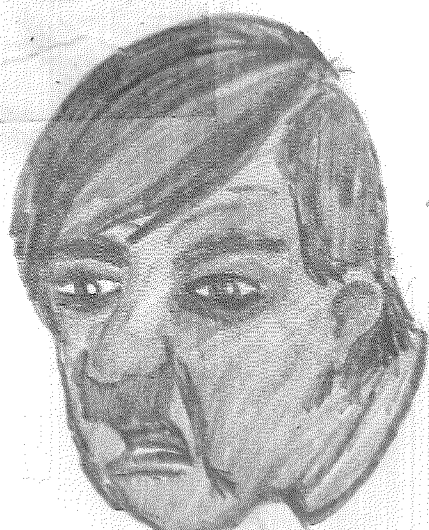
Quantum Mechanics

Indiana University

R.J. Marks II Class Notes

(1975)



VEN I VAS A
BOI IN GEMANY,
DEY SAW ME ON
DA STREET STANDING
UND SACH "VY ARE U
LOOKING DA VAY U R
LOOKING UND VIE R
U ACKTING DA VAY U
R ACTING UND ICH
SAGA ICH NICHT
DEUTCH GESPRECHEN
ABER DU BIST EINER
GRÖSSER GANOSE
GERSNÖTEN UND SIE
MACHT MIR STARB.
UND ICH WAR IN
MEINER HEAD
GESTARBEN

QUANTUM MECHANICS

Syllabus: Physics 6[illegible]1

Quantum Mechanics

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Spring, 1975

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I. INTRODUCTION

A. SCHRÖDINGER'S EQ'N FOR ONE PARTICLE

1. $H = \frac{p^2}{2m} + V(r)$: HAMILTONIAN OPERATOR
2. $p = \frac{\hbar}{i}\nabla$: MOMENTUM OPERATOR
3. $H\,\phi_n(x) = E_n\,\phi_n(x)$: EIGENVALUE PROBLEM

   a. EIGEN FUNCTION PROPERTIES
   - $\int_{-\infty}^{\infty} \phi_n \phi_m^* d^3r = \delta_{mn}$: ORTHOGONALITY
   - $\sum_n \phi_n^*(r)\phi_m(r')\,d^3r = \delta(r-r')$: COMPLETENESS

   b. ORTHONORMAL EXPANSIONS
   - $\psi(x) = \sum_n a_n \phi_n(x)$
   - $a_n = \int_{-\infty}^{\infty} \psi(x)\phi_n(x)$
   - $\sum_n |a_n|^2 = 1$

   c. $\psi(r,t) = \sum_n a_n \phi_n(x) e^{-itE_n/\hbar}$: WAVE FUNCTION

   d. $|\psi(r,t)|^2 = \rho(r)$: PROBABILITY DENSITY FUNCTION

   e. STATISTICAL INTERPRETATION
   - $a_n = e^{-E_n/kT} / \sum_n e^{-E_n/kT}$

C. EXPECTATION VALUES

1. $\langle F(r,t)\rangle = \int d^3r\; F(r)\rho(r,t)$: OF A FUNCTION

   a. $\langle r(t)\rangle = \int d^3r\; r\,\rho(r,t)$

   b. $\langle V(r)\rangle = \int d^3r\; V(r)\rho(r,t)$

   c. $\frac{\delta}{\delta t}\langle r\rangle = \frac{\langle p\rangle}{m}$ (Pg. 3)

2. $\langle O(r)\rangle = \int dr^3\; \psi^*(r,t)\,O(r)\,\psi(r,t)$: OF AN OPERATOR

   a. $\frac{\delta}{\delta t}\langle O\rangle = \frac{i}{\hbar}\langle [H,O]\rangle$ (Pg. 4)

D. REPRESENTATIONS

1. OF OPERATORS A & B

a. $[A,B] \triangleq AB - AB = -[B,A]$: COMMUTOR

- IF $[A,B]=0$, OPERATORS COMMUTE (MAY USE SAME EIGENFUNCTIONS) (Pg 9)
- $[x, p_x] = [x, \frac{\hbar}{i}\frac{d}{dx}] = i\hbar$; $[p_x, H] = 0$ (Pg 5)

b. $\{A,B\} = AB + BA$; ANTI-COMMUTOR

2. MATRIX REPRESENTATION

a. $\langle n | f(x) | \ell \rangle \triangleq \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\, f(x)\, \phi_\ell(x)$

b. $\langle n | \ell \rangle = \delta_{nm}$ c. $|n\rangle = \psi_n$

c. HERMITIAN CONJUGATE:

$(AB)^+ = B^* A^*$

$\langle n | f | \ell \rangle^+ = \langle \ell | f^+ | m \rangle$; $a|m\rangle^+ = \langle m | a^+$

d. $\langle n | f g | \ell \rangle = [\langle n | f][g | \ell \rangle]$

E. PLANE WAVE STATES

FOR $V=0$: $H = \frac{p^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2$

$\Rightarrow \underline{\psi}(x) = e^{i\vec{k}\cdot\vec{r}}$

$k = (k_x, k_y, k_z)$; $r = (x, y, z)$

$E = \hbar^2 k / 2m$

F. CURRENT OPERATOR: CONTINUITY

$\frac{\delta \rho}{\delta t} + \nabla \cdot J = 0$; EQUATION OF CONTINUITY

$J = \frac{\hbar}{2mi}[\psi^* \nabla \psi - \psi \nabla \psi^*]$: CURRENT OPERATOR (Pg 3)

G. MISC.

1. ANGULAR MOMENTUM OPERATOR

$L_z = x p_y - y p_x$; $L_x = y p_z - z p_y$; $L_z = x p_z - z p_y$

$[p^2, L] = [p_x^2, L_z] + [p_y^2, L_z] + [p_z^2, L_z] = 0$ (pg 5)

2. FEYMAN'S THEM. (Pg 12)

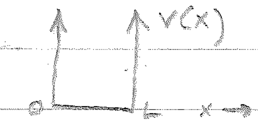
a. $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$, WHERE A & B ARE OPERATRS.

AND $[F,A] = [F,B] = 0$ WHERE $F = [A,B]$

b. $e^L a e^{-L} = a + [L,a] + \frac{1}{2!}[L,[L,a]] + \frac{1}{3!}[L[L[L,a]]] + \ldots$

II. ONE DIMENSIONAL SOLUTION TO SCHRÖ'S EQ'N.

A. BOX POTENTIAL (Pg 7)



$$V(x) = \begin{cases} 0 & ; \ 0 \le x \le L \\ \infty & ; \ x < 0 \text{ OR } x > 0 \end{cases}$$

1. SOLUTION

a. $\left[\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} - E\right]\psi(x) = 0 = \left[\frac{\delta^2}{\delta x^2} - k^2\right]\psi(x); \ 0 < x \le L$

$\psi(x) = A e^{ikx} + B e^{-ikx} \quad ; \ k^2 = \frac{2mE}{\hbar^2}$

b. BOUNDRY CONDITIONS:

- $\psi(0) = 0 \Rightarrow A = -B \Rightarrow \psi(x) = A' \sin kx$
- $\psi(L) = 0 \Rightarrow \sin kL = 0 \Rightarrow k = \frac{n\pi}{L} \Rightarrow \psi(x) = A' \sin \frac{n\pi x}{L}$
- $\int_0^L \psi_n(x)\psi_m(x)\,dx = \delta_{nm} \Rightarrow |A'|^2 \int_0^L \sin^2 \frac{n\pi x}{L} = \frac{1}{2} A'^2 L$

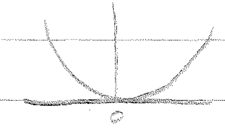
  $\Rightarrow A' = \sqrt{L/2}$

  $\therefore \psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

2. VALUES:

$E = \frac{k^2\hbar^2}{2m} = \left(\frac{n\pi}{L}\right)^2 \frac{\hbar^2}{2m} \leftarrow$ BOUND STATE

B. HARMONIC OSCILLATOR



$$V(x) = \frac{1}{2} k x^2$$

1. SOLUTION

(Pg. 8)

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{k}{2}x^2 - E \right]\psi(x) = 0 \qquad \text{; SCHRO'S EQ'N}$$

LET:

$$\omega = \sqrt{\frac{k}{m}}$$

$$x_0 = \sqrt{\hbar / m\omega}$$

$$\xi = x / x_0$$

$$\Rightarrow \left[\frac{d^2}{d\xi^2} - \xi^2 + \frac{2E}{\hbar\omega} \right]\psi(\xi) = 0$$

SOLUTION IS:

$$\psi_n(\xi) = N_n e^{-\xi^2/2} H_n(\xi) \quad ; \int_{-\infty}^{\infty} \psi_n \psi_m \, d\xi = \delta_{nm}$$

$$N_n = \left[2^n n! \sqrt{\pi} \right]^{-1/2}$$

$$E_n = \hbar\omega(n + \tfrac{1}{2}) \leftarrow \text{BOUND STATE}$$

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \qquad \text{; HERMITE POLYNOMIALS}$$

2. PROPERTIES OF HERMITE POLYNOMIALS AND WAVE FUNCTION

a. $\xi H_n = n H_{n-1} + \frac{1}{2} H_{n+1}$; $\xi \psi_n = \sqrt{\frac{n}{2}}\,\psi_{n-1} + \sqrt{\frac{n+1}{2}}\,\psi_{n+1}$

$$\frac{d}{d\xi}\psi_n = \sqrt{\frac{n}{2}}\,\psi_{n-1} - \sqrt{\frac{n+1}{2}}\,\psi_{n+1}$$

b. a AND a^+ OPERATORS:

(Pg. 11)

- $a = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$: LOWERING OR DESTRUCTION OPERATOR

  $$a\psi_n(\xi) = \sqrt{n}\,\psi_{n-1}(\xi)$$

- $a^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)$: RAISING OR CREATING OPERATOR

  $$a^+\psi_n(\xi) = \sqrt{n+1}\,\psi_{n+1}(\xi)$$

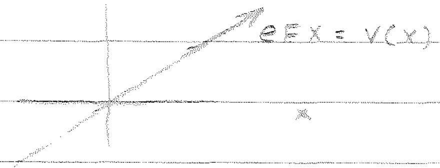
- $(a)^+ = a^+$: HERMITIAN CONJUGATES (Pg. 11)
- $[a, a^+] = 1$

c. SOME MATRIX VALUES

- $\langle n|x|\ell\rangle = x_0\left[\sqrt{\frac{n}{2}}\,\delta_{\ell,n-1} + \sqrt{\frac{n+1}{2}}\,\delta_{\ell,n+1}\right]$ (Pg. 10)
- $\langle n|p_x|\ell\rangle = \frac{\hbar}{i x_0}\left[\sqrt{\frac{n}{2}}\,\delta_{\ell,n-1} - \sqrt{\frac{n+1}{2}}\,\delta_{\ell,n+1}\right]$ (Pg. 10)

(SEE ALSO FIRST HOMEWORK SET & Pg 13 FOR
$\langle n|x^2|m\rangle$, $\langle n|p^2|m\rangle$, $\langle n|e^{iqx}|m\rangle$)

C. LINEAR POTENTIAL



1. SOLUTION

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + eFx - E\right]\psi(x) = 0$$

$$\left[\frac{\hbar^2}{2meF}\frac{\partial^2}{\partial x^2} - \left(x - \frac{E}{eF}\right)\right]\psi(x) = 0$$

LET $\xi = \left(x - \frac{E}{eF}\right)\left(\frac{2meF}{\hbar^2}\right)^{1/3}$

$$\Rightarrow \left(\frac{d^2}{d\xi^2} - \xi\right)\psi(\xi) = 0 \qquad \text{; AIRY'S EQN}$$

SOLUTION IS:

$$\psi(x) = C_1 A_i(\xi) + C_2 B_i(\xi)$$

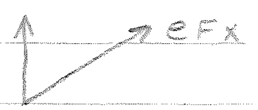
$$A_i(\xi) = \frac{1}{\pi}\int_0^\infty dt \cos\left(\xi t + \frac{t^3}{3}\right)$$

$$B_i(\xi) = \frac{1}{\pi}\int_0^\infty \left[e^{z\xi - \frac{1}{3}z^3} + \sin\left(z\xi + \frac{1}{3}z^3\right)\right]dz$$

BOUNDARY CONDITION: $\psi(+\infty) = 0 \Rightarrow C_2 = 0$

$\therefore \psi(\xi) = A_i(\xi)$

2. BOUND STATE



$$V(x) = \begin{cases} eFx & ; x > 0 \\ \infty & ; x < 0 \end{cases}$$

D. EXPONENTIAL POTENTIAL

$$V(x) = \lambda e^{-2x/a} = \lambda Y^2 \quad (Y = e^{-x/a})$$

SCHRO'S EQ'N:

$$\left[-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + \lambda e^{-2x/a} - E\right]\psi(x) = 0$$

OR $$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} - \frac{2ma^2\lambda^2}{\hbar^2}Y^2 + \frac{2ma^2E}{\hbar^2}\right]\psi(Y) = 0$$

1. CASE 1: $\lambda > 0$ (NO BOUND STATES) (Pg 15)

$$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} - 2a^2K_0^2Y^2 + 2a^2K^2\right]\psi(Y) = 0$$

$$K^2 = 2mE/\hbar^2 \;;\; K_0^2 = \frac{2m\lambda}{\hbar^2}$$

a. SOLUTION IS

$$\psi(Y) = C_1 I_{ika}(aK_0Y) + C_2 I_{-ika}(aK_0Y)$$

$$I_\nu(x) = \sum_{K=0}^{\infty}\frac{1}{K!\,\Gamma(n+\nu+1)}\left(\frac{x}{2}\right)^{\nu+2n}$$

b. BOUNDRY CONDITIONS DICTATE:

$$\lim_{x\to-\infty}\psi(x) = \lim_{Y\to\infty}\psi(Y) = 0$$

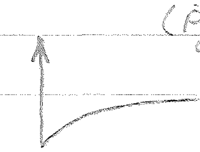
$$\lim_{z\to\infty} I_\nu(z) = \frac{1}{\sqrt{2\pi z}}e^{z}\left[1 + O\left(\frac{1}{z}\right)\right] \Rightarrow C_1 = -C_2$$

$$\therefore \psi(Y) = C_1\left[I_{ika}(aK_0Y) + I_{-ika}(aK_0Y)\right]$$

c. THRU DELTA-FUNCTION NORMAL: $|C_1| = |\Gamma(1+ika)|/\sqrt{2\pi}$

2. CASE 2: $\lambda < 0$ (Pg 17)

$$V(x) = \begin{cases} -|\lambda| e^{-2x/a} & ; x > 0 \\ \infty & ; x < 0 \end{cases}$$



$$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} + \frac{2ma^2}{\hbar^2}E + \frac{2ma^2}{\hbar^2}|\lambda|\right]\psi(Y) = 0$$

a. SOLUTION IS:

$$\psi(Y) = C_1 J_{ika}(K_0aY) + C_2 J_{-ika}(K_0aY)$$

$$J_\nu(x) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!\,\Gamma(n+\nu+1)}\left(\frac{x}{2}\right)^{\nu+2n}$$

BOUNDRY CONDITIONS DICTATE:

$$\psi(x=0) = \psi(Y=1) = 0$$

$$\therefore \frac{C_2}{C_1} = -J_{ika}(K_0a)/J_{-ika}(K_0a)$$

b. BOUND STATES $(E<0)$

$$\alpha^2 = -{}^{2mE}/\hbar^2 > 0$$

$$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} + \alpha^2 a^2 + K_0^2 a^2\right]\psi(Y) = 0$$

$$\psi(Y) = C_1 J_{\alpha a}(K_0 a Y) + C_2 J_{-\alpha a}(K_0 a Y)$$

$$\psi(X=\infty) = \psi(Y=0) = 0 \qquad \text{: BOUNDRY CONDITION}$$

$$\lim_{z\to 0} J_\nu(z) = \frac{1}{\Gamma(1+\nu)} z^\nu$$

$$\therefore \lim_{Y\to 0}\psi(Y) = C_1 \frac{1}{\Gamma(1+\alpha a)}(K_0 a Y)^{\alpha a} + C_2 \frac{1}{\Gamma(1-\alpha a)}(K_0 a Y)^{-\alpha a}$$

$$= C_1'\left(K_0 a e^{-X/a}\right)^{\alpha a} + C_2'\left(K_0 a e^{-X/a}\right)^{\alpha a}$$

C_2' TERM BLOWS UP $\Rightarrow C_2' = 0$

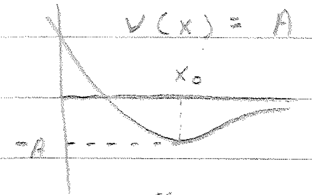
$$\Rightarrow \psi(Y) = C_1 J_{\alpha a}(K_0 a Y)$$

$$\psi(X=0) = \psi(Y=1) = 0 \qquad \text{: BOUNDRY CONDITION}$$

$$\therefore J_{\alpha a}(K_0 a) = 0 \Leftarrow \text{BOUND STATE CONDITION}$$

$$E_i = \frac{\hbar^2}{2m}\alpha_i^2$$

E. MORSE POTENTIAL (pg 36)



$$V(x) = A\left[e^{-2(x-x_0)\alpha} - 2e^{-(x-x_0)\alpha}\right]$$

$$Y = e^{-\alpha(x-x_0)}$$

$$\Rightarrow V(Y) = A\left[Y^2 - 2Y\right]$$

SCHÖ'S EQ'N:

$$\left\{Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} + \frac{2m}{\hbar^2\alpha^2}\left[E - AY^2 + 2AY\right]\right\}\psi(Y) = 0$$

a. SOLUTION IS FOR $t^2 = -\frac{2mE}{\alpha^2\hbar^2}$; $S^2 = \frac{2mA}{\hbar^2\alpha^2}$

$$\psi(Y) = C_1 e^{-SY} Y^{it} F\left[\tfrac{1}{2} + it - s,\ 1 + i2t,\ 2SY\right]$$
$$+ C_2 e^{-SY} Y^{-it} F\left[\tfrac{1}{2} - it - s,\ 1 - i2t,\ 2SY\right]$$

b. CONFLUENT HYPERGEOMETRIC FUNCTION (pg 54)

$$F(a,b;z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \dots = \frac{\Gamma(b)}{\Gamma(a)}\sum_{n=0}^{\infty}\frac{z^n}{n!}\frac{\Gamma(a+n)}{\Gamma(b+n)}$$

$$\lim_{z\to\infty} F(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^{z}$$

c. BOUND STATE $(E<0)$

$$s = \sqrt{\frac{2mA}{\hbar^2\alpha^2}} \quad ; \quad t^2 = \frac{-2mE}{\hbar^2\alpha^2}$$

$$\psi(Y) = C_1 e^{-sY} Y^{t} F\left[\tfrac{1}{2} + t - s,\ 1 + 2t;\ 2sY\right]$$
$$+ C_2 e^{-sY} Y^{-t} F\left[\tfrac{1}{2} - t - s,\ 1 - 2t;\ 2sY\right]$$

BOUNDRY CONDITIONS:

$$\psi(x\to\infty) = \psi(Y=0) = 0 \Rightarrow C_2 = 0$$

$$\therefore \psi(Y) = C_1 e^{-sY} Y^{t} F\left[\tfrac{1}{2} + t - s,\ 1 + 2t;\ 2sY\right]$$

$$\psi(x\to-\infty) = \psi(Y\to\infty) = 0$$

$$\Rightarrow a = \tfrac{1}{2} + t - s = -n$$

$t = s - \frac{1}{2} - n$ $\Leftarrow$ BOUND STATE CONDITION

$$E_n = -A\left[1 - \frac{(n+\frac{1}{2})}{s}\right]^2 \quad ; \quad n \le s - \tfrac{1}{2}$$

F. DELTA FUNCTION POTENTIAL

$V(x) = -\lambda\,\delta(x)\ ;\ \lambda > 0$

SOLUTION

$$\psi(x) = A e^{-\alpha|x|}$$

BOUNDRY CONDITION:

$$\left(\frac{\delta\psi}{\delta x}\right)_{0^+} - \left(\frac{\delta\psi}{\delta x}\right)_{0^-} = \frac{-2m\lambda}{\hbar^2}\psi(0)$$

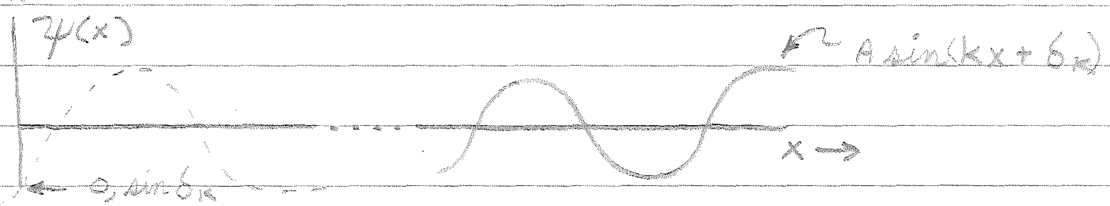
$$\Rightarrow \alpha = \frac{m\lambda}{\hbar^2} \Rightarrow E = \frac{-m\lambda^2}{\hbar^2} \Leftarrow \text{ONE BOUND STATE}$$

$A = \sqrt{\alpha}$

G. MISC.

1. PHASE SHIFT, δ_k

DEFN'



a. FOR EXPONENTIAL $(\lambda > 0)$

WAVE EQ'N WAS

$$\psi(x) = c_1 \left[I_{ika}(a K_0 Y) - I_{-ika}(a K_0 Y) \right] \quad ; \quad Y = e^{-x/a}$$

$$\lim_{z \to 0} I_\nu(z) = z^\nu / \Gamma(1+\nu)$$

YIELDS: $\psi(x) = c_1' \sin(kx + \delta_k)$

$$e^{i2\delta_k} = (K_0 a)^{-i2ka} \frac{\Gamma(1+ika)}{\Gamma(1-ika)}$$

b. FOR EXPONENTIAL $(\lambda < 0)$

$$\psi(x) = c_1 J_{-ika}(K_0 a Y) + c_2 J_{ika}(K_0 a Y)$$

$$\psi(x=0) = \psi(Y=1) = 0$$

$$\Rightarrow \frac{c_2}{c_1} = - J_{ika}(K_0 a) / J_{-ika}(K_0 a)$$

$$\psi(x) = c_1 \left[J_{-ika}(K_0 a e^{-x/a}) - \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} J_{ika}(K_0 a e^{-x/a}) \right]$$

$$\lim_{z \to 0} J_\nu(z) = \left(\frac{z}{2}\right)^\nu / \Gamma(1+\nu)$$

$$\therefore \lim_{\substack{Y \to 1 \\ x \to \infty}} \psi(Y) = c_1 \left[\frac{\left(\frac{K_0 a}{2}\right)^{ika}}{\Gamma(1+ika)} e^{ikx} - \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} \frac{\left(\frac{K_0 a}{2}\right)^{-ika}}{\Gamma(1-ika)} e^{-ikx} \right]$$

$$\Rightarrow e^{i2\delta} = \left(\frac{K_0 a}{2}\right)^{-i2ka} \frac{\Gamma(1+ika)}{\Gamma(1-ika)} \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)}$$

C. FOR MORSE POTENTIAL

$$\psi(x) = C_1 e^{-sY} Y^{it} F\left[\tfrac{1}{2} + it - s, 1 + i2t; 2sY\right]$$
$$+ C_2 e^{-sY} Y^{-it} F\left[\tfrac{1}{2} - it - s, 1 - i2t; 2sY\right]$$

BOUNDARY CONDITION: $\psi(x \to -\infty) = \psi(Y \to \infty) = 0$

$$\lim_{z \to \infty} F(a, b; z) = \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^{z}$$

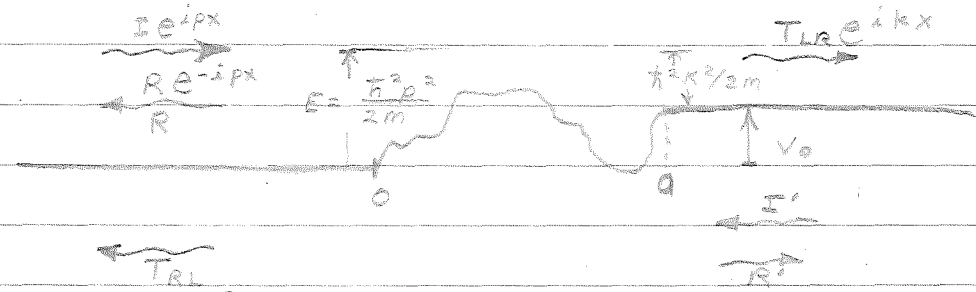
GIVES:

$$\frac{C_2}{C_1} = -\frac{\Gamma(1 + i2t)}{\Gamma(1 - i2t)} \frac{\Gamma(\tfrac{1}{2} - it - s)}{\Gamma(\tfrac{1}{2} + it - s)} (2s)^{i2t}$$

$$\lim_{\substack{x \to \infty \\ Y \to 0}} \psi(Y) = C_1 Y^{it} + C_2 Y^{-it} \quad ; \quad Y = e^{-\alpha(x - x_0)}$$
$$= C_1 e^{ikx_0} \left[e^{ikx} + \frac{C_2}{C_1} e^{ikx} e^{-ik2x_0} \right]$$

$$\therefore \quad e^{i2\delta} = e^{-i2kx_0} \frac{C_2}{C_1}$$

2. TRANSMISSION COEFFICIENT



$E = \frac{\hbar^2 p^2}{2m} > V_0$

WAVE EQ'N: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - E\right]\psi_1(x) = 0$

$$\psi_1(x) = \begin{cases} I e^{ipx} + R e^{-ipx} & ; x < 0 \\ T_{RL} e^{ikx} & ; x > a \end{cases}$$

THEN: $\begin{cases} |I|^2 = |R|^2 + \frac{k}{p}|T_{LR}|^2 \\ |I'|^2 = |R'|^2 + \frac{p}{k}|T_{RL}|^2 \end{cases}$

AND: $\frac{T_{RL}}{I'}\,p = \frac{T_{LR}}{I}\,k$

COMBINING: $\frac{R'}{I'} = -\frac{R^*}{I}\frac{T_{LR}}{T_{RL}}$

3. FUNCTION REPRESENTATIONS AND LIMITS

a. HERMITE POLYNOMIALS

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^n}$$

b. AIRY FUNCTIONS

$$A_i(\xi) = \frac{1}{\pi} \int_0^\infty dt \cos\left(\xi t + \frac{t^3}{3}\right)$$

$$B_i(\xi) = \frac{1}{\pi} \int_0^\infty dt \left[e^{t\xi - \frac{1}{3}t^3} + \sin\left(t\xi + \frac{1}{3}t^3\right)\right] dt$$

c. BESSEL FUNCTIONS

– OF THE FIRST KIND

$$J_\nu(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,\Gamma(\nu+n+1)} \left(\frac{z}{2}\right)^{\nu+2n}$$

$$\lim_{z \to 0} J_\nu(z) = \frac{1}{\Gamma(1+\nu)} \left(\frac{z}{2}\right)^\nu$$

$$\lim_{z \to \infty} J_\nu(z) = \sqrt{\frac{2}{\pi z}} \cos\left[z - \frac{\nu\pi}{2} - \frac{\pi}{4}\right]$$

– OF THE SECOND KIND

$$I_\nu(z) = \sum_{n=0}^{\infty} \frac{1}{n!\,\Gamma(\nu+n+1)} \left(\frac{z}{2}\right)^{\nu+2n}$$

$$\lim_{z \to 0} I_\nu(z) = \frac{1}{\Gamma(\nu+1)} \left(\frac{z}{2}\right)^\nu$$

$$\lim_{z \to \infty} I_\nu(z) = \frac{1}{\sqrt{2\pi z}} e^z \left[1 + O\left(\frac{1}{z}\right)\right]$$

d. CONFLUENT HYPERGEOMETRIC FUNCTIONS

$$F(a,b;z) = 1 + \frac{a}{b} \cdot z + \frac{a(a+1)}{b(b+1)} \frac{z^2}{2!} + \cdots$$

$$= \frac{\Gamma(b)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{z^n}{n!} \frac{\Gamma(a+n)}{\Gamma(b+n)}$$

$$F(a,b;0) = 1$$

$$\lim_{z \to \infty} F(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^z$$

e. GAMMA FUNCTION

$$\Gamma(1+a) = a\,\Gamma(a)$$

$$\Gamma(a-1) = a!$$

$$\lim_{z \to \infty} \Gamma(z) = \sqrt{2\pi}\, z^{z-\frac{1}{2}} e^{-z}$$

III. WAVE FUNCTION NORMALIZATION

A. BOUND STATES

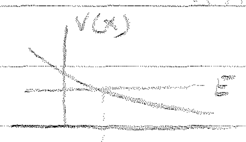
$$\int_{-\infty}^{\infty} \psi_n(x)\,\psi_m(x)\,dx = \delta_{mn}$$

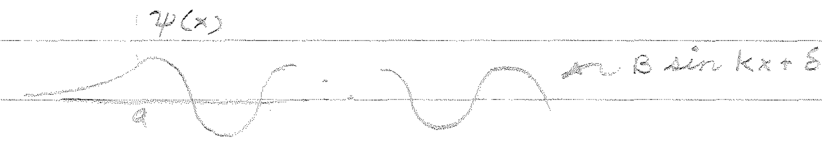
$$\int_{-\infty}^{\infty} \psi_{nm\ell}(r)\,\psi_{n'm'\ell'}\,d^3r = \delta_{nn'}\,\delta_{mm'}\,\delta_{\ell\ell'}$$

B. DELTA FUNCTION NORMALIZATION : $\int_{-\infty}^{\infty} \psi_k^*(x)\,\psi_{k'}(x)\,dx = \delta(k-k')$

$$\int_{-\infty}^{\infty} dx\, e^{ix(k-k')} = 2\pi\,\delta(k-k')$$

GENERAL:





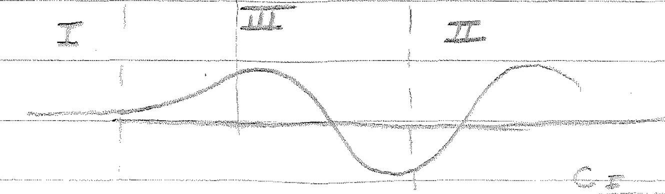
FOR $x \gg a$, $\psi(x) = B \sin(kx+\delta) \Rightarrow \underline{B = \sqrt{\tfrac{2}{\pi}}}$

C. BOX NORMALIZATION (Pp. 31-2)

$$\lim_{L\to\infty} \frac{L}{2\pi}\,\delta_{n,m} = \delta(k-k')$$

IV. WKBJ (QUASICLASSICAL APPROXIMATION) (Pg 35)

A. GENERAL



IN REGION I: $\psi(x) = \dfrac{C_I}{\sqrt[4]{2m(V-E)}}\, e^{\frac{\sqrt{2m}}{\hbar}\int_b^x \sqrt{V-E}\,dx}$

IN REGION II: $\psi(x) = \dfrac{C_{II}}{\sqrt[4]{2m(E-V)}} \sin\left[\dfrac{\sqrt{2m}}{\hbar}\int_b^x \sqrt{E-V}\,dx + \dfrac{\pi}{4}\right]$

$$C_I = \tfrac{1}{2} C_{II}$$

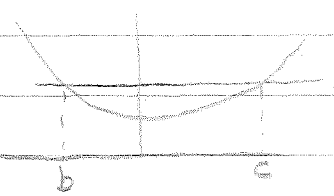
IN REGION III: $\psi(x) = C_0 A_i(-\xi)$; $\xi = (x-b)\left(\dfrac{2mF}{\hbar^2}\right)^{\frac{1}{3}}$ (pg 42)

NOTE: OMIT $\frac{\pi}{4}$ PHASE TERM FOR ∞ POTENTIALS:

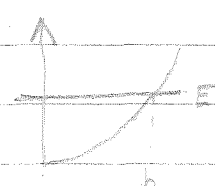
B. BOUND STATES

BOHR SOMMERFIELD CONDITION:

$$P(x) = \sqrt{2m(E-V)}$$



$\Rightarrow \int_b^c dx\, p(x) = \hbar\left(n+\tfrac{1}{2}\right)\pi$



$\int_0^b dx\, p(x) = \hbar\left(n+\tfrac{3}{4}\right)\pi$

C. PHASE

$$\delta_{WKBJ} = \lim_{x\to\infty}\left[\frac{\sqrt{2m}}{\hbar}\int_b^x \sqrt{E-V(x)}\,dx - kx + \frac{\pi}{4}\right]$$

FOR ∞ POTENTIALS, OMIT $\frac{\pi}{4}$ TERM

POTENTIAL	PHASE-SHIFT	BOUND STATE	NORMALIZATION
BOX	N.A.	YES (Pg. 3)	YES (Pg. 3)
HARMON. OSC.	N.A.	YES (Pg 4)	YES (Pg 4)
LINEAR	NO	YES (Pg. 5)	YES (Pg. 5)
EXP. ($\lambda > 0$)	YES (Pg. 10)	NONE	YES (Pg. 6)
($\lambda < 0$)	YES (Pg 10)	YES. (Pg. 7)	NO
MORSE	YES (Pg 11)	YES (Pg. 8)	NO ✓
DELTA	NO	YES (Pg 9)	YES (Pg 9)

d. IN THREE DIMENSIONS

- $\psi(r) = Y_\ell^m R(r)$

$\chi(r) = r R(r)$

BOUNDRY CONDITION: $\chi(r=0) = 0$

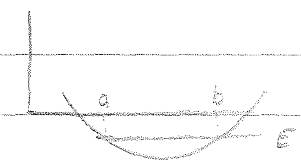
$p^2(r) = 2m[E - V(r)] + \frac{1}{r^2}(\ell + \frac{1}{2})^2 \hbar^2$

$$\Rightarrow \left[\frac{d^2}{dr^2} + p^2(r)/\hbar^2\right]\psi(r) = 0$$

WKBJ IS:

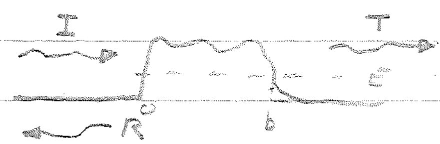
$$\chi(r) = \begin{cases} \frac{C}{\sqrt{p(r)}} \sin\left[\frac{1}{\hbar}\int_b^r dr'\,p(r') + \frac{\pi}{4}\right] \\ \frac{C}{2\sqrt{p}} \exp\left[-\frac{1}{\hbar}\int_b^x dr'\,|p(r')|\right] \end{cases}$$

- FOR BOUND STATES



$$\int_a^b dr\,p(r) = \begin{cases} \pi\hbar(n + \frac{1}{2}) & \text{: SOFT POTEN.} \\ \pi\hbar(n + \frac{3}{4}) & \text{: ABRUPT POTEN} \end{cases}$$

e. TRANSMISSION COEFFICIENT



$$T = e^{-\frac{2}{\hbar}\int_a^b \sqrt{2m(V-E)}\,dx}$$

V. THE HYDROGEN ATOM

A. EXACT SOLUTION

$V(r) = \frac{-Ze^2}{r}$ (HYDROGEN ATOM: $Z=1$)

$\psi(r) = R_{n\ell}(r)\, Y_\ell^m(\theta,\phi)$ (Y_ℓ^m on pg. 50)

$\chi(r) = r R(r)$

$$\left[\frac{-\hbar^2}{r2m}\frac{d^2}{dr^2}r + \frac{\hbar^2}{2m}\frac{(\ell+1)\ell}{r^2} - \frac{Ze^2}{r} - E\right]R(r) = 0$$

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{(\ell+1)\ell}{r} - \frac{Ze^2}{r} - E\right]\chi(r) = 0$$

LET
- $a = \frac{\hbar^2}{me^2} = 0.529\times 10^{-8}$ cm : BOHR RADIUS
- $\frac{e^2}{a} = \frac{me^4}{\hbar^2} = 27.2$ eV : HARTREE

  $1\ \text{eV} = 1.6\times 10^{-12}$ ERG
- $\rho = r/a$
- $\epsilon = \frac{Ea}{e^2}$

$$\Rightarrow \left[\frac{\delta^2}{\delta\rho^2} + \frac{2Z}{\rho} - \frac{\ell(\ell+1)}{\rho^2} + 2\epsilon\right]\chi(\rho) = 0$$

1. BOUND STATES

$E < 0 \Rightarrow -\alpha^2 = 2\epsilon$

$$\left[\frac{\delta^2}{\delta\rho^2} + \frac{2Z}{\rho} - \frac{\ell(\ell+1)}{\rho^2} - \alpha^2\right]\chi(\rho) = 0$$

LET $\chi(\rho) = \rho^{\ell+1} e^{-\alpha\rho} F(\rho)$

$$\Rightarrow \left[\rho\frac{d^2}{d\rho^2} + \{2(\ell+1) - 2\alpha\rho\}\frac{d}{d\rho} + \{2Z - 2\alpha(\ell+1)\}\right]F(\rho) = 0$$

$\therefore F(\rho) = F\left(\ell+1-\frac{Z}{\alpha}, 2\ell+2, 2\rho\alpha\right)$

$\psi(\rho) = \rho^{\ell+1} e^{-\alpha\rho} F\left[\ell+1-\frac{Z}{\alpha}, 2\ell+2; 2\alpha\rho\right]$

CONFLUENT HYPERGEOMETRIC FUNCTION

MUST BE TRUNCATED AT $\ell+1-\frac{Z}{\alpha} = -n_r$

$\therefore \alpha = \frac{Z}{n_r+\ell+1} \Rightarrow E_n = -\left(\frac{e}{2a}\right)\frac{Z^2}{(n_r+\ell+1)^2}$

- n_r: RADIAL QUANTUM #
- ℓ: ORBITAL QUANTUM #
- $n = n_r+\ell+1$: PRINCIPLE QUANTUM #
- $E_{RYD} = \frac{e^2}{2a} = 13.6$ eV : RYDBERG

$$\chi_n(\rho) = \rho^{\ell+1}e^{-\alpha\rho}F[-n_r, 2\ell+2, 2\alpha\rho] = \rho^{\ell+1}e^{-\alpha\rho}L^{2\ell+1}_{n_r+\ell}(2\alpha\rho)$$

(FOR VARIOUS χ_n SEE PG. 58)

