Distribution**

- $\checkmark$  square of the wave function
- ✓ probability of finding an electron at a given position
- Radial probability distribution is the probability distribution in each spherical shell.

Two Representations of the Hydrogen 1s, 2s, and 3s Orbitals









Fig. 13.15. Radial eigenfunctions  $R_{n\ell}(r)$ , their squares  $R_{n\ell}^2(r)$ , and the functions  $r^2 R_{n\ell}^2(r)$  for the lowest eigenstates of the electron in the hydrogen atom and the lowest angular-momentum quantum numbers  $\ell = 0, 1, 2$ . Also shown are the energy eigenvalues as horizontal dashed lines, the form of the Coulomb potential V(r), and, for  $\ell \neq 0$ , the forms of the effective potential  $V_{\ell}^{\text{eff}}(r)$ . The eigenvalue spectra are degenerate for all  $\ell$  values, except that the minimum value of the principal quantum number is  $n = \ell + 1$ .

From The Picture Book of Quantum Mechanics, S. Brandt and H.D. Dahmen, 3rd ed., © 2001 by Springer-Verlag New York.

1s, 2s, 3s, 4s, 5s







### 3d, 4d, 5d





Fig. 13.15. Radial eigenfunctions  $R_{n\ell}(r)$ , their squares  $R_{n\ell}^2(r)$ , and the functions  $r^2 R_{n\ell}^2(r)$  for the lowest eigenstates of the electron in the hydrogen atom and the lowest angular-momentum quantum numbers  $\ell = 0, 1, 2$ . Also shown are the energy eigenvalues as horizontal dashed lines, the form of the Coulomb potential V(r), and, for  $\ell \neq 0$ , the forms of the effective potential  $V_{\ell}^{\text{eff}}(r)$ . The eigenvalue spectra are degenerate for all  $\ell$  values, except that the minimum value of the principal quantum number is  $n = \ell + 1$ .

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http://itl.chem.ufl.edu/4412\_aa/radwfct.html

START TO SOLVE

make equation dimensionless r -> p  $a_0 = \frac{hL}{mol} \qquad BOHR RADIUS = 0.52 Å$ length p= n/ao  $E_0 = \frac{k^2}{2ma^2} = 13.6 \text{ ev} \text{ RYDBERG}$ E > 12  $\lambda^2 = E_m/E_0$  $\frac{2ma_0^2}{\hbar^2} \left[ -\frac{\hbar^2}{2mn} \frac{2^2}{2n^2} + \frac{\hbar^2 \ell(\ell+1)}{2mn^2} - \frac{\ell^2}{n} \right] Rn\ell = E_m R_m \ell$  $n \neq - \frac{a_0^2}{n} \frac{\partial^2}{\partial n^2} n \neq \left(\frac{a_0^2}{n^2}\right) e(e+i) - \frac{2me^2}{t^2} \frac{a_0^2}{n} Rme = \lambda^2 Rme$  $-\frac{\partial^{2}}{\partial \left(\frac{n}{2}\right)^{2}} + \frac{\mathcal{L}(\mathcal{L}+i)}{\rho^{2}} - \left(\frac{2}{\alpha_{0}}\right)\left(\frac{\alpha_{0}^{2}}{n}\right)$ 2 S= r Kml

 $\left[\frac{\lambda^2}{dp^2} - \frac{\ell(\ell+1)}{p^2} + \frac{\ell}{p} - \lambda^2\right] S(p) = 0$ 



$$\frac{d}{d\rho} \left[ -\lambda e^{-\lambda\rho} Y + e^{-\lambda\rho} \frac{dY}{d\rho} \right]$$

$$+\lambda^{L} e^{-\lambda\rho} Y - \lambda e^{-\lambda\rho} \frac{dY}{d\rho} - \lambda e^{-\lambda\rho} \frac{dY}{d\rho} + e^{-\lambda\rho} \frac{d^{L}Y}{d\rho^{L}}$$

$$-2\lambda \dots$$

$$e^{-\lambda\rho} \left[ \frac{dL}{d\rho^{L}} - 2\lambda \frac{d}{d\rho} + \lambda^{L} - \frac{2(L+i)}{\rho^{L}} + \frac{2}{\rho} - \lambda^{L} \right] Y(\rho) = 0$$
went to aster this squation and stat  $\Psi(n) \rightarrow 0$  to  $n \rightarrow 0$ 

$$V(\rho) = \rho^{m} \sum_{m=0}^{\infty} Cm \rho^{m} = \sum_{m=0}^{\infty} Cm \rho^{m+m}$$

$$\int_{m=0}^{\infty} m^{m} \sum_{m=0}^{\infty} Cm \rho^{m+m} = \sum_{m=0}^{\infty} Cm \rho^{m+m}$$

$$\frac{d}{d\rho} = \frac{d}{d\rho} \left[ \sum Cm \rho^{m+m} \right] = \sum_{m=0}^{\infty} (m+m) Cm \rho^{(m+m-i)}$$

$$\frac{d^{L}Y}{d\rho^{L}} = \frac{d}{d\rho} \left[ \sum (m+m) Cm \rho^{(m+m-i)} \right] = \sum_{m=0}^{\infty} (m+m) (m+m-i) Cm \rho^{m+m-L}$$

