QM 4/13/15 (MATT)

1. GENERAL SCHRÖDINGER EQN. FOR SPHERICALLY SYMMETRIC POTENTIALS

- $$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(r)\,\psi(\vec{r}) = E\,\psi(\vec{r})$$

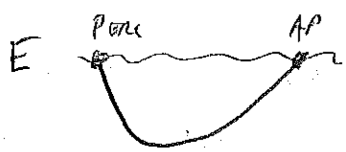
- DO SEPARATION OF VARIABLES, $\psi(\vec{r}) = R(r)\cdot Y(\theta,\phi)$
  FIND SPHERICAL HARMONICS SOLUTIONS,
  WITH $L^2 = \hbar^2 \cdot \ell(\ell+1)$

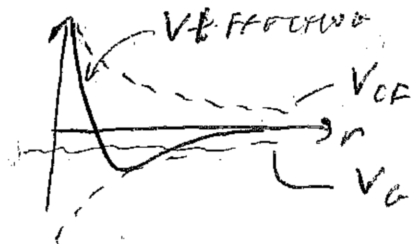
- GIVES RADIAL EQN.
$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + V(r)\,R(r) + \frac{\hbar^2\,\ell(\ell+1)}{2mr^2}R = ER$$

2. CONCEPTUALLY, $\frac{\hbar^2\ell(\ell+1)}{2mr^2}$ IS "CENTRIFUGAL BARRIER".
   FOR LARGE ℓ, IT IS HARDER FOR A PARTICLE TO HAVE A SMALL RADIUS.

- $V(r) + \frac{\hbar^2\,\ell(\ell+1)}{2mr^2}$ IS "EFFECTIVE POTENTIAL".

  e.g. WITH PLANETS,





FOR A GIVEN ENERGY, PERIHELION AND APHELION FOR $\dot{r} = 0$
($KE_{RADIAL} = 0$, ONLY $KE_{ROTATIONAL}$)

3. ODE IS EASIER TO SOLVE USING $u \equiv r\cdot R$.
- SO $R = \frac{1}{r}u$, $R' = \frac{1}{r}u' - \frac{1}{r^2}u$

$$r^2R' = (ru' - u)$$
$$(r^2R')' = u' + ru'' - u' = ru''$$

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

4. MUCH OF QM IS SOLVING THIS EQUATION FOR DIFFERENT CHOICES OF $V(r)$, ANALOGOUS TO WHAT YOU DID IN 1-DIMENSION
   - 3-D WELL
   - 3-D HARMONIC OSCILLATOR
   - 3-D H-ATOM

   } EMILY'S SPROJ (for the first two)

5. 3-D SPHERICAL WELL $V(r) = \begin{cases} 0 & r<a \\ \infty & r>a \end{cases}$

$$\frac{d^2u}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2\right]u$$

- For $l=0$, $u = \sin/\cos(kr)$
- For $l>0$, u MORE COMPLICATED BUT SIMILAR (BESSEL)

AS ALWAYS IN QM, QUANTIZATION COMES FROM APPLYING THE BOUNDARY CONDITIONS, IN THIS CASE THAT $u(ka)=0$.

$u(ka)=0$ MEANS ka IS A ZERO OF THE BESSEL FN. (FIGURE 4.2)
THIS DETERMINES k, AND $\boxed{\frac{\hbar^2 k^2}{2m} = E}$

GET QUANTIZED ENERGIES.

6. YOU CAN EXTEND TO FINITE WELL, SOLVE IT NUMERICALLY (EMILY AGAIN)

7. H-ATOM: FUNDAMENTAL TEST CASE FOR QM

8. ON WEDNESDAY, MAYA WILL DISCUSS THE OBSERVED LINE SPECTRA

$$\frac{1}{\lambda} = R\left[\frac{1}{n^2} - \frac{1}{n'^2}\right] \qquad R = 0.01097\ nm^{-1}$$

(RYDBERG)

9. WHAT NEEDS TO BE EXPLAINED BY A THEORY:

1. WHY DOESN'T H-ATOM ALWAYS RADIATE
2. WHAT IS THE PROCESS OF EMISSION OR ABSORPTION OF LIGHT?
3. WHY THESE PARTICULAR λ'S AND ONLY THESE?

10. 3 LEVELS OF 'ANSWERS'; SOME SIMILARITIES.