2. CONTINUUM STATES

$$\alpha = ik \Rightarrow E = \frac{k^2 e^2}{a}$$

$$\chi(\rho) = c_1 \rho^{\ell} e^{-ik\rho} F\left[\ell+1+\frac{z}{ik}, 2\ell+2, -i2k\rho\right] + c_2 \rho^{\ell} e^{ik\rho} F\left[\ell+1-\frac{z}{ik}, 2\ell+2, i2k\rho\right]$$

3. REPULSIVE COULOMB POTENTIAL

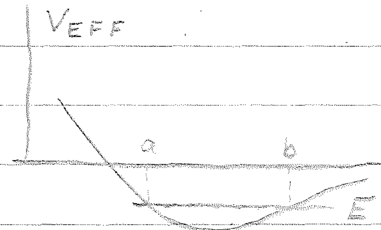
$$V(r) = Ze^2/r^2$$

$$Z \to -Z$$

$$\chi(\rho) = c_1 \rho^{\ell} e^{-ik\rho} F\left[\ell+1-\frac{z}{ik}, 2\ell+2, -i2k\rho\right] + c_2 \rho^{\ell} e^{ik\rho} F\left[\ell+1+\frac{z}{ik}, 2\ell+2, i2k\rho\right]$$

4. WKBJ BOUND STATE SOLUTION

$$V_{EFF} = \frac{-Ze^2}{r} + \frac{\hbar^2}{2m}\frac{(\ell+\frac{1}{2})^2}{r^2}$$



$$\int_a^b dr\, p(r) = \pi\hbar(n+\tfrac{1}{2})$$

$$p^2(r) = 2m\left[E + \frac{Z^2e^2}{r}\right] - \hbar^2(\ell+\tfrac{1}{2})^2/r^2$$

$$\int_a^b p(r)dr = \pi\hbar(n+\tfrac{1}{2}) = \int_a^b \sqrt{2m\left[E+\frac{Z^2e^2}{r}\right] - \hbar^2(\ell+\tfrac{1}{2})^2/r^2}\, dr$$

$$\rho = \frac{r}{a_B}, \quad E_{RYD} = \frac{\hbar^2}{2ma_B^2} = \frac{e^2}{2a_B} = 13.6\,eV$$

$$\Rightarrow \pi(n+\tfrac{1}{2}) = \int_{a/a_B}^{b/a_B} \sqrt{\frac{E}{E_{RYD}} + \frac{2Z}{\rho} - \frac{1}{\rho^2}(\ell+\tfrac{1}{2})^2}\, d\rho$$

$$= \int_{a/a_B}^{b/a_B} \frac{d\rho}{\rho}\left[\rho^2\alpha^2 + 2Z\rho - (\ell+\tfrac{1}{2})^2\right]^{1/2} d\rho \,;\ \alpha^2 = \frac{E}{E_{RYD}}$$

$$= \alpha \int_{a'}^{b'} \frac{d\rho}{\rho}\sqrt{(\rho-a')(\rho-b')}\, d\rho$$

$$= \alpha\pi\left[\frac{a'+b'}{2} - \sqrt{a'b'}\right]$$

$$a'+b' = \frac{2Z}{\alpha^2} \quad ; \quad -a'b' = \frac{-(\ell+\frac{1}{2})^2}{\alpha^2}$$

GIVES: $E = -E_{RYD} Z^2 / (n_r+\ell+1)^2$

B. HYDROGEN-LIKE ATOMS (Pg. 71)

$n^* = n - \delta \quad \ni \quad \delta =$ QUANTUM DEFECT

$E_n = \frac{-Z^2 E_{RYD}}{n^{*2}}$

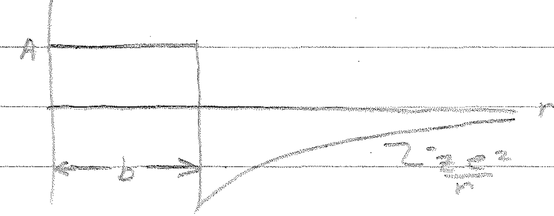
WKBJ: $\varphi_T = \frac{1}{\hbar}\int dr\, p(r) + \frac{\pi}{2} + \pi\delta$

$\psi(r) = R(r)\, Y_\ell^m(\theta, \phi)$

$R(r) = W_{n^*, \ell+\frac{1}{2}}\left(\frac{2r}{a_0 n^*}\right); r > b \leftarrow$ WHITTIKER'S FUNCTION

$\langle r^2 \rangle = \frac{n^{*2} a_0^2}{2}\left[5n^{*2} + 1 - 3\ell(\ell+1)\right]$

A IS LINEAR WITH E (BOUND)



FOR $r < b$

$$\chi_\ell(r) = \sqrt{r}\left[A_1 J_{\ell+\frac{1}{2}}(\alpha r) + B_1 J_{-\ell-\frac{1}{2}}(\alpha r)\right]$$

$$\alpha^2 = \frac{2m}{\hbar^2}(A + E)$$

FOR $r > b$

$$\chi_u(r) = A\, e^{-kr}\, r^{\ell+1}\, U\left(\ell + 1 - \frac{(bk_0)^2}{2k}, 2\ell+2, 2kr\right)$$

$$k^2 = \frac{-2mE}{\hbar^2} \quad ; \quad k_0^2 = \frac{2mA}{\hbar^2}$$

C. PSEUDOPOTENTIALS (Pg. 75)

$$A = \sum_\alpha (E - E_\alpha)\, \phi_\alpha(r) \cdot \langle \alpha | \chi \rangle > 0$$

$\alpha =$ CORE STATES WITH SAME SPIN

USUALLY LET $\chi = \chi(0)$

VI. SPIN AND ANGULAR MOMENTUM

A. EIGENSTATES:

GIVEN: $[M_Y, M_Z] = i\hbar M_X$

$[M_Z, M_X] = i\hbar M_Y$

$[M_X, M_Y] = i\hbar M_Z$

DEFINE: $M^2 = M_X^2 + M_Y^2 + M_Z^2$

$L^+ = M_X + i M_Y$

$L^- = M_X - i M_Y$

THEN $[M^2, M_Z] = 0$

$\Rightarrow M^2 |jm\rangle = M_j^2 |jm\rangle$

$M_Z |jm\rangle = \hbar m |jm\rangle$

GIVES $-j \leq m \leq j$

j = INTEGERS OR $\frac{1}{2}$ INTEGERS

$L^- |jm\rangle = \hbar \sqrt{j(j+1) - m(m-1)}\ |j, m-1\rangle$

$L^+ |jm\rangle = \hbar \sqrt{j(j+1) - m(m+1)}\ |j, m+1\rangle$

$M^2 |jm\rangle = \hbar^2 j(j+1) |j, m\rangle$

B. CLEBSH GORDON COEFFICIENTS

EX. $\frac{1}{2} \otimes \frac{1}{2}$ $\qquad -j \leq m \leq j$

$j_1 = \frac{1}{2} \qquad m_1 = -\frac{1}{2}, \frac{1}{2}$

$j_2 = \frac{1}{2} \qquad m_2 = -\frac{1}{2}, \frac{1}{2}$

$\left.\begin{array}{ll} \alpha_1 = |\frac{1}{2}, \frac{1}{2}\rangle & \alpha_2 = |\frac{1}{2}, \frac{1}{2}\rangle \\ \beta_1 = |\frac{1}{2}, -\frac{1}{2}\rangle & \beta_2 = |\frac{1}{2}, -\frac{1}{2}\rangle \end{array}\right\} |j, m\rangle$

m'S ALWAYS ADD.

$J = j_1 + j_2 = 1 \qquad |1, 1\rangle \quad \alpha_1 \alpha_2$

$\Rightarrow M = -1, 0, 1 \qquad |1, 0\rangle \quad \alpha_1 \beta_2 \quad \alpha_2 \beta_1$

$|1, -1\rangle \quad \beta_1 \beta_2$

$J = j_1 - j_2 = 0 \qquad |0, 0\rangle \quad \alpha_1 \beta_2, \alpha_2 \beta_1$

$\Rightarrow M = 0$

$$L|j\,m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\,|j, m\rangle$$

$$L|1, 1\rangle = \sqrt{2}\,|1, 0\rangle = L(\alpha_1 \alpha_2)$$

$$= \alpha_1 L(\alpha_2) + \alpha_2 L(\alpha_1)$$

$$= \alpha_1 \beta_2 + \alpha_2 \beta_1$$

$$\Rightarrow |1, 0\rangle = \frac{1}{\sqrt{2}}(\alpha_1 \beta_2 + \alpha_2 \beta_1)$$

	ϕ_1^1	ϕ_1^0	ϕ_1^0	ϕ_1^{-1}
$\alpha_1 \alpha_2$	1			
$\alpha_1 \beta_2$		$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	
$\alpha_2 \beta_1$		$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	
$\beta_2 \beta_1$				1

VII. VARIATIONAL CALCULATION

A. STATEMENT OF METHOD

1. LIMITATIONS: USEFULL ONLY IN GROUND STATE ENERGIES
2. USEFUL RELATIONSHIPS:

$$\nabla^2 = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{d}{d\theta} + \frac{1}{r^2}\frac{d^2}{d\theta^2} + \frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}$$

$$\int d^3r\, \Theta \Phi R = \int_0^{\pi} \Phi\, d\phi \int_0^{2\pi} \Theta \sin\theta\, d\theta \int_0^{\infty} r^2 R\, dr$$

$$\int_0^{\infty} r^n e^{-r/a} = n!\, a^{n+1}$$

$$H = \frac{\hbar^2 \nabla^2}{2m} + V(r)$$

3. CHOOSE $\phi(x)$ WITH VARIATIONAL PARAMETERS α

$$E(\alpha) = \frac{\int d^3r\, \phi^*(r) H \phi(r)}{d^3r\, \phi^*(r)\phi(r)} \geq E_0$$

MINIMIZE E_α

B. HELIUM ATOM

$$H = \frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{|r_1 - r_2|}$$

ASSUME: $\psi(r_1, r_2) = A\, e^{-z^*(r_1 + r_2)/a_B}$

NORMALIZATION: $\int d^3r_1 \int d^3r_2\, \psi(r_1, r_2) = \left(\frac{\pi A^2 a_B^{\,2}}{z^{*3}}\right)^2$

NUCLEUS: $-2\int d^3r_1\, \phi^2(r_1)\, \frac{e^2}{r_1} \int d^3r_2\, \phi^2(r_2)$

$$= -2\left(\frac{\pi A^2 a_B^{\,3}}{z^3}\right) \frac{e^2 z}{a_B}\left(\frac{\pi A^2 a_B}{z^3}\right)$$

ELEC/ELEC: $\int d^3r_1 \int d^3r_2\, \phi_1^2(r_1)\phi_2^2(r_2)\, \frac{e^2}{|r_1 - r_2|}$

$$= \left(\frac{\pi A^2 a_B^{\,3}}{z^3}\right)^2 \frac{5}{4} z \frac{e^2}{2a_B}$$

(P_5 - 22)

GIVES $E(z) = E_{RYD}\left[2z^2 - 8z + \frac{5}{4}z\right]$

$$E_0 \simeq -5.7\, E_{RYD}$$

EXPERIMENTALLY, $-1.8 E_{RYD}$ = TO TAKE OUT 1^{ST} e

$-4\, E_{RYD}$ = " " " 2^{nd} "

$-5.8\, E_{RYD}$

VIII. PERTURBATIONS INDEP. OF TIME

A. SECOND ORDER PERTURBATION

$$H = H_0 + V$$

H_0 HAS SOLUTIONS $\psi_n^{(0)}$ AND $E_n^{(0)}$

THEN

$$E_L = E_L^{(0)} + V_{LL} + \sum_{m \neq L} \frac{|V_{Lm}|^2}{E_L^{(0)} - E_m^{(0)}}$$

$$\psi_L = \psi_L^{(0)} + \sum_{m \neq L} \frac{\psi_m^{(0)} V_{mL}}{E_L^{(0)} - E_m^{(0)}}$$

$$V_{ij} = \langle i | V | j \rangle$$

EX) HARMONIC OSCILLATOR IN E FIELD

$$H = \frac{p^2}{2m} + \frac{K}{2} x^2 + Fx$$

$$H_0 = \frac{p^2}{2m} + \frac{K}{2} x^2$$

$$E_n^{(0)} = \hbar\omega(n + \tfrac{1}{2}) \quad ; \quad \psi_n^{(0)} \sim \text{HARMONIC OSC (Pg 4)}$$

THEN:

$$E_n = \hbar\omega(n + \tfrac{1}{2}) + \langle n | Fx | n \rangle + \sum_{m \neq n} \frac{|\langle n | Fx | m \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

FROM Pg. 4:

$$\langle n | x | m \rangle = x_0 \left[\sqrt{\tfrac{n}{2}}\, \delta_{m,n-1} + \sqrt{\tfrac{n+1}{2}}\, \delta_{m,n+1} \right]$$

$$\Rightarrow \sum_{m \neq n} \frac{|\langle n | Fx | m \rangle|^2}{E_n^{(0)} - E_m^{(0)}} = \sum_{m \neq n} \frac{\left[x_0 F \left(\sqrt{\tfrac{n}{2}}\, \delta_{m,n-1} + \sqrt{\tfrac{n+1}{2}}\, \delta_{m,n+1} \right) \right]^2}{\hbar\omega(n-m)}$$

$$= \sum_{m \neq n} \frac{x_0^2 F^2 \left(\frac{n}{2} \delta_{m,n-1} + \frac{n+1}{2} \delta_{m,n+1} \right)}{\hbar\omega(n-m)}$$

$$= \sum_{m \neq n} \frac{x_0^2 F^2}{2\hbar\omega} \left[\frac{n\, \delta_{m,n-1}}{(n-m)} + \frac{(n+1)\, \delta_{m,n+1}}{(n-m)} \right]$$

$$= \frac{x_0^2 F^2}{2\hbar\omega} \left[\frac{n}{n-(n-1)} + \frac{(n+1)}{n-(n+1)} \right]$$

$$= \frac{x_0^2 F^2}{2\hbar\omega} \left[n - (n+1) \right] = -\frac{x_0^2 F^2}{2\hbar\omega} = -\frac{F^2}{2m\omega^2}$$

$$\therefore E_n = \hbar\omega(n + \tfrac{1}{2}) - \frac{F^2}{2m\omega^2}$$

$$= \hbar\omega(n + \tfrac{1}{2}) - \frac{F^2}{2K} \Leftarrow \text{EXACT SOLUTION}$$

B. ATOMIC POLARIZABILITY

CONSIDER ATOM IN AN E FIELD:

$$H = H_0 + eF\Sigma x_i$$

$$E_n = E_n^{(0)} + \langle n|eF\Sigma x_i|n\rangle + \sum_{m\neq n} \frac{|\langle n|eF\Sigma x_i|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

DIPOLE MOMENT $= d_n = e\sum_i \langle n|x_i|n\rangle$

POLARIZABILITY $= \alpha_n$

$$= -2e^2 \sum_{m\neq n} \frac{|\langle n|\Sigma x_i|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\therefore E_n = E_n^{(0)} + Fd_n - \tfrac{1}{2}F^2\alpha_n$$

EX) HYDROGEN : $\alpha = \frac{9}{2}a^3$

$$\alpha_{1s} = -2e^2 \sum_{m\neq n} \frac{|\langle 1s|z|n, \ell=0, m=0\rangle|^2}{-E_{RYD} + E_{RYD}/m^2}$$

$$\simeq \frac{2e^2}{\frac{3}{4}E_{RYD}} |\langle 1s|z|2p\rangle|^2$$

$$\psi_{1s} = \frac{1}{\sqrt{4\pi}} c\, e^{-r/a} \quad (= Y_0^0 R_0^1)$$

$$c^2\int_0^\infty r^2 e^{-2r/a} dr = 1 = c^2\, 2\left(\frac{a}{2}\right)^3 = c^2 \cdot \frac{a^3}{4} \Rightarrow c = \frac{2}{\sqrt{a^3}}$$

$$\psi_{1s} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \quad (= Y_0^0 R_0^1)$$

$$\psi_{2p} = \sqrt{\frac{3}{4\pi}} \cos\theta\, c\, r\, e^{-r/2a}$$

$$c^2\int_0^\infty r^4 \cdot e^{-r/a} dr = 1 = c^2\, 24 (a)^5 \Rightarrow c = \frac{1}{\sqrt{24a^5}}$$

$$\psi_{2p} = \sqrt{\frac{1}{32\pi a^5}}\, r\, e^{-r/2a} \cos\theta \,(= Y_1^0 R_1^2)$$

$$\langle 1s|z = r\cos\theta|2p\rangle = \frac{1}{\pi a^4}\frac{1}{\sqrt{32}} \int d^3r\, r^2 e^{-3r/2a} \cos^2\theta$$

GIVES $\alpha_{1s} \simeq 2.7a^3$

C. STARK EFFECT IN HYDROGEN

EX: $n=2$

4 STATES $\ell = 0$ $\qquad$ $\ell = 1$

$m=0$	$m=-1$	$m=0$	$m=1$
$2S_0$	$2P_{-1}$	$2P_0$	$2P_1$

APPLY E FIELD IN z DIRECTION

ONLY STATES WITH SAME m MIX

$$\begin{array}{c|cccc} & 2S_0 & 2P_0 & 2P_{-1} & 2P_{+1} \\ \hline 2S_0 & -\Delta E & \lambda & 0 & 0 \\ 2P_0 & \lambda & -\Delta E & 0 & 0 \\ 2P_{-1} & 0 & 0 & -\Delta E & 0 \\ 2P_{+1} & 0 & 0 & 0 & -\Delta E \end{array}$$

$$\lambda = \langle 2S_0 | eFz | 2P_0 \rangle = eF \langle 2S_0 | r\cos\theta | 2P_0 \rangle$$

$2S_0 \Rightarrow (n=2, \ell=0, m=0)$ $\qquad$ $2P_0 \Rightarrow (n=2, \ell=1, m=0)$

$$\therefore \psi_{2S_0} = R_0^2 Y_0^0 = \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{8\pi a^3}} e^{-r/2a}\left(1 - \frac{r}{2a}\right)$$

$$\psi_{2P_0} = R_1^2 Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta \frac{1}{\sqrt{32\pi a^3}} e^{-r/2a}$$

$$\lambda = eF \int d^3r\, \psi_{2S_0}^* \, r\cos\theta \, \psi_{2P_0}$$

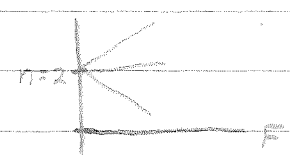
$$= -3a\,eF$$

TAKING MATRIX DETERMINANT GIVES

$$\Delta E = \pm\lambda, 0$$

FOR HYDROGEN, $E_n = \dfrac{E_{RYD}}{n^2}$

$$\Rightarrow E + \Delta E \rightarrow \begin{array}{l} \frac{1}{4}E_{RYD} - 3a\,eF \\ \frac{1}{4}E_{RYD} + 3a\,eF \\ \frac{1}{4}E_{RYD} \end{array}$$



$n=3$ WORKED IN #1, HOMEWORK #3

D. VAN-DER-WAALS INTERACTION

$$O \xleftarrow{\quad R \quad} \!\!\rightarrow O \qquad V(r) = \frac{C_6}{R^6} \leftarrow \text{EXPERIMENT}$$

LONDON'S FORMULA (pg. 101, 105)

$$C_6 = e^4 \sum_{n,m} \frac{(r_{nA} \cdot \phi \cdot r_{mB})(r_{mB} \cdot \phi \cdot r_{na})}{E_{nA} + E_{nB}}$$

E. SPIN-ORBIT INTERACTION (pg. 112)

WITH E FIELD → (pg. 115)

F. ZEEMAN EFFECT

$$H = \frac{p^2}{2m} - \underbrace{\frac{2e}{2mc} p \cdot A}_{\text{PARAMAGNETIC}} + \underbrace{\frac{e^2}{2mc^2} A^2}_{\text{DIAMAGNETIC}}$$

FROM ADDED MAGNETIC FIELD H_0

$$A = \frac{1}{2} \underset{\sim}{H_0} \times \underset{\sim}{r} \qquad \nabla \times \tilde{A} = H_0$$

G. CONTINUUM STATES PERTURBED BY LOCAL POTENTIAL

CONSIDER A CONTINUUM STATE VIA BOX NORMALIZATION:

$$\psi(r) = \frac{1}{\sqrt{\Omega}} e^{i k \cdot r}$$

THEN FOR A PERTURBATION V:

$$\langle k | V | k' \rangle = \frac{1}{\Omega} \int d^3 r \, e^{-i k \cdot r} \, V(r) \, e^{i k \cdot r}$$
$$= \frac{1}{\Omega} \mathcal{V}(k - k')$$

WHERE $\mathcal{V}(q) = \int d^3 r \, V(r) \, e^{i r \cdot q}$

IS THE FOURIER TRANSFORM OF $V(r)$

PERTURBATION THEORY GIVES

$$E_n = E_n^{(0)} + \langle k | V | k \rangle + \sum_{k' \neq k} \frac{1}{E_k^{(0)} - E_{k'}^{(0)}} |\langle k | V | k' \rangle|^2$$
$$= \frac{\hbar^2 k^2}{2m} + \frac{1}{\Omega} \mathcal{V}(0) + \sum \frac{1}{\Omega^2} \frac{2m}{\hbar^2} \frac{1}{k^2 - k'^2} \mathcal{V}^2(k - k')$$

NOW

$$\lim \sum_{k'} f(k') \longrightarrow \frac{\Omega}{(2\pi)^3} \int d^3 k' \, f(k')$$

THUS

$$E_n = \frac{\hbar^2 k^2}{2m} + \frac{1}{\Omega} \left[\mathcal{V}(0) + \frac{2m}{\hbar^2 (2\pi)^3} \int d^3 k' \, \frac{\mathcal{V}^2(k - k')}{k^2 - k'^2} \right]$$

$$\lim_{\Omega \to \infty} E_n = \frac{\hbar^2 k^2}{2m}$$

$\therefore$ CONTINUUM STATE ENERGYS ARE NOT EFFECTED

FOR WAVE EQUATION: (Pg 11)

$$\psi_k(r) = \psi_k^{(0)} + \sum_{k' \neq k} \frac{\psi_{k'} \langle k | V | k' \rangle}{E_k^{(0)} - E_{k'}^{(0)}}$$
$$= \frac{1}{\sqrt{\Omega}} e^{i k \cdot r} + \frac{\hbar^2}{2m \Omega^{3/2}} \sum \frac{1}{k^2 - k'^2} \mathcal{V}(k - k') e^{i k' \cdot r}$$
$$= \frac{1}{\sqrt{\Omega}} \left[e^{i k \cdot r} + \frac{2m}{\hbar^2 (2\pi)^3} \int d^3 k' \, \frac{1}{k^2 - k'^2} e^{i k \cdot r} \mathcal{V}(k - k') \right]$$

EXAMPLE: $V(r) = \frac{\lambda}{r} e^{-k_s r}$ (YUKAWA POTENTIAL)

$$V(q) = \frac{4\pi\lambda}{q^2 + k_s^2}$$

FOR $k = 0$

$$\psi(r) = \frac{1}{\sqrt{\Omega}} \left[1 - \frac{4\lambda m}{\hbar^2 k_s^2 r} \left(1 - e^{-k_s r} \right) \right]$$

IX. TIME DEPENDENT PERTURBATION THEORY

A. (FERMI'S) GOLDEN RULE & BORN APPROXIMATION

1. $w_{\ell m}$ = RATE OF CHANGE FROM STATE ℓ TO m

   a. BOUND STATES

   $$w_{\ell m} = \frac{2\pi}{\hbar} |V_{\ell m}|^2 \, \delta\left[E_\ell^{(0)} - E_m^{(0)}\right] \quad \text{(BORN APPROX.)}$$

   b. CONTINUUM STATES (BOX NORMALIZATION Ω_0)

   $$w_{k \to k'} = \frac{2\pi}{\hbar} \frac{1}{(2\pi)^3} \frac{1}{\Omega_0} \frac{k m}{\hbar^4} \int d\Omega \, |\mathcal{V}^2(k - k')|$$

   $$\begin{cases} E_k^{(0)} = \frac{\hbar k^2}{2m} = pc & \text{; NON-RELATIVISTIC} \\ E_k^{(0)} = \sqrt{p^2c^2 + m^2c^4} & \text{; } p = \hbar k \quad \text{RELATIVISTIC} \end{cases}$$

   FOURIER

   $$\mathcal{V}(q) = \int d^3r \, V(r) \, e^{i r \cdot q}$$

   $$\text{EX: } V(r) = \frac{\lambda}{r} e^{-k_s r} \to V(q) = \frac{4\pi\lambda}{q^2 + k_s^2}$$

   $E =$

   FOR FREE PARTICLES $|V_{\ell m}|^2 = \frac{1}{\Omega} \mathcal{V}^2(k - k')$

   $E_k = \sqrt{p^2c^2 + m^2c^4}$; $p = \hbar k$ ⟸ RELATIVISTIC

2. $\frac{d\sigma}{d\Omega}_{k \to k'}$ = DIFFERENTIAL CROSS SECTION

   $$= \frac{1}{4\pi^2} \frac{m^2}{\hbar^2} |\mathcal{V}(k - k')|^2$$

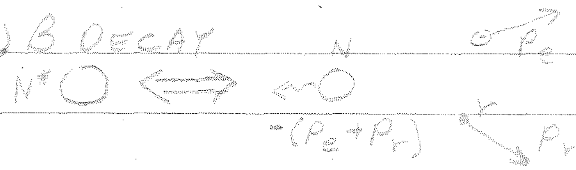
   σ = TOTAL CROSS SECTION

   $$= \frac{1}{4\pi^2} \frac{m^2}{\hbar^2} \int d\Omega_{k'} |\mathcal{V}(k - k')|^2$$

$$|k - k'|^2 = k^2 + k'^2 - 2kk' \cos\theta$$

B. PARTICLE DECAY

EX) β DECAY



Δ = EXCESS KINETIC ENERGY

$$= \underbrace{\frac{\hbar^2}{2m}\left(p_e^2+p_\nu^2\right)}_{\text{NUCLEUS}} + \underbrace{cp_\nu}_{\text{NEUTRINO}} + \underbrace{\sqrt{cp_e^2+m^2c^4}}_{\text{ELECTRON}}$$

$$\simeq cp_\nu + \sqrt{cp_e^2+m^2c^4}$$

$$\omega = \sum_{\substack{p_e\\ p_\nu}} \frac{2\pi}{\hbar} |M|^2 \, \delta\left(E_n^{(0)} - E_m^{(0)}\right) \Leftarrow \text{FERMI'S GOLDEN RULE}$$

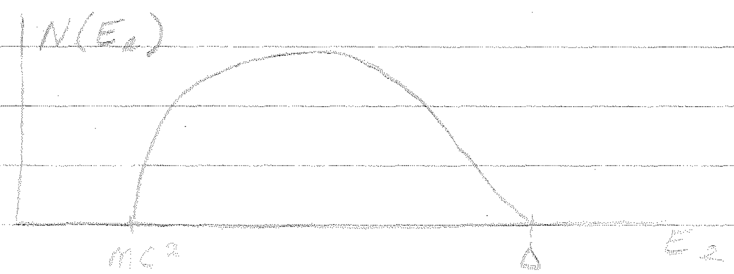
FERMI SAID: ASSUME M CONSTANT

$$\omega = \frac{2\pi}{\hbar}\frac{1}{(2\pi)^6}|M|^2 \int d^3p_e \int d^3p_\nu \, \delta\left[\Delta - cp_\nu - \sqrt{cp_e^2+m^2c^4}\right]$$

LET $\quad E_e = \sqrt{m^2c^4+c^2p_e^2} \quad \left(E_e\,dE_e = c^2p_e^2\,dp_e\right)$

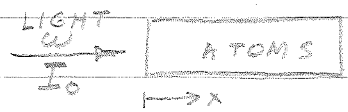
$$\Rightarrow \frac{d\omega}{dE_e} = \text{CONST.}\,(\Delta - E_e)^2\left(E_e^2 - m^2c^4\right)^{\frac{1}{2}}$$

$$= \frac{\text{\# OF ELECTRONS}}{\text{UNIT ENERGY}}$$



C. SEMICLASSICAL RADIATION THEORY (Pg. 137)

1. BEER'S LAW



$$I = I_0 e^{-\alpha(\omega) x} \quad \left(\frac{dI}{dx} = -\alpha I \right)$$

n = REFRACTIVE INDEX $= \sqrt{\mu \epsilon}$

N_A = # OF ATOMS

$$\alpha(\omega) = 4\pi^2 \left(\frac{N_A}{V} \right) \frac{e^2}{m^2 n c\, \omega_K} \sum_f (\underset{\sim}{n} \cdot P_{fi}) \delta[E_i + \hbar\omega - E_f]$$

F_K = FLUX $= {N_K}/{V} \; \frac{c}{n}$

$\omega_K = ckn$

2. OSCILLATOR STRENGTH (Pg. 142, 152)

$$f_{ij} = \frac{2(\hat{n} \cdot x_{ij})^2 m \omega_{fi}}{\hbar} = \frac{2(\hat{n} \cdot P_{ij})^2}{m \hbar \omega_{if}}$$

$$\alpha_e(\omega) = \frac{4\pi^2 e^2}{2mna} \left(\frac{N_a}{V} \right) \sum_n f_{ne} \delta[\hbar\omega - \hbar \omega_{en}]$$

$$\int_0^\infty d\omega \; \alpha(\omega) = \frac{4\pi^2 e^2}{2mnc} \left(\frac{N_a}{V} \right) \sum_n f_{en}$$

3. f-SUM OR THOMUS-KUHN RULE

Z = # OF ELECTRONS $= \sum_n f_n$

4. POLARIZABILITY (Pg. 156)

$\alpha(\omega)$ = POLARIZABILITY

$$= \frac{2e^2}{\hbar^2} \sum_n (\underset{\sim}{r}_{ni} \cdot \underset{\sim}{r}_{in}) \frac{\omega_{ni}}{\omega_{ni}^2 - \omega_K^2}$$

D. LIGHT SCATTERING

1. RALEIGH SCATTERING (ELASTIC / BOUND PARTICLES)

BOTH FOR CLASSICAL (pg. 160) AND Q.M. (pg. 161)

$$\frac{d\sigma}{d\Omega} = \frac{\omega^4}{c^2}\langle \hat{n}_k \cdot \alpha \cdot \hat{n}_{k'} \rangle$$

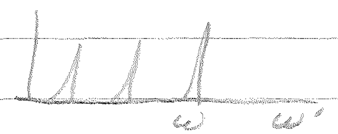
$$= \frac{\omega^4}{c^2}\langle \hat{n}_k \cdot \hat{n}_{k'} \rangle^2 \quad \text{FOR ISOTROPIC MEDIA}$$

2. RAMAN SCATTERING (pg. 164) (INELASTIC / BOUND)

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi\hbar c}\int_0^\infty k'^2 dk' \, \delta\left[\hbar c(k-k') + E_i - E_f\right](MV)^2$$

$$\frac{d\sigma^2}{d\Omega d\omega'} = \frac{\omega'^2}{4\pi^2\hbar^2 c^4}\,\delta\left[\omega - \omega' - \frac{E_f - E_i}{\hbar}\right]|MV|^2$$

M GIVEN ON pg. 164



FOR 2 PHOTON SCATTERING, M ON pg. 166

3. COMPTON SCATTERING (INELASTIC / FREE)

$$\frac{d\sigma}{d\Omega} = \frac{(\hbar\omega')^2}{4\pi^2\hbar^4 c^4}\left|V(k-k')\right|^2$$

IN CLASSICAL LIMIT

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2(\hat{n}_k \cdot \hat{n}_{k'}) \leftarrow \text{THOMPSON CROSS SECTION}$$

APP. I. NUMERICAL SOLUTION TO SCHRÖDINGER'S EQ'N (92)

A. $\psi(r,\theta,\phi) = R(r)\,Y_l^m(\theta,\phi)$; $\chi(r) = r R(r)$

$$A(r) = \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}\left[V(r) - E\right]$$

$$\frac{d^2}{dr^2}\chi = A(r)\,\chi(r) \Leftarrow \text{SCHRÖ'S EQ'N}$$

Δ = INCREMENT OF r

χ_i = VALUE OF χ AT $r = i\Delta$

A_i = " " A " "

$$Y_i = \chi_i - \frac{\Delta^2}{12} A_i \chi_i$$

THEN, TO ORDER Δ^6:

$$Y_{i+1} = Y_i\left[2 + \frac{A_i\Delta^2}{1 - \frac{A_i\Delta^2}{12}}\right] - Y_{i-1}$$

ASSUME Y_1. $Y_0 = 0$. χ GENERATED TO NORMALIZATION FACTOR

B. PHASE SHIFT (δ) AND NORMALIZATION FACTOR (D)

$$\tan\delta = -\frac{\chi_m \sin kr_i - \chi_i \sin kr_m}{\chi_m \cos kr_i - \chi_i \cos kr_m}$$

$$k = \sqrt{2mE/\hbar^2}$$

$$D = \chi_i / \sin(kr_i + \delta)$$

Y_ℓ^m

$Y_0^0 = \frac{1}{\sqrt{4\pi}}$

$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$

$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{\pm i\phi}$

$Y_2^0 = \sqrt{\frac{5}{16\pi}} \left[3\cos^2\theta - 1\right]$

$Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta \, e^{\pm i\phi}$

$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, e^{\pm i2\phi}$

$R_\ell^n \quad , \rho = \frac{r}{a}$

$R_0^1 = e^{-\rho}$

$R_0^2 = \left(1 - \frac{\rho}{2}\right) e^{-\rho/2}$

$R_1^2 = \rho \, e^{-\rho/2}$

$R_1^3 = \rho \, e^{-\rho/3} \left(1 - \frac{\rho}{6}\right)$

$R_2^3 = \rho^2 e^{-\rho/3}$

$$\begin{cases} \ell = 0, & 1, & 2, & \ldots \\ \downarrow & \downarrow & \downarrow & \\ s, & p, & d, & \ldots \end{cases}$$

THREE QUANTUM NUMBERS:

n

$\ell = 0, 1, 2, \ldots, n-1$

$m = 0, \pm 1, \pm 2, \ldots, \pm \ell$

A PARTICULAR STATE IS SIGNIFIED BY

$n \, \ell_m$

FOR EXAMPLE

$2s_1, 3s_0, 3d_{-1}$

CLEBSCH - GORDON COEFFICIENTS

Notation for basis states

$j = 1/2 \quad m = 1/2 \quad \alpha$

$\qquad\qquad -1/2 \quad \beta$

$j = 1 \quad m = 1 \quad U = -(x+iy)/\sqrt{2} = \sin\theta\, e^{i\phi}$

$\qquad\qquad 0 \quad V = z = \cos\theta$

$\qquad\qquad -1 \quad W = (x-iy)/\sqrt{2} = \sin\theta\, e^{-i\phi}$

$j > 1 \quad m \quad \chi(m)$

$1 \times \frac{1}{2}$	$\phi^{3/2}_{3/2}$	$\phi^{1/2}_{3/2}$	$\phi^{1/2}_{1/2}$	$\phi^{-1/2}_{3/2}$	$\phi^{-1/2}_{1/2}$	$\phi^{-3/2}_{3/2}$
$U\alpha$	1					
$U\beta$		$\sqrt{1/3}$	$\sqrt{2/3}$			
$V\alpha$		$\sqrt{2/3}$	$-\sqrt{1/3}$			
$V\beta$				$\sqrt{2/3}$	$\sqrt{1/3}$	
$W\alpha$				$\sqrt{1/3}$	$-\sqrt{\frac{2}{3}}$	
$W\beta$						1

$1/2 \times 1/2$	ϕ^1_1	ϕ^0_1	ϕ^0_0	ϕ^{-1}_1
$\alpha_1\alpha_1$	1			
$\alpha_1\beta_2$		$\sqrt{1/2}$	$\sqrt{1/2}$	
$\beta_1\alpha_2$		$\sqrt{1/2}$	$-\sqrt{1/2}$	
$\beta_1\beta_2$				1

m

ℓ

$|1,1\rangle = U$

$|1,0\rangle = V$

$|1,-1\rangle = W$

1×1	ϕ^2_2	ϕ^1_2	ϕ^1_1	ϕ^0_2	ϕ^0_1	ϕ^0_0	ϕ^{-1}_2	ϕ^{-1}_1	ϕ^{-2}_2
U_1U_2	1								
U_1V_2		$\sqrt{\frac{1}{2}}$	$\sqrt{1/2}$						
V_1U_2		$\sqrt{1/2}$	$-\sqrt{1/2}$						
U_1W_2				$\sqrt{1/6}$	$\sqrt{1/2}$	$\sqrt{1/3}$			
V_1V_2				$\sqrt{2/3}$	0	$-\sqrt{1/3}$			
W_1U_2				$\sqrt{1/6}$	$-\sqrt{1/2}$	$\sqrt{1/3}$			
V_1W_2							$\sqrt{1/2}$	$\sqrt{1/2}$	
W_1V_2							$\sqrt{1/2}$	$-\sqrt{1/2}$	
W_1W_2									1

P 6111

MAHAN RM. 161, OFFICE HOURS EVERY AFTERNOON

TEXT: QUANTUM MECHANICS, DAVYDOV, NEO PRESS

1/14/75

OTHER QUANTUM TEXTS:

1) LANDAU & LIFTSCHITS "NON-RELATIVISTIC QUANTUM MECHANICS"

2) SCHIFF "QUANTUM MECHANICS

3) MESSIAH, VOL I & II, "Q.M."

HAMILTONIAN OPERATOR

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

ASSUMPTIONS

1) ONE PARTICLE

2) $V(r)$ IS A FUNCTION OF ONLY r (POSITION)

3) $p = \frac{\hbar}{i}\nabla$

4) NON-RELATIVISTIC

SCHROEDINGER'S EQUATION

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = H\psi(r,t)$$

$\psi(r,t)$ = WAVE FUNCTION

IF ONE CAN SOLVE

$$H\phi_n(r) = E_n\phi_n(r)$$

(EIGENVALUE PROBLEM)

E_n = EIGEN VALUE

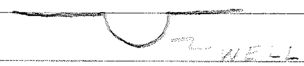
ϕ_n : VECTOR SPACES

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E_n\right]\phi_n(r) = 0$$

$$\psi(r,t) = \sum_n a_n\phi_n(r)\, e^{-itE_n/\hbar}$$

PLUG INTO SCHROEDINGER'S EQ.