lowest power of p in (m-2) TH. (pl+m)(pl+m-1) Cop<sup>m-2</sup> -  $\frac{2(2+1)}{p^2}$  Cop<sup>m</sup>  $[m(m-1) - l(l+1)] c_0 = 0 = m = l+1$ m = -lcoefficient of the (m+m-2) TH TERM  $\sum_{m=0}^{\infty} (m+m)(m+m-1) Cm \rho = 2\lambda(m+m) Cm \rho$  $+ \frac{2}{p!} c_m p^{(m+m)-1} - \frac{L(L+1)!}{p!!} c_m p^{(m+m)-2}$ = 0  $[(m+m)(m+m-1) - l(l+1)] Cm + [-2\lambda (m-1+m) + 2] Cm-1 = 0$  $\int (m+\ell+1) (m+\ell) - \ell(\ell+1) \int Cm = 2 [(m+\ell)\lambda - 1] Cm-1$  $m \left[ m + 2k + i \right] Cm = 2 \left[ (m + 2)\lambda - i \right] Cm - i$ special values of A terminale  $C_{m} = \frac{2\left[\left(m+2\right)\lambda - i\right]}{n\left[m+2k+i\right]} C_{m-1}$ series TWO CONPITIONS 12 1) POLYNOMIAL STARTS WITH P finite 410) POLYNOMIAL STOPS WITH P M+R finite energy 2)

l= m-1

$$Lignereques$$

$$L_{m} = \frac{2 \left[ \left( m + 2 \right) \lambda - 1 \right]}{m \left( m + 2 \lambda + 1 \right)} Cm - 1$$

$$(m + 2) \lambda - 1 = 0$$

$$\lambda = \left( \frac{1}{m + 2} \right) = \frac{1}{14^{2} + 2^{2}}$$

$$mangy \qquad \lambda^{2} = \frac{E_{m}}{E_{0}}$$

$$Em = \frac{1}{14^{2} + 2^{2}} E_{0}$$

$$\frac{Em = \frac{1}{m^{2}} E_{0}}{\left[ \frac{Em}{2m} - \frac{1}{m^{2}} \frac{E_{0}}{2m} \right]}$$

$$W_{m,2,m} (\lambda^{2}) = R_{m,2} (\lambda_{1}) Y_{2,m} (\theta, \theta) = \frac{e^{-\lambda \beta}}{\epsilon_{0} \beta} Y_{m,2} (\beta) Y_{2,m} (\theta, \theta)$$

$$= N = e^{-\beta Im} \left[ \frac{Y_{m,2} (\beta)}{\beta} \right] Y_{2,m} (\theta, \theta)$$

$$Y = pine form E \dots m$$

$$[] = que form E - 1 \dots m - 1$$

Probability distribution  

$$P(\vec{x}) = | \Psi_{mem}(\vec{x}) |^{2} d^{3}n.$$

$$|R_{me}(n)|^{2} n^{2} dn$$

$$|Y_{em}(\theta, \varphi)|^{2} dn.$$

$$E_{L} = -\frac{H.C}{2^{2}}$$

$$R_{10} \qquad E_{L} = -\frac{H.C}{2^{2}}$$

$$E_{1} = -H.C$$

$$E_{1} = -H.C$$

$$R_{21} \qquad p \ 142 \ panking$$

$$p \ 266 \ Eisting.$$

$$R_{21}$$

: Angulor dependence

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

phase changes so you go sound 2 spice but the prob does not change 10(0)<sup>2</sup>

Polar plat



Figure of revolution

around & apic

p 271 272 Eisberg



$$R_{30} = \frac{1}{2\sqrt{27}} 3^{1/2} \left(1 - \frac{1}{2} 3^{2} + \frac{1}{27} 3^{1} n^{2}\right) e^{-\frac{3}{2} n/3}$$

$$R_{31} = \frac{9}{27\sqrt{67}} 3^{3/2} \left(\frac{3}{2} - \frac{1}{6} 3^{2} n^{1}\right) e^{-\frac{3}{2} n/3}$$

$$R_{32} = \frac{4}{91\sqrt{767}} 3^{3/2} n^{2} e^{-\frac{3}{2} n/3}$$

$$R_{32} = \frac{4}{91\sqrt{767}} 3^{3/2} n^{2} e^{-\frac{3}{2} n/3}$$

$$R_{32} = \frac{4}{91\sqrt{767}} 3^{3/2} n^{2} e^{-\frac{3}{2} n/3}$$

$$R_{33} = \frac{2}{2} n/3 e^{-\frac{3}{2} n/3}$$

$$R_{33} = \frac{4}{91\sqrt{767}} 3^{3/2} n^{2} n^{2} e^{-\frac{3}{2} n/3}$$

$$R_{33} = \frac{4}{91\sqrt{767}} n^{2} n^{2} e^{-\frac{3}{2} n/3}$$

$$R_{33} = \frac{4}{91\sqrt{767}} n^{2} e^{-\frac{3}{2} n/3}$$

$$R_{33} = \frac{4}{91\sqrt{767}} n^{2} e^{-\frac{3}{2} n/3}$$