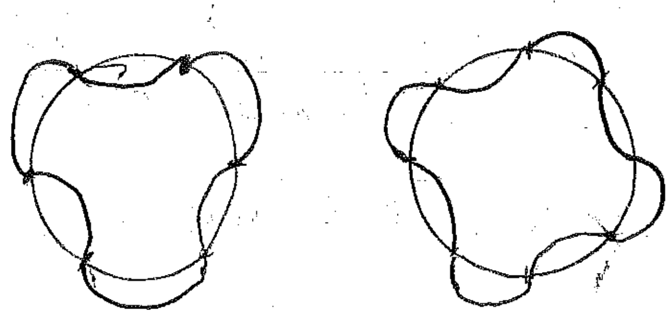
11. BOHR: (1): THERE ARE STABLE ORBITS WHEN $L = n\hbar$ (TALK THROUGH DERIVATION ON HANDOUT)

(2) ELECTRON TRANSITION $E_\gamma = \Delta E_e = |E_n - E_{n'}|$

(3) DERIVATION GIVES RYDBERG FORMULA FROM $\frac{1}{\lambda} = \frac{E_\gamma}{hc}$

12. DEBROGLIE: (1) STABLE ORBITS ARE DUE TO STANDING WAVES.

(2), (3) SAME ANSWER AS BOHR.



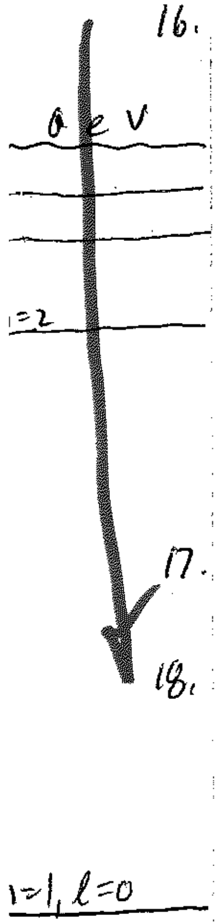
13. QM: ① WHEN A SYSTEM IS IN AN ENERGY EIGENSTATE, IT DOES NOT LOSE ENERGY
② SAME ANSWER AS BOHR AND DeBROGLIE
③ SOLVE SCHRÖDINGER EQN. FOR EIGENSTATES

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

14. FINDING POLYNOMIAL SOLUTIONS (SHEET $\boxed{3}$)

15. LAGUERRE POLYNOMIALS IN CONTEXT OF EARLIER SOLUTION SETS
- SIN/COS IN 1-D SQ. WELL
- HERMITE POLYS IN 1-D HARMONIC OSCILLATOR
- BESSEL FNS IN 3-D SPHERICAL WELL

DIDN'T GET TO THIS



16. COMPLETE SOLUTIONS

$n = 1, 2, 3, \ldots$

$l = n, n+1, n+2, \ldots$

$m = -l, -l+1, \ldots, 0, \ldots, l-1, l$

E_n	n, l, m	d
-0.85 eV	4s, 4p, 4d, 4f	(16)
-1.51 eV	3s, 3p, 3d	(9)
-3.40 eV	2s, 2p	(4)
-13.6 eV	1s	(1)

$$\psi_{nlm}(r,\theta,\phi) = \left[\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)^3}\right]^{1/2} e^{-r/na} \cdot \left(\frac{2r}{na}\right)^l \cdot L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right) \cdot Y_l^m(\theta,\phi)$$

17. QUALITATIVE DISCUSSION OF WAVE FNS.

18. NOTICE: $E(n)$ ONLY, NOT l OR m.
- SPHERICAL SYMMETRY ⇒ m-DEGENERACY
- MORE SUBTLE SYMMETRY ⇒ l-DEGENERACY.

HYDROGEN ATOM - POLYNOMIAL SOLN

1. SPH. SYM. POT $\Rightarrow$ $u(r) \equiv r \cdot R(r)$

SPH. HARM $\Rightarrow$ $V_L = \dfrac{\hbar^2 \ell(\ell+1)}{2mr^2}$ CONTRIBUTION TO EFFEC. POT.

H-ATOM $$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-k_e\frac{1}{r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]u = Eu \qquad \underline{E<0}$$

2. $\dfrac{\hbar^2}{2m}$ HAS UNITS $E \cdot L^2$, SO DEFINE A ~~CHARACTERISTIC~~ LENGTH $1/K$

$$K^2 \equiv \frac{-E}{\frac{\hbar^2}{2m}} \Rightarrow K \equiv \frac{\sqrt{-2mE}}{\hbar} \qquad \left[= \frac{1}{a_0},\ \text{IT WILL TURN OUT}\right]$$

$$\therefore \frac{1}{K^2}\frac{d^2u}{dr^2} = \left[1 - \frac{2mk_e}{\hbar^2 K}\left(\frac{1}{Kr}\right) + \frac{\ell(\ell+1)}{(Kr)}\right]u$$