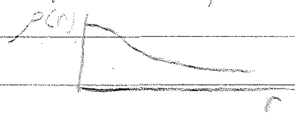
a_n'S DETERMINED BY INITIAL CONDITIONS & BNDRY CONDITIONS

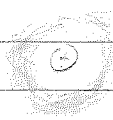


STATISTICALLY: $a_n = \dfrac{e^{-E_n/k_BT}}{\sum_n e^{-E_n/kT}}$

$|\psi(x,t)|^2 = \psi(x,t)\psi^*(r,t) = \rho(r,t)$ ⇐ PROBABILITY DENSITY

CONSIDER ATOM





$1 = \int \rho(r,t)\, d^3r$ ⇐ NORMALIZING WAVE FUNCTION

EIGEN FUNCTION PROPERTIES:

1. $\phi_n(r)$ FORMS ORTHONORMAL SET

$$\int \phi_n^*(r)\phi_m(r)\, d^3r = \begin{Bmatrix} 1 & ; n=m \\ 0 & ; \text{OTHERWISE} \end{Bmatrix} = \delta_{nm}$$

2. COMPLETENESS:

$$\sum_n \phi_n^*(r)\,\phi_n(\underset{\sim}{r}')\, d^3r = \begin{Bmatrix} 0 & ; r \neq r' \\ \infty & ; r = r' \end{Bmatrix} = \delta(r-r')$$

THEN ANY FUNCTION $f(r) = \sum_n b_n \phi_n(r)$

$$b_n = \int d^3r'\, f(r')\,\phi_n^*(r)$$

$$\Rightarrow f(r) = \sum_n \int d^3r' f(r')\,\phi_n^*(r)\;\phi_n(r)$$

$$= \sum_n \int d^3r'\, f(r')\left[\phi_n^*(r')\,\phi_n(r)\right]$$

$$= \begin{Bmatrix} 0 & ; r \neq r' \\ f(r) & ; r = r' \end{Bmatrix}$$

WAVE FUNCTION AGAIN:

$$1 = \sum_{nm} a_n^* a_m\, e^{\frac{-it}{\hbar}(E_n - E_m)} \int \phi_n^*(r)\phi_m(r)\, d^3r$$

$$\Rightarrow 1 = \sum_n |a_n|^2$$

$$\Rightarrow \psi(r,t) = \sum_n a_n \phi_n e^{-itE_n/\hbar}$$

KNOWING a_n & ϕ_n, WE CAN GET

1. $\rho(r,t)$
2. EXPECTATION VALUES

$$\langle F(r,t)\rangle = \int d^3r\, F(r)\rho(r,t)$$

EX: 1. $\langle r(t)\rangle = \int d^3r\, \underset{\sim}{r}\, \rho(r,t)$

2. $\langle V(r)\rangle = \int d^3r\, V(r)\rho(r,t) \Rightarrow$ V IS POTENTIAL ENERGY

3. CONSIDER:

$$\left\langle \frac{dr}{dt}\right\rangle = \int d^3r \left(\frac{\delta r}{\delta t}\right)\rho(r,t) \Leftarrow \text{NOT DEFINED}$$

$$\frac{d}{dt}\langle r\rangle = \text{VELOCITY}$$

$$= \int d^3r\, \underset{\sim}{r}\, \frac{\delta}{\delta t}\rho(r,t)$$

$$\frac{\delta}{\delta t}\rho(r,t) = \frac{\delta}{\delta t}\psi\psi^* = \left(\frac{\delta}{\delta t}\psi^*\right)\psi + \psi^*\left(\frac{\delta\psi}{\delta t}\right)$$

FROM SCHR. EQ: $\frac{\delta\psi}{\delta t} = \frac{1}{i\hbar}H\psi$

$\frac{\delta\psi^*}{\delta t} = -\frac{1}{i\hbar}H\psi^*$ (FOR OUR PURPOSE $H=H^*$ & $V=V^*$)

$$\therefore \frac{\delta}{\delta t}\rho(r,t) = \frac{-1}{i\hbar}\left[\psi H\psi^* - \psi^* H\psi\right]$$

$$= -\frac{1}{i\hbar}\left[\psi\left(\frac{p^2}{2m}+V\right)\psi^* - \psi^*\left(\frac{p^2}{2m}+V\right)\psi\right]$$

$$= -\frac{i\hbar}{2m}\left[\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right]$$

$$= -\frac{i\hbar}{2m}\nabla\cdot\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right]$$

EQUATION OF CONTINUITY

$$\Rightarrow \frac{\delta\rho}{\delta t} + \nabla\cdot J = 0$$

$$\Rightarrow J = \frac{\hbar}{2mi}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]$$

PARTICLE CURRENT OPERATOR

BACK TO FINDING $\frac{d}{dt}\langle r\rangle$

$$\frac{\delta}{\delta t}\langle r\rangle = \int d^3r\, \underset{\sim}{r}\, \frac{\hbar}{2mi}\left[\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right]$$

$$\int d^3r\, A\nabla^2 B = \int d^3 B\nabla^2 A + \underbrace{\text{SURFACE INTEGRALS}}_{\to 0}$$

$$A = r\psi\ ;\ B = \psi^*$$

$$\int d^3r\, \nabla\cdot(A\nabla B) = \int d^3r\left[\nabla A\cdot\nabla B + A\nabla^2 B\right]$$

(NOTE $\nabla^2 r = 0$)

$$(\nabla\psi\cdot\nabla)r = \nabla\psi$$

+ GARBAGE

$$\frac{\delta}{\delta t}\langle r\rangle = \frac{\hbar}{mi}\int d^3r\,\psi^*\nabla\psi = \frac{1}{m}\int d^3r\,\psi^*\frac{\hbar\nabla}{i}\psi$$

$$p = \hbar\nabla/i$$

$$\Rightarrow \frac{\delta}{\delta t}\langle r\rangle = \frac{\langle p\rangle}{m} = \text{VELOCITY}$$

SCHROEDINGER REPRESENTATION

a. WAVE FUNCTIONS DEPEND ON TIME.

b. OPERATORS DO NOT DEPEND ON TIME

HEISENBURG REPRESENTATION

a. WAVE FUNCTIONS DO NOT DEPEND ON TIME

b. OPERATORS DO DEPEND ON TIME

SCHRO: $\psi(r,t) = \sum_n a_n \phi_n(r) e^{-i t E_n/\hbar}$.

HEISEN: $= \psi(r,t) = e^{-i \frac{H}{\hbar} t} \sum_n a_n \phi_n(r)$

$$\Rightarrow e^{-i \frac{H}{\hbar} t} = \sum_l \frac{1}{l!} \left(-\frac{it}{\hbar} H\right)^l$$

$$H^l \phi_n = E_n^l \phi_n$$

$\langle O \rangle \Rightarrow O$ IS ANY OPERATOR

$$\langle O \rangle = \int d^3r\, \psi^*(r,t)\, O\, \psi(r,t)$$

$$\psi(r,t) = e^{-iHt/\hbar} \psi(r) \Rightarrow \psi(r) = \psi(r,0)$$

$$\psi(r) = \sum_n a_n \phi_n(r)$$

$(ABCD)^\dagger = D^* C^* B^* A^* \Rightarrow \dagger$ DENOTES HERMITIAN CONJUGATE

$$\psi^*(r,t) = \psi^*(r) e^{iHt/\hbar}$$

THUS:

$$\langle O \rangle = \int d^3r\, \psi^*(r,t)\, O\, \psi(r,t) \quad \leftarrow (\text{SHRO})$$

$$= \int d^3r\, \psi^*(r)\, O(t)\, \psi(r) \quad \leftarrow (\text{HEISEN})$$

$$\Rightarrow O(t) = e^{iHt/\hbar}\, O\, e^{-iHt/\hbar}$$

CONSIDER: $\frac{\delta}{\delta t} \langle O \rangle = \int dr^3\, \psi^*(r)\, e^{iHt/\hbar} \left[\frac{iH}{\hbar} O - O\frac{iH}{\hbar}\right] e^{\frac{-itH}{\hbar}} \psi(r)$

$(H e^{iH} = e^{i \cdots} H)$

$$\Rightarrow \frac{\delta}{\delta t} \langle O \rangle = \frac{i}{\hbar} \langle [H, O] \rangle$$

$$[A, B] = AB - BA$$

$$\{A, B\} = AB + BA$$

FOR HEIS: $O(t) = e^{iHt/\hbar}\, O\, e^{-iHt/\hbar}$

$$\frac{\delta O}{\delta t} = \frac{i}{\hbar} e^{iHt/\hbar} [H, O] e^{-itH/\hbar} = \frac{i}{\hbar} [H, O(t)]$$

$$\Rightarrow \frac{\delta}{\delta t} \langle O \rangle = \left\langle \frac{\delta}{\delta t} O \right\rangle$$

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REVIEW

S. EQ $\Rightarrow i\frac{\delta}{\delta t}\psi = H\psi$

$$\rho(r,t) = |\psi(r,t)|^2$$

$$J(r,t) = \frac{\hbar}{2mi}\left[\psi^* \nabla \psi - \psi \nabla \psi^*\right]$$

$$\langle F \rangle = \int d^3r \ \psi^*(r,t)\, F(r)\, \psi(r,t)$$

NON-COMMUTING OPERATORS

EX: $x, \quad p_x = \frac{\hbar}{i}\frac{\delta}{\delta x}$

$[x, p_x] = i\hbar \Rightarrow$ ANY FUNCTION OF $x \quad f(x)$,

$[x, p_x] f$

$$x \frac{\hbar}{i}\frac{\delta}{\delta x} f - \frac{\hbar}{i}\frac{d}{dx} x f = \frac{x\hbar}{i}\frac{df}{dx} - \frac{\hbar}{i}\left[x \frac{d}{dx} f + f\right] = i\hbar$$

EX. $q(x, p_x) = \sqrt{a x^2 + b p_x^2}$

$$= \sqrt{b}\, p_x \left[1 + \frac{a^2}{b p_x}\right]^{1/2}$$

$$= 1 + \frac{1}{2}\frac{a}{b}\frac{x^2}{p_x^2} + \dots$$

$$\frac{x^2}{p_x^2} = \frac{x^2}{d^2/dx^2} = \ ?$$

UNDEFINED

EX: $e^{ax + bp_x} = 1 + (ax + bp) + \frac{1}{2!}(ax + bp_x)^2 + \dots$

PLANE WAVE: $H = \frac{p^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2$

$$\psi = e^{i k \cdot r}$$

$$k = (k_x, k_y, k_z)$$

$E = \hbar^2 k^2 / 2m \quad \Leftarrow$ SOLVES $H\psi = E\psi$

IF TWO OPERATORS COMMUTE, THEN ONE CAN DEFINE SIMULTANEOUS EIGENVALUES & EIGENVECTORS

EX: $p_x = \frac{\hbar}{i}\frac{\delta}{\delta x}$

$[p_x, H] = 0$ ie (p_x & H COMMUTE)

$$p_x \psi = \hbar k_x \psi$$

EX: ANGULAR MOMENTUM OPERATOR:

$$L_z = x p_y - y p_x$$

$$L_x = y p_z - z p_y$$

$$L_z = x p_z - z p_x$$

PROOVE: $0 = [p^2, L_z] = [p_x^2, L_z] + [p_y^2, L_z] + [p_z^2, L_z]$

NO z's

(CONT)

$$[p_x^2, L_z] = p_x^2 L_z - L_z p_x^2 + p_x L_z p_x - p_x L_z p_x$$
$$= p_x [p_x, L_z] + [p_x, L_z] p_x$$

NOW $[x, p_x] = i\hbar$

$[p_x, x] = -i\hbar$

$$\Rightarrow [p_x^2, L_z] = -2i\hbar\, p_x p_y$$

SIMILARLY:

$$[p_y^2, L_z] = 2i\hbar\, p_x p_y$$
$$\Longrightarrow [p^2, L_z] = 2i\hbar\, p_x p_y$$

THUS:

$$[H, L_z] = 0$$
$$[p_x, L_z] \neq 0$$
$$[p_x, H] = 0$$

SPHERICAL CO-ORDINATES

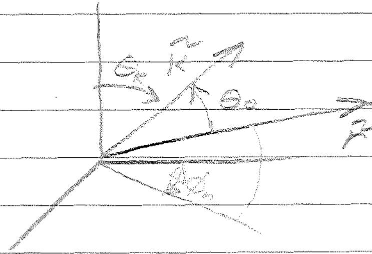
$$x = r \sin\theta \cos\phi$$
$$y = r \sin\theta \sin\phi$$
$$z = r \cos\theta$$

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum i^l (2l+1) \times P_l(\cos\theta_0)\, J_l(kr)$$

AT (IT TURNS OUT);

$$L_z = \frac{\hbar}{i}\frac{\delta}{\delta\phi}$$

$$L_z e^{im\phi} = \hbar m e^{im\phi}$$



$$(2l+1) P_l(\cos\theta_0) = \sum_{m=-l}^{l} Y_{lm}(\theta_r, \phi_r) Y^*_{lm}(\theta_k, \phi_k)$$

P_l : LEGENDRE

l	
0	1
1	$\cos\theta$
2	$\frac{1}{2}(3\cos^2\theta - 1)$

$$Y_{lm} = N_{lm}\, e^{im\phi}\, P_l^{|m|}(\cos\theta)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\phi\, Y_{lm}^2 = 1$$

$\psi_{k\ell m} = J_\ell(kr)\, Y_{\ell m}(\theta,\phi)$

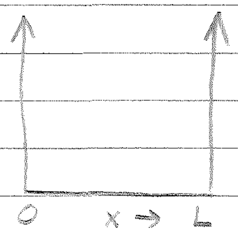
$H\psi = E\psi$

$L_z\psi = \hbar m\psi$

$e^{ik\cdot r} = \sum_{\ell m} C_{\ell m}\, J_\ell(kr)\, Y_{\ell m}(\theta_r,\phi_r)$

ONE DIMENSIONAL EX

(1)



$V(x) = 0$ IF $0 \leq x \leq L$
$= \infty$ IF $x<0,\ x>0$

$\frac{\hbar}{2m}\frac{\delta^2}{\delta x^2}\psi(x) = E\psi(x)$ IF $0<x<L$

SOLUTION:

$\psi(x) = Ae^{ikx} + Be^{-ikx}$; $E = \frac{\hbar^2 k^2}{2m}$

OUTSIDE BOX, $\psi(x) = 0$

$\psi(L) = \psi(0) = 0$

CONSIDER, THEN

$\psi(x) = A\sin(kx) \Rightarrow \psi(0) = 0$

$\sin(kl) = 0 \Rightarrow k = \frac{n\pi}{\ell} \Rightarrow \psi(L) = 0$

LET $\psi_n(x) = A\sin(n\pi x/L)$

NOW

$\int_0^L dx\, \psi_n(x)\,\psi_m(x) = \delta_{ij}$

$A^2\int_0^L dx \sin^2(kx) = \frac{1}{2}A^2L = 1 \Rightarrow A = \sqrt{2/L}$

THEN: $\psi_n = \sqrt{2/L}\,\sin\left(\frac{n\pi x}{L}\right)$

$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$

$$\psi_{klm} = J_l(kr)\, Y_{lm}(\theta,\phi)$$

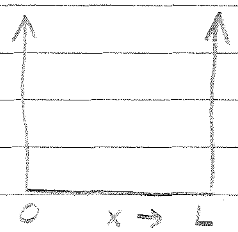
$$H\psi = E\psi$$

$$L_z\psi = \hbar m \psi$$

$$e^{ik\cdot r} = \sum_{lm} C_{lm} J_l(kr)\, Y_{lm}(\theta_r, \phi_r)$$

ONE DIMENSIONAL EX

(1)



$$V(x) = 0 \quad \text{IF} \quad 0 \le x \le L$$
$$= \infty \quad \text{IF} \quad x < 0,\ x > 0$$

$$\frac{\hbar}{2m}\frac{\delta^2}{\delta x^2}\psi(x) = E\psi(x) \qquad \text{IF} \quad 0 < x < L$$

SOLUTION:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \,;\quad E = \frac{\hbar^2 k^2}{2m}$$

OUTSIDE BOX $\psi(x) = 0$

$$\psi(L) = \psi(0) \overset{!}{=} 0$$

CONSIDER, THEN

$$\psi(x) \overset{!}{=} A \sin(kx) \Rightarrow \psi(0) = 0$$

$$\sin(kl) = 0 \Rightarrow k = \frac{n\pi}{L} \Rightarrow \psi(L) = 0$$

LET $\psi_n(x) = A \sin(n\pi x/L)$

NOW

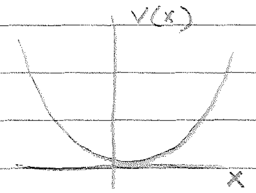
$$\int_0^L dx\, \psi_n(x)\, \psi_m(x) = \delta_{ij}$$

$$A^2\int_0^L dx \sin^2(kx) = \tfrac{1}{2}A^2 L = 1 \Rightarrow A = \sqrt{2/L}$$

THEN: $\psi_n = \sqrt{2/L}\,\sin\left(\frac{n\pi x}{L}\right)$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

② HARMONIC OSCILLATOR



$$V(x) = \frac{K}{2} x^2$$

$$\left[\frac{-\hbar^2}{2m} \frac{\delta^2}{\delta x^2} + \frac{K}{2} x^2 \right] \psi(x) = E\,\psi(x)$$

LET $\omega = \sqrt{K/m}$ $\qquad \frac{K}{m} = \frac{erg}{cm^2\,gm} = \frac{gm\,cm^2}{sec^2\,gm}\frac{1}{cm^2} = \frac{1}{sec^2}$

$\Rightarrow K = \omega^2 m$ $\qquad \hbar \sim erg \times sec$

$x_0 = \sqrt{\hbar/m\omega} = \left[\frac{\hbar^2}{mK} \right]^{1/4}$ $\qquad \frac{gm\,cm^2}{sec\;gm^2/sec} = cm$

$$\xi = x/x_0$$

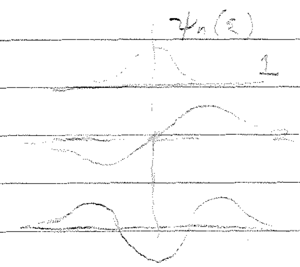
$$\left[\frac{-\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + \frac{\omega^2 m}{2} - E \right] \psi = 0$$

$$\left[-\frac{1}{2}\frac{\hbar}{m\omega}\frac{\delta^2}{\delta x^2} + \frac{1}{2}\frac{\omega m}{\hbar} - \frac{E}{\hbar\omega} \right] \psi = 0$$

$$\left[-\frac{1}{2} x_0^2 \frac{\delta^2}{\delta x^2} + \frac{1}{2}\frac{x^2}{x_0^2} - \frac{E}{\hbar\omega} \right] \psi = 0$$

$$\left[-\frac{\delta^2}{\delta \xi^2} + \xi^2 - \frac{2E}{\hbar\omega} \right] \psi = 0$$

GIVES SOLUTION:



$$\psi_n(\xi) = N_n e^{-\xi^2/2} H_n(\xi)$$

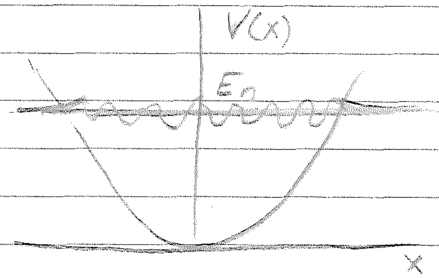
$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$N_n = \frac{1}{\sqrt{2^n\, n!\, \sqrt{\pi}}}$$

n	$H_n(\xi)$ → HERMITE POLYNOMIALS
0	1
1	2ξ
2	$4\xi^2 - 2$
⋮	⋮
n	$(-1)^n e^{\xi^2} \frac{\delta^n}{\delta\xi^n} e^{-\xi^2}$

(CONT)

NOW: $\int_{-\infty}^{\infty} d\xi \, \psi_n(\xi)\psi_m(\xi) = \delta_{nm}$ ← IS TRUE



a. MATRIX ELEMENT

$$\langle n | x | \ell \rangle = \int_{-\infty}^{\infty} dx \; \phi_n(x) \, x \, \phi_\ell(x)$$

ACTUAL EIGEN FUNCTION $\rightarrow \phi_n(x) = \frac{1}{\sqrt{x_0}} \psi_n(x/x_0) = \psi_n(\xi)$

$$\int_{-\infty}^{\infty} dx \; \phi_n(x)\phi_\ell(x) = \int_{-\infty}^{\infty} d\xi \, \psi_n(\xi)\,\psi_\ell(\xi) = \delta_{n\ell}$$

$$= \int_{-\infty}^{\infty} \frac{dx}{x_0} \psi_n(\xi)\,\psi_\ell(\xi)$$

$$H_{n+1}(\xi) = (-1)^{n+1} e^{\xi^2} \frac{d^{n+1}}{d\xi^{n+1}} e^{-\xi^2}$$

$$= (-1)^{n+1} e^{\xi^2} \frac{d^n}{d\xi^n}\left[\frac{d}{d\xi} e^{-\xi^2}\right]$$

$$= (-1) e^{\xi^2} \frac{d^n}{d\xi^n} (-2)\xi e^{-\xi^2}$$

$$= (-1)^{n+1}(-2) \, e^{\xi^2} \frac{d^n}{d\xi^n}\left(\xi e^{-\xi^2}\right)$$

NOW $\frac{d}{d\xi} \xi e^{-\xi^2} = e^{-\xi^2} + \xi \frac{d}{d\xi} e^{-\xi^2}$

$$\frac{d^2}{d\xi^2} \xi e^{-\xi^2} = \frac{d}{d\xi}\left[\quad\right]$$

$$= 2\frac{d}{d\xi} e^{-\xi^2} + \xi \frac{d}{d\xi^2} e^{-\xi^2} \quad \text{ETC}$$

$$\vdots$$

$$\frac{d^n}{d\xi^n} \xi e^{-\xi^2} \triangleq n \frac{d^{n-1}}{d\xi^{n-1}} e^{-\xi^2} + \xi \frac{d^n}{d\xi^n} e^{-\xi^2}$$

PUT IT ALL TOGETHER:

$$H(\xi) = -2(-1)^{n+1}\left[n e^{\xi^2} \frac{d^{n-1}}{d\xi^{n-1}} e^{-\xi^2} + \xi e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}\right]$$

$$\therefore \xi H_n = n H_{n-1} + \frac{1}{2} H_{n+1}$$

BACK TO

$$\langle n|x|\ell\rangle = x_0\int_{-\infty}^{\infty}\frac{dx}{x_0}\,\psi_n(\xi)\;\frac{x}{x_0}\,\psi_\ell(\xi)$$

$$= x_0\int d\xi\,\psi_n(\xi)\;\xi\;\psi_\ell(\xi)$$

NOW $\xi\psi_n(\xi) = N_n e^{-\xi^2/2}\,\xi H_n(\xi)$

$$= N_n e^{-\xi^2/2}\left[n H_{n-1} + \tfrac{1}{2} H_{n+1}\right]$$

$$= \sqrt{\tfrac{n}{2}}\,\psi_{n-1} + \sqrt{\tfrac{n+1}{2}}\,\psi_{n+1}$$

$$\therefore \langle n|x|\ell\rangle = x_0\int_{-\infty}^{\infty} d\xi\left[\sqrt{\tfrac{n}{2}}\,\psi_{n-1} + \sqrt{\tfrac{n+1}{2}}\,\psi_{n+1}\right]\psi_\ell \leftarrow \psi_n \text{ ORTHONORMAL!}$$

$$= x_0\left[\sqrt{\tfrac{n}{2}}\,\delta_{\ell,n-1} + \sqrt{\tfrac{n+1}{2}}\,\delta_{\ell,n+1}\right]$$

b. MATRIX ELEMENT

$$\langle n|p_x|\ell\rangle = \frac{\hbar}{i x_0}\int d\xi\,\psi_n\,\frac{\delta}{\delta\xi}\,\psi_\ell$$

$$\frac{\delta}{\delta\xi}H_n(\xi) = (-1)^n\frac{d}{d\xi}\left(e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2}\right)$$

$$= (-1)^n\left[2\xi e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2} + e^{\xi^2}\frac{d^{n+1}}{d\xi^{n+1}}e^{-\xi^2}\right]$$

$$= 2\xi H_n - H_{n+1} - 2n H_{n-1}$$

NOW $\xi H_n = n H_{n-1} + \tfrac{1}{2} H_{n+1}$

$$\frac{\delta}{\delta\xi}\psi_n(\xi) = \sqrt{n/2}\,\psi_{n-1} - \sqrt{\tfrac{n+1}{2}}\,\psi_{n+1}$$

$$\therefore \langle n|p|\ell\rangle = \frac{\hbar}{i x_0}\left[\sqrt{n/2}\,\delta_{\ell,n-1} - \sqrt{\tfrac{n+1}{2}}\,\delta_{\ell,n+1}\right]$$

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REVIEW

$$\xi = x/x_0 \Rightarrow x_0 = \sqrt{\hbar/m\omega} \; ; \; \omega = \sqrt{k/m}$$

THEN

$$\xi \psi_n(\xi) = \sqrt{\tfrac{n}{2}}\, \psi_{n-1}(\xi) + \sqrt{\tfrac{n+1}{2}}\, \psi_{n+1}(\xi)$$

$$\frac{d}{d\xi} \psi_n(\xi) = \sqrt{n/2}\, \psi_{n-1}(\xi) - \sqrt{\tfrac{n+1}{2}}\, \psi_{n+1}(\xi)$$

ADDING:

$$\left(\xi + \frac{d}{d\xi}\right) \psi_n(\xi) = \sqrt{2n}\, \psi_{n-1}(\xi)$$

LET $a = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right) \Rightarrow \underline{a\psi_n(\xi) = \sqrt{n}\, \psi_{n-1}(\xi)}$

a IS CALLED $\begin{cases} \text{LOWERING OPERATOR} \\ \text{DESTRUCTION OPERATOR} \end{cases}$

SUBTRACTING:

$$\left(\xi - \frac{d}{d\xi}\right) \psi_n(\xi) = \sqrt{2(n+1)}\, \psi_{n+1}(\xi)$$

LET $a^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right) \Rightarrow \underline{a^+ \psi_n(\xi) = \sqrt{n+1}\, \psi_{n+1}(\xi)}$

a^+ IS CALLED $\begin{cases} \text{RAISING OPERATOR} \\ \text{CREATING OPERATOR} \end{cases}$

(a^+ IS THE HERMITIAN CONJUGATE OF a)

$$a\psi_0 = 0$$
$$a^+ \psi_0 = \psi_1$$
$$(a^+)^2 \psi_0 = a^+(a^+\psi_0) = a^+\psi_1 = \sqrt{2}\, \psi_2$$
$$\vdots$$
$$(a^+)^n \psi_0 = \sqrt{n!}\, \psi_n \Rightarrow \underline{\psi_n = \frac{1}{\sqrt{n!}} (a^+)^n \psi_0}$$

NOTATION: $\psi_0 = |0\rangle$

$\psi_n = |n\rangle$

PROOF: $\xi = \frac{1}{\sqrt{2}}(a + a^+) = \frac{x}{x_0}$

$$\Rightarrow x = \frac{x_0}{\sqrt{2}}(a + a^+)$$

$$a = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + x_0 \frac{\partial}{\partial x}\right) = \frac{1}{\sqrt{2}} x_0 \left(\frac{x}{x_0^2} + \frac{i}{\hbar} p_x\right)$$

$$a = \frac{1}{\sqrt{2}} \frac{i}{\hbar} \sqrt{\hbar/m\omega}\, (p_x - i m\omega x)$$

AND $a^+ = \frac{-i}{\sqrt{2\hbar m\omega}}(p_x + i m\omega x)$

NOW $x = x^+$ & $p_x^+ = p_x \Leftarrow$ BOTH HERMITIAN

CONSIDER

$$\langle n|x|m\rangle^* = \langle m|x^+|n\rangle = \langle m|x|n\rangle \Rightarrow x \text{ IS HERMITIAN}$$

TO SHOW p IS HERMIT. CONJ. WE GOTTA SHOW

$$\langle n|p|m\rangle^* = \langle m|p|x\rangle$$

$$\langle n|p|m\rangle = \int dx (\psi_n\, p\, \psi_m)$$ ← DONE BY PARTS INTEGR. THE SURFACE

$$= \tfrac{\hbar}{i}\int dx\, \psi_n^* (\tfrac{d}{dx}\psi_m) = -\tfrac{\hbar}{i}\int dx\, \psi_m \tfrac{d}{dx}\psi_n^*$$

$$\langle n|p|m\rangle^* = \hbar/i \int dx\, \psi_m^* (\tfrac{d}{dx}\psi_n)$$

$$= \langle m|p|n\rangle$$

NOTE: $\frac{d}{dx}$ IS NOT HERMITIAN $(\frac{d}{dx}^+ = -\frac{d}{dx})$

$(ABC)^+ = C^+B^+A^+$ IF A IS FUNCTION, $A^+ = A^*$

$$\langle n|p|m\rangle = \int dx\, [\psi_n^* p\, \psi_m]^+ = \int dx\, \psi_m^*\, p^+\, \psi_n$$

NOTE: $(a^+)^+ = a$

FEYNMAN'S THEM

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$$ ⇒ A & B ARE OPERATORS

$$F = [A,B]$$

TRUE IF: $[F,A] = [F,B] = 0$

COMMON CASE: F = CONSTANT

PROOF:

$$e^{A+B} = 1 + (A+B) + \tfrac{1}{2}(A+B)(A+B) + \ldots$$

$$= 1 + A + B + \tfrac{1}{2}(A^2 + B^2 + BA + AB) + \ldots$$

$$= 1 + A + B + \tfrac{1}{2}(A^2 + B^2 + 2AB + BA - AB) + \ldots$$

$$= 1 + A + \tfrac{1}{2}A^2 + B + \tfrac{1}{2}B^2 + AB - \tfrac{1}{2}[A,B] + \ldots$$

$$= [1 + A + \tfrac{1}{2}A^2 + \ldots][1 + B + B^2/2 + \ldots][1 - \tfrac{1}{2}[A,B] + \ldots]$$

$$= e^A e^B e^{-\frac{1}{2}[A,B]}$$

$$\Rightarrow \langle n|e^{iqx}|m\rangle$$

$$x = \tfrac{x_0}{\sqrt{2}}(a + a^+)$$

$$\Rightarrow iqx = i\left(\tfrac{x_0 q}{\sqrt{2}}\right)(a + a^+)$$

$$= i\lambda(a + a^+)$$

$A = i\lambda a^+,\ B = i\lambda a$

$$[A,B] = i\lambda^2 [a, a^+] = \lambda^2$$

$$\Rightarrow e^{i\lambda(a+a^+)} = e^{-\frac{1}{2}\lambda^2} e^{i\lambda a^+} e^{i\lambda a}$$

PROOF: $[a, a^+] = \left[\frac{1}{\sqrt{2\hbar m\omega}}(p - im\omega x), \frac{1}{\sqrt{2\hbar m\omega}}(p + im\omega x)\right]$

$= \frac{1}{2\hbar m\omega}\left[im\omega[p_x, \overset{-i\hbar}{x}] - im\omega[x, \overset{i\hbar}{p}]\right] = 1$

$$e^{i\lambda a}|m\rangle = \sum_{\ell=0}^{\infty} \frac{(i\lambda)^\ell}{\ell!} a^\ell |m\rangle$$

$a^\ell |m\rangle = ?$

$a|m\rangle = \sqrt{m}\,|m-1\rangle$

$a^2|m\rangle = \sqrt{m(m-1)}\,|m-2\rangle$

$\vdots$

$a^\ell|m\rangle = \sqrt{\frac{m!}{(m-\ell)!}}\,|m-\ell\rangle$ FOR $m \geq \ell$

$$e^{-\frac{\lambda^2}{2}}\langle n|e^{i\lambda a^+} e^{i\lambda a}|m\rangle$$

$\left[e^{-i\lambda a}|n\rangle\right]^+ = \langle n|e^{i\lambda a^+}$

$\left[\sum_n \frac{(-i\lambda)^\alpha}{\alpha!}\frac{\sqrt{n!}}{\sqrt{(n-\alpha)!}}|n-\alpha\rangle\right]^+ = \sum_{\alpha=0} \frac{(i\lambda)^\alpha}{\alpha!}\sqrt{\frac{n!}{(n-\alpha)!}}\langle n-\alpha|$

$= e^{-\lambda^2/2}\sum_{\alpha\ell}\frac{(i\lambda)^{\alpha+\ell}}{\alpha!\,\ell!}\sqrt{\frac{m!}{(m-\ell)!}}\sqrt{\frac{n!}{(n-\alpha)!}}\langle n-\alpha|m-\ell\rangle$

$\langle n-\alpha|m-\ell\rangle = \delta_{n-\alpha, m-\ell} = \int \psi_{n-\alpha}\psi_{m-\ell}$

FOR $n > m$, $\alpha = n - m + \ell$

$= e^{-\lambda^2/2}\sum_\ell \frac{(i\lambda)^{\ell+n-m+\ell}}{\ell!\,(n-m+\ell)!}\sqrt{\frac{n!\,m!}{(m-\ell)!^2}}$

$= (i\lambda)^{n-m} e^{-\lambda^2/2}\sqrt{m!/n!}\; L_m^{n-m}(\lambda^2)$

L_m^{n-m} IS A LAGUERRE POLYNOMIAL

③ LINEAR POTENTIAL

TYPICALLY IN CONSTANT EL. FIELD F

$$V(x) = eFx$$

IN GRAVITATIONAL POTENTIAL

SCH. EQ:

$$\left[-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + eFx - E\right]\psi(x) = 0$$

$$\left[\frac{\hbar^2}{2meF}\frac{\delta^2}{\delta x^2} - \left(x - \frac{E}{eF}\right)\right]\psi(x) = 0$$

LET $\xi = \left(x - \frac{E}{eF}\right)\left(\frac{2meF}{\hbar^2}\right)^{\frac{1}{3}}$

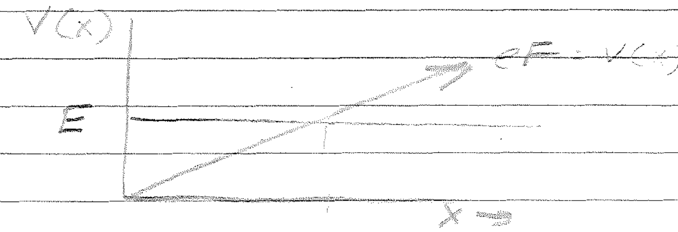
$$\left(\frac{d^2}{d\xi^2} - \xi\right)\psi = 0 \Leftarrow \text{AIRY'S EQ'N}$$

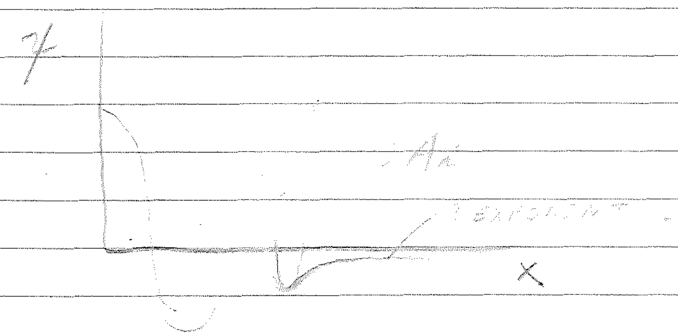
GENERATES AIRY FUNCTIONS:

$$\psi(x) = c_1 A_i(\xi) + c_2 B_i(\xi)$$

$$A_i(\xi) = \frac{1}{\pi}\int_{-\infty}^{\infty} dt \cos\left(\xi t + t^3/3\right) \sim$$

B_i IS PHYSICALLY UNREASONABLE





$$B_i(\xi) = \frac{1}{\pi}\int_0^{\infty}\left[e^{z\xi - \frac{1}{3}z^3} + \sin\left(z\xi + \frac{1}{3}z^3\right)\right]dz$$

SHOW THAT $c_i A_i = \psi$ SATISFIES D.E.

$$\frac{d}{d\xi} A_i = \frac{-1}{\pi}\int_0^\infty dt\; t \sin(\xi t + t^3/3)$$

$$\frac{d^2}{d\xi^2} A_i = -\frac{1}{\pi}\int_0^\infty dt\; t^2 \cos(\xi t + t^3/3)$$

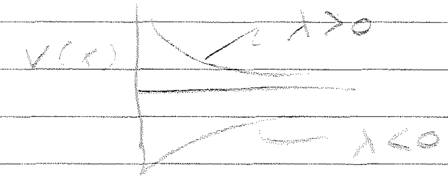
$$\left(\frac{d^2}{d\xi^2} - \xi\right) A_i = -\frac{1}{\pi}\int_0^\infty dt\,(t^2-\xi)\cos(\xi t + t^3/3)$$

$$= \frac{d}{dt}\sin(\xi t + t^3/3)$$

$$= -\frac{1}{\pi}\sin(\xi t + t^3/3)\Big|_0^\infty = 0$$

④ EXPONENTIAL POTENTIAL

$$V(x) = \lambda e^{-2x/a} \quad \Rightarrow$$



$$\left[-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + \lambda e^{-2x/a} - E\right]\psi(x) = 0$$

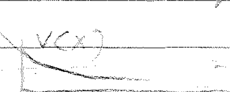
TRICK IS TO LET $Y = e^{-x/a}$; $\frac{d}{dx} = \frac{dY}{dx}\frac{d}{dY} = -\frac{Y}{a}\frac{d}{dY}$

$$\frac{d^2}{dx^2} = \frac{d}{dx}\left(-\frac{Y}{a}\frac{d}{dY}\right) = \frac{Y^2}{a^2}\frac{d^2}{dY^2} + \frac{Y}{a^2}\frac{\delta}{\delta Y}$$

SUBSTITUTING GIVES

$$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} - \frac{2ma^2\lambda Y^2}{\hbar^2} + \frac{2ma^2E}{\hbar^2}\right]\psi(x) = 0$$

a. FOR $\lambda > 0 \Rightarrow$



NO SOLUTIONS FOR $E<0$

THUS, WE MUST HAVE $E \geq 0$

FOR LARGE X, $V(x) \approx 0$, AND SOLUTION IS $\sin kx$ OR $\cos kx$ $\ni k^2 = 2mE/\hbar^2$

ψ WILL DECAY WHEN $V(x) \geq E$

$$k^2 = 2m\;E/\hbar^2 \qquad k_0^2 = 2m\;\lambda/\hbar^2$$

$$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} - 2a^2k_0^2Y^2 + 2a^2k^2\right]\psi(x) = 0$$

$$\psi = C_1 I_{ika}(ak_0Y) + C_2 I_{-ika}(ak_0Y)$$

BOUNDRY CONDITIONS

1. AS $x \to -\infty$, $\psi = 0$, $Y = e^{-x/a} \to +\infty$

$$\lim_{z\to\infty} I_\nu(z) = \frac{e^{z}}{\sqrt{2\pi z}}\left[1 + O\left(\frac{1}{z}\right)\right]$$

THE B.C. GIVES

$$\psi = C_1\left[I_{ika}(ak_0Y) - I_{-ika}(ak_0Y)\right]$$

2. AS $x \to \infty$; $Y \to 0$

$$\lim_{z\to 0} I_\nu(z) = \frac{z^\nu}{\Gamma(1+\nu)}$$

$$\psi(x) = C_1\left[\frac{(k_0 a e^{-x/a})^{ika}}{\Gamma(1+ika)} - \frac{(k_0 a e^{-x/a})^{-ika}}{\Gamma(1-ika)}\right]$$

$$= \frac{C_1 (k_0 a)^{ika}}{\Gamma(1+ika)}\left[e^{-ikx} - e^{+ikx}(k_0 a)^{-2ika}\frac{\Gamma(1+ika)}{\Gamma(1-ika)}\right]$$

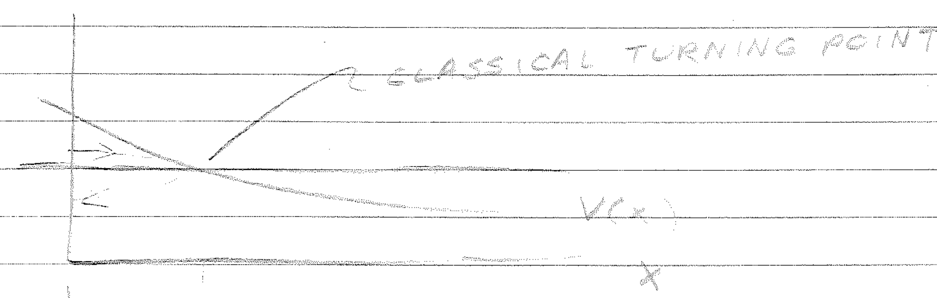
$$e^{2i\delta} = (k_0 a)^{-2ika}\frac{\Gamma(1+ika)}{\Gamma[1-ika)}$$

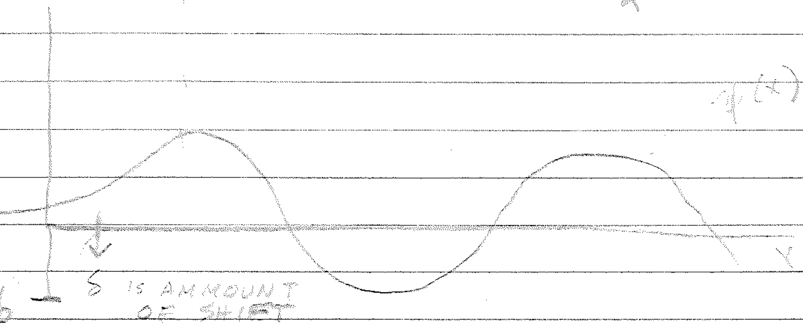
$$\Gamma(z) = \rho e^{i\theta} \qquad \Gamma(z^*) = \rho e^{-i\theta}$$

$$\therefore \psi(x) = e^{i\delta}(\quad)\left[e^{-ikx-i\delta} - e^{ikx+i\delta}\right]$$

$$= e^{i\delta}(\quad)\sin(kx+\delta)\,(-i2)$$

δ IS CALLED THE PHASE SHIFT





NOW

$$\underset{\sim}{p}' = \hbar(\underset{\sim}{k} - \underset{\sim}{k}')$$

$$\hbar c k = \hbar c k' + \frac{p'^2}{2m}$$

$$= \hbar c k' + \frac{\hbar^2}{2m}(\underset{\sim}{k} - \underset{\sim}{k}')^2$$

LET $K_0 = \frac{mc}{\hbar}$

$$\Rightarrow 2K_0(K - K') = (\underset{\sim}{K} - \underset{\sim}{K}')^2 = K^2 + K'^2 - 2KK'\cos\theta$$

GIVES

$$K' = K\cos\theta - K_0 + \sqrt{K^2 + 2KK_0(1-\cos\theta) - K^2(1-\cos\theta)}$$

NON RELATIVISTIC ASSUMPTION:

$$K_0 >> K, K'$$

GIVES

$$K' = K\cos\theta \overset{-K_0}{+} K_0\left[1 - \frac{2K}{K_0}(1-\cos\theta) + \ldots\right]$$

$$\simeq K\cos\theta - K_0 + K_0\left[1 + \frac{K}{K_0}(1-\cos\theta) + O\left(\frac{K^2}{K_0^2}\right)\right]$$

$$= K + O\left(\frac{\hbar^2 K}{2m^2c^2}\right)$$

CROSS SECTION (NON-RELATIVISTIC) IS

$$\frac{d\sigma}{d\Omega} = \frac{\hbar^2\omega'^2}{4\pi^2\hbar^4 c^4}\,\frac{e^4\,4\pi^2\hbar^2}{m^2\omega^2}\,(\hat{n}_k \cdot \hat{n}_{k'})^2$$

$$= \left(\frac{e^2}{mc^2}\right)^2 (\hat{n}_k \cdot \hat{n}_{k'}) \leftarrow \text{CLASSICAL COMPTON RESULT}$$

THOMPSON CROSS SECTION

$\frac{e^2}{mc^2}$ = CLASSICAL ELECTRON RADIUS $= 2.8 \times 10^{-13}$ cm

$$\Rightarrow \frac{d\sigma}{d\Omega} \sim 10^{-25} \quad \text{(NOT TO BIG)}$$

IF

$$A \sin kx + B \cos kx = C \sin(kx + \delta)$$

$$A = C \cos \delta$$

$$B = C \sin \delta$$

RECALL: CURRENT OPERATOR

$$J = \frac{\hbar}{2mi}\left[\psi^* \frac{\delta}{\delta x}\psi - \psi \frac{\delta}{\delta x}\psi^*\right]$$

FOR $\psi = e^{-ikx}$

$J = -\hbar k/m$

SAYS WAVE IS GOING TO LEFT ←

CONSIDER:

IF OTHER THAN PHASE, PARTICLE WOULD BE SWALLOWED

$$e^{-ikx} - e^{ikx} e^{2i\delta}$$

$(\longleftarrow) \quad (\longrightarrow)$

1-23-75

GRADER: MR. KNIGHT

REVIEW:

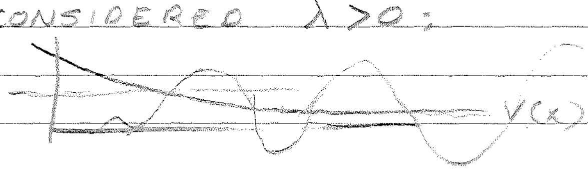
$V(x) = \lambda e^{-2x/a}$

$Y = e^{-x/a}$

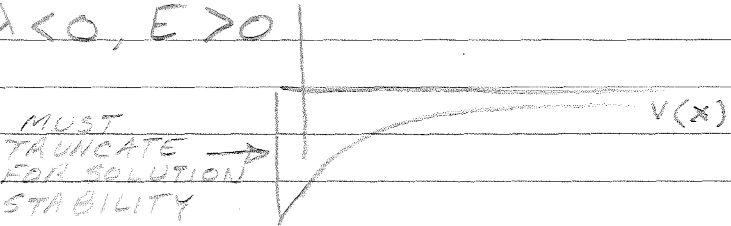
$$\left[Y^2 \frac{d^2}{dY^2} + Y \frac{d}{dY} + \frac{2ma^2}{\hbar^2} E - \frac{2ma^2}{\hbar^2}\lambda\right]\psi(x) = 0$$

BESSEL'S EQUATION

WE CONSIDERED $\lambda > 0$:



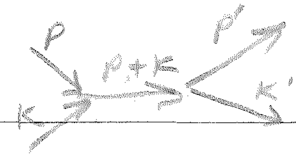
b. FOR $\lambda < 0$, $E > 0$



THUS, LET $V(x) = -|\lambda| e^{-\frac{2x}{a}}$; $x > 0$

$= \infty$; $x < 0$

$\Rightarrow \psi(0) = 0$

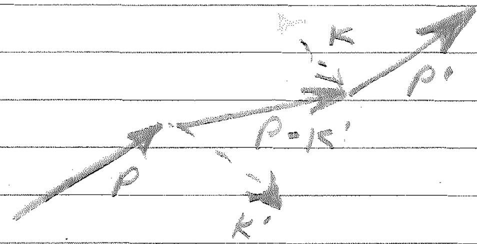


$\Leftarrow$ 1ST TERM

p·A TERM:

$$\frac{e^2}{m^2c^2}\;\frac{2\pi\hbar c^2}{V\sqrt{\omega\omega'}}\left[\frac{\hat{n}_k\cdot(p+k)\,(n_k\cdot p)}{\frac{\hbar^2}{2m}(p+k)^2-\frac{\hbar^2}{2m}p^2-\hbar\omega}\right.$$

$$\left.-\frac{n_k\cdot(p-k')\,n_{k'}\cdot p}{\frac{\hbar^2}{2m}(p-k')^2-\frac{\hbar^2 p^2}{2m}+\hbar\omega'}\right]$$



$\Leftarrow$ SECOND TERM

THIS TERM IS NEGLIGIBLE FOR NON-RELATIVISTIC TREATMENT

$\omega=\omega'$ IS NON-RELATIVISTIC LIMIT (ASSUME $p=0$ VIA COORDINATE CHANGE)

PUTTING IN EQ. GIVES

$$\left[Y^2 \frac{d^2}{dY^2} + Y\frac{d}{dY} + \frac{2ma^2}{\hbar^2} E + \frac{2ma^2}{\hbar^2} |\lambda| \right] \psi(Y) = 0$$

STILL A BESSELL'S EQ'N GIVES

$$\psi(Y) = C_1 J_{ika}(K_0 a Y) + C_2 J_{-ika}(K_0 a Y); \; E > 0$$

$$K_0^2 = \frac{2m}{\hbar} |\lambda| \qquad K^2 = \frac{2m}{\hbar^2} E$$

@ $x = 0$, $\psi(x) = 0$ OR $Y = 1$

$$\Rightarrow 0 = C_1 J_{ika}(K_0 a) + C_2 J_{-ika}(K_0 a)$$

SOLVE FOR EITER C_1 OR C_2

OTHER IS SOLVED BY NORMALIZATION

$$\lim_{z \to 0} J_\nu(z) = \left(\frac{z}{2}\right)^\nu / \Gamma(1+\nu)$$

c. CONSIDER $\lambda < 0$; $E < 0$ (BOUND STATES)

$$\alpha^2 = -E2m/\hbar^2$$

GOING THRU BESSELS EQ. YIELDS

$$C_1 J_{\alpha a}(K_0 a Y) + C_2 J_{-\alpha a}(K_0 a Y) = \psi(x)$$

CONDITIONS

1. $X \to \infty \Rightarrow Y \to 0 \quad \psi \to 0$

$$\psi(x) = C_1 \left(K_0 a e^{-x/a}\right)^{\alpha a} + C_2 \underbrace{\left(K_0 a e^{-x/a}\right)^{-\alpha a}}_{\text{FOR LARGE } X \; \to \; \infty}$$

(CANNOT USE)

THUS $C_2 = 0$ AND

$$\psi(x) = C_1 J_{\alpha a}(K_0 a Y)$$

2. $X = 0$, $Y = 1 \Rightarrow \psi = 0$

$\Rightarrow J_{\alpha a}(K_0 a) = 0 \Leftarrow$ EIGENVALUE CONDITION

GIVEN: a & $K_0^2 = \lambda 2ma^2/\hbar^2$,

WE NEED TO KNOW α

(WILL BE A # OF α_i SOLUTIONS. CHOOSE

α SUCH THAT

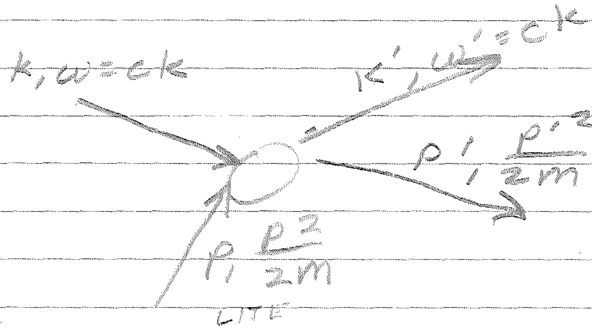
$$E_i = \frac{\hbar^2}{2m} \alpha_i^2$$

COMPTON SCATTERING (A RAMAN PROCESS)

SCATTERING OF LIGHT BY FREE PARTICLES

1) NON-RELAVISTIC TREATMENT (ELECTRONS)

e^- HAS p ∋ $E = p^2/2m$



$$\underset{\sim}{p}' + \hbar \underset{\sim}{k}' = \underset{\sim}{p} + \hbar \underset{\sim}{k}$$

$$\frac{p'^2}{2m} + \hbar c k' = \frac{p^2}{2m} + \hbar c k$$

∴ THE CROSS SECTION IS

$$\frac{d\sigma}{d\Omega} = \frac{(\hbar\omega')^2}{4\pi^2\hbar^4 c^4} \left| V(k-k') \right|^2$$

$$\psi(r) = \frac{1}{\sqrt{V}} e^{ip\cdot r}$$

$A^2 \longrightarrow 1^{ST}$ ORDER

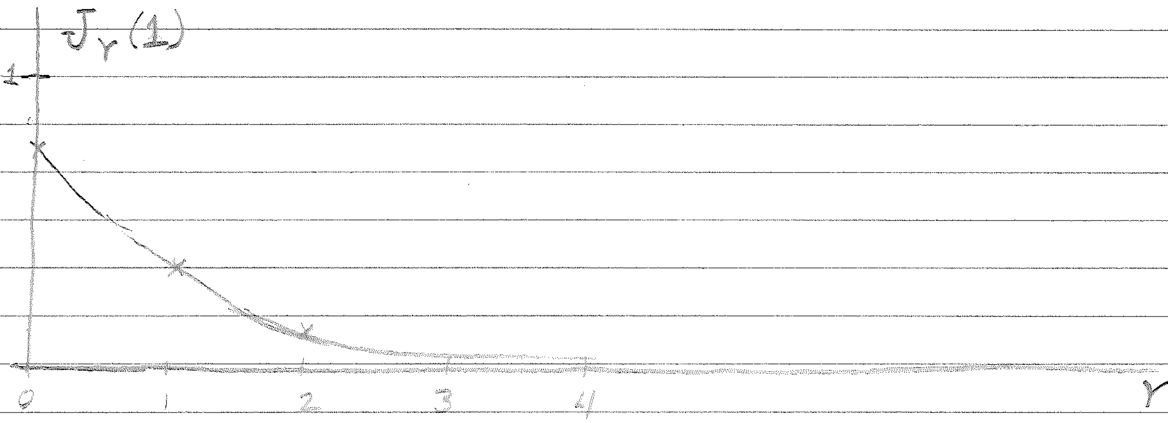
$p\cdot A \longrightarrow 2^{nd}$ ORDER

$$A^2_{TERM} \rightarrow \frac{e^2}{2mc^2} \langle f | A^2 | i \rangle = \frac{e^2}{2mc^2} \frac{2\pi \hbar c^2}{V\sqrt{\omega\omega'}}$$

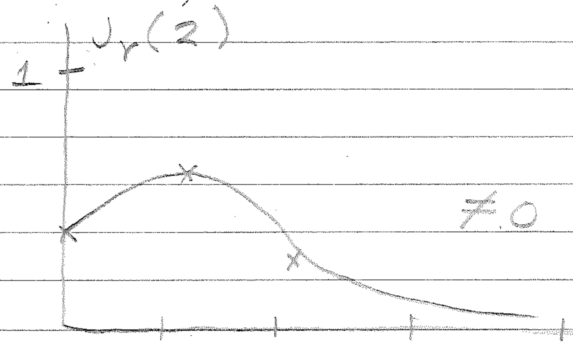
$$\times\, 2\, \hat{n}_k \cdot \hat{n}_{k'} \langle \underset{\sim}{p}' | e^{ir\cdot(k-k')} | \underset{\sim}{p} \rangle$$

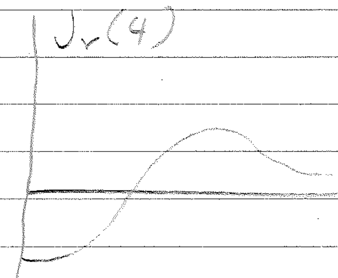
$$\langle p' | e^{ir\cdot(k-k')} | \underset{\sim}{p} \rangle = \delta_{p'+k',\, p+k}$$

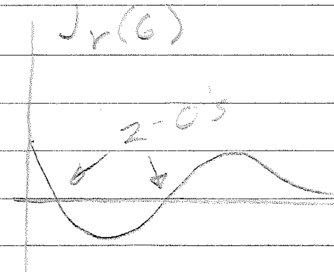
TABLES GIVE $J_n(x) \ni n$-INTEGER ~ $0 \leq x \leq 10$

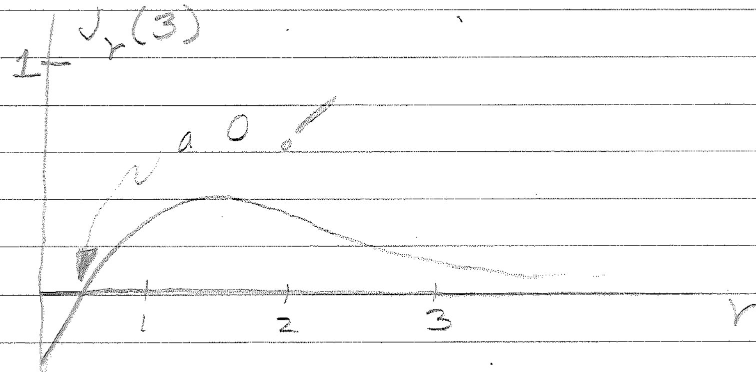


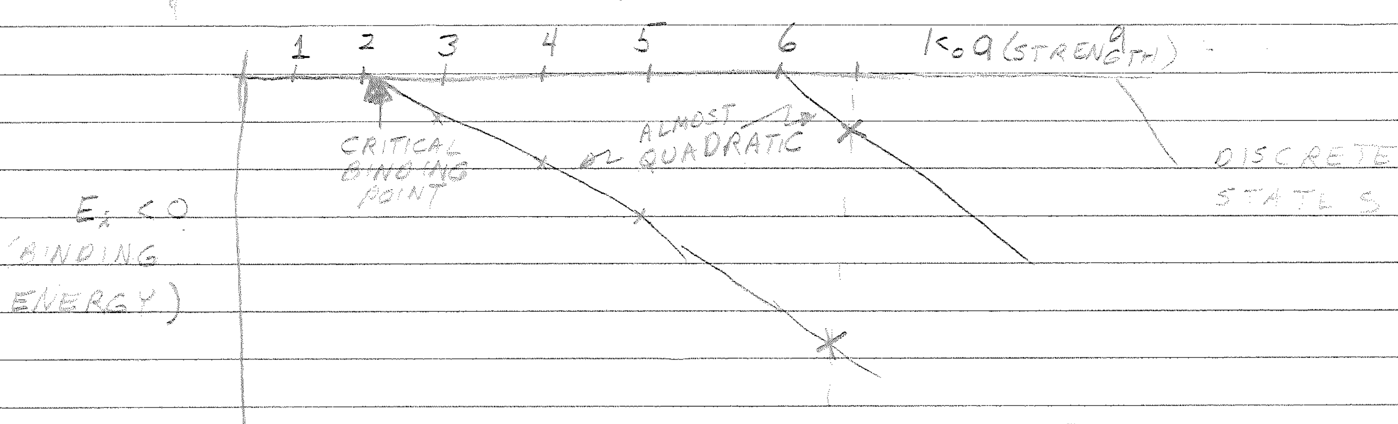
IF $K_0 a = 1$ NO BOUND STATES





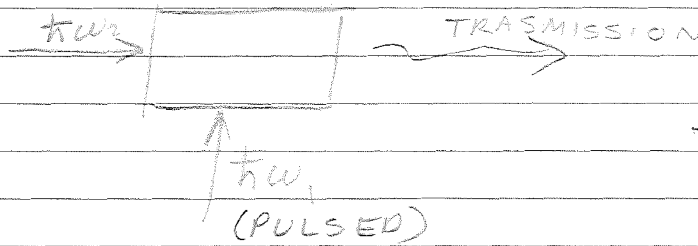




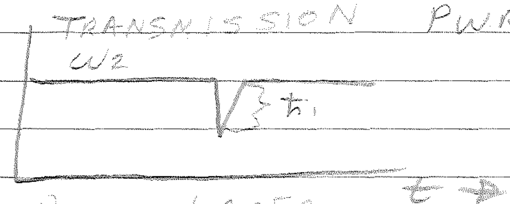


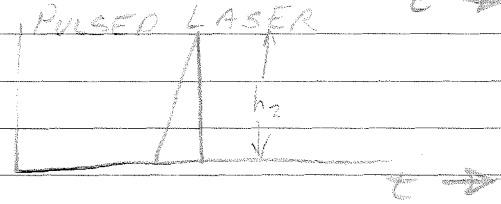
TWO BOUND STATES

MOST POTENTIALS HAVE FINITE # OF BOUND STATES (EXCEPTION: $V(x) = \frac{C}{x}$ HAS ∞ # OF BOUND STATES FOR ANY STRENGTH C.



$\hbar\omega_2 > \hbar\omega_1$

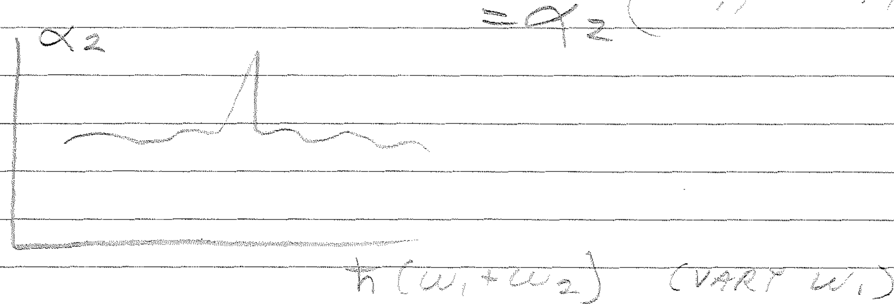


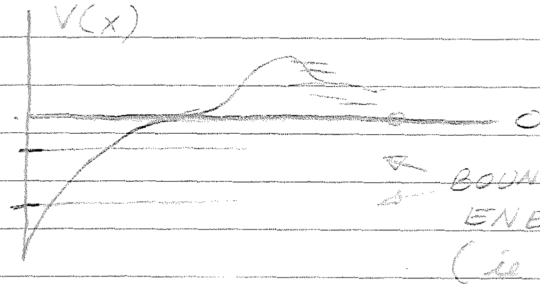


IS PROPORTIONAL TO

TWO PHOTON ABSORPTION $\propto$ LASER PWR

$= \alpha_2($ " " $)$





UNBOUND (CONTINUUM) FOR $E > 0$

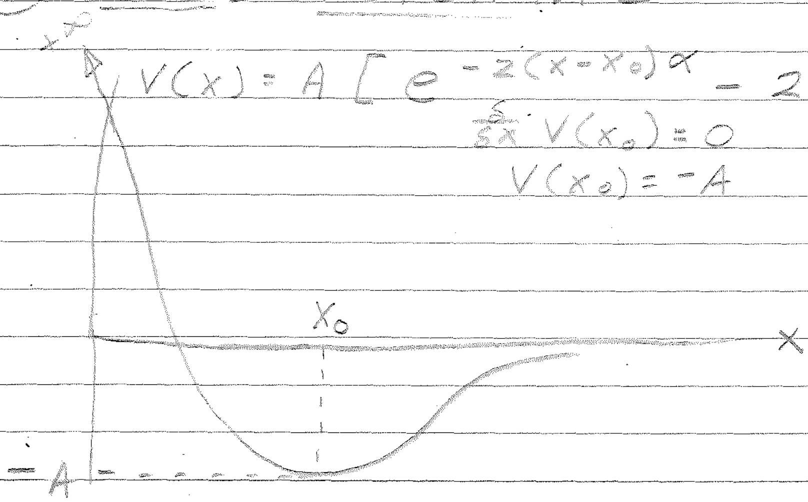
BOUND STATES: ONLY NEGATIVE ENERGY'S ALLOWED (ie DISCRETE)

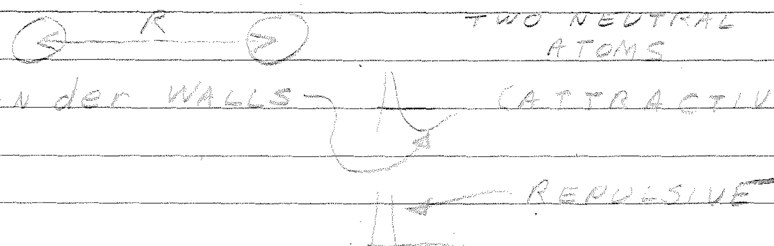
(5) MORSE POTENTIAL

$$V(x) = A\left[e^{-2(x-x_0)\alpha} - 2e^{-(x-x_0)\alpha}\right]$$

$$\frac{\delta}{\delta x} V(x_0) = 0$$

$$V(x_0) = -A$$





TO SOLVE, LET $Y = e^{-\alpha(x-x_0)}$

$$\frac{\delta}{\delta x} = -\alpha Y \frac{d}{dY}$$

$$\frac{\delta^2}{\delta x^2} = \alpha^2 Y \frac{d}{dY} + \alpha^2 Y^2 \frac{d^2}{dY^2}$$

PUTTING IN SCHRÖ EQ'N: $\quad (V(x) = A(Y^2) - 2AY$

$$\left(Y^2 \frac{d^2}{dY^2} + Y\frac{d}{dY} + \frac{2m}{\hbar^2\alpha^2}\left[E - AY^2 + 2AY\right]\right)\psi(x) = 0$$

SOLUTION IS (GET THIS NOW)
CONFLUENT HYPERGEOMETRIC FUNCTION

PARITY AND SYMMETRY

EVEN PARITY $\Rightarrow \ell = 0, 2, 4, \ldots$

ODD " $\Rightarrow \ell = 1, 3, 5, \ldots$

$\langle \ell | \hat{\pi} \cdot p | i \rangle$

$s \to p$

$1s \to 2p$

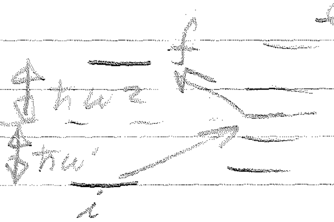
p HAS ODD PARITY

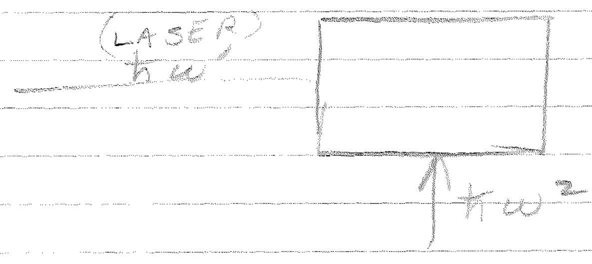
$p \to s, d$

ONE PHOTON ABSORBTION CAUSES SYSTEM TO CHANGE PARITY!

THUS, IN RAMAN SCATTERING $(i \to \ell \to f)$ PARITY DOES NOT CHANGE.

TWO PHOTON EXPERIMENT





ELECTRONS ADD. TO GIVE (COMPARE WITH RAMAN)

$$M = \frac{e}{mc} \frac{2\pi\hbar c}{V\sqrt{\omega\omega'}} \sum_{\ell} \Big\{ \big(\qquad \big) + \big(\qquad \big) \Big\}$$

ONLY CHANGE

CONFLUENT HYPERGEOMETRIC FUNCTIONS

$$F(a,b;z) = 1 + \frac{az}{b} + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{z^3}{3!} + \dots$$

$$\left[z\frac{d^2}{dz^2} + (b-z)\frac{d}{dz} - a\right]F(a,b;z) = 0 \Leftarrow$$ WILL BE A HMWRK PROB

$$\lim_{z\to\infty} F(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^{z}$$
(a & b NOT)

BACK TO MORSE POTENTIAL

NOTE: $E=0$ IS CHOSEN $\Rightarrow \lim_{x\to\infty}\psi = 0$

FOR BOUND STATES ($E<0$)

LET $s = \sqrt{2mA/\hbar^2\alpha^2}$ (SIMILAR TO $k_0 a$)

FOR LARGE s, LARGE POTENTIAL

α SCALES

$$t^2 = -2mE/\hbar^2\alpha^2$$

GIVEN s, WE LOOK FOR A t

SOL'N OF SCHRÖ EQ'N IS

$$\psi(\ ) = C_1 e^{-sy} y^{t} F\left[\tfrac{1}{2}+t-s,\ 1+2t;\ 2sy\right] + C_2 e^{-sy} y^{-t} F\left[\tfrac{1}{2}-t-s,\ 1-2t;\ 2sy\right]$$

BOUNDRY CONDITIONS:

1) $x\to\infty,\ \psi\to 0$
($y\to 0$)

SINCE $y^{-t}\to\infty$, LET $C_2 = 0$

$$\Rightarrow \psi = C_1 e^{-sy} y^{t} F\left[\tfrac{1}{2}+t-s;\ 1+2t;\ 2sy\right]$$

2) $x\to -\infty\quad \psi\to 0$
$y\to +\infty$

$$e^{-st} e^{2st} \to \infty$$

$a = \frac{1}{2}+t-s = -n \Leftarrow$ SERIES IS FINITE, &

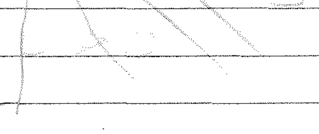
$\lim_{x\to -\infty}\psi = 0$ SINCE $e^{-sy}y^{n}\to 0$

EIGEN VALUE CONDITION

$$t = s - \tfrac{1}{2} - n = s\left[1 - \frac{n+\frac{1}{2}}{s}\right]$$

$$\therefore E = -\frac{\hbar^2}{2m\alpha^2}t^2 = -\frac{\hbar^2}{2m\alpha^2}s^2\left[1 - \frac{(n+\frac{1}{2})}{s}\right]^2$$

$$\Rightarrow E_n = -A\left[1 - \frac{(n+\frac{1}{2})}{s}\right]^2$$



n IS LIMITED BY THE CONDITION

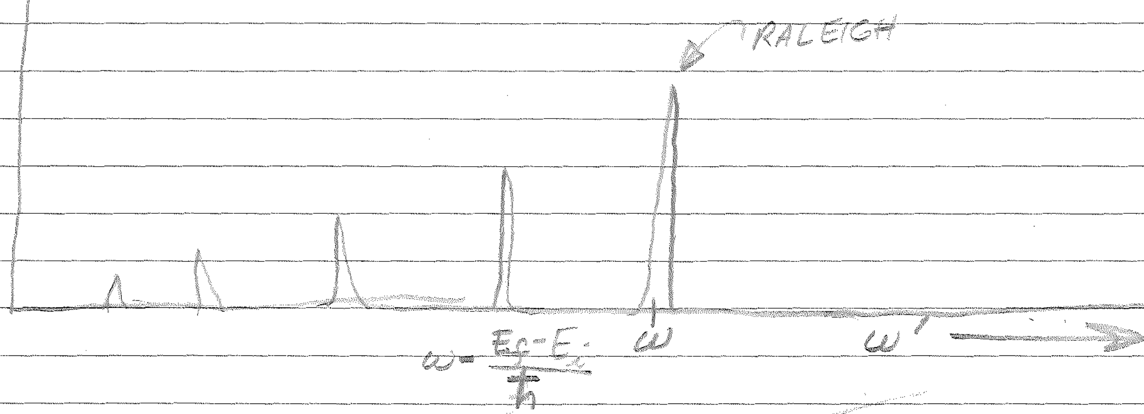
$t > 0 \Rightarrow n \leq s - \frac{1}{2}$

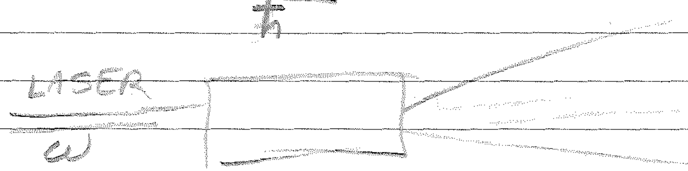
DEFINE

$$\frac{d^2\sigma}{d\Omega\, d\omega'} \ni \frac{d\sigma}{d\Omega} = \int d\omega' \frac{d^2\sigma}{d\Omega\, d\omega'}$$

SINCE $k' = \frac{\omega'}{c}$

$$\frac{d^2\sigma}{d\Omega\, d\omega'} = \frac{\omega'^2}{4\pi^2\hbar^2 c^4}\, \delta\left[\omega - \omega' - \frac{E_f - E_i}{\hbar}\right] |M_V|^2$$





AGAIN: $\psi = e^{-sY} Y^t F$

$$\frac{d\psi}{dY} = -s\psi + t\frac{\psi}{Y} + e^{-sY} Y^t \frac{dF}{dY}$$

$$\frac{d^2\psi}{dY^2} = s^2\psi + t(t-1)\psi/Y^2 - \frac{2st\psi}{Y}$$
$$+ e^{-st} Y^t \left[\frac{d^2F}{dY^2} + \frac{2t}{Y}\frac{dF}{dY} - 2s\frac{dF}{dY}\right]$$

SCHRÖ. EQ. WAS:

$$Y^2 \frac{d^2\psi}{dY^2} + Y\frac{d\psi}{dY} - \left[t^2 - s^2(Y^2 - 2Y)\right]\psi = 0$$

THUS

$$e^{-st} Y^t \Big\{ \left[\cancel{s^2Y^2} + t(t-1) - 2sYt\right] F$$
$$+ \left[Y^2 \frac{d^2F}{dY^2} + 2tY\frac{dF}{dY} - 2sY^2\frac{dF}{dY}\right]$$
$$- sYF + tF + Y\frac{dF}{dY} - F\left(t^2 + \cancel{s^2Y^2} - 2s^2Y\right) \Big] = 0$$

$$= e^{-st} Y^t \left[Y^2 \frac{d^2F}{dY^2} + \frac{dF}{dY}\left(2tY - 2sY^2 + Y\right) + F\left(-2sYt - sY + 2s^2Y\right)\right]$$

$$= \left[Y\frac{d^2F}{dY^2} + \frac{dF}{dY}\left(2t - 2sY + 1\right)\frac{dF}{dY} + F\left(-2st - s + 2s^2\right)\right)$$

LET $Z = 2sY$

$$\Rightarrow \left[Z\frac{d^2}{dZ^2} + (1 + 2t - Z)\frac{d}{dZ} - \left(\frac{1}{2} + t - s\right)\right] F = 0$$

LET $a = \frac{1}{2} + t - s$, $b = 1 + 2t$

THIS IS D.E. FROM WHICH C.H.F. ARE GENERATED.

RAMAN SCATTERING

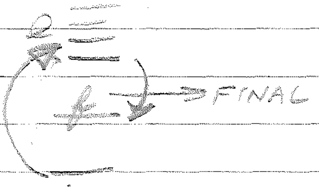
- ELECTRONIC (E LEFT IN ELECTRONS) $\Delta\hbar \sim 1\,eV$
- VIBRATIONAL

N_2 VIBRATIONAL ENERGY

REQUIRES 3^{RD} ORDER PERT.