3. DEFINE DIM. LESS RADIUS VARIABLE: $\rho \equiv Kr$

FOR P.E. TERM: $\rho_0 = \dfrac{2mk_e}{\hbar^2 K}$ MAGIC

$$u'' = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right]u$$

4. COULD JUST TRY $u = \sum a_n \rho^n$, BUT NOT CLEANEST (IT TURNS OUT)

- $\rho \gg 1, \rho_0$ $\quad u'' \approx u$

$$u = Ae^{-\rho} + Be^{+\rho} \qquad BC \Rightarrow B=0.$$

- $\rho \to 0$, $\quad u'' \approx \dfrac{\ell(\ell+1)}{\rho^2}u$

$$u = \rho^\alpha \Rightarrow \alpha(\alpha+1) = \ell(\ell+1)$$

$\therefore \alpha = -\ell$ OR $\alpha = +(\ell+1)$

BC $\Rightarrow$ ONLY $(\ell+1)$

$$\therefore u(\rho) = \rho^{\ell+1} e^{-\rho} \cdot v(\rho)$$

SOLVE FOR THIS $v(\rho)$

5. $\rho v'' + 2(\ell+1-\rho)v' + [\rho_0 - 2(\ell+1)]v = 0$

TRY $v(\rho) = \sum_0 a_j \rho^j$

$$v' = \sum (j+1) a_{j+1} \rho^j \qquad \rho v' = \sum j a_j \rho^j$$

$$\rho v'' = \sum j(j+1) a_{j+1} \rho^j$$

ρ^j: $j(j+1) a_{j+1} + 2(\ell+1)(j+1) a_{j+1} - 2j a_j + [\rho_0 - 2(\ell+1)] a_j = 0$

$$a_{j+1} = \left[\frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)}\right] a_j$$

RECURSION RELN.

6. IF $j \gg \ell$, $a_{j+1} \sim \frac{2j}{j^2} \Rightarrow v \sim e^{2\rho}$

BUT THEN $u = A\rho^{\ell+1} e^{+\rho}$ DIVERGES.

DIDN'T GET TO THIS

SO SERIES HAS TO TERMINATE

FOR SOME j, $2(j+\ell+1) - \rho_0 = 0$.

DEFINE $n = j_{max} + \ell + 1$, $\rho_0 = 2n$ $\boxed{\ell \geq n-1}$

$$E_n = -\frac{\hbar^2 k^2}{2m} = -\frac{1}{2}(mc^2)\left(\frac{ke}{\hbar c}\right)^2 \cdot \frac{1}{n^2}$$

$$= -13.6\,\text{eV} \cdot \frac{1}{n^2}$$

$E = \frac{1}{2} PE$ $\therefore -\frac{1}{2}\frac{ke}{r_0} = -13.6\,\text{eV} \Rightarrow r_0 = a_0$

7. DISCUSS DIFF

PASSED OUT
AND SKIMMED
THROUGH IT

Bohr Atom "Derivation"

Classical Circular Orbits

$$\frac{k_e}{r^2} = \frac{mv^2}{r} \qquad \left(\text{with } k_e \equiv \frac{e^2}{4\pi\varepsilon_0}\right)$$ Centripetal Force for a Circular Orbit

$$\frac{k_e}{r} = mv^2$$

$$E = \left(\tfrac{1}{2}mv^2 - \frac{k_e}{r}\right) = \left(-\tfrac{1}{2}mv^2\right) = \left(-\tfrac{1}{2}\frac{k_e}{r}\right)$$ Total Energy = Kinetic + Potential

$$|\vec{L}| = |\vec{r}\times\vec{p}| = rmv$$ Angular Momentum for Circular Orbit

$$E = \left(-\frac{L^2}{2mr^2}\right) = \left(-\tfrac{1}{2}\frac{k_e}{r}\right)$$

Bohr Quantization

$$L_n = n\hbar$$ Bohr's Quantization Condition

$$\frac{k_e}{r_n} = \frac{(n\hbar)^2}{mr_n^2}$$

$$r_n = \left(\frac{\hbar^2}{k_e m}\right) n^2 = a\,n^2$$ Quantized Orbital Radii

$$E_n = \left(-\tfrac{1}{2}\frac{k_e}{r_n}\right) = -E_1\frac{1}{n^2}$$ Quantized Energy Levels

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Numerical Values

Useful Constants: $\boxed{\hbar c = 197.37 \text{ eV}\cdot\text{nm} \qquad mc^2 = 511{,}000 \text{ eV} \qquad \frac{k_e}{\hbar c} = \frac{1}{137.04}}$

Bohr Radius: $$a \equiv \left(\frac{\hbar^2}{k_e m}\right) = (\hbar c)\left(\frac{\hbar c}{k_e}\right)\left(\frac{1}{mc^2}\right) = 0.0529 \text{ nm}$$

Lowest Energy: $$E_1 \equiv \tfrac{1}{2}\frac{k_e}{a} = \tfrac{1}{2}\frac{k_e^2 m}{\hbar^2} = \tfrac{1}{2}\left(\frac{k_e}{\hbar c}\right)^2 (mc^2) = 13.6 \text{ eV}$$