$\Delta\hbar \sim 0.010\,eV$

FOR ELECTRONIC RAMAN:



$\hbar\omega \neq E_{li}$

GOES VIRTUALLY FROM i TO l

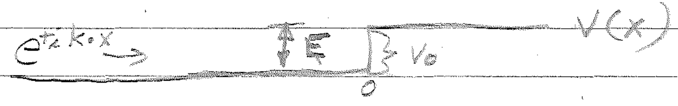
IF PHOTON STAYS @ l FOR A WHILE: FLOURESCENCE

$$M = \frac{e}{mc}\frac{2\pi\hbar c^2}{V\sqrt{\omega\omega'}}\sum_l \left\{ \frac{\langle f|\hat{n}_{k'}\cdot p|l\rangle\langle l|\hat{n}_k\cdot p|i\rangle}{E_i-\hbar\omega} + \frac{\langle f|\hat{n}_k\cdot p|l\rangle\langle l|n_{k'}\cdot p|i\rangle}{E_l-E_i+\hbar\omega} \right\}$$

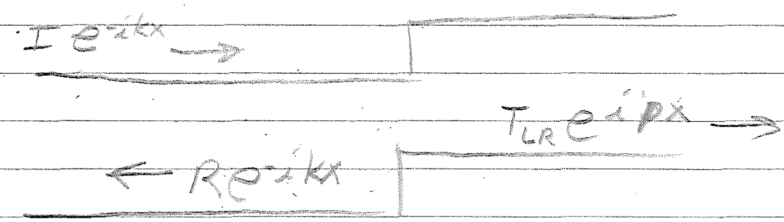
TURNS OUT THAT CROSS SECTION IS

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2\hbar c}\int_0^\infty k'^2\,dk'\,\delta\left[\hbar ck-\hbar ck'+E_i-E_f\right](MV)^2$$

TRANSMISSION COEFFICIENTS



[NOTE $J[e^{ikx}] = \hbar k/m > 0 \Rightarrow e^{ikx}$ GOES TO THE RIGHT]

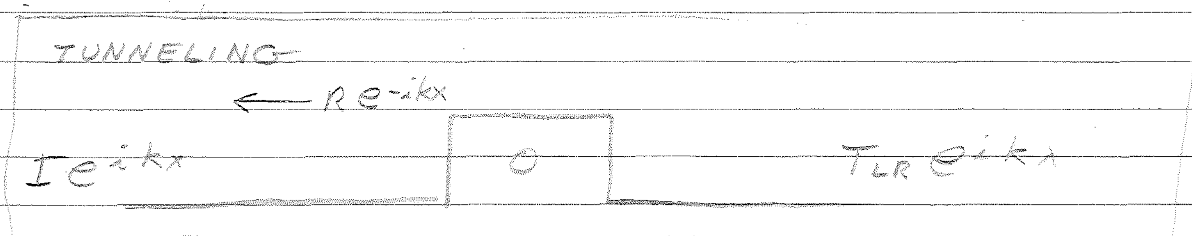


$(p \neq k)$

FOR

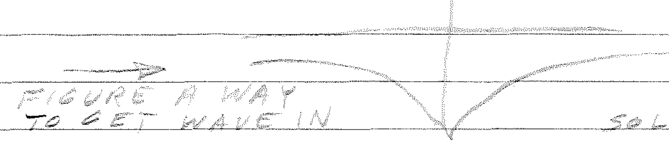
1) $E < V_0$, $p = i\alpha = i\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

$|R| = |I|$, $T_{RL} = Te^{-\alpha x}$



2) $E > 0$, $p = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$

ON HOMEWORK:



SOLUTION: $C_1 I_{ik} + C_2 I_{-ik}$

APPLY BNDRY CNDITIONS

4/29/75

HOMEWORK #10

(1). $\frac{d\sigma}{d\Omega} = \frac{E^2}{4\pi\hbar^4 c^4} |V(p-p')| \Rightarrow E = \sqrt{c^2p^2 + m^2c^4}$

FOR RALEIGH, $m \to 0$ & $E = cp$

(2) $\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^4}\left(\frac{4\pi^2 e^2}{(p-p')^2}\right)^2$; $(\underset{\sim}{p}-\underset{\sim}{p}')^2\Big|_{p=p'} = 2p^2(1-\cos\theta)$

$= 4p^2 \sin^2\frac{\theta}{2}$

SAME AS RUTHERFORD FORMULA

(3) $N^* \to N + e^- + e^+$

ANSWER IS

$$\frac{dw}{dE_e} = E_N E_p \sqrt{E_e^2 - m^2c^4}\ \sqrt{E_p^2 - m^2c^4}$$

$$E_p = \Delta - E_e$$

(4)

$$f = \frac{2m}{\hbar^2}(\Delta E)\langle x\rangle^2$$

a. HYDROGEN

$$f = \frac{2m}{\hbar^2}\left[\frac{3}{4}\frac{e^2}{2a}\right]\left[\frac{2^{15/2}}{3^5}a\right]$$

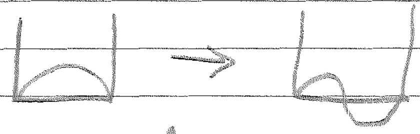
$$= \left(\frac{me^2}{\hbar^2}\frac{a^2}{a}\right)\left(\frac{2^{13}}{3^9}\right) = 0.42$$

b. HARMONIC OSCILLATOR

$f = 1$ $\quad\quad \langle n|p|m\rangle = c\,\delta_{m,n+1}$

$$f = \frac{2m}{\hbar^2}(\hbar\omega)\left(\frac{\hbar}{2m\omega}\right) = 1$$

c. BOX



$$\langle x\rangle = \frac{2}{L}\int_0^L \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) x\,dx = \frac{16}{9\pi^2}L$$

$$f = \frac{2m}{\hbar^2}\left[\frac{\hbar^2}{2m}\right]\left[\left(\frac{2\pi}{L}\right)^2 - \left(\frac{\pi}{L}\right)^2\right]\left(\frac{16L^2}{9\pi^2}\right)^2$$

$$= \frac{256}{27\pi^2} = 0.96$$

1-28-75

FIRST HOMEWORK SET SOLUTION ERGS, GMS

① a. $\lambda = h/p = \frac{h}{\sqrt{2mE}}$ (ELECTRON)

$E = 100\,eV = 1.6 \times 10^{-10}$ ERGS

$m = 0.9 \times 10^{-27}$ GMS $\Rightarrow \lambda = \frac{6.6 \times 10^{-27}}{[2(1.6)(0.9) \times 10^{-37}]^{1/2}} \simeq 1\frac{1}{2}\,\mathring{A}$

b. (NEUTRON) $T = 300\,°K$

$kT = 4.2 \times 10^{-14}$ ERGS $\quad (k = 1.4 \times 10^{-16} \frac{ERGS}{°K})$

$\Rightarrow \lambda \simeq 2\,\mathring{A}$

② PROVE $e^{L} a e^{-L} = a + [L,a] + \frac{1}{2!}[L,[L,a]] + \ldots$

LET $f(\lambda) = e^{\lambda L} a e^{-\lambda L} = f_0 + \lambda \left(\frac{df}{d\lambda}\right)_0 + \frac{\lambda^2}{2!}\left(\frac{d^2 f}{d\lambda^2}\right)_0 + \ldots$

$e^{L} a e^{-L} = f(1) = 1 + \left(\frac{df}{d\lambda}\right)_0 + \frac{1}{2!}\left(\frac{d^2 f}{d\lambda^2}\right)_0 + \ldots$

$f(0) = a$

$f'(\lambda)_0 = \left[e^{\lambda L} L a e^{-\lambda L} + e^{\lambda L} a (-L) e^{-\lambda L}\right]_0$

$= \left[e^{\lambda L} [L,a] e^{-\lambda L}\right]_{\lambda=0}$

$= [L,a]$

$f''(\lambda)_0 = \left[e^{\lambda L}\{L[L,a]\} - \{[L,a]L\} e^{-\lambda L}\right]_0$

$= \left[e^{\lambda L} [L,[L,a]] e^{-\lambda L}\right]_0$

$= [L,[L,a]]$

③ PROVE $\frac{d}{dt}\langle F \rangle = \frac{1}{i\hbar}\langle [H,F] \rangle = \frac{1}{i\hbar}\langle n | [H,F] | n \rangle$

$= \frac{1}{\hbar i}\langle n | (HF - FH) | n \rangle$

$= \frac{E_n - E_n}{i\hbar}\langle n | F | n \rangle$

$= 0$

NOTE: WORKS FOR CONT. EIGENFUNCTION ALSO

④ $\frac{1}{m i\hbar}\langle p \rangle = \langle [x,H] \rangle$

$\rightarrow 0 \Leftarrow$ FROM ABOVE

$\therefore \langle p \rangle = 0$

TAKING INTO ACCOUNT OTHER TERM

$$M_{KK'} = \frac{e^2 2\pi\hbar c^2}{mc^2\omega_i}\hat{\mathcal{E}}_K \cdot \hat{\mathcal{E}}_{K'} \langle a_K a_{K'}^\dagger \rangle$$

$$+ \frac{\langle F | \frac{eP\cdot A}{mc} | M \rangle \langle M | \frac{eP\cdot A}{mc} | I \rangle}{E_M - E_I}$$

$|M\rangle$ = EXITED STATES OF ATOMS

CAN ATTACK IN TWO WAYS

a) 1^{ST} STEP: OPERATE a_K & DESTROY PHOTON IN K

2^{nd} STEP: OPERATE $a_{K'}^\dagger$ & CREATE PHOTONS IN K'

b) 1^{ST} STEP: CREATE K' : $a_{K'}^\dagger$

2^{nd} STEP: DESTROY K ; a_K

$$\frac{2\pi e^2}{\omega m}\left[\hat{\mathcal{E}}_K \cdot \mathcal{E}_{K'} + \frac{1}{m}\sum_{n\neq i}\left[\frac{P_{in}\cdot\hat{\mathcal{E}}_{K'}\, P_{ni}\cdot\hat{\mathcal{E}}_K}{E_{ni} - \hbar\omega_K} + \frac{P_{in}\cdot\hat{\mathcal{E}}_K\, P_{ni}\cdot\mathcal{E}_K}{E_{ni} + \hbar\omega_K}\right]\right] = \alpha(\omega)$$

RECALL: $\frac{P_{in}}{m} = \frac{r_{in} E_{ni}}{i\hbar}$

AFTER MANIPOLATING MANIPULATIONS:

$$\frac{d\sigma}{d\Omega} = \frac{(\hbar\omega)^2}{4\pi^2\hbar^4 c^4}|M|^2 = \frac{\omega^4}{c^4}(n\cdot\alpha\cdot n')^2$$

⑤ a. $\langle n|x^2|m\rangle$

WE SHOWED $\quad x = \sqrt{\frac{\hbar}{2m\omega}}\,(a+a^+)$

$$x^2 = \frac{\hbar}{2m\omega}(a+a^+)(a+a^+)$$
$$= \frac{\hbar}{2m\omega}(aa + a^+a^+ + a^+a + aa^+)$$

$[a,a^+]=1$
$\Rightarrow aa^+ = a^+a+1$

$$a|m\rangle = \sqrt{m}\,|m-1\rangle$$
$$a^+|m\rangle = \sqrt{m+1}\,|m+1\rangle$$

$$\therefore\ x^2|m\rangle = \frac{\hbar}{2m\omega}\left[aa|m\rangle + a^+a^+|m\rangle + a^+a|m\rangle + aa^+|m\rangle\right]$$

$$= \frac{\hbar^2}{2m\omega}\Big[\sqrt{m(m-1)}\,|m-2\rangle + \sqrt{(m+1)(m+2)}\,|m+2\rangle$$
$$+ m|m\rangle + (m+1)|m\rangle\Big]$$

$$\Rightarrow \langle n|x^2|m\rangle = \frac{\hbar^2}{2m\omega}\Big[\sqrt{(m)(m-1)}\,\delta_{n,m-2} + \sqrt{(m+1)(m+2)}\,\delta_{n,m+2}$$
$$+ (2m+1)\,\delta_{n,m}\Big]$$

b. $\langle n|p^2|m\rangle$ (SAME IDEA)

FOR ISOTROPIC SYSTEM

$$\underset{\approx}{\alpha} = \alpha\, \delta_{\mu\nu}$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{\omega^4}{c^4}\left(n_k \cdot n_{k'}\right)^2$$

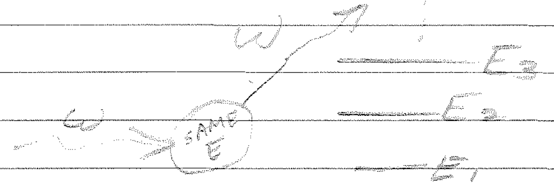
Q.M. GIVES SAME RESULT.

PROOF:

QUANTUM THEORY OF RALEIGH SCATTERING

H.W. $\Rightarrow$ $$\frac{d\sigma}{d\Omega} = \frac{(\hbar\omega)^2}{4\pi^2\hbar^4 c^4}\left|M_{kk'}\right|^2$$

$$H_I = \frac{e\,p\cdot A}{mc} + \frac{e^2}{2mc^2}A^2$$



$$M_{kk'} = \langle F \,|\, \underline{m} \,|\, I \rangle$$

$|I\rangle$ = ATOM IN GROUND STATE
n_k PHOTON IN k

$|F\rangle$ = ATOM IN GROND STATE,
ONE MORE PHOTON mk', $n_k - 1$ IN k

$$\frac{e^2}{2mc^2}A^2 = \frac{e^2}{2mc^2}\left[\sum_k \hat{\varepsilon}_k \sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\left[a_n e^{-i\omega_n t} + a_n^{+} e^{i\omega_n t}\right]\right]$$

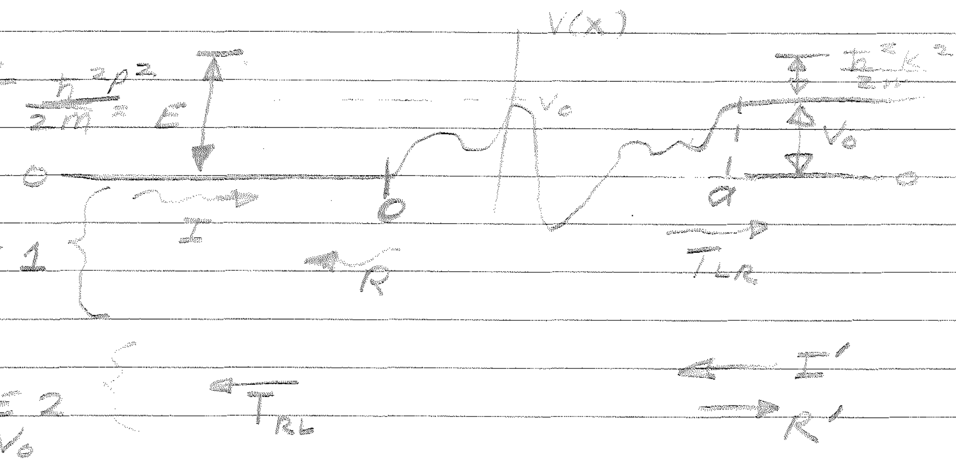
$$= \frac{e^2}{2mc^2}\;\frac{2\pi\hbar c^2}{\sqrt{\omega_k \omega_{k'}}}\left[2a_k a_{k'}^{+}\, e^{i r\cdot(k-k')}\right]$$

$$M_{kk'} = \frac{e^2\, 2\pi\hbar c^2}{mc^2\omega_i}\left\langle i \right| e^{i r\cdot(k-k')} \left| i \right\rangle \times \langle a_k a_{k'}^{+}\rangle\, \hat{\varepsilon}_k \cdot \hat{\varepsilon}_{k'}$$

$$\langle i | e^{i r\cdot(k-k')} | i \rangle \simeq 1$$

NOTES: TRANSMISSION & REFLECTION COEFFICIENTS

A GENERAL CASE: $\frac{\hbar^2 p^2}{2m} = E$



CASE 1

CASE 2

ASSUME $E > V_0$

$E = \frac{\hbar^2 p^2}{2m}$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - E \right] \psi_1(x) = 0$$

$\psi = e^{\pm ipx} \Leftarrow$ PLANE WAVE WITH $E = \frac{\hbar^2 p^2}{2m}$

ON RIGHT: $\left[\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0 - E \right] \psi(x) = 0$

$$\psi = e^{\pm ikx} \quad ; \quad k^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$$\begin{pmatrix}\text{CASE}\\1\end{pmatrix} \quad \psi_1(x) = \begin{cases} I e^{ipx} + R e^{-ipx} & x < 0 \\ T_{LR} e^{ikx} & x > a \end{cases}$$

$$\begin{pmatrix}\text{CASE}\\2\end{pmatrix} \quad \psi_2(x) = \begin{cases} I' e^{-ikx} + R' e^{ikx} \\ T_{RL} e^{-ipx} \end{cases}$$

THEOREM 1: $|I|^2 = |R|^2 + \frac{k}{p}|T_{LR}|^2$

$$|I'|^2 = |R'|^2 + \frac{p}{k}|T_{RL}|^2$$

APPLYING CONSERVATION OF FLUX (PARTICLE)

j = CURRENT OPERATOR = $\frac{\hbar}{2mi}\left[\psi^* \frac{d}{dx}\psi - \psi \frac{d\psi^*}{dx} \right]$

FIND $j(x)$ FOR $x < 0$

CASE 1 $\Rightarrow \frac{d}{dx}\psi = ip\left[I e^{ipx} - R e^{-ipx} \right]$

$$\psi^* \frac{d}{dx}\psi = ip\left[I^* e^{-ipx} + R^* e^{ipx} \right]\left[I e^{ipx} - R e^{-ipx} \right]$$

$$= ip\left(\left[|I|^2 - |R|^2 + I R^* e^{2ipx} \right] - [\quad]^* \right)$$

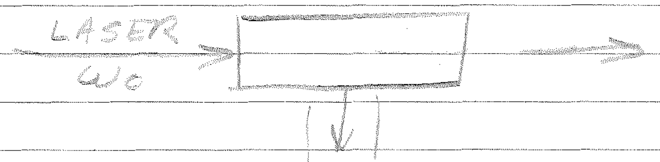
(CONT)

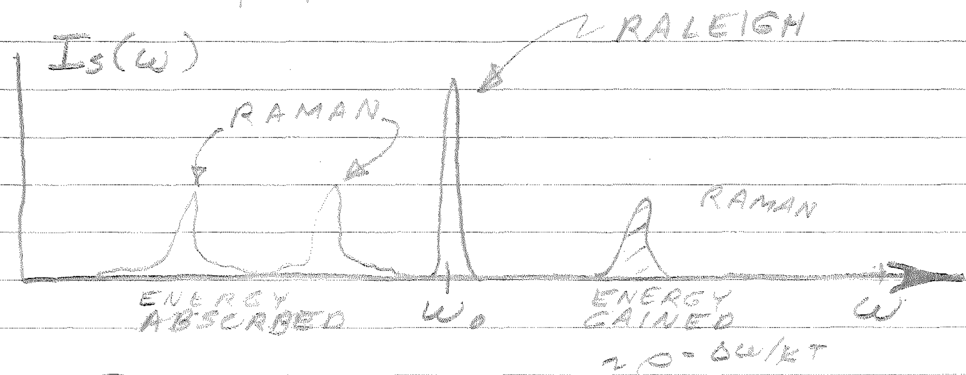
$|I^2| = \#$ IN

$|R^2| = \#$ OUT

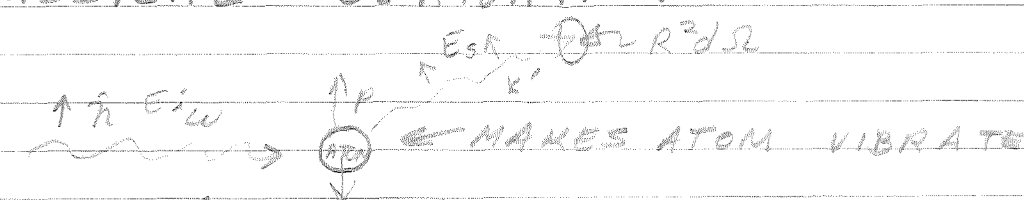
LIGHT SCATTERING

- RALEIGH " → ELASTIC OF BOUND PARTICLES
- RAMAN " → INELASTIC " " "
- COMPTON " → " " FREE "





THEORY FOR RALEIGH SCATTERING
CLASSICAL DERIVATION



$$E = \hat{n} E_i e^{-i\omega t}$$

$$P = \alpha(\omega) \cdot \hat{n} E_i e^{-i\omega t}$$

WISH TO CALCULATE RESULTING RADIATION

FAR-FIELD:

$$E_s = \frac{e^{ikR}}{R} \frac{\omega^2}{c^2} n_k \cdot (n_k \cdot P)$$

$$\frac{|E_s|^2}{|E_i|^2} R^2 d\Omega = \% \text{ IN } d\Omega \text{ DIRECTION}$$

$$= d\Omega \frac{\omega^4}{c^4} \langle n_k \cdot \alpha \cdot n_{k_0} \rangle^2 = d\sigma$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{\omega^4}{c^4} \langle \hat{n}_k \cdot \alpha \cdot n_{k_0} \rangle^2$$

ALSO; WE GOTTA FIND $j(x)$ FOR $X > a$

$$j_R(x) = \frac{\hbar}{2im}\left[|T_{LR}|^2 - (-ik)\right]$$
$$= \frac{\hbar k}{m}|T_{LR}|^2$$
$$j_L(x) = \frac{\hbar p}{m}\left[|I|^2 - |R|^2\right]$$

PROVED BY EQUATING $j_R(x)$ AND $j_L(x)$

$$\Rightarrow |I|^2 - |R|^2 = \frac{k}{p}|T_{LR}|^2$$

THEOROM 2: $\frac{T_{RL}}{I'}\, p = \frac{T_{LR}}{I}\, k$

(COUPLED WITH THEM 1 GIVES $R'/I' = (-R^*/I)(T_{LR}/T_{LR}^*)$)

PROOF.

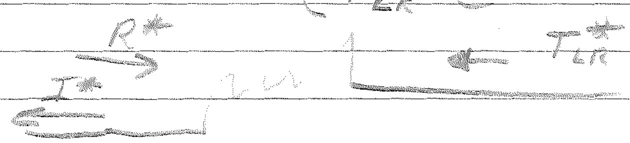
TIME REVERSAL OPERATOR, K, OPERATING ON A WAVE FUNCTION:

a. COMPLEX CONJUGATE

b. SPIN FLIP (S_x) ← (WON'T CONSIDER HERE)

$\therefore K\psi_1(x) = \psi_1^*(x)$

$$= \begin{cases} I^* e^{-ipx} + R^* e^{ipx} & ; x<0 \\ T_{LR}^* e^{-ikx} & ; x>a \end{cases}$$



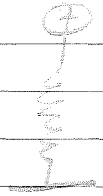
$$\frac{I(K\psi_1) - R^*\psi_1}{T_{LR}^*} = \begin{cases} \dfrac{e^{ipx}(IR^* - R^*I) + e^{-ipx}\left[|I|^2 - |R|^2\right]}{T_{LR}^*} & ; x<0 \\ e^{ikx}\left(\dfrac{-R^* T_{LR}}{T_{LR}^*}\right) + e^{-ikx} & ; X>a \end{cases}$$

$= \psi_2$ QED!

USING THEM 1:

$$|I|^2 - |R|^2 = \frac{|T_{LR}|^2}{T_{LR}^*}\cdot\frac{k}{p} = \frac{k}{p}T_{LR}$$

RECALL CLASSICALLY



$$\ddot{x} + \omega_0^2 x = \frac{e}{m} E_0 e^{-i\omega t}$$

$$x = \frac{e}{m} \frac{1}{\omega_0^2 - \omega^2} E$$

$$p = ex \Rightarrow \alpha = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega^2}$$

COMPARE WITH Q.M. DEFINITION

DIELECTRIC FUNCTION

$$\varepsilon(\omega) = 1 + 4\pi\alpha$$

α = POLARIZABILITY

IF n = INDEX OF REFRACTION

K = EXTINCTION CO-EFFICIENT

$$\varepsilon(\omega) = (n + iK)^2$$

$$e^{ikz} \rightarrow k = (n + iK)\omega/c$$

$$I = e^{-\frac{2K\omega}{c}z}$$ ← INTENSITY

$$\alpha = \frac{2K\omega}{c}$$ ← ABSORBTION COEFFICIENT

POL: $\alpha_{\mu\nu} = \mathrm{Re}\,\alpha + i\,\mathrm{Im}\,\alpha$ (COMPLEX)

$$\alpha_{\mu\nu}(\omega) = \frac{e^2}{m} \sum_n \frac{f_{ni}\,\delta_{\mu\nu}}{\omega_{ni}^2 - (\omega + i\delta)^2}$$

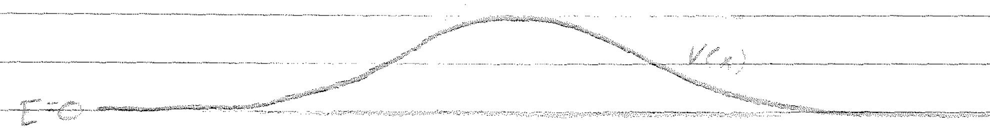
$$K = 2\pi\,\mathrm{Im}\,\alpha / n$$

α = ABS. COEF $= \frac{4\pi}{nc}\,\mathrm{Im}\,\alpha$

$$= \frac{4\pi^2 e^2}{mnc} \sum_n f_{ni} \frac{\delta(\omega_{ni} - \omega)}{2\omega}$$

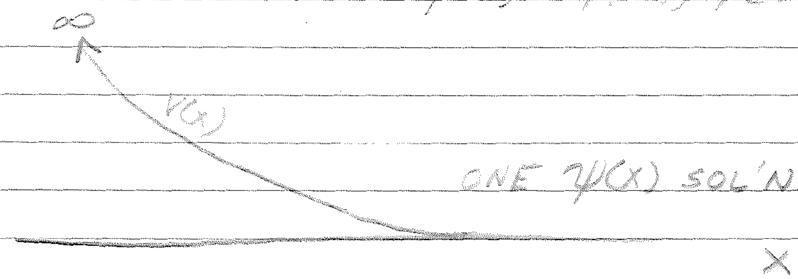
SAME AS TWO LECTURES AGO

SUMMARY:

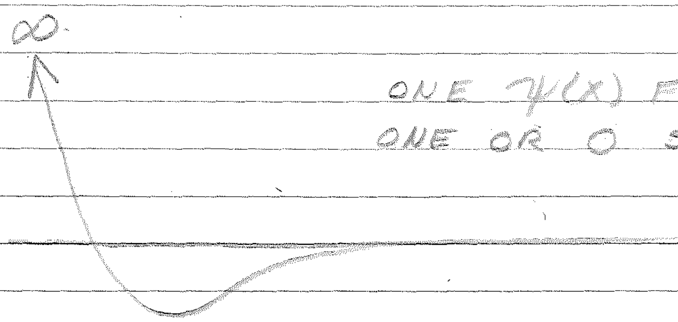


E>0 GIVES $\psi(x) = e^{ikx}\ e^{-ikx}$ w/o BULGE

$\psi(x) = \psi_1(x), \psi_2(x)$ ie 2 SOLUTIONS



ONE $\psi(x)$ SOL'N



ONE $\psi(x)$ FOR EACH $E>0$

ONE OR 0 SOL'N FOR EACH E

RECALL

$$\frac{i\hbar p}{m} = [x, H]$$

$$\frac{p_{ni}}{m} = \frac{-1}{i\hbar} \underset{\sim}{r}_{ni} E_{ni}$$

GIVES:

$$P(t) = \frac{e^2}{i^2 \hbar c} \sum_n \left\{ A_K e^{i\omega_K t} \left[\frac{-2\omega_{ni}\omega_K}{\omega_{ni}^2 - \omega_K^2} \right] \right.$$

$$\left. + A' e^{i\omega t} \left[\frac{2\omega_{ni}\omega_K}{\omega_{ni}^2 - \omega_K^2} \right] \right\}$$

$$= 2e^2 \sum_n \left(\underset{\sim}{r}_{ni} \underset{\sim}{r}_{in} \frac{\omega_{ni}}{\omega_{ni}^2 - \omega_K^2} \right) \left(\frac{\omega \hat{E}_n}{c} \left(A_K e^{-i t \omega_K} \right. \right.$$

$$\left. - A_K' e^{i\omega_K t} \right]$$

$$= \frac{2e^2}{\hbar} \sum_n \left(r_{ni} r_{in} \frac{\omega_{ni}}{\omega_{ni}^2 - \omega_K^2} \right) E$$

$$\boxed{\Rightarrow \alpha(\omega) = \frac{2e^2}{\hbar} \sum_n \underset{\sim}{r}_{ni} \underset{\sim}{r}_{in} \frac{\omega_{ni}}{\omega_{ni}^2 - \omega_K^2}}$$

NOTE IT LOOKS GOOD @ $\omega = 0$

GENERALLY

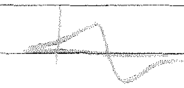
$$\alpha_{\mu\nu}(\omega) = \frac{2e^2}{\hbar} \sum_n \frac{\langle i | r_\mu | n \rangle \langle n | r_\nu | i \rangle \omega_{ni}}{\omega_{ni}^2 - \omega^2}$$

$$= \frac{e^2}{m} \sum_n \frac{f_{ni}}{\omega_{ni}^2 - \omega^2}$$

NORMALIZATION OF WAVE FUNCTIONS

1) BOUND STATES

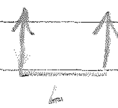
$\psi(x)$ IS BOUND IN SPACE



ALWAYS REAL

$$\int \psi_n \psi_m^* dx = \int \psi_n \psi_m dx = \left\{ \begin{matrix} 0 & \text{IF } n \neq m \\ 1 & \text{IF } n = m \end{matrix} \right\} = \delta_{n,m}$$

EX:



$$\psi_n = \sqrt{2/L} \sin \frac{n\pi x}{L}$$

IN 3D: $\int \psi_{nm\ell}(r)\, \psi_{n'm'\ell'}(r)\, d^3r$

$$= \delta_{nn'}\, \delta_{mm'}\, \delta_{\ell\ell'}$$

$\Longrightarrow$ CONSIDER: $\psi(x) = e^{ikx}$

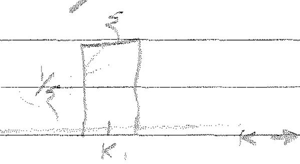
THEN $\int \rho\, dx = \infty$

2. DELTA FUNCTION NORMALIZATION

$$\int_{-\infty}^{\infty} dx\, \psi_k^*(x)\, \psi_{k'}(x)\, dx$$; k & k' ARE CONTINUOUS

$$= \left\{ \begin{matrix} 0 & ; k \neq k' \\ \infty & ; k = k' \end{matrix} \right\} = \delta(k-k')$$

$$\delta(k-k') = \lim_{\epsilon \to 0}$$



LET $\psi_k(k) = C e^{ikx}$ $\ni$ C IS CONSTANT

$$\Rightarrow \delta(k-k') = |C|^2 \int_{-\infty}^{\infty} dx\, e^{ix(k'-k)}$$

$$\int_{-\infty}^{\infty} dx\, e^{ix(k'-k)} = 2\pi\, \delta(k-k')$$

$$\Longrightarrow |C|^2 = \frac{1}{2\pi} \quad \text{OR} \quad |C| = \frac{1}{\sqrt{2\pi}}$$

$$C = \frac{1}{\sqrt{2\pi}} e^{i\delta}$$

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FINDING C_n:

$$C_n = \int_0^t dt'\, V(t') = \frac{e}{mc}\frac{\hat{\varepsilon}_n \cdot p_{ni}}{i}\left[\frac{A_k\left[e^{it(\omega_{ni}-\omega_k)}-1\right]}{\omega_{ni}-\omega_k} + \frac{A_k'\left[e^{i(\omega_{ni}+\omega_k)t}-1\right]}{\omega_{ni}+\omega_n}\right]$$

THUS:

$$\psi_g = \psi_i(r)e^{-i\omega_i t} + \sum_{n\neq i} C_n(t)\psi_n(t)e^{-it\omega_n}$$

$$\langle g|e\Sigma r_i|g\rangle = \left\{\langle\psi_i|e^{i\omega_i t} + \sum_n C_n^+ e^{i\omega_n t}\langle n^+|\right\} \times er\left\{|\psi_i\rangle e^{i\omega_i t} + \sum_m \psi_m C_m e^{-i\omega_m t} + \dots\right\}$$

LIMITING TO TERMS LINEAR IN C_n (IN E_n)

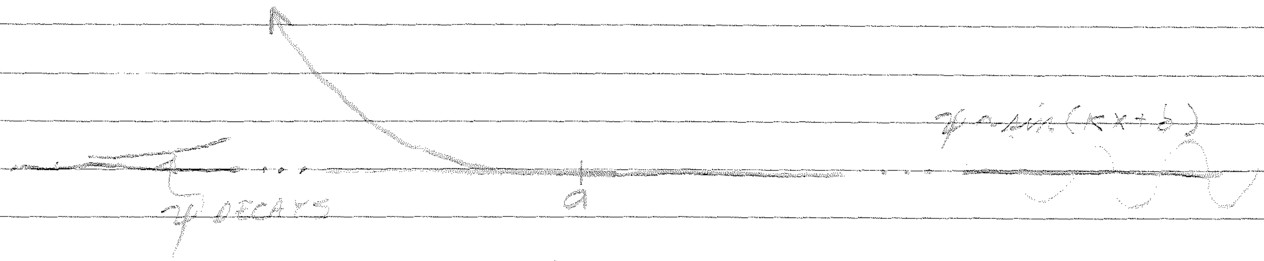
$$\langle g|e\Sigma r_i|g\rangle = \langle\psi_i|er|\psi_i\rangle + \sum_n\left[e^{it\omega_{in}}\langle i|er|n\rangle C_n + e^{it\omega_{ni}}C_n^+\langle i|er|n\rangle\right]$$

GIVES POLARIZATION:

$$P(t) = \frac{e}{mci}\sum_n\left[\left\{A_k\frac{e^{-it\omega_k}}{\omega_{ni}-\omega_k} + \frac{A'e^{it\omega}}{\omega_{ni}+\omega_n}\right\}r_{in}\,\hat{\varepsilon}\cdot p_{ni} + \hat{\varepsilon}\cdot p_{in}\, r_{ni}\left\{\frac{A_k^+e^{it\omega}}{\omega_{ni}-\omega_k} + \frac{A'^+e^{-it\omega}}{\omega_{ni}+\omega_k}\right\}\right]$$

NOW

$$A_k' = A_k^+ \qquad A_k = \sqrt{\frac{2\pi\hbar c^2}{V\omega}}\,a$$



LET $\psi_K(x) = B \sin(KX + \delta_K)$ FOR $X \geq a$

$$B = \sqrt{\frac{2}{\pi}}$$

THEN $\int_{-\infty}^{\infty} dx\, \psi_K^*(x)\psi_{K'}(x) = \delta(K-K')$

PROOF:

$$\int_{-\infty}^{\infty} dx\, \psi_K(x)\psi_{K'}(x) = \int_{-\infty}^{a} + \int_{a}^{\infty}$$

$$\int_a^{\infty} = \int_a^{\infty} B^2 \sin(KX+\delta_K)\sin(K'X+\delta_K)$$

WILL GIVE A δ FUNCTION

$\int_{-\infty}^{a}$ IS FINITE

$\therefore$ WE ONLY GOTTA LOOK @ $\int_a^{\infty}$.

$$B^2\int_a^{\infty} = B^2\int_a^{\infty} dx \sin[K(x-a)+\bar{\delta}_K]\sin[K'(x-a)+\bar{\delta}']$$

LET $Y = X - a$

$$= B^2\int_0^{\infty} = \int dY \sin(KY + \bar{\delta}_K)\sin(K'Y + \bar{\delta}'_K)$$

$$= B^2 \frac{\pi}{2}\delta(K-K')$$

PROOF

$$\int_0^{\infty}\frac{B^2}{4}\left[e^{i(KY+\delta_K)} - e^{-i(KY+\delta_K)}\right]\left[e^{i(K'Y+\delta_K')} - e^{-i(K'Y+\delta)}\right]$$

$$= \frac{B^2}{4} 2\pi\,\delta(K-K')$$

IT TURNS OUT $B = \sqrt{\frac{2}{\pi}}$

RECALL

$$\psi(x) = C\left[I_{iKa}(K_0 a e^{-x}) - I_{-iKa}(K_0 a e^{-x})\right]$$

@ $X \to \infty$, $\psi = \sqrt{2/\pi}\sin(KX+\delta)$

4/24/75

POLARIZABILITY

$$\underset{\sim}{p} = \underset{\approx}{\alpha} \cdot \underset{\sim}{E}$$

BEFORE: $\alpha \cong 2e^2 \sum_{\ell} \frac{|X_{\ell i}|^2}{\hbar \omega_{\ell i}}$

ONLY GOOD @ 0 FREQUENCY: $\omega = 0$

CONSIDER THE MORE GENERAL CASE

$$\underset{\sim}{p}\, e^{-i\omega t} = \underset{\approx}{\alpha}(\omega)\, \underset{\sim}{E}\, e^{-i\omega t}$$

NOW

$$\underset{\sim}{p} = \langle g | \sum e r_i | g \rangle$$

ASSUME IF $E = 0$, THEN $P = 0$

$$g = \psi_g(r,t) = \sum_n c_n(t)\, \psi_n(r)\, e^{-itE_n/\hbar}$$

$$c_n \cong \frac{1}{i\hbar} \int_0^t dt'\, V_{ni}(t')$$

$$V \sim \frac{e p \cdot A}{mc}$$

ASSUME $A = \hat{\varepsilon}_k \left[A_k e^{i(k\cdot r - \omega t)} + A_k' e^{-i(k\cdot r - \omega_k t)} \right)$

$$\underset{\sim}{E} = -\frac{1}{c}\frac{d}{dt} A$$

$$= \frac{-i\omega_k}{c} \varepsilon_n \left[A_k e^{i(\ )} - A' e^{-i(\ )} \right]$$

$$V = \frac{e}{mc} p \cdot A\, e^{i\omega_{ni} t}$$

$$\Rightarrow V(t) = \frac{e}{mc} P_{ni} \cdot \varepsilon_k \left[A_k e^{it(\omega_{ni} - \omega_k)} + A_k' e^{it(\omega_{ni} + \omega_k)} \right]$$

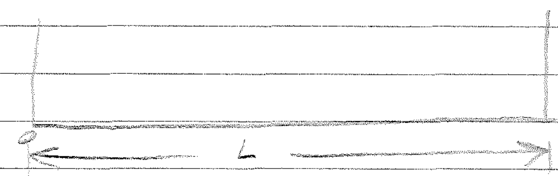
1-30-75

DELTA FUNCTION NORMALIZATION

$$\int_{-\infty}^{\infty} dx\, \psi_K^*(x)\, \psi_{K'}(x) = \delta(K-K')$$

K MUST BE CONTINUOUS.

3. Box Normalization



PUT WAVE FUNCTION (PLANE WAVE) IN A BOX

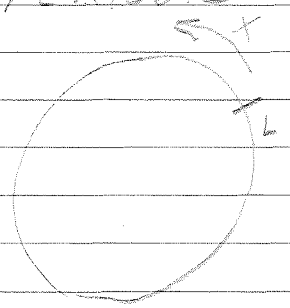
$$\Rightarrow \psi_n(x) = \sqrt{\tfrac{2}{L}}\, \sin\left(\frac{n\pi x}{L}\right)$$

LET $K_n = \frac{n\pi}{L}$ (K IS DISCRETE)

$$\Rightarrow \psi_n(x) = \sqrt{2/L}\, \sin(K_n x)$$

$$\int_0^L \psi_n(x)\, \psi_m(x) = \delta_{n,m} \quad ; \quad E_n = \frac{\hbar^2 K_n^2}{2m}$$

$\Rightarrow$ PERIODIC BOUNDRY CONDITIONS



$\leftarrow$ PLANE WAVE FUNCTION IS CONFINED TO CIRCLE WITH CIRCUMFERENCE L

(PER

$$\psi_K(x) = A e^{\pm iKx}$$

NOW

$$\psi_K(0) = \psi_K(L) \quad \text{(PERIODIC SYSTEM)}$$

$$\therefore 1 = e^{\pm iKL}$$

$$\Rightarrow KL = 2n\pi$$

$$K_n = \frac{2\pi n}{L}$$

$$\int_0^L dx\, \psi_n^*(x)\, \psi_m(x) = \delta_{n,m}$$

FOR $n=m$

$$A^2 L = 1 \Rightarrow A = \frac{1}{\sqrt{L}}$$

$$\therefore \psi_n(x) = \frac{1}{\sqrt{L}}\, e^{iK_n x}$$

b. $\mathcal{E} \perp Z \qquad (\mathcal{E} = x)$

$$\frac{\hbar}{i}\frac{d}{dx}(1s) = \frac{x}{r} e^{-r/a}$$

$$Y_1^1 = \sin\theta \, e^{i\phi} = \frac{1}{\sqrt{2}}(x + iY)$$

ABSORBTION SPECTRA STAYS THE SAME

EXTENSION TO THREE DIMENSIONS

FOR PERIODIC BOUNDARY

$\psi(x,y,z)$

$\psi(0,y,z) = \psi(L,y,z)$

$\psi(x,0,z) = \psi(x,M,z)$

$\psi(x,y,0) = \psi(x,y,N)$

$$K_{xn} = \frac{2n\pi}{L}, \quad K_{ym} = \frac{2m\pi}{M}, \quad K_{zn'} = \frac{2n'\pi}{N}$$

LET $\underset{\sim}{K} = (K_{xn}, K_{ym}, K_{zn'})$ $\Rightarrow$ STILL DISCRETE

THEN $\psi_K(x,y,z) = \frac{1}{\sqrt{LMN}} e^{i\underset{\sim}{K}\cdot\underset{\sim}{r}}$

VOLUME OF BOX $= V = LMN$

$$\Rightarrow \underline{\psi_K(\underset{\sim}{r}) = 1/\sqrt{V}\, e^{iK\cdot r}} \leftarrow \text{NORMALIZED}$$

BACK TO ONE DIMENSION:

$$\int_0^L dx \frac{e^{-ik_n x}}{\sqrt{L}} \frac{e^{ik_m x}}{\sqrt{L}} dx = \delta_{n,m} = \int \psi_n^* \psi_m dx$$

$$\lim_{L\to\infty} \int_0^L dx \frac{e^{-ik_n x} e^{ik_m x}}{L}$$

$$= \int_{-\infty}^{\infty} \lim_{L\to\infty} \frac{e^{-ik_n x} e^{ik_m x}}{L}$$

$$= \lim dx\, e^{-ik_n x} e^{ik_m x} = \lim \delta_{n,m} \frac{L}{2\pi}$$

AS $L \to \infty$, $k_{n+1} - k_n \to 0$

$$\underline{\lim_{L\to\infty} \frac{L}{2\pi} \delta_{n,m} = \delta(K-K')}$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iKx} e^{iK'x} dx = \delta(K-K')$$

RECALL STARK EFFECT $(n=2)$

$$eFz \rightarrow \begin{array}{l} \text{—— (1) } 3eaF \\ \text{—— (2) } 0 \\ \text{—— (3) } -3eaF \end{array}$$

a. $\vec{E} \parallel z$

$$f = \frac{2|\langle i | p_z | f \rangle|^2}{m \hbar \omega}$$

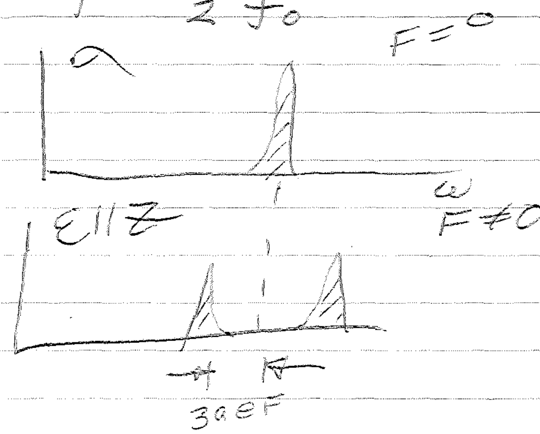
$\langle i | \Rightarrow \langle 1s |$

$$|f\rangle \Rightarrow \psi_{2p_{+1}},\ \psi_{2p_{-1}},\ \overbrace{\frac{1}{\sqrt{2}}(\psi_{2s} + \psi_{2p})}^{3eaF},$$

$$\underbrace{\frac{1}{\sqrt{2}}(\psi_{2s} - \psi_{2p_z})}_{-3eaF}$$

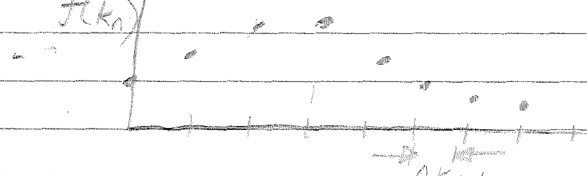
$$\frac{d}{dz}|1s\rangle = \frac{z}{ar} e^{-r/a}$$

$$f = \frac{1}{2} f_0$$



ANOTHER PROOF:

FINITE L: $f(k_n) = \sum_m f(k_m)\,\delta_{n,m}$



$$k_m = \frac{2m\pi}{L}$$

$$\Delta m = \Delta(k_n)\frac{L}{2\pi}$$

$$\sum_m f(k_m)(\Delta m) = \frac{L}{2\pi}\sum_m (\Delta k_m)\, f(k_m)$$

$$\lim_{L\to\infty} \sum_{k_m} f(k_m) = \frac{L}{2\pi}\int dk'\, f(k')$$

$$\lim_{L\to\infty} \sum_{k_m} f(k_m)\,\delta_{nm} = \frac{L}{2\pi}\int dk'\, f(k')\,\delta_{n,m} = f(k)$$

$$\therefore \boxed{\lim_{L\to\infty} \frac{L}{2\pi}\delta_{n,m} \longrightarrow \delta(k-k')}$$

NOTE $\left[\delta(\text{DIMENSION})\right] = \left[\frac{1}{\text{DIMENSION}}\right]$

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THEN FOR CONTINUUM STATES AND BOUND STATES

$$\alpha_e(\omega) = \frac{4\pi^2 e^2}{2m\hbar c}\left(\frac{N_a}{V}\right)\Big[\sum_n f_{ne}\,\delta(\hbar\omega - \hbar\omega_{en})$$

$$+ \int \frac{d^3k}{(2\pi)^3}\tilde{f}_k\,\delta\left(\hbar\omega - \frac{\hbar^2 k^2}{2m} + \omega_e \hbar\right)\Big]$$

~~FOR~~

$$\int_0^\infty d\omega\,\alpha(\omega) = \frac{4\pi^2 e^2}{2m\hbar c}\left(\frac{N_a}{V}\right)\sum_n f_{en}$$

THEOREM: f - SUM RULE OR THOMAS-KUHN RULE

$$\cancel{Z} = \text{NUMBER OF ELECTRONS} = \sum_n f_n$$

PROOF: WE WISH TO PROVE

$$Z = \sum_n \frac{2(\hat{\varepsilon}\cdot P_{en})^2}{m\hbar\omega_{ne}}$$

$$= \sum_n \frac{(\hat{\varepsilon}\cdot P_{en})^2}{m\hbar\omega_{ne}} + \frac{(\hat{\varepsilon}\cdot P_{em})^2}{m\hbar\omega_{ne}}$$

$$[x, H] = \frac{p}{m} i\hbar$$

$$\Rightarrow x_{en}\hbar\omega_{en} = \frac{i\hbar P_{en}}{m}$$

$$\Rightarrow Z = \sum_n \frac{\varepsilon\cdot P_{en} * \varepsilon\cdot P_{ne}}{m\hbar\omega_{ne}} + \frac{\varepsilon P_{en}\,\varepsilon\cdot P_{ne}}{m\hbar\omega_{ne}}$$

$$= \sum_n -\frac{i}{\hbar}\varepsilon\cdot X_{ne}\,\varepsilon\cdot P_{en} + \frac{i}{\hbar}\varepsilon\cdot X_{en}\,\varepsilon\cdot P_{ne}$$

$$= \frac{i}{\hbar}\sum_n\left\{\varepsilon\cdot P_{en}\,\varepsilon\cdot X_{ne} - \varepsilon\cdot X_{en}\,\varepsilon\cdot P_{ne}\right\}$$

$$= \frac{i}{\hbar}\sum_n\Big[\langle e|\varepsilon\cdot p|n\rangle\langle n|\varepsilon\cdot r|e\rangle - \langle e|\varepsilon\cdot r|n\rangle\langle n|\varepsilon\cdot p|e\rangle\Big]$$

$$= \frac{i}{\hbar}\sum\langle e|\varepsilon\cdot p\,\varepsilon\cdot r - \varepsilon\cdot r\,\varepsilon\cdot p|e\rangle = 1$$

$$= \text{"}Z\text{"}$$

SCHÖ'S EQ:

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar^2}\left[V(x)-E\right]\psi^*(x)$$

#1) $\psi(x)$ IS CONTINUOUS

#2) $d\psi(x)/dx$ IS CONTINUOUS IF $V(x)$ HAS NO DELTA FNCTION

PROOF:

$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{2m}{\hbar^2}\int_{x_0-\epsilon}^{x_0+\epsilon} dx\left[V(x)-E\right]\psi(x)$$

$$\left(\frac{d\psi}{dx}\right)\Big|_{x_0+\epsilon} - \left(\frac{d\psi}{dx}\right)\Big|_{x_0-\epsilon} = \frac{2m}{\hbar^2}2\epsilon\left[V(x_0)-E\right]\psi(x_0)$$

$$\lim_{\epsilon\to 0}\left[\qquad\qquad\right] = 0$$

$\therefore \frac{d\psi}{dx}$ IS CONTINUOUS = $\delta(x)$

NOTE: [NO #1 BY EVALUATING $\int_{x_0-\epsilon}^{x_0+\epsilon}\frac{d\psi}{dx}$]

EX $V=0$

$$\Rightarrow \frac{d^2}{dx^2}\psi = -\frac{2m}{\hbar^2}E\psi =$$

$E<0$, $\psi = C_1 e^{\alpha x} + C_2 e^{-\alpha x}$; $\alpha^2 = -\frac{2m}{\hbar^2}E$

BOTH BLOW UP $\Rightarrow C_1 = C_2 = 0$

DELTA FUNCTION POTENTIAL:

$$V(x) = -\lambda\,\delta(x) \quad ; \lambda > 0$$

THEN $x_0 = 0$; $\left(\frac{d\psi}{dx}\right)_{\epsilon} - \left(\frac{d\psi}{dx}\right)_{-\epsilon} = \frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon} dx(-\lambda\delta(x))\psi(x)$

$$= -\frac{2m\lambda}{\hbar^2}\psi(0)$$

$\Rightarrow \frac{d\psi}{dx}$ IS NOT CONTINUOUS

SOL'N IS:

$$\psi(x) = Ae^{-\alpha x} \qquad x>0$$
$$\psi(-x) = Ae^{\alpha x} \qquad x<0$$

THEN

$$-\alpha A - \alpha A = -\frac{2m\lambda}{\hbar^2}A$$

$$\Rightarrow \boxed{\alpha = \frac{m\lambda}{\hbar^2}}$$

$$E = -\frac{\hbar^2\alpha^2}{2m} = -\frac{m\lambda^2}{2\hbar^2} \qquad \lambda \sim erg\cdot cm$$

$A = \sqrt{\alpha}$ $\Rightarrow$ 1 BOUND STATE

5. $V(r) = \dfrac{\lambda e^{-k_s r}}{r}$

$$V(q) = \int d^3r\, e^{i q\cdot r} V(r) = \frac{4\pi\lambda}{q^2 + k^2}$$

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^2}\left| V_{k-k'}\right|^2$$

$$q^2 = k^2 + k'^2 - 2k\cdot k' = 2k^2\left[1 - \cos 2\theta\right]$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^2}\left[\frac{4\lambda\pi}{k_s^2 + 2k^2(1-\cos\theta)}\right]^2$$

$$\sigma = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, \frac{d\sigma}{d\Omega}$$

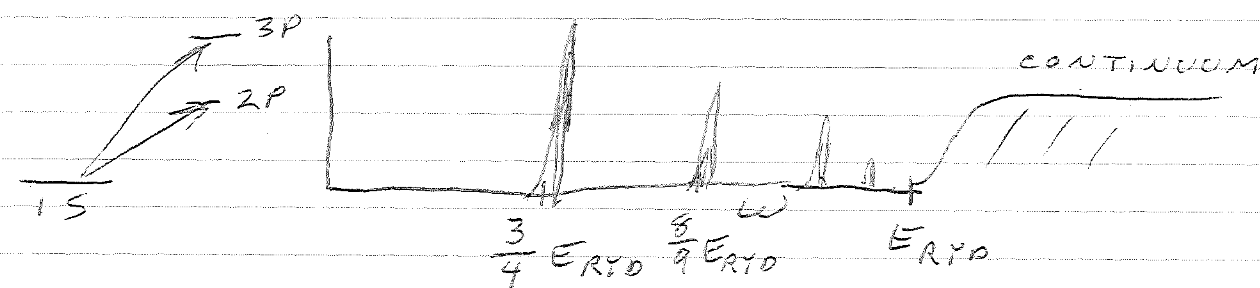
NOTES

OSCILLATOR STRENGTH

$$f = \frac{1}{\hbar} 2m\omega_{en}\langle \hat{\varepsilon}\cdot \hat{r}_{en}\rangle = \frac{2}{m\hbar\omega_{em}}\langle \hat{\varepsilon}\cdot \hat{P}_{en}\rangle^2$$

ABSORBSION COEFFICIENT:

$$\alpha_e(\omega) = \frac{4\pi^2 e^2}{2mnc}\left(\frac{N_e}{V}\right)\sum_n f_{ne}\,\delta(\hbar\omega - \hbar\omega_{en})$$



$$r_{en} = \int \psi_n^* \, r\, \psi_e$$

FOR CONTINUUM $(E > 0)$, THEN IF V = VOLUME OF BOX

$$\psi_k = \frac{1}{\sqrt{V}}\phi_k$$

$$\Rightarrow r_{ek} = \frac{1}{\sqrt{V}}\int d^3r\, \phi_k^* \, r\, \phi_e = \frac{1}{\sqrt{V}}\tilde{r}_{ke}$$

APPROXIMATION METHODS

[MIDTERM ON FEB 18, 1975 (TUESDAY) 1 HR EXAM]

WENTZEL
KRAMERS
BRILLOUIM
JEFFRIES $\longrightarrow$ WKBJ (A LIKEABLE METHOD)
OR QUASICLASSICAL APPROXIMATION

AGAIN: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right]\psi(x) = 0$

GIVEN: $\psi(x) = e^{i\sigma(x)/\hbar}$

THEN $\frac{d\psi}{dx} = \frac{i}{\hbar}\frac{d\sigma}{dx}e^{i\sigma/\hbar}$

$= \frac{i}{\hbar}\sigma' e^{i\sigma/\hbar}$

$\frac{d^2\psi}{dx^2} = \left(\frac{i}{\hbar}\sigma'' - \left(\frac{\sigma'}{\hbar}\right)^2\right)e^{i\sigma/\hbar}$

SCHRÖ EQ'N BECOMES

$\therefore \boxed{(\sigma')^2 - i\hbar\sigma'' + 2m[V(x) - E] = 0}$

CLASSICAL LIMIT IS $\hbar \to 0$

ASSUMPTION: $\sigma(x,\hbar) = \sigma_0(x) + \frac{\hbar}{i}\sigma_1(x) + \frac{\hbar^2}{i^2}\sigma_2(x) + \ldots$

$$\left(\sigma_0' + \frac{\hbar}{i}\sigma_1' + \frac{\hbar^2}{i^2}\sigma_2'\right)^2 - i\hbar\left(\sigma_0'' - \frac{\hbar}{i}\sigma_1''\right) + 2m(V - E) = 0$$

$\hbar^0$ SOLUTION $(\sigma_0')^2 + 2m[V(x) - E] = 0$

$$\Rightarrow \sigma_0' = \pm\sqrt{2m[E - V(x)]}$$

THEN:

$$\sigma_0(x) = \pm\int_a^x dx'\sqrt{2m[E - V(x')]}$$

$\hbar'$ SOLUTION: $2\sigma_0'\sigma_1' + \sigma_0'' = 0$

$$\frac{d\sigma_1}{dx} = \sigma_1' = -\frac{1}{2}\frac{\sigma_0''}{\sigma_0'} = -\frac{1}{2}\frac{d}{dx}\ln\sigma_0'$$

$$\Rightarrow \sigma_1 = \frac{1}{2}\ln\sigma_0' + C$$

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④ $i\hbar \dot{a}_n = \sum_\ell a_\ell V_{m\ell}\, e^{it\omega_{m\ell}}$

$i\hbar \dot{a}_m^{(0)} = 0$

$i\hbar \dot{a}_m^{(1)} = \sum_\ell a_\ell^{(0)} V_{m\ell}\, e^{it\omega_{m\ell}}$

$i\hbar \dot{a}_m^{(2)} = \sum_\ell a_\ell^{(1)} V_{m\ell}\, e^{it\omega_{m\ell}}$

$a_m^{(1)} = \frac{1}{i\hbar}\int_0^t dt'\, e^{i\omega_{mL}t'}$ INTO

GIVES

$a_m^{(2)} = \frac{1}{i\hbar}\sum_\ell V_{m\ell}\int_0^t dt\, a\, e^{it\omega_{m\ell}}$

$\times \int_0^{t'} dt''\, e^{it''\omega_{\ell L}}$

$= \frac{1}{(i\hbar)^2}\sum_\ell V_{m\ell}V_{\ell L}\int_0^t dt\, e^{it'\omega_{m\ell}}\frac{1}{i\omega_{\ell L}}\left[e^{it'\omega_{\ell L}} - 1\right]$

$\times\ \frac{e^{it'\omega_{mL}} - e^{it'\omega_{m\ell}}}{i\omega_{\ell L}}$

$= \frac{1}{(i\hbar)^2}\frac{1}{i^2}\sum_\ell \frac{V_{m\ell}V_{\ell L}}{\omega_{\ell L}}\left[\frac{e^{it\omega_{mL}} - 1}{\omega_{mL}} - \cancel{\frac{e^{it\omega_{m\ell}} - 1}{\omega_{m\ell}}}\right]$ $\to 0$

GIVES

$$w_{L\to m} = \frac{2\pi}{\hbar}\delta\left[E_m - E_L\right]\left[V_{mL} - \sum_{\ell\neq L} V_{m\ell}V_{\ell L}\left(\frac{1}{E_\ell - E_L}\right)\right]^2$$

EXACT

$H_0 = \psi_n^{(0)},\ E_n^{(0)}$

$H_0 + V \Rightarrow \phi_n, \mathcal{E}_m$

$$w_{EXACT} = \frac{2\pi}{\hbar}\delta(\mathcal{E}_m - \mathcal{E}_L)\,|T_{m\ell}|^2$$

$$= \int d^3r\, \phi_m(r)\, V(r)\, \psi_L^{(0)} r$$

$$T_{Lm}^* = T_{m\ell} = \int d^3r\, \phi_\ell(r) V(r)\, \psi_m^{(0)}(r)$$

$$\psi(x) = e^{\frac{i}{\hbar}\sigma(x)} = e^{\frac{i}{\hbar}\sigma_0 + \sigma_1 + \frac{\hbar}{i}\sigma_2 + \frac{\hbar^2}{i^2}\sigma_3^3 + \ldots}$$

$$\lim_{\hbar \to 0} \psi(x) \simeq e^{\frac{i}{\hbar}\sigma_0 + \sigma_1}$$

$$\therefore \psi(x) = e^{\pm\frac{i}{\hbar}\int^{x'} dx' \sqrt{2m[E - V(x')]}} \times e^{-\frac{1}{2}\ln \sigma_0'}$$

$$= \frac{e^{\pm\frac{i}{\hbar}\int^{x'} dx' \sqrt{2m[E - V(x')]}}}{(2m[E - V(x)])^{1/4}} \times \text{CONSTANT}$$

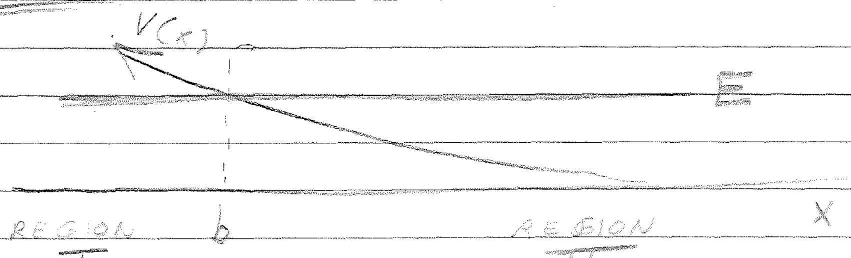
THE GENERAL WKBJ SOLUTION IS

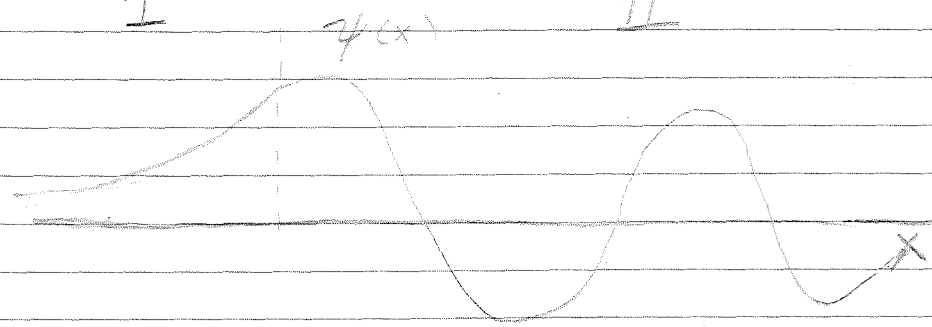
$$\psi(x) = \frac{1}{(2m[E - V(x)])^{1/4}}\Big[C_1 e^{+\frac{i}{\hbar}\int^{x'} dx' \sqrt{2m[E - V(x')]}}$$

$$+ C_2 e^{-\frac{i}{\hbar}\int^{x'} dx \sqrt{2m[E - V(x')]}}\Big]$$

LET $p(x) = \sqrt{2m(E - V(x))}$

EXAMPLE





b = TURNING POINT

IN REGION I : $\psi(x) = \dfrac{C' e^{-1/\hbar \left|\int_b^x dx' \sqrt{2m[V(x) - E]}\right|}}{[2m[V(x) - E]]^{1/4}}$ $\to E<V$

IN REGION II : $\psi(x) = \dfrac{C}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_b^x dx'\, p(x') + \alpha\right]$ $(E>V)$

C' & α ARE CONSTANTS

$\alpha = \frac{\pi}{4}$, $C' = \frac{1}{2}C$

WAVE FUNCTION BEHAVES BADLY @ $p = 0$ $(x = b)$

$$H = \frac{p_z^2}{2m} + (n+\tfrac{1}{2})\hbar\omega_c - \tfrac{1}{2}m\omega_c^2(\quad)$$

③ $H = -\mu_0 \underset{\sim}{l} \cdot \underset{\sim}{H}_0 - e\underset{\sim}{F}\cdot\underset{\sim}{r}$

a. $\underset{\sim}{H}_0 \parallel \underset{\sim}{F}$ CHOOSE z DIRECTION

$-\mu_0 l_z H_0$; $l_z|m\rangle = m\hbar|m\rangle$

$|2S\rangle = 0$
$|2P_z\rangle = 0$
$|2P_{\pm 1}\rangle = \pm 1$

$\Rightarrow 2P_{\pm 1} \Rightarrow E_\pm \pm \mu_0 H_0$

$eFz \} P_{2z} + P_{2s} \Rightarrow E = \pm 3aeF$

SO 4 STATES ALTOGETHER

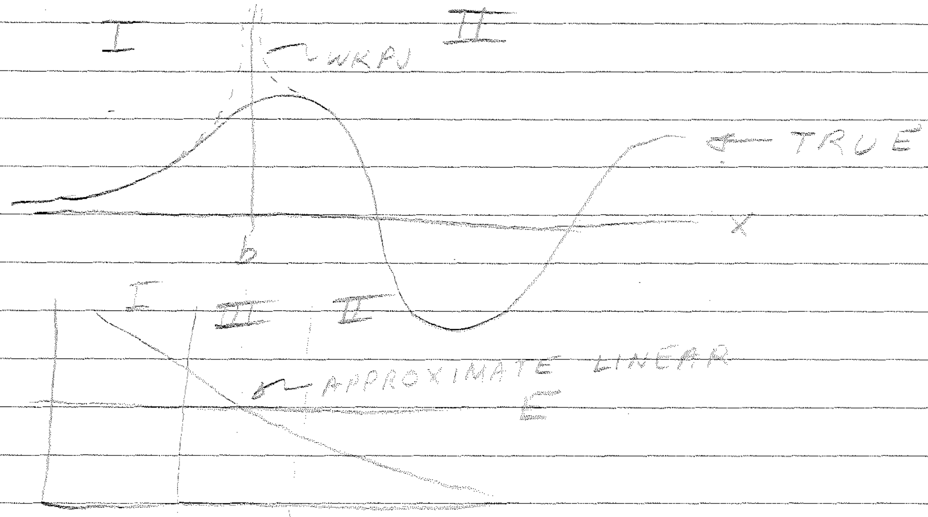
b. $\underset{\sim}{H}_0 \perp \underset{\sim}{F}$

F IN z DIREC
H IN X "

$$l_x = \tfrac{1}{2}(l^+ + l^-)$$

$$l_x Y_{l=1}^{m=0} = \frac{1}{\sqrt{2}}\left[Y_{l=1}^{m=1} + Y_1^{-1}\right]$$

$$\begin{array}{c} \begin{array}{cccc} ~~2S~~ & 2P_z & 2P_{+1} & 2P_{-1} \end{array} \\ \left(\begin{array}{cccc} 0 & 3eFa & 0 & 0 \\ 3eFa & 0 & \frac{1}{\sqrt{2}}\mu_0 H_0 & \frac{1}{\sqrt{2}}\mu_0 H_0 \\ 0 & \frac{1}{\sqrt{2}}\mu_0 H_0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}\mu_0 H_0 & 0 & 0 \end{array}\right) \end{array} \begin{array}{l} 2S \\ 2P_z \\ 2P_{+1} \\ 2P_{-1} \end{array} \Rightarrow E = \pm\sqrt{+(3aeF)^2 + \mu_0^2 H_0^2},\ 0,\ 0$$



IN REGION III (NEAR b)

$$V(x) = V(b) + (x-b)\frac{dV}{dx} + \ldots$$

$$V(b) = E \qquad \frac{dV}{dx} = -F = \text{CONSTANT}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (x-b)F\psi = 0$$

2-3-75

2nd HOMEWORK SET SOLUTIONS

1a. SHOW $H = \hbar\omega\left(a^+a + \frac{1}{2}\right)$

$$= \frac{p^2}{2m} + \frac{k}{2}x^2 \quad ; \quad k = m\omega^2 \quad ; \quad \omega = \sqrt{k/m}$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+)$$

$$p = i\sqrt{\frac{\hbar m\omega}{2}}\,(a - a^+)$$

$$\Rightarrow x^2 = \frac{\hbar}{2m\omega}\left(a^2 + a^{+2} + aa^+ + a^+a\right)$$

$$p^2 = -\frac{\hbar m\omega}{2}\left(a^2 + a^{+2} - aa^+ - a^+a\right)$$

$$\Rightarrow H = \frac{\hbar\omega}{4}\left[a^2 + a^{+2} + aa^+ + a^+a\right] - \frac{\hbar\omega}{4}\left[a^2 + a^{+2} - aa^+ - a^+a\right]$$

$$= \frac{\hbar\omega}{2}\left[aa^+ + a^+a\right] \qquad , \quad [a, a^+] = 1$$

$$= \frac{\hbar\omega}{2}\left[a^+a + 1 + a^+a\right]$$

$$= \hbar\omega\left[a^+a + \frac{1}{2}\right]$$

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4/22/75

HOMEWORK #9

1. $m\dot{\underset{\sim}{v}} = -\left[F_x + \frac{1}{c}\, \underset{\sim}{v} \times \underset{\sim}{H_z}\right]$

AS COMPONENTS:

$$\dot{v}_x = -\frac{e}{m}F_x + \frac{eH_0}{mc}v_y$$

$$\dot{v}_y = \qquad\qquad -\frac{eH_0}{mc}v_x$$

$$\dot{v}_z = 0 \Rightarrow v_z = \text{CONSTANT} = v_z(0)$$

$$\ddot{v}_x = -\omega_c \dot{v}_y = -\omega_c^2 v_x$$

$$v_x = A\sin\omega_c t + B\cos\omega_c t$$

$$v_y = -\frac{\dot{v}_x}{\omega_c} + \frac{cF}{H_0}$$

$$= A\cos\omega_c t - B\sin\omega_c t + \frac{cF}{H_0}$$

2. $\nabla \times A = H_0 \hat{z}$

$A_y = xH_0$ EQUIVALENTLY $A_x = -yH_0$

$A_x = 0$ $A_y = 0$

$A_z = 0$ $A_z = 0$

GIVES

$$H = \left(\frac{p_x^2}{2m} + \frac{p_z^2}{2m} + \left(p_y - \frac{e}{mc}xH_0\right)^2\right) + eFx$$

CONSTANTS OF MOTION

$$[p_y, H] = 0 = [p_z, H]$$

SUGGESTS

$$\psi = \phi(x)\, e^{i(k_y y + k_z z)}$$

$$\frac{p_x^2}{2m} + \frac{\hbar^2 k_z^2}{2m} + \frac{\left(\hbar k_y - \frac{e}{c}xH_0\right)^2}{2m} + eFx$$

$$\cancel{= \frac{p_x^2}{2m} + \frac{\hbar^2 k_z^2}{2m} +} \qquad b = \frac{\left(\frac{e}{c}H_0\right)^2}{2m}$$

$$= \frac{p_z^2}{2m} + \frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2(x-b) + eFx$$

$$= \frac{p_z^2}{2m} + \frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2\left(x - b + \frac{eF}{\omega_c m}\right)$$

$$-\frac{1}{2}m\omega_c^2\left(\frac{e^2F^2}{m^2\omega_c^2} - \frac{2beF}{m\omega_c}\right)$$

$$x_0 = b - \frac{eF}{m\omega_c^2} = \frac{1}{\omega_c}\left[v_y - \frac{cF}{H_0}\right]$$

b. $[a, H] = \hbar\omega\,[a, a^+a]$

$= \hbar\omega\,\big[[a, a^+]a + a^+\cancel{[a, a]}^{\,0}\big]$

$[a^+, H] = -[a, H]^+ = -\hbar\omega a^+$

c. $e^{sH} a e^{-sH} = a + s[H, a] + \frac{s^2}{2!}[H, [H, a]] + \dots$

$[H, a] = -\hbar\omega a$

$\Rightarrow e^{sH} a e^{-sH} = a - s\hbar\omega a + \frac{(\hbar\omega s)^2}{2!} a + \dots + (-1)^n \frac{(\hbar\omega s)^n}{n!} a$

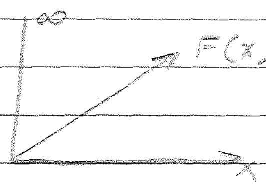
$= a e^{-s\hbar\omega}$

$e^{sH} a^+ e^{-sH}$

Now $[e^{sH} a e^{-sH}]^+ = e^{-sH} a^+ e^{sH} = a^+ e^{-s\hbar\omega}$

$\Rightarrow e^{sH} a^+ e^{-sH} = a^+ e^{s\hbar\omega}$

2.



$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + Fx - E\right]\psi(x) = 0$$

$$\xi = -\left(\frac{E}{F} + x\right)\left(\frac{2mF}{\hbar^2}\right)^{-1/3}$$

$$\left(\frac{\partial^2}{\partial\xi^2} - \xi\right)\psi(\xi) = 0$$

BLOWS UP

$$\Rightarrow \psi(\xi) = aA_i(\xi) + b\cancel{B_i(\xi)}$$

$$\psi(\xi) = cA_i(\xi)$$

B.C. $\rightarrow \psi(x=0) = 0 = \psi\left[\xi_0 = -\frac{E}{F}\left(\frac{2mF}{\hbar^2}\right)^{\frac{1}{3}}\right] = 0$

$\Rightarrow$ EIGENVALUE CONDITION:

$$A_i(\xi_0) = 0$$

$E = \frac{1}{c}\dot{A} + \nabla\phi \; ; \; P = \frac{-E}{4\pi}$

$\frac{1}{c}\dot{A}$ IS PERPUNDICULAR (USUALLY) TO $\nabla\phi$

$$\Rightarrow P^2 = \frac{\left(\frac{1}{c}\dot{A}\right)^2 + (\nabla\phi)^2}{16\pi^2}$$

$$\Rightarrow P \cdot \nabla\phi = (\nabla\phi)^2 \times \frac{1}{4\pi}$$

$$\int (\nabla\phi)^2 \, dr = -\int \phi \nabla^2 \phi \, dr = 4\pi \int \rho \phi \, dr$$

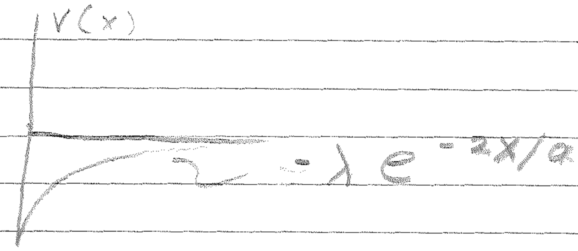
COMBING THE WHOLE MESS GIVES

$$H = \overbrace{\frac{1}{2m} \sum_i \left(P_i + \frac{e}{c} A(r_i)\right)^2}^{K.E.}$$

$$+ \underbrace{\sum_K \hbar\omega_K \left(a_K^{\dagger} a_K + \frac{1}{2}\right)}_{E.M.\ PART} + \underbrace{\frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}}}_{COULOMB}$$

DIFFERENT DERIVATION ALSO IN CHAPT. 14 OF SCHIFF

3.



$$\psi(x) = c_1 J_{-ika}(k_0 a e^{-x/a}) + c_2 J_{ika}(k_0 a e^{-x/a})$$

$$\psi(x=0) = 0 = c_1 J_{ika}(k_0 a) + c_2 J_{-ika}(k_0 a)$$

$$\Rightarrow \frac{c_2}{c_1} = -\frac{J_{ika}(k_0 a)}{J_{-ika}(k_0 a)}$$

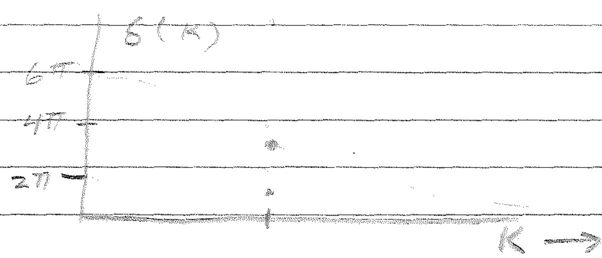
$$\therefore \psi(x) = c_1 \Big[J_{ika}(k_0 a e^{-\frac{x}{a}}) - J_{-ika}(k_0 a e^{-\frac{x}{a}}) \times \frac{J_{ika}(k_0 a)}{J_{-ika}(k_0 a)} \Big]$$

$x \to \infty$ $(\nu \to 0)$

$$\lim_{z \to 0} J_\nu(z) = \left(\frac{z}{2}\right)^\nu \Big/ \Gamma(1+\nu)$$

$$\lim_{x\to\infty} \psi(x) = c_1 \left[\frac{\left(\frac{k_0 a}{2}\right)^{ika}}{\Gamma(1+ika)} e^{-ikx} - \frac{e^{ikx}\left(\frac{k_0 a}{2}\right)^{2ikx}}{\Gamma(1-ika)} \frac{J_{ika}}{J_{-ika}} \right]$$

$$e^{2i\delta} = \left(\frac{k_0 a}{2}\right)^{-2ika} \frac{\Gamma(1+ika)}{\Gamma(1-ika)} \cdot \frac{J_{ika}(k_0 a)}{J_{-ika}(k_0 a)}$$



2. FIELD COORDINATES

$$e\sum_i\left[\phi(r_i)-\frac{1}{c}\dot{r}_i\cdot A(r_i)\right]$$

$$=\int d^3r\left[\rho(r)\phi(r)-\frac{j(r)}{c}\cdot A(r)\right]$$

$$\rho(r)=e\sum_i\delta(r-r_i)$$

$$j(r)=e\sum_i V_i\ \delta(r-r_i)$$

THEN

$$\mathcal{L}=\frac{1}{8\pi}\left[E^2-H^2\right]+\rho\phi-j\frac{A}{c}$$

$$\frac{\delta\mathcal{L}}{\delta\phi}=\rho\quad;\quad\frac{\delta\mathcal{L}}{\delta\dot\phi}=0$$

$$\frac{\delta\mathcal{L}}{\delta\left(\frac{\delta\phi}{\delta x}\right)}=\qquad\qquad\nabla\cdot E=4\pi\rho$$

$$\frac{\delta\mathcal{L}}{\delta\left(\dot{A}_x/c\right)}=\dot{j}_x$$

$$\nabla\times\dot{H}=\frac{1}{c}\dot{E}+\frac{4\pi j}{c}$$

$$H=\sum_i\dot{r}_i\cdot p_i+\int d^3r\ P(r)\cdot\frac{1}{c}\frac{\delta A}{\delta t}-L$$

REMEMBER: $p_i=m\dot{r}_i-\frac{e}{c}A(r_i)=\frac{\delta L}{\delta\dot{r}_i}$

$$\Rightarrow\dot{r}_i=\frac{1}{m}\left(p+\frac{e}{c}A(r_i)\right)$$

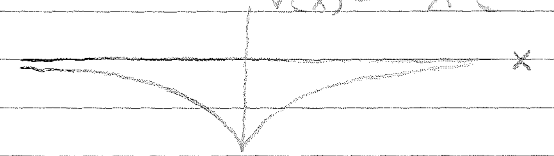
$$H=\sum_i\left\{\frac{p_i}{m}\cdot\left(p_i+\frac{e}{c}A\right)-\frac{1}{2m}\left(p+\frac{e}{c}A\right)^2+\frac{e}{mc}A\cdot\left[p+\frac{e}{c}A\right]\right\}$$

$$=\sum_i\frac{1}{2m}\left[p_i+\frac{e}{c}A(r_i)\right]^2-e\sum_i\phi(r_i)$$

$$+\int d^3r\left[2\pi P^2+\frac{1}{8\pi}(\nabla\times A)^2-P\cdot\nabla\phi\right]$$

$V(x) = -\lambda e^{-2|x|/a}$

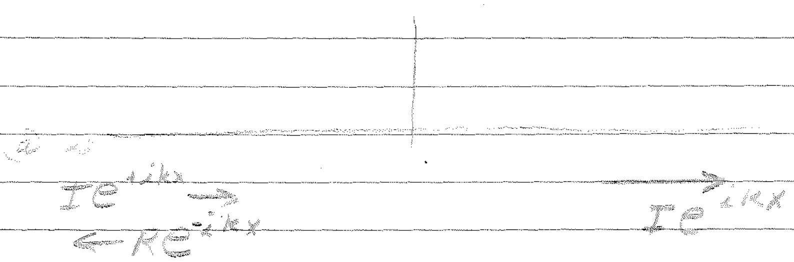
4.



WAVE FUNCTION ON RIGHT,

$$\psi_R(x) = c_1 J_{ika}(k_0 a e^{-x/a}) + c_2 J_{-ika}(k_0 a e^{-x/a})$$

ON LEFT: $\psi_L(x) = c_3 J_{ika}(k_0 a e^{x/a}) + c_4 J_{-ika}(k_0 a e^{x/a})$



$C_1 = 0$ USING ASYMYTOTIC LIMIT

$$\lim_{\substack{z\to\infty \\ (0)}} J_\nu(z) = \left(\frac{z}{2}\right)^\nu \Big/ \Gamma(1+\nu)$$

FOR LEFT

$$\lim_{x\to-\infty} \psi_L(x) = \underbrace{\frac{c_3\left(\frac{k_0 a}{2}\right)^{ika}}{\Gamma(1+ika)}}_{\to I} e^{ikx}$$

$$\lim_{x\to\infty} \psi_R(x) = \underbrace{c_2 \frac{\left(\frac{k_0 a}{2}\right)^{-ika}}{\Gamma(1-ika)}}_{\to T_{LR}} e^{ikx}$$

THEN: $$\frac{T_{RL}}{I} = \left(\frac{c_2}{c_3}\right)\left(\frac{k_0 a}{2}\right)^{-2ika}\frac{\Gamma(1+ika)}{\Gamma(1-ika)}$$

$$[A_\mu(r), P_\nu(r')]$$

$$= \frac{1}{4\pi c^2} \sum_{kk'} A_k A_{k'} \Omega_{k\mu} \Omega_{k'\nu}$$

$$\left[-[a_k, a_{k'}] e^{i(k\cdot r - k'\cdot r')} + [a_k^\dagger, a_{k'}] \right]$$

$$\text{IF } A_k^2 = \frac{2\pi \hbar c^2}{\sqrt{\omega_k}}$$

IT TURNS OUT

$$H = \int d^3r \left[\sum_{kk'} 2\pi P_{rH} + \frac{1}{8\pi} (\nabla \times A)^2 \right]$$

$$= \sum_k \hbar \omega_k [a_k^\dagger a_k + \tfrac{1}{2})$$

$$E = -\frac{1}{c} \frac{\delta A}{\delta t} + \nabla \phi$$

$$H = \nabla \times A$$

$$L = \int d^3r \frac{1}{8\pi} [E^2 - H^2] + \tfrac{1}{2} m \sum_i \dot{r}_i^2$$

$$+ e \sum_i \left[\phi(r_i) - \frac{1}{c} \dot{r}_i \cdot A(r_i) \right]$$

1) PARTICLE COORDINATES

$$x_i) \quad \frac{\delta L}{\delta x_i} = e \frac{\delta \phi}{\delta x_i} - \frac{e}{c} \dot{r}_i \cdot \frac{\delta}{\delta x_i} A(r_i)$$

$$P_i = \frac{\delta L}{\delta \dot{x}_i} = m \dot{x}_i - \frac{e}{c} A(r_i)$$

$$0 = \frac{\delta L}{\delta x} - \frac{\delta}{\delta t} \frac{\delta L}{\delta \dot{x}_i}$$

$$= e \frac{\delta \phi}{\delta x_i} - \frac{e}{c} \dot{r}_i \frac{\delta A}{\delta x_i} - m \ddot{x}$$

$$+ \frac{e}{c} \left[\frac{\delta A}{\delta t} + \underbrace{\frac{\delta A}{\delta r} \frac{\delta r}{\delta t}}_{V \cdot \nabla A_x} \right]$$

$$\Rightarrow m \ddot{x} = e \left[E + \frac{1}{c} v \times H \right]$$

@ $x=0$, $\psi_L(0) = \psi_R(0)$

$$\Rightarrow C_2 J_{-ika}(k_0 a) = C_3 J_{ika}(k_0 a) + C_4 J_{-ika}(k_0 a)$$

$$\frac{d}{dx} J_\nu(z) = J'_\nu(z)\frac{dz}{dx}$$

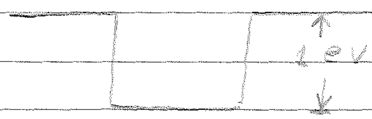
$$\psi'_L(0) = \psi'_R(0)$$

$$\Rightarrow \frac{k_0 a}{2}\left[-C_2 J'_{-ika} = C_3 J'_{ika} + C_4 J'_{-ika}\right]_{x=0}$$

CAN GET OTHER C'S VALUE FROM NORMALIZATION

$$\therefore \frac{C_2}{C_3} = \frac{J_{ika} J'_{ika} - J'_{ika} J_{-ika}}{-2 J_{-ika} J'_{-ika}}$$

5. ANSWER IS $-0.17\,eV$



$\Rightarrow$ $1 > E_L > 0$
(WORKED IN BOOK)

STATEMENTS (Q.M.)

$$H = P \cdot \frac{1}{c}\frac{\delta A}{\delta t} - \mathcal{L}$$

$$\left[\frac{1}{c}A_\mu(r), P_\nu(r')\right] = i\hbar\,\delta_{\mu\nu}\,\delta(r-r')$$

$$\mathcal{H} = P\cdot\underbrace{\left[\frac{1}{c}\dot{A} + \nabla\phi\right]}_{4\pi P} - P\cdot\nabla\phi - 2\pi P^2 + \frac{1}{8\pi}(\nabla\times A)^2$$

$$= 2\pi P^2 + \frac{1}{8\pi}(\nabla\times A)^2 - P\cdot\nabla\phi$$

HAVE HARMONIC OSCILLATOR IN FIRST 2 TERMS.
IT TURNS OUT THAT $P\cdot\nabla\phi = 0$

$$H = \int d^3r\,\mathcal{H}(r)$$

$$= \int d^3r\,P\cdot\nabla\phi = \int d^3r\,\phi\,\nabla\cdot P = \nabla\cdot E = 0$$

THUS

$$H = \int d^3r\,\mathcal{H}(r) = \int d^3r\left[2\pi P^2 + \frac{1}{8\pi}(\nabla\times A)^2\right]$$

ASSUME THAT $A(r,t) = \sum \hat{\eta}_k A_k\left[a_k e^{ik\cdot r}e^{-i\omega_k t} + a_k^\dagger e^{-ik\cdot r}e^{+i\omega_k t}\right]$

$$a_k|n_k\rangle = \sqrt{n}\,|n_k - 1$$

WITHOUT ϕ

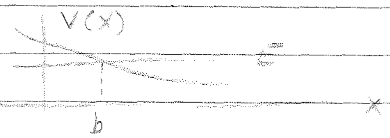
$$P = \frac{1}{4\pi c}\frac{\delta A}{\delta t} = \frac{-1}{4\pi c}\sum_{k} i\omega_k A_{k'}\hat{\eta}_{k'}$$

$$\times\left[a_{k'}e^{ik'\cdot r}e^{-i\omega_k t} + a_{k'}^\dagger e^{-ik'\cdot r}e^{i\omega_k t}\right]$$

$$[a_k, a_{k'}^\dagger] = \delta_{kk'}$$

NOTES:

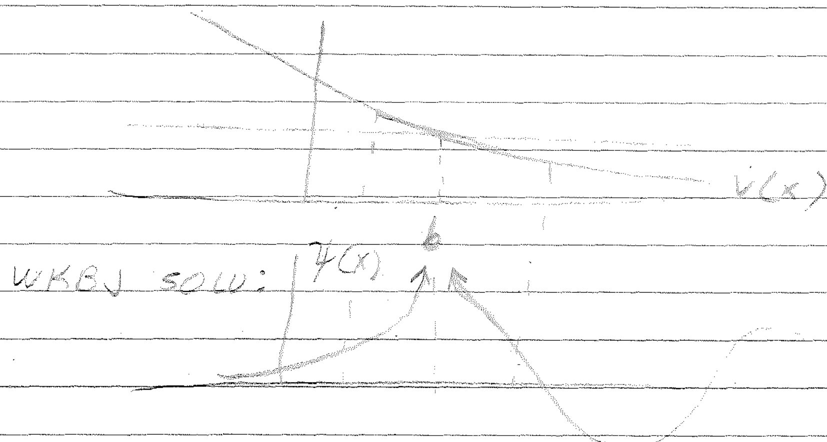
WKBJ



$$x > b \Rightarrow \psi(x) = \frac{C}{\sqrt{p}} \sin \frac{1}{\hbar}\int_b^a dx'[p(x') + \alpha]$$

$$p = \sqrt{2m[E - V(x)]} \qquad \alpha = \pi/4$$

$$x < b \Rightarrow \psi(x) = \frac{C'}{|p|^{1/2}} e^{-\frac{1}{\hbar}\int_x^b dx' \sqrt{2m[V(x') - E]}}$$



IN BLOW UP REGION, APPROXIMATE V(x) BY LINE

TAYLOR SERIES

$$V(x) = V(b) + (x-b)\left(\frac{\delta V}{\delta x}\right)_b + \ldots$$

$$= V(b) - F(x-b) \quad \Rightarrow \quad \left.\frac{\delta V}{\delta x}\right|_{x=b} = -F$$

THEN

$$= 0 \text{ (SINCE } V(b) = E)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - E + V(b) + F(x-b)\right]\psi(x) = 0$$

AIRY FUNCTION SOLUTION:

$$\psi(x) = C_0 A_i(-\xi)$$

$$\xi = (x-b)\left(\frac{2mF}{\hbar^2}\right)^{1/3}$$

CONSIDER NOW A_x AS A PRIMARY VARIABLE

$$(\nabla \times A)^2 = \left(\frac{\delta}{\delta x} A_y - \frac{\delta}{\delta y} A_x\right)^2 + \left(\frac{\delta A_z}{\delta y} - \frac{\delta A_y}{\delta z}\right)^2 + \left(\frac{\delta A_x}{\delta z} - \frac{\delta A_z}{\delta x}\right)^2$$

$$\frac{\delta \mathcal{L}}{\delta (A_x/c)} = 0$$

$$\frac{\delta \mathcal{L}}{\delta \left(\frac{\dot{A}}{c}\right)} = \frac{1}{4\pi}\left[\frac{\dot{A}_x}{c} + \frac{\delta \phi}{\delta x}\right] = P_x$$

$$\frac{\delta \mathcal{L}}{\delta \left(\frac{\delta A_x}{\delta x}\right)} = 0$$

$$\frac{\delta \mathcal{L}}{\delta \left(\frac{\delta A_x}{\delta y}\right)} = -\frac{1}{4\pi}\left(\frac{\delta A_x}{\delta y} - \frac{\delta A_y}{\delta x}\right)$$

$$\frac{\delta \mathcal{L}}{\delta \left(\frac{\delta A_x}{\delta z}\right)} = -\frac{1}{4\pi}\left(\frac{\delta A_x}{\delta z} - \frac{\delta A_z}{\delta x}\right)$$

PLUGGING INTO LAG'S EQN

$$0 = -\frac{1}{4\pi c}\frac{\delta}{\delta t}\left[\frac{1}{c}\dot{A}_x + \frac{\delta \phi}{\delta x}\right] + \frac{1}{4\pi}\frac{\delta}{\delta y}\underbrace{\left[\frac{\delta A_x}{\delta y} - \frac{\delta A_y}{\delta x}\right]}_{H_z}$$

$$+ \frac{1}{4\pi}\frac{\delta}{\delta z}\underbrace{\left[\frac{\delta A_x}{\delta z} - \frac{\delta A_z}{\delta x}\right]}_{-H_y}$$

CORRESPONS TO ④: $\nabla \times H = \frac{1}{c}\dot{E}$

WISH TO MATCH UP REGIONS.

FIND $\lim x-b \to \infty$ $[\xi >> 1]$
(WANT WIGGLES IN A_i SAME AS FOR $b > 0$)

$$\lim_{\xi\to\infty} C_0 A_i(-\xi) = \frac{C_0}{\sqrt{\pi}} \frac{1}{\xi^{1/4}} \sin\left[\frac{2}{3}\xi^{3/2} + \pi/4\right]$$

WKBJ RESULT (SAME APPROX.): $V(x) = V(b) - F(x-b)$

$$p(x) = \sqrt{2m[E - V(b) + F(x-b)]} = \sqrt{2mF(x-b)}$$

$$\int \frac{1}{\hbar} dx' \sqrt{2mF} \sqrt{x'-b} = \sqrt{\frac{2mF}{\hbar^2}} \frac{2}{3}(x-b)^{3/2}$$

$$= \frac{2}{3}\xi^{3/2}$$

$\therefore$ FOR $x > b$

$$\psi(x) = \frac{c}{p^{1/2}} \sin\left[\frac{1}{\hbar}\int_b^x dx[p(x') + \alpha]\right]$$

$$= \frac{c}{p^{1/2}} \sin\left[\frac{2}{3}\xi^{3/2} + \alpha\right]$$

$$\Rightarrow \alpha = \pi/4$$

LET $C_0 = \dfrac{C\sqrt{\pi}}{(2mF\hbar^2)^{1/6}}$ $\qquad p^{\frac{1}{2}} \approx \xi^{\frac{1}{4}}$

$$\lim_{x\to-\infty} C_0 A_i(-\xi) = \frac{C_0}{2\sqrt{\pi}} \frac{1}{|\xi|^{1/4}} e^{-\frac{2}{3}|\xi|^{3/2}}$$

WKBJ COMPARISON IS SIMILAR, GIVING
$C' = \frac{1}{2}C$

$\therefore$ FOR LINEAR POT:

$$x > b, \quad \psi(x) = \frac{c}{p^{1/2}} \sin\left[\frac{1}{\hbar}\int_b^x dx'\, p(x') + \frac{\pi}{4}\right]$$

$$x < p, \quad \psi(x) = \frac{c}{2|p|^{1/2}} e^{-\frac{1}{\hbar}\int_x^b dx' \sqrt{2m[V(x')-E]}}$$

THIS IS TRUE FOR OTHERS TOO

DERIVATION WITH NO SOURCES OR CURRENTS,

MAXWELL'S EQ'NS:

① $\nabla \cdot E = 0$

② $\nabla \cdot H = 0$

③ $\nabla \times E = -\frac{1}{c}\dot{H}$

④ $\nabla \times H = \frac{1}{c}\dot{E}$

② $\nabla \cdot H = 0 \Longrightarrow H = \nabla \times A$

PUT INTO ③:

$$\nabla \times \left(E + \frac{1}{c}\frac{dA}{dt}\right) = 0$$

NOW, IF $\nabla \times C = 0$ THEN $C = \nabla \phi$

$$\left.\begin{aligned} \Rightarrow E &= -\frac{1}{c}\frac{dA}{dt} - \nabla\phi \\ H &= \nabla \times A \end{aligned}\right\}$$

CONSIDER NOW A LAGRANGIAN:

$$\mathcal{L}\left[A_x, A_y, A_z, \phi, \dot{A}_x, \dot{A}_y, \dot{A}_z, \dot{\phi}, \ldots\right]$$

IT TURNS OUT THAT

$$\mathcal{L} = \frac{1}{8\pi}\left[\frac{1}{c}\frac{\delta A}{\delta t} + \nabla\phi\right]^2 - \frac{1}{8\pi}(\nabla \times A)^2$$

$$\left(= \frac{1}{8\pi}\left(E^2 - H^2\right)\right)$$

NOW $\frac{d\mathcal{L}}{\delta\phi} = 0$

$$\frac{\delta\mathcal{L}}{\delta\dot{\phi}} = 0 \qquad (= P_\phi)$$

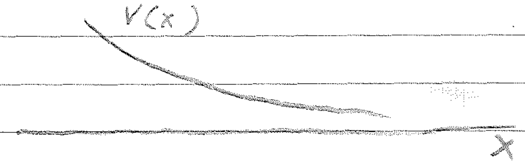
$$\frac{\delta\mathcal{L}}{\delta\left(\frac{\delta\phi}{\delta x}\right)} = \frac{1}{\pi}\left[\frac{\delta\phi}{\delta x} + \frac{1}{c}\dot{A}_x\right]$$

FROM EQ'N ON PRECEEDING PAGE:

$$0 = \frac{1}{4\pi}\left[\frac{\delta}{\delta x}\left[\frac{\delta\phi}{\delta x} + \frac{1}{c}\dot{A}_x\right] + \frac{\delta}{\delta y}\left[\frac{\delta\phi}{\delta y} + \frac{1}{c}\dot{A}_y\right] + \frac{\delta}{\delta z}\left[\quad\right]\right]$$

CORRESPONDS TO ① $\nabla \cdot E = 0$

IF $V(x) \to 0$ FOR LARGE x



$$\delta_{WKBJ} = \lim_{x\to\infty}\left[\frac{\cancel{\sqrt{2m}}}{\hbar}\int_b^x dx'\left[p(x') - kx\right]\right] + \frac{\pi}{4}$$

EXAMPLE:

CONSIDER $\quad V(x) = \lambda e^{-2x/a}$

$$E = \lambda e^{-2b/a}$$

$$\ln \lambda/E = 2b/a \Rightarrow b = \frac{a}{2}\ln\left(\lambda/E\right) \Leftarrow \text{TURNING POINT}$$

$$\frac{\sqrt{2m}}{\hbar}\int_b^x dx'\sqrt{E - \lambda e^{-2x'/a}}$$

$$z = e^{-2x/a} \Rightarrow dx = -\frac{a}{2}\frac{dz}{z}$$

$$\Rightarrow \frac{\sqrt{2m}}{\hbar}\int_b^x dx'\sqrt{E-\lambda e^{-2x'/a}} = -\sqrt{\frac{2m}{\hbar^2}}\left(\frac{a}{2}\right)\int_{E/\lambda}^{e^{-2x/a}}\frac{dz}{z}\sqrt{E-\lambda z}$$

$$= -\frac{1}{2}\left[2\sqrt{E-\lambda z} + \sqrt{E}\,\ln\left|\frac{\sqrt{E-\lambda z}-\sqrt{E}}{\sqrt{E-\lambda z}+\sqrt{E}}\right|\right]_{E/\lambda}^{e^{-2x/a}}$$

$$= -\sqrt{\frac{2ma^2E}{\hbar^2}}\left[\sqrt{1-\frac{\lambda}{E}e^{-2x/a}} + \frac{1}{2}\ln\left|\frac{1-\sqrt{1-\frac{\lambda}{E}e^{-2x/a}}}{1+\sqrt{1+\frac{\lambda}{E}e^{-2x/a}}}\right|\right]$$

$$= -\sqrt{\frac{2ma^2E}{\hbar^2}}\left[\sqrt{1-\alpha} + \frac{1}{2}\ln\left|\frac{1-\sqrt{1-\alpha}}{1+\sqrt{1+\alpha}}\right|\right] ;\ \alpha = \frac{\lambda}{E}e^{-\frac{2x}{a}}$$

$$\lim_{x\to\infty} = \lim_{\alpha\to 0}$$

$$\lim_{\alpha\to 0}\sqrt{1-\alpha} = 1 - \frac{\alpha}{2}$$

$$\Rightarrow \lim\left[\quad\right] = 1 - \frac{1}{2}\ln\frac{\alpha}{4}$$

$$\Rightarrow \lim_{x\to\infty}\frac{\sqrt{2m}}{\hbar}\int dx'\sqrt{E-\lambda e^{-2x'/a}} = -\sqrt{\frac{2ma^2E}{\hbar^2}}\left[1 - \frac{x}{a} - \frac{1}{2}\ln\frac{\lambda}{4E}\right]$$

$$= kx - ka\left[1 + \ln\sqrt{\lambda/4E}\right]$$

$$\Rightarrow \delta^{WKBJ} = \frac{\pi}{4} - ka\left[1 + \ln\sqrt{\lambda/4E}\right]$$

(CONT)

QUANTIZING EM FIELDS

RECALL LAGRANGIAN:

$$L = T - V = \frac{1}{2} m \dot{x}^2 - V(x)$$

THEN

$$\frac{\delta L}{\delta x_i} - \frac{d}{dt}\frac{\delta L}{\delta \dot{x}_i} = 0 \quad \leftarrow \text{LAGRAN'S EQ'N}$$

$$-\frac{\delta V}{\delta x} - m\ddot{x}_i = 0$$

$$\frac{\delta L}{\delta \dot{x}_i} = P_i = \text{MOMENTUM}$$

$$H = \sum_i P_i \dot{x}_i - L = \sum_i \frac{p^2}{2m} + V$$

$$[x_i, p_i] = i\hbar$$

CONSIDER FIELDS $E(r)$, $H(r)$

$$L = \int d^3r\, \mathcal{L}(r) \qquad \mathcal{L}(r) \Rightarrow \text{LAGRAN. DENSITY}$$

EXAMPLE:

FOR $\mathcal{L}(c, \nabla c, \dot{c}, t)$

THEN $$\frac{\delta \mathcal{L}}{\delta c} - \frac{d}{dt}\frac{\delta \mathcal{L}}{\delta \dot{c}} = \sum_{xyz} \frac{\delta}{\delta x} \frac{\delta \mathcal{L}}{\delta\left(\frac{\delta c}{\delta x}\right)}$$

$$P(r) = \frac{\delta \mathcal{L}}{\delta \dot{c}}$$

GIVES

$$\mathcal{H}(r) = \dot{c}P - \mathcal{L} \quad ; \quad H = \int d^3r\, \mathcal{H}(r)$$

IN Q.M.:

$$[C(r), P(r')] = i\hbar\, \delta(\underset{\sim}{r} - \underset{\sim}{r}')$$

EXACT ANSWER WAS

$$e^{2i\delta^{EXACT}} = (ka)^{-i2ka}\frac{\Gamma(1+ika)}{\Gamma(1-ika)}$$

NOW

$$\Gamma(1+z) = z\Gamma(z)$$

$$\therefore \Gamma(1+ika) = ika\,\Gamma(ika)$$

$$\lim_{z\to\infty}\Gamma(z) = z^{z+1/2}e^{-z} \qquad \sqrt{2\pi}$$

(TURNS OUT WKBJ IF $ka >> 1$)

GENERALLY:
WKBJ WORKS IF:

1) $ka >> 1$
2) $V(x)$ IS SMOOTH

2-17-75

$$\alpha = \frac{4\pi^2 e^2}{m^2 n c \omega}\left(\frac{N_a}{V}\right)\sum_f (\hat{\eta}\cdot P_{fc})^2\,\delta[E_i + \hbar\omega - E_f]$$

OSCILLATOR STRENGTH:

$$f_{ij} = \frac{2(\vec{\eta}\cdot P_{if})^2}{m\hbar\omega_{if}} \Rightarrow \text{NO DIMENSIONS}$$

RECALL THAT

$$[\mathcal{H}, x] = -\frac{i\hbar P_x}{m}$$

$$\mathcal{H} = \frac{p_x^2}{2m} + V(r)$$

THEN

$$\langle i|[H,x]|j\rangle = (E_i - E_f)\langle i|x|j\rangle$$

$$= -\frac{i\hbar}{m}\langle i|P_x|j\rangle$$

$$(E_i - E_f) = \hbar\omega_{if}$$

$$\Rightarrow f_{ij} = \frac{2(\eta\cdot X_{ij})^2 m\,\omega_{fi}}{\hbar}$$

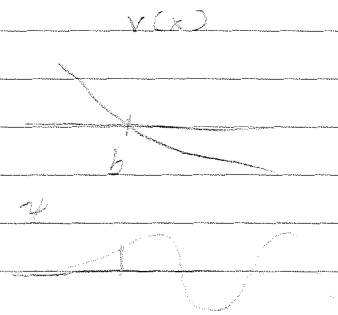
2-5-75

HOMEWORK $\frac{1}{4}$ OF GRADE

OPEN NOTE ? TEST

RM. 153'S BOX

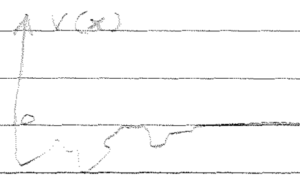
WKBJ



$$x > b \Rightarrow \psi(x) = \frac{C}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_b^x dx'\,p(x') + \frac{\pi}{4}\right]$$

$$p = \sqrt{2m(E - V(x))}$$

CONSIDER



$$\psi(0) = 0$$

$$\Rightarrow \psi(x) = \frac{C}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_0^x dx'\,p(x')\right]$$

(NO $\frac{\pi}{4}$ PHASE)

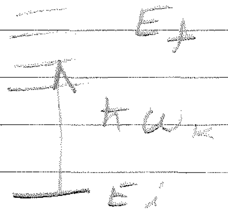
FOR STEEP POTENTIAL $\qquad$), $0 < \delta < \frac{\pi}{4}$

AND WKBJ WON'T WORK.

$$w = \frac{2\pi}{\hbar}\sum_f \left|\langle f|\frac{e\,p\cdot A}{mc}|i\rangle\right|^2 \Big[\delta\left[E_i + \hbar\omega_\lambda - E_f\right) + \delta\left[E_i - \hbar\omega_k - E_f\right)\Big]$$

ABSORPTION

$\delta\left[E_i - \hbar\omega_k - E_f\right) \to 0$ SINCE $E_f > E_i$



$$\langle f|V|i\rangle = \sum_{k\lambda} \frac{e}{mc} A_{k\lambda} \left\{ \langle f|\hat{\eta}\cdot p\, e^{ik\cdot r}|i\rangle e^{-i\omega_k t} + \langle f|\eta_0 p\, e^{-ik\cdot r}|i\rangle e^{i\omega_k t} \right\}$$

ABSORPTION OF LIGHT

FOR LIGHT, $e^{ik\cdot r}$ IS INSIGNIFICANT $\sim e^{i10^{-5}}$

$$P_{fi} = \langle f|\eta\cdot p|i\rangle = \int \psi_f(r)\, \underset{\sim}{p}\, \psi_i(r)\, d^3r$$

$$\langle f|V|i\rangle = \sum_k \frac{e}{mc} \underset{\sim}{P_{fi}} \cdot \hat{\eta}_k A_k$$

$$w = \frac{N_A 2\pi}{\hbar}\sum_f \left(\frac{e}{mc}\right)^2 (\hat{\eta}\cdot \underset{\sim}{P_{fi}})^2 \frac{2\pi}{\varepsilon_1}\frac{\hbar c^2}{\omega_k}\frac{N_k}{V}$$ (FOR SYS

$$w = dN_k/dt$$ FOR AN ATOM, N_A = TOTAL # ATOMS

$$= \frac{Vn}{c}\frac{dF_k}{dt}$$

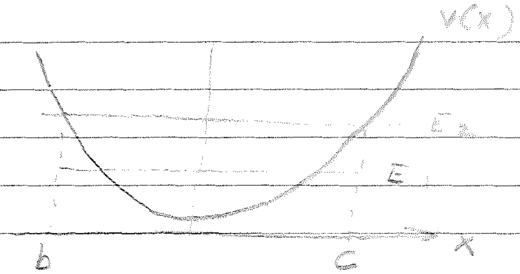
$$= V\frac{dF_k}{dx}$$

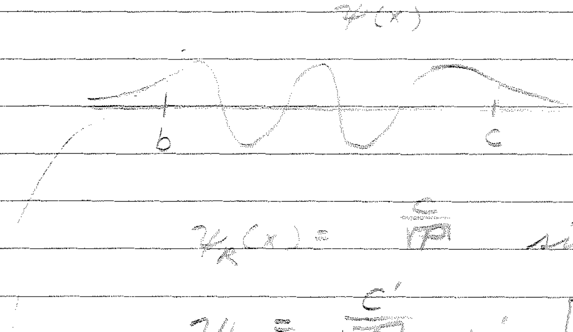
GIVES BEER'S LAW

$$\Rightarrow \frac{dF}{dx} = -\alpha F_k$$ WHERE α IS IN w EQ.

$$\boxed{\alpha(\omega) = 4\pi^2\left(\frac{N_A}{V}\right)\frac{e^2}{m^2 n c\,\omega_k}\sum_f (\underset{\sim}{\eta}\cdot \underset{\sim}{P_{fi}})\,\delta[E_i + \hbar\omega - E_f]}$$

BOUND STATES





$$\psi_R(x) = \frac{C}{\sqrt{p}} \sin\Big[\overbrace{\frac{1}{\hbar}\int_b^x dx'\, p(x') + \frac{\pi}{4}}^{\rho_R}\Big] \quad ; \quad b < x < c$$

$$\psi_L = \frac{C'}{\sqrt{p}} \sin\Big[\underbrace{\frac{1}{\hbar}\int_x^c dx'\, p(x') + \frac{\pi}{4}}_{\rho_L}\Big] \qquad c > x > b$$

$$\therefore \quad \psi_R = \psi_L$$

(WE GOTTA EQATE sin ARGUMENTS)

$$\rho_T = \rho_{TOTAL} = \rho_L + \rho_R = \int_b^c \frac{dx'\, p(x')}{\hbar} + \frac{\pi}{2}$$

$$\psi_L = \frac{C'}{\sqrt{p}} \sin \rho_L = \frac{C'}{\sqrt{p}} \sin(\rho_T - \rho_R)$$

$$= \frac{C'}{\sqrt{p}} \big[\sin \rho_T \cos \rho_R - \cos \rho_T \sin \rho_R\big)$$

$$= \psi_R = \frac{C}{\sqrt{p}} \sin \psi_R$$

NOW, LET $\rho_T = \pi(n+1)$ ← EIGEN VALUE CONDITION

$\sin \rho_T = 0$, $\cos \rho_T = (-1)^{n+1}$ $(n = 0, 1, 2, \ldots)$

$$\Rightarrow \psi_L = \frac{C'(-1)^{n+1}}{\sqrt{p}} \sin \rho_R$$

$$\pi(n+1) = \frac{1}{\hbar}\int_b^c dx'\, p(x') + \pi/2$$

$$\boxed{\Rightarrow \int_b^c dx'\, p(x') = \hbar\left(n + \tfrac{1}{2}\right)\pi}$$ ← BOHR-SOMMERFIELD CONDITION

SOMETIMES WRITTEN $\oint dx\, p(x) = 2\pi\hbar\left(n+\tfrac{1}{2}\right) = h\left(n+\tfrac{1}{2}\right)$

DERIVATION

$$\underline{H} = \underline{\nabla} \times \underline{A} = i \sum_{k,\lambda} \underset{\sim}{k} \times \hat{\eta}_k \left[A e^{i(\;)} - A' e^{-i(\;)} \right]$$

$$E = -\frac{1}{c} \frac{dA}{dt}$$

$$= -\frac{i}{c} \sum_{\lambda\lambda'} \eta_k \, \omega_\lambda \left[A e^{i(\;)} - A' e^{-i(\;)} \right]$$

$$\text{TOTAL E.M. ENERGY} = \frac{1}{8\pi} \int d^3r \left[\epsilon E^2 + \mu H^2 \right]$$

$$= \sum_{k\lambda} \left(N_{k\lambda} + \frac{1}{2} \right) \hbar \omega_{k\lambda} \leftarrow \text{SUM OF ALL } k\lambda \text{ HARMONIC OSCILLATOR}$$

WHY IS EACH A HARMONIC OSCIL? TUNE IN NEXT LECTURE!

ANYWAY

$$\epsilon \int E^2 d^3r = \sum_{kk'} \cdot \underbrace{\int d^3r \, e^{i r \cdot (k - k')}}_{V \delta_{k=k'}}$$

$$= \sum_k (\omega_k / c)^2 [V\epsilon] \left[A_k^2 + A_k'^2 - \cancel{2 A_k A_k'} \right]$$

$$= \mu (\underset{\sim}{\eta} \times \underset{\sim}{k})^2 V \left[A_k^2 + A_k'^2 \right]$$

$$= \mu k^2 V \left[A_k^2 + A_k'^2 \right]$$

$$\omega_k = ck \sqrt{\mu / \epsilon} \quad ; \quad \sqrt{\frac{\mu}{\epsilon}} = \text{REF. INDEX}$$

A_k' AND A_k FALL OUT

THEN WE GOT:

$$\int_{Y_-}^{Y_+} \frac{dY}{Y} \sqrt{(Y_+ - Y)(Y - Y_-)}$$

$$= \frac{\pi}{2} \left[Y_+ + Y_- - 2\sqrt{Y_+ Y_-} \right]$$

FOR OUR CASE, $Y_+ + Y_- = 2$, $Y_+ Y_- = -E/A$

$$\int_{Y^-}^{Y^+} [\quad] = \frac{\pi}{2} \left[2 - 2\sqrt{-\frac{E}{a}} \right]$$

(NOTE: FOR BND STATES, $E<0$)

FINALLY:

$$+\frac{1}{\alpha}\sqrt{2mA} \cdot \frac{\pi}{2}\left[2 - 2\sqrt{-E/A}\right] = \pi\hbar\left(n + \frac{1}{2}\right)$$

$$\sqrt{-\frac{E}{A}} = \frac{-\hbar}{\sqrt{2mA}}\left(n + \frac{1}{2}\right) + 1$$

$$\therefore \quad E = -A\left[1 - \left(n + \frac{1}{2}\right)\sqrt{\frac{\hbar^2\alpha^2}{2mA}}\right]^2$$

$$\frac{1}{s^2} = \frac{\hbar^2\alpha^2}{2mA}$$

$$E = -A\left[1 - \frac{(n + 1/2)}{s}\right]^2 \Leftarrow \text{AGAIN, EXACT SOLUTION.}$$

SEMICLASSICAL RADIATION THEORY

1. TREAT E-M FIELDS CLASSICALLY AND TREAT
2. EVERTHING ELSE BY QUANTUM MECHANICS

REPLACE $\frac{p^2}{2m}$ BY $\frac{(p-\frac{e}{c}A)^2}{2m}$

$$\frac{(p-\frac{e}{c}A)^2}{2m} = \frac{p^2}{2m} - \underbrace{\frac{e}{c}\frac{p \cdot A}{m}}_{\text{"P DOT A" TERM}} + \underbrace{\frac{e^2}{2mc^2}A^2}_{\text{A SQUARED TERM}} \quad (A \text{ \& } P \text{ COMMUTE})$$

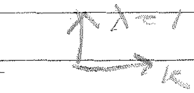
$$\underset{\sim}{A}(\underset{\sim}{r},t) = \sum_{K\lambda} \hat{\eta}_{K\lambda}\left[A_{\lambda K}\, e^{i(\underset{\sim}{k}\cdot\underset{\sim}{r}-\omega_\lambda t)} + A'_{K\lambda}\, e^{-i(k\cdot r-\omega_\lambda t)}\right]$$

ANS. IS

$$A_{K\lambda} = \sqrt{\frac{2\pi\hbar c^2}{\varepsilon V \omega_{K\lambda}}(N_K+1)}$$

$$A'_{K\lambda} = \sqrt{\frac{2\pi\hbar c^2}{\varepsilon V \omega_{K\lambda}} N_K}$$

$\eta \rightarrow$ POLARIZATION VECTOR

$[p, A] = k \cdot \eta_{\kappa} = 0$ FOR 

THREE DIMENSIONS:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E\right]\psi(r) = 0$$

ASSUME $V(r)$ IS SPHERICALLY SYMMETRIC

i.e. $V(\underset{\sim}{r}) = V(|\underset{\sim}{r}|)$

$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

IN SPHERICAL COORDINATES

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) + \frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}\right]$$

BECAUSE OF SPHERICAL SYMMETRY:

$$\psi(r,\theta,\phi) = R(r)\,Y_{\ell m}(\theta,\phi) = R(r)\,Y_\ell^m(\theta,\phi)$$

$$Y_\ell^m = \epsilon\left[\frac{2\ell+1}{4\pi}\,\frac{(\ell-|m|)!}{(\ell+|m|)!}\right]^{1/2} P_\ell^{|m|}(\cos\theta)\,e^{im\phi}$$

$$\epsilon = \begin{cases} 1 & \text{IF } m \geq 0 \\ -1 & \text{IF } m \leq 0 \end{cases}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, Y_\ell^{m}(\theta,\phi)\, Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell\ell'}\delta_{mm'}$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$$

$$Y_{1,\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}$$

$$Y_{2,0} = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$$

$$Y_{2\pm1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_{2,\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm i2\phi}$$

CONSIDER

$$H_0, \quad V = \Theta(t) \sum_\lambda V_\lambda \, e^{i\omega_\lambda t}$$

ANSWER IS

$$\omega = \frac{2\pi}{\hbar} \sum_\lambda |\langle n|V_\lambda|e\rangle|^2 \, \delta(E_n^{(0)} - E_e^{(0)} - \hbar\omega_\lambda)$$

ASSUME:

$$\psi = \sum_n a_n(t) \, e^{-it\frac{E_n^{(0)}}{\hbar}} \psi_n^{(0)}(t)$$

WE GET

$$i\hbar \frac{da_n}{dt} = \sum_\lambda \langle n|V_\lambda|e\rangle a_e(t) \times e^{it(E_n^{(0)} - E_e^{(0)} - \omega_\lambda\hbar)/\hbar}$$

$$i\hbar \dot{a}_n^{(1)} = \sum_\lambda \langle n|V_\lambda|e\rangle e^{it(\quad)/\hbar}$$

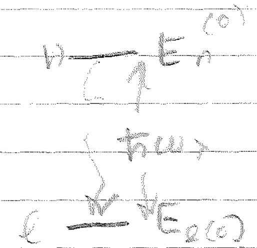
$$|a_m^{(1)}(t)|^2 = \left| \sum_\lambda \langle n|V_\lambda|e\rangle \frac{e^{it(\omega_\lambda - \omega_{ne})} - 1}{\omega_{ne} - \omega_\lambda} \right|^2$$

$$\omega_{ne} = \frac{E_n^{(0)} - E_e^{(0)}}{\hbar}$$

TURNS OUT THAT $\lambda = \lambda'$ GIVES ONLY RELAVENT (NON e^{i}) TERMS.

$$|a_m^{(1)}(t)| = \sum_\lambda |\langle n|V_\lambda|e\rangle|^2 \left| \frac{e^{-it(\omega_{ne} - \omega_\lambda)} - 1}{\omega_{ne} - \omega_\lambda} \right|^2$$

TAKE $\frac{d}{dt}$ AND LIMIT GIVES ANSWER



$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}+\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}\right]Y_{\ell m}=-\ell(\ell+1)Y_{\ell,m}$$

SCHRO'S EQ. BECOMES

MULTIPLY OUT

$$\left(-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}\right]+V(r)-E\right)R(r)\cancel{Y_\ell^m}=0$$

NOW,

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{dR}{dr}\right]=\frac{2}{r}\frac{dR}{dr}+\frac{d^2R}{dr^2}$$

AND $$\frac{1}{r}\frac{d^2}{dr^2}(rR)=\frac{2}{r}\frac{dR}{dr}+\frac{d^2R}{dr^2}\longrightarrow \therefore \text{EQUAL}$$

SCHRÖ'S EQ:

$$\left[-\frac{\hbar^2}{2m}\left\{\frac{1}{r}\frac{d^2}{dr^2}r-\frac{\ell(\ell+1)}{r^2}\right\}+V(x)-E\right]R(r)=0$$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(rR)}+\underbrace{\left[\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}+V(r)-E\right]}(rR)=0$$

NOTE SIMILARITY TO ONE DIMENSIONAL CASE

DEFINE $\chi(r)=rR(r)$

GIVES: $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V_{eff}(r)-E\right]\chi(r)=0$$

$$V_{eff}=V+\frac{\hbar^2}{2mr^2}\ell(\ell+1)$$

BOUNDRY CONDITIONS

@ $r=0$, $\psi(r)$ MUST BE FINITE $\Rightarrow R(0)$ IS FINITE

$$\Rightarrow \underline{\chi(0)=0}$$

CHANGE VARIABLES:

$$E_e = \sqrt{m^2c^4 + c^2p_e^2}$$

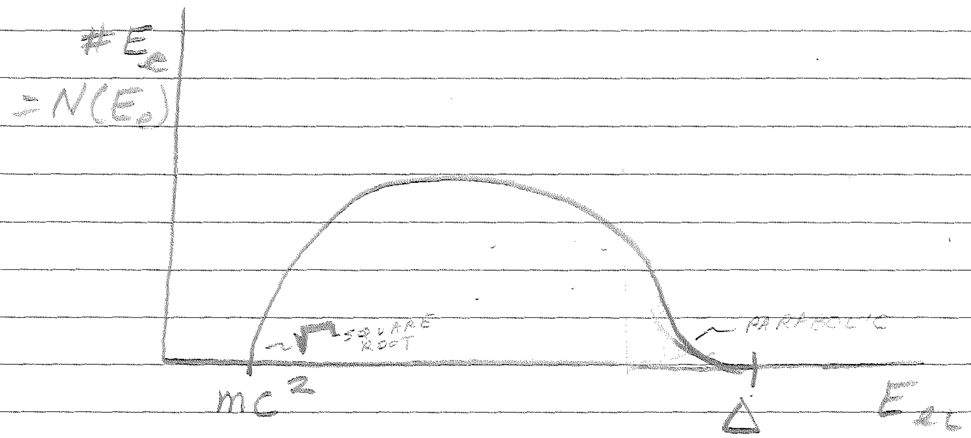
$$E_e\,dE_e = c^2 p_e\,dp_e$$

$$\omega = C\int dE_e\,(\Delta - E_e)^2\,(E_e^2 - m^2c^4)^{1/2}$$

FROM THIS RELATIONSHIP

$$\frac{\#\ \text{ELECTRONS}}{\text{UNIT ENERGY}} = \frac{d\omega}{dE_e}$$

$$= C\,(\Delta - E_e)^2\,(E_e^2 - m^2c^4)^{1/2}$$



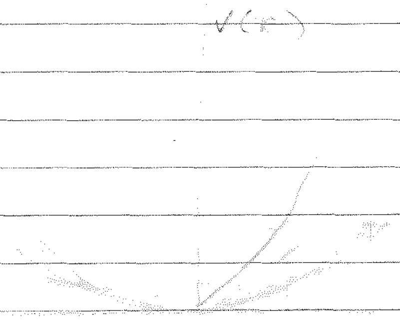
ℓ = ORBITAL QUANTUM NUMBER

m = AZIMUTHAL " "

(k_x, k_y, k_z) (k, ℓ, m) (k, k_ρ, m)

RECTANG. SPHR. CYLINDICAL

RELEM 3-D HARMONIC OSCILLATOR:



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{k}{2}r^2 - E\right]\psi(r)$$

RECTANG. APPROACH

$$r^2 = x^2 + y^2 + z^2$$

$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

$$\Rightarrow [H_x + H_y + H_z - E]\psi = 0$$

$$H_x = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{k}{2}x^2$$

$$\psi(x, y, z) = \phi_\alpha(x)\,\phi_\beta(y)\,\phi_\gamma(z)$$

$$E = \hbar\omega\left[(\alpha + \tfrac{1}{2}) + (\beta + \tfrac{1}{2}) + (\gamma + \tfrac{1}{2})\right]$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}\frac{\hbar^2}{2m} + \frac{k}{2}r^2 - E\right)\chi_n = 0$$

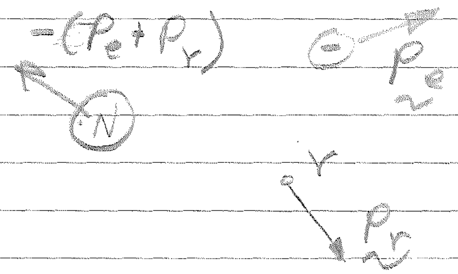
$$E = \hbar\omega\,(n_r + 3/2)$$

TURNS OUT TO BE SAME ANSWER

$m_\nu = 0$ = NEUTRINO MASS

$E_\nu = \hbar c k_\nu$

CALCULATION EMPLOYING NEUTRINO



$$\Delta = \overset{\text{NUCLEUS}}{\frac{\hbar^2}{2M}(\underset{\sim}{P_e} + \underset{\sim}{P_\nu})^2} + \overset{\text{NEUTRINO}}{c\underset{\sim}{p_\nu}} + \overset{\text{ELEC}}{\sqrt{c\underset{\sim}{p_e}^2 + m^2c^4}}$$

$\frac{\hbar^2}{2M}(\underset{\sim}{P_e} + \underset{\sim}{P_\nu})^2$ IS SMALL

$$\Rightarrow \Delta \simeq cp_\nu + \sqrt{c\underset{\sim}{p_e}^2 + m^2c^4}$$

NOW THE CALCULATION:

FROM FERMI:

$$\omega = \sum_{\underset{\sim}{P_e}, \underset{\sim}{P_\nu}} \frac{2\pi}{\hbar} |M|^2 \, \delta\left[\Delta - cp_\nu - \sqrt{c^2p_e^2 + m^2c^4}\right]$$

ASSUME $|M|$ CONSTANT

$$\omega = \frac{2\pi}{\hbar}|M|^2 \int d^3 p_e$$

$$\times \int d^3 p_\nu \, \delta\left[\Delta - cp_\nu - \sqrt{m^2c^4 + c^2p_e^2}\right]$$

$$= (4\pi)^2 \frac{2\pi}{\hbar^2}|M|^2 \int p_e^2 \, dp_e$$

$$\int p_\nu^2 \, dp_\nu \, \delta\left[\Delta - cp_\nu - \sqrt{mc^2 + c^2p_e^2}\right]$$

$$= \frac{2\pi (4\pi)^2}{\hbar (2\pi)^6} |M|^2 \int p_e^2 \, dp_e \, \frac{\Delta - \sqrt{m^2c^4 + c^2p_e^2}}{c^3}$$

EXAMPLE: $V(r) = 0$

THEN

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\hbar^2}{2mr^2} \ell(\ell+1) - E \right] R(r) = 0$$

$$R(r) = \underbrace{j_\ell(kr)}_{\text{SPHERICAL BESSEL FUNCTIONS}} \; ; \; k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$j_\ell(z) = \sqrt{\frac{\pi}{2z}}\, J_{\ell+\frac{1}{2}}(z)$$

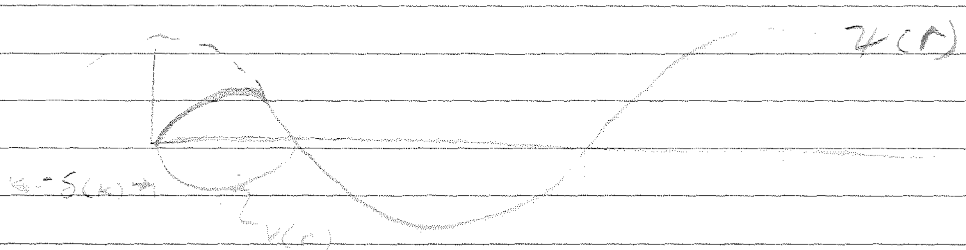
$$j_0(z) = \frac{\sin z}{z}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}$$

$$\lim_{z\to\infty} j_\ell(z) = \frac{1}{z} \sin\left[z - \frac{\pi}{2}\ell\right]$$

GENERALLY,

$$\lim_{r\to\infty} R(r) = \frac{1}{kr} \sin\left[kr - \frac{\pi\ell}{2} + \delta_\ell(k)\right]$$



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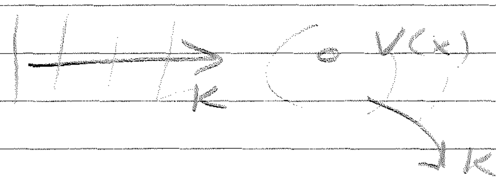
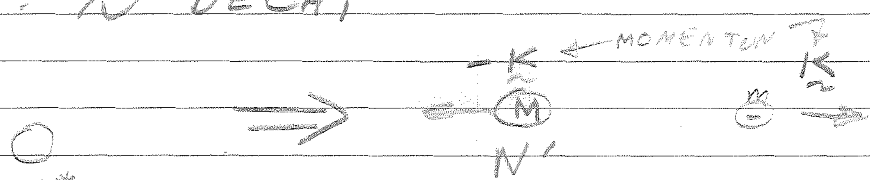
FERMI'S GOLDEN RULE

$$w_{n\to l} = \frac{2\pi}{\hbar}|M_{nl}|^2 \delta(E_n^{(0)} - E_l^{(0)})$$

PREVIOUS EXAMPLE



EXAMPLE: β DECAY



K.E. $\Rightarrow$ $\frac{\hbar^2 k^2}{2m}$ $\qquad$ $\frac{\hbar^2 k^2}{2M}$

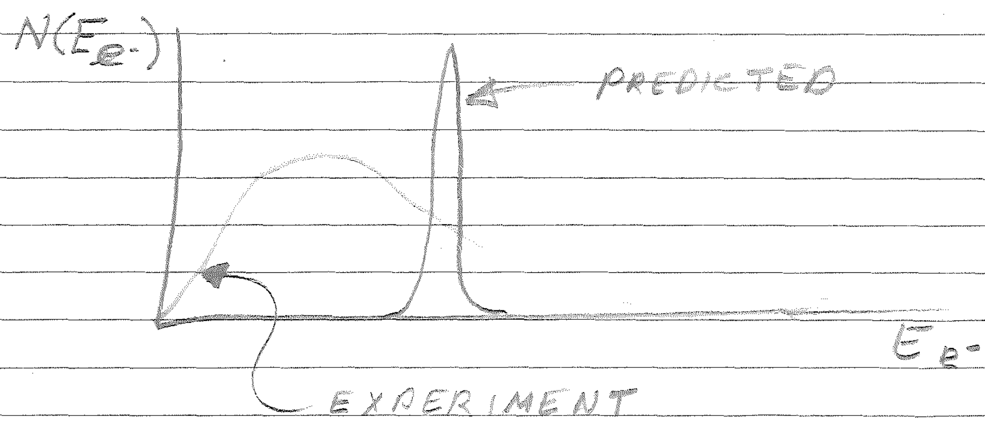
TOTAL K.E: $\frac{\hbar^2 k^2}{2\mu}$ $\Rightarrow \frac{1}{\mu} = \frac{1}{m} + \frac{1}{M}$

$$\frac{\hbar^2 k^2}{2\mu} = \Delta - mc^2$$

NOW $\hbar^2 k^2 = 2\mu(\Delta - mc^2)$

$$E_{e^-} = \frac{\mu}{m}(\Delta - mc^2) = \text{CONSTANT}$$

$\Delta - mc^2$ = EXCESS K.E.



DIFFERENCE DUE TO NEUTRINO ν

$$N^* \to N + e^- + \nu$$

2-11-75

EXAM IN 1 WEEK

HOMEWORK SET # 3

1. $\psi(x) = c[I_{ika}(k_0aY) - I_{-ika}(k_0aY)]$ (REPULSIVE EXP. POTENTIAL)

FIND $C \ni \psi(x) \xrightarrow[x\to\infty]{} \sqrt{\frac{2}{\pi}}\sin(kx+\delta)$

$x\to\infty,\ Y\to 0,\ C_1 I_{ika}(k_0aY) \to C\left(\frac{k_0a}{2}\right)^{ika}\frac{e^{-ika}}{\Gamma(1+ika)}$ PHASE

$\therefore\ |C_1| = |\Gamma(1+ika)|/\sqrt{2\pi}$ (ETC?)

(USE CONDITION $\psi(x) \xrightarrow[x\to\infty]{} \sqrt{\frac{2}{\pi}}\sin(kx+\delta)$)

2. FIND δ_k FOR MORSE POTENTIAL

$t = \sqrt{\frac{2mE}{\hbar^2\alpha^2}}$

$$\psi(x) = C_1 e^{-sY} Y^{it} F[\tfrac{1}{2}+it-s, 1+i2t; 2sY]$$

$$+ C_2 e^{-sY} Y^{-it} F[\tfrac{1}{2}-it-s, 1-i2t; 2sY]$$

$x\to-\infty \Rightarrow Y\to+\infty \Rightarrow \psi(x)\to 0$

$$\lim_{z\to\infty} F(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^{z}$$

$$0 \doteq \lim_{x\to-\infty}\psi(x) = e^{-sY}\Big[C_1 Y^{it}\frac{\Gamma(1+i2t)}{\Gamma(\frac{1}{2}+it-s)}(2sY)^{-\frac{1}{2}-it-s}e^{2sY}$$

$$+ C_2 Y^{-it}\frac{\Gamma(1-i2t)}{\Gamma(\frac{1}{2}-it-s)}(2sY)^{-\frac{1}{2}+it-s}e^{2sY}\Big]$$

$$= e^{sY}Y^{-\frac{1}{2}-s}(2s)^{-\frac{1}{2}-s}\underbrace{\Big[C_1\frac{\Gamma(1+i2t)}{\Gamma(\frac{1}{2}+it-s)}(2s)^{-it} + C_2\frac{\Gamma(1-i2t)}{\Gamma(\frac{1}{2}-it-s)}(2s)^{it}\Big]}_{=0}$$

$$\therefore\ \frac{C_2}{C_1} = -\frac{\Gamma(1+i2t)\,\Gamma(\frac{1}{2}-it-s)}{\Gamma(1-i2t)\,\Gamma(\frac{1}{2}+it-s)}\times(2s)^{-2it}$$

$$\lim_{\substack{x\to\infty\\ Y\to 0}}\psi(x) = C_1Y^{it} + C_2Y^{it} \quad ;\ Y = e^{-\alpha(x-x_0)}$$

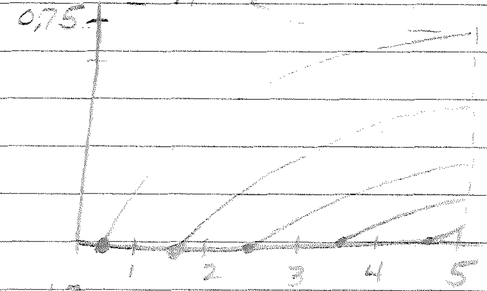
$t = k/\alpha$

$$= C_1 e^{ikx_0}\left[e^{-ikx} + \frac{C_2}{C_1}e^{ikx}e^{-i2kx_0}\right]$$

$$\Rightarrow e^{i2\delta} = e^{-i2kx_0}\frac{C_2}{C_1}$$

3. $$E = -A\left[1 - \frac{(n+\frac{1}{2})}{S}\right]^2$$

$$S > n + \tfrac{1}{2}$$



4. SHOW $$\left[z\frac{d^2}{dz^2} + (b-z)\frac{d}{dz} - a\right]F(a,b;z) = 0$$

$$F(a,b,z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \cdots$$

n^{TH} TERM $$\frac{a(a+1)\cdots(a+n)}{b(b+1)\cdots(b+n)}\frac{z^n}{n!} = \frac{\Gamma(a+n)\,\Gamma(b)}{\Gamma(a)\,\Gamma(b+n)}\frac{z^n}{n!}$$

$$F(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)}\sum_{n=1}^{\infty}\frac{z^n}{n!}\frac{\Gamma(a+n)}{\Gamma(b+n)}$$

$$\frac{dF}{dz} = \frac{\Gamma(b)}{\Gamma(a)}\sum\frac{n z^{n-1}}{n}\frac{\Gamma(a+n)}{\Gamma(b+n)} = \sum\frac{\Gamma(a)}{\Gamma(b)}\frac{z^{n-1}}{(n-1)!}\frac{\Gamma(a+n)}{\Gamma(b+n)}$$

$$\frac{d^2F}{dz^2} = \frac{\Gamma(a)}{\Gamma(b)}\sum\frac{n(n-1)}{n!}z^{n-2} = \frac{\Gamma(a)}{\Gamma(b)}\sum\frac{z^{n-2}}{(n-2)!}\frac{\Gamma(a+n)}{\Gamma(b+n)}$$

$$\sum_n\frac{\Gamma(a+n)}{\Gamma(b+n)}\left[\frac{z^{n-1}}{(n-2)!} - \frac{b z^{n-1}}{(n-1)!} - \frac{z^n}{(n-1)!} - \frac{a z^n}{n!}\right]$$

LET $m = n-1$ $\qquad m = n-1 \qquad m = n$

$$= \sum_m z^m\left[\frac{\Gamma(a+m+1)}{(m-1)!\,\Gamma(b+m+1)} + \frac{b}{m!}\frac{\Gamma(a+m+1)}{\Gamma(b+m+1)} - \frac{\Gamma(a+m)}{\Gamma(b+m)}\frac{1}{(m-1)!}\right.$$
$$\left. - \frac{a}{m!}\frac{\Gamma(a+m)}{\Gamma(b+m)}\right]$$

$$= \sum_m\frac{z^m\,\Gamma(a+m)}{m!\,\Gamma(b+m)}\left[\frac{(a+m)m}{b+m} + \frac{b(a+m)}{b+m} - m - a\right]$$

$$= \sum_m\frac{z^m\,\Gamma(a+m)}{m!\,\Gamma(b+m)}\left[m+b-(b+m)\right] = 0$$

CONSIDER

$$V(r) = -Ze^2/r \qquad (Z=1 \Rightarrow \text{HYDROGEN ATOM})$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E\right]\psi(r) = 0$$

DUE TO SPHERICAL SYMMETRY (RADIAL FORM)

$$\psi(r) = R_{nl}(r)\,Y_l^m(\theta,\phi)$$

THEN

$$\left[-\frac{\hbar^2}{2mr}\frac{d^2}{dr^2}r + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r) - E\right]R(r) = 0$$

$$\chi(r) = rR$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{(l+1)l}{r^2} + V(r) - E\right]\chi(r) = 0$$

$$a = \frac{\hbar^2}{me^2} \quad (\text{LENGTH}) \Rightarrow \frac{(erg)^2 sec^2}{gm \cdot erg \cdot cm} = cm$$

$$= 0.529 \times 10^{-8}\ cm \qquad (\text{BOHR RADIUS})$$

$$\frac{e^2}{a} = \text{ENERGY} = \frac{me^4}{\hbar^2} = 27.2\ eV \qquad (\text{HARTREE})$$

$E_R = \frac{e^2}{2a}$

$$1\ eV = 1.6 \times 10^{-12}\ erg$$

LET'S GO INTO DIMENSIONLESS UNITS

$$\rho = r/a$$

$$\left[-\frac{\hbar^2}{2ma^2}\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2}\right] - \frac{Ze^2}{a}\frac{1}{\rho} - E\right]\chi(\rho) = 0$$

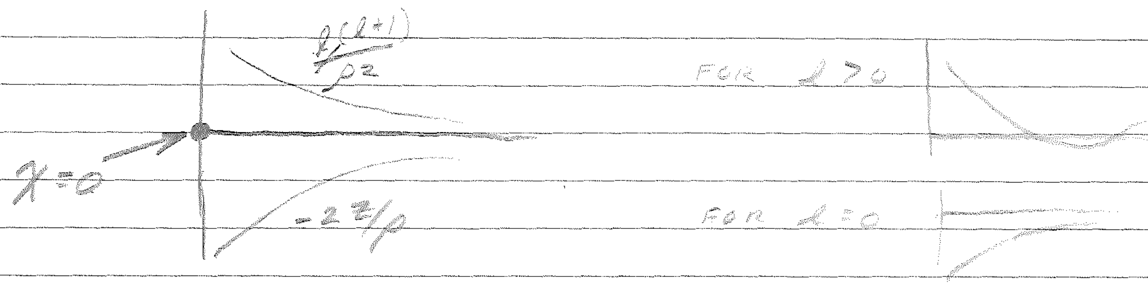
$$\frac{\hbar^2}{2ma^2} = \frac{e^4 m}{\hbar^2}$$

$$\left[-\frac{\delta^2}{\delta\rho^2} + \frac{l(l+1)}{\rho^2} - \frac{2Z}{\rho} - \frac{2Ea}{e^2}\right]\chi(\rho) = 0$$

$$\epsilon = \frac{Ea}{e^2}$$

$$\left[\frac{\delta^2}{\delta\rho^2} + \frac{2Z}{\rho} - \frac{l(l+1)}{\rho^2} + 2\epsilon\right]\chi(\rho) = 0$$

BOUND STATE SOLUTION:



FOR $E<0$, LET $2E = -\alpha^2$

$$@\ \rho\to\infty,\quad \left(\frac{d^2}{d\rho^2} - \alpha^2\right)\chi(\rho) = 0$$

$$\Rightarrow \chi = A e^{-\alpha\rho} + B \underbrace{e^{\alpha\rho}}_{\text{BLOWS UP}}$$

$$@\ \rho\to 0\ (l\neq 0) \rightarrow \left(\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right)\chi = 0$$

$$\chi = \rho^{l+1},\ \cancel{\rho^{-l}}\ \text{NO GOOD}$$

TRY $\chi(\rho) = \rho^{l+1} e^{-\alpha\rho} F(\rho)$

$$\Rightarrow \frac{d}{d\rho}\chi(\rho) = \left[(l+1)\rho^{l} F - \alpha\rho^{l+1} F + \rho^{l+1}\frac{dF}{d\rho}\right] e^{-\alpha\rho}$$

$$\frac{d^2}{d\rho^2}\chi(\rho) = (l+1)l\,\rho^{l-1} F e^{-\alpha\rho} + \alpha^2 \rho^{l+1} F e^{-\alpha\rho}$$

$$- 2\alpha(l+1)\rho^{l} F e^{-\alpha\rho}$$

$$+ \frac{dF}{d\rho} e^{-\alpha\rho}\left[\rho^{l}\,2(l+1) - 2\alpha\rho^{l+1}\right]$$

$$+ e^{-\alpha\rho}\rho^{l+1}\, d^2F/d\rho^2$$

$$e^{-\alpha\rho}\rho^{l+1}\left[\frac{d^2F}{d\rho^2} + \frac{dF}{d\rho}\left\{\frac{2(l+1)}{\rho} - 2\alpha\right\}\right.$$

$$\left. + F\left\{\frac{2Z}{\rho} - \frac{2\alpha(l+1)}{\rho}\right\}\right] = 0$$

$$\Rightarrow \rho\frac{d^2F}{d\rho^2} + \left(2(l+1) - 2\alpha\rho\right)\frac{dF}{d\rho} + \left(2Z - 2\alpha(l+1)\right)F = 0$$

GIVES: $F\left(l+1-\frac{Z}{\alpha},\ 2l+2,\ 2\rho\alpha\right)$ AS SOLUTION

$$\rho\frac{d^2F}{d\rho^2} + (b - c\rho)\frac{dF}{d\rho} + (d) = 0 \Rightarrow F\left(\frac{d}{c}; b; c\rho\right)$$

$$\therefore \chi(\rho) = \rho^{\ell+1} e^{-\alpha\rho} F\left[\ell+1-\frac{Z}{\alpha}, 2\ell+2; 2\alpha\rho\right]$$

IS THIS A WAVE FUNCTION

$$\rho \to 0, \quad \chi \to \rho^{\ell+1} \to 0$$

$$\rho \to \infty, \quad F \to \frac{\Gamma(2\ell+2)}{\Gamma(\ell+1-Z/\alpha)} (2\alpha\rho)^{a-b} e^{2\alpha\rho} \to \infty$$

NO!

IT'S GOTTA GO TO ZERO

$\therefore$ WE GOTTA TRUNCATE SERIES WITH

$$\ell+1-\frac{Z}{\alpha} = -n_r$$

$$\Rightarrow \alpha = \frac{Z}{n_r+\ell+1}$$

$$\frac{-2Ea}{e^2} = \alpha^2 = \frac{Z^2}{(n_r+\ell+1)^2}$$

$$\therefore \boxed{E_n = -\left(\frac{e^2}{2a}\right)\frac{Z^2}{(n_r+\ell+1)^2}}$$

n_r = RADIAL QUANTUM #

ℓ = ORBITAL " "

$n = n_r+\ell+1$ = PRINCIPLE QUANTUM #

$e^2/2a = 13.6\,eV = 1$ RYDBERG

NOW $\chi(\rho) = \rho^{\ell+1} e^{-\alpha\rho} F[-n_r, 2\ell+2, 2\alpha\rho]$

$$= \rho^{\ell+1} e^{-\alpha\rho} L^{2\ell+1}_{n_r+\ell}(2\alpha\rho)$$

					R
$n_r=0$,	$\ell=0$,	$n=1$,	1S	STATE	$e^{-\rho}$
$n_r=1$,	$\ell=0$,	$n=2$,	2S	"	$(1-\frac{\rho}{2})e^{-\rho/2}$
$n_r=0$,	$\ell=1$,	$n=2$	2p	"	$\rho e^{-\rho/2}$
$n_r=1$,	$\ell=1$,	$n=3$	3p		$\rho e^{-\rho/3}[1-\frac{\rho}{6}]$
$n_r=0$,	$\ell=2$,	$n=3$	3d		$\rho^2 e^{-\rho/3}$

CONTINUUM STATES $(E>0)$

LET $\alpha = ik \Rightarrow E = k^2 e^2/a$

THEN

$$\chi(\rho) = c_1 \rho^{\ell} e^{-ik\rho} F\left[\ell+1+\frac{Z}{ik}, 2\ell+2, -2ik\rho\right]$$

$$+ c_2 \rho^{\ell} e^{ik\rho} F\left[\ell+1-\frac{Z}{ik}, 2\ell+2, i2k\rho\right]$$

WHAT ABOUT REPULSIVE COULOMB POTENTIAL:

$$V(r) = +Ze^2/r$$

[YOU REPLACE Z BY $-Z$ IN $\chi(\rho)$]

Q: WHAT ARE THE PHASE SHIFTS FOR COULOMB POTENTIAL

A: IT IS NOT DEFINED

2-13-74

HOMEWORK SET #3

5. $V(x) = \left(\frac{\delta\psi}{\delta x}\right)_{0+} - \left(\frac{\delta\psi}{\delta x}\right)_{0-} = \frac{2m}{\hbar^2}\lambda\,\psi(0)$

$$\psi_1(k,x) = \begin{cases} \frac{1}{\sqrt{2\pi}}\left[e^{ikx} + Re^{-ikx}\right] & x<0 \\ \frac{1}{\sqrt{2\pi}}\,T e^{ikx} & x>0 \end{cases}$$

THUS $1+R=T$

NOW $ikT - ik(1-R) = \frac{2m\lambda T}{\hbar^2}$

$T-(1-R) = \frac{2m\lambda T}{ik\hbar^2} = \frac{2m}{k}\alpha T$

$\psi_B = \sqrt{\alpha}\,e^{-\alpha|x|}$

$R = -\alpha/\alpha+ik$

$T = k/\alpha+ik$

$$\psi_2(x,k) = \begin{cases} \frac{1}{\sqrt{2\pi}}\left[e^{-ikx} + Re^{ikx}\right]; & x>0 \\ \frac{1}{\sqrt{2\pi}}\,T e^{-ikx}; & x<0 \end{cases}$$

SHOW

$\int_{-\infty}^{\infty} \psi_2(k,x)\,\psi_1(k',x) = 0$

CONSIDER $\psi(k,x) = \sqrt{\frac{2}{\pi}}\sin kx$

$\psi(k,x) = \sqrt{\frac{2}{\pi}}\cos\left[k|x| + \delta\right]$

$\left(\frac{d\psi}{dx}\right)_{x>0} = \sqrt{\frac{2}{\pi}}\frac{d}{dx}\cos(kx+\delta) = -k\sqrt{\frac{2}{\pi}}\sin(kx+\delta)$

$\frac{\delta\psi}{\delta x}_{x<0} = \sqrt{\frac{2}{\pi}}\frac{d}{dx}\cos(-kx+\delta) = k\sqrt{\frac{2}{\pi}}\sin(-kx+\delta)$

$2k\sqrt{2/\pi}\sin\delta = -2\alpha\sqrt{2/\pi}\cos\delta$

$\Rightarrow \tan\delta = \alpha/k$

$\psi_B = \sqrt{\alpha}\,e^{-\alpha|x|}$

$\int_{-\infty}^{\infty}\psi_1\psi_B = \int_{-\infty}^{0} e^{\alpha x}\sin kx + \int_0^{\infty} e^{-\alpha x}\sin kx = 0$

$\int_{-\infty}^{\infty}\psi_2\psi_B = \sqrt{\frac{2\alpha}{\pi}}\left[\int_{-\infty}^{0} dx\,e^{\alpha x}\cos(-kx+\delta) + \int_0^{\infty} dx\,e^{-\alpha x}\cos(kx+\delta)\right]$

$= C\,\frac{1}{2}\left(\frac{e^{i\delta}}{\alpha - ik} + \frac{e^{-i\delta}}{\alpha+ik}\right)$

$= \frac{1}{2}\sqrt{\alpha^2+k^2}\left[e^{i\delta}e^{i\tan^{-1}\left(\frac{k}{\alpha}\right)} + \text{c.c.}\right]$

$\delta = \tan^{-1}\frac{\alpha}{k}$, $\tan^{-1}(a) + \tan^{-1}\left(\frac{1}{a}\right) = \frac{\pi}{2}$

$\Rightarrow \int_{-\infty}^{\infty}\psi_2\psi_B = 0$

$\therefore$ THEY ARE ORTH. TO BOUND STATE

ARE THEY COMPLETE? IF SO

$$\Sigma\, \psi(x)^* \psi(x') = \delta(x-x')$$

$$\therefore \delta(x-x') = \psi_0(x)\psi_0(x') + \int_0^\infty dx \left[\psi_1^*(k,x)\,\psi_1(k,x') + \psi_2^*(k,x)\,\psi_2(k,x') \right]$$

FOUR POSSIBILITIES

$x>0,\ x'>0$

$x<0,\ x'>0$

$x<0,\ x'<0$

$x>0,\ x'<0$

TO SHOW FOR $x>0,\ x'>0$

$$\psi_0 = \sqrt{\alpha}\, e^{-\alpha|x|}$$

$$\Rightarrow \text{ONE TERM} = \alpha e^{-\alpha(x+x')} + \frac{2}{\pi}\int_0^\infty dk \left[\sin kx \sin kx' + \sin(kx+\delta)\sin(kx'+\delta)\right]$$

$$= \alpha e^{-\alpha(x+x')} + \frac{2}{\pi}\int_0^\infty dk \left[\frac{1}{4}\left(e^{ik(x-x')} + e^{-ik(x-x')} - e^{ik(x+x')} - e^{-ik(x+x')}\right)\right.$$

$$+ \frac{1}{4}\left(e^{ik(x-x')} + e^{-ik(x-x')} + e^{ik(x+x')+i2\delta}\right.$$

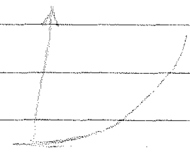
$$\left. + e^{-ik(x+x')}\, e^{-i2\delta} \right]$$

$$= \alpha e^{-\alpha(x+x')} + \frac{1}{2\pi}\int_{-\infty}^\infty dk \left[2e^{ik(x-x')} - e^{ik(x+x')}(1-e^{i2\delta})\right.$$

PTEWEE

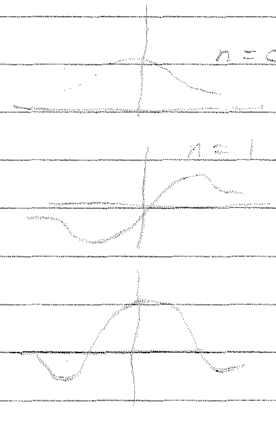
HOMEWORK SET #4

1.



FOR NORMAL HAR OSC: $E = \hbar\omega(n + \frac{1}{2})$

$n = 0, 1, 2, \ldots$



$\Leftarrow$ NO GOOD FOR $\frac{1}{2}$ SPACE

$\Leftarrow$ OKAY

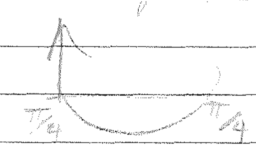
$\Leftarrow$ NO GOOD

$\therefore$ ONLY ODD ONES WORK. LET $n = 2m+1$

$\Rightarrow E = 2\hbar\omega(m + 3/4)$

FOR WKB)

$\int dx\, p(x) = \hbar(n + \frac{1}{2})\pi$, BUT NOT FOR THIS CASE



$\varphi_L = \frac{1}{\hbar}\int_a^x p(x')\,dx$

$\varphi_R = \frac{1}{\hbar}\int_x^b dx'\, p(x)$

$\Rightarrow \frac{1}{\hbar}\int_a^b dx\, px + \frac{\pi}{4} = \pi(n+1)$

$\Rightarrow E = 2\hbar\omega(m + 3/4)\pi$

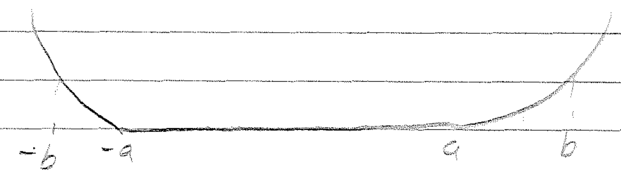
AND $\int dx\, p(x) = \sqrt{2m}\int_a^b dx\left[E - \frac{k}{2}x^2\right]dx$

$= \frac{\pi}{2}\sqrt{\frac{m}{k}}\,E$

$\therefore E = 2\hbar\sqrt{\frac{k}{m}}(n + 3/4) = 2\hbar\omega(n + 3/4)$

$\frac{\pi}{2\omega}E = \frac{\pi}{2\omega}2\hbar\omega(n + \frac{3}{4})$

2.



$$\int_{-b}^{b} dx\,\sqrt{2m(E-V(x))} = \pi\hbar\left(n+\tfrac{1}{2}\right)$$

NOW

$$\int_{-a}^{a} dx\,p(x) = \sqrt{2mE}\,(2a)$$

$$\int_{-b}^{b} p(x)\,dx = \sqrt{2mE}\,2a + \pi\sqrt{\frac{m}{k}}\,E = \pi\hbar\left(n+\tfrac{1}{2}\right)$$

SOLVE FOR $\sqrt{E} > 0$

3. $$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}\phi + \phi\left[V(r)-E\right] = 0$$

$$\phi = e^{i\sigma/\hbar}$$

$$r\frac{d\phi}{dr} = \frac{ri\sigma'}{\hbar}e^{i\sigma/\hbar}$$

$$\frac{d}{dr}r\frac{d}{dr}\phi = \frac{i}{\hbar}e^{i\sigma/\hbar}\left[\sigma'' r + \sigma' + \frac{i}{\hbar}(\sigma')^2 r\right]$$

END UP WITH

$$(\sigma')^2 + \hbar i\left(\sigma'' + \frac{\sigma'}{r}\right) + p(x)^2 = 0 \quad \Rightarrow p^2 = 2m(E-V)$$

$$\sigma = \sigma_0 + \frac{\hbar}{i}\sigma_1 + \frac{\hbar}{i^2}\sigma_2 + \ldots$$

$$(\sigma_0')^2 = p(x)^2 \Rightarrow \sigma_0 = \pm\int^{x} p(x')\,dx'$$

$$\frac{2\hbar}{i}\sigma_0'\sigma_1' - \frac{\hbar}{i}\left(\sigma_0'' + \frac{\sigma_0'}{r}\right) = 0$$

$$\Rightarrow \sigma_1' = -\frac{1}{2}\left[\frac{1}{r} + \frac{\sigma_0''}{\sigma_0'}\right]$$

$$\sigma_1 = -\frac{1}{2}\ln r - \frac{1}{2}\ln\sigma_0'$$
$$= -\frac{1}{2}\ln r - \frac{1}{2}\ln p$$

$$\Rightarrow e^{\frac{i}{\hbar}\left(\sigma_0 + \frac{\hbar}{i}\sigma_1\right)} = e^{\frac{i\sigma_0}{\hbar}}e^{\sigma_1} = \frac{e^{i\sigma_0/\hbar}}{\sqrt{r\,p(r)}}$$

4. $V(x) = \frac{\hbar^2}{2mx^2}\lambda^2$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar^2}{2mx^2}\lambda^2 - \frac{\hbar^2 k^2}{2m}\right]\phi = 0$$

$$\Rightarrow \left[\frac{d^2}{dx^2} - \frac{\lambda^2}{x^2} + k^2\right]\phi = 0$$

HINT WAS $\phi = \sqrt{x}\left[A J_\nu(x) + B J_{-\nu}(x)\right]$

GIVES $\nu = \sqrt{\lambda^2 + 1/4} > \frac{1}{2}$

$J_{-\nu}$ BLOWS UP, THUS $B = 0$

$$\phi = A\sqrt{x}\,J_\nu(x)$$

$$kx \to \infty,\ \sqrt{x}\,J_\nu(kx) \to \frac{1}{\sqrt{k}}\cos\left(kx - \frac{\pi}{4} - \frac{\nu\pi}{2}\right)$$

$$\Rightarrow \phi \to \sin\left(kx + \frac{\pi}{4} - \frac{\nu\pi}{2}\right)$$

$$\Rightarrow \delta = \frac{\pi}{4} - \frac{\pi}{2}\sqrt{\lambda^2 + \tfrac{1}{4}}$$

BY WKBJ, WE GET

$$\sin\left[\frac{1}{\hbar}\int_b^x dx\sqrt{2m(E - V(x))} + \frac{\pi}{4}\right]$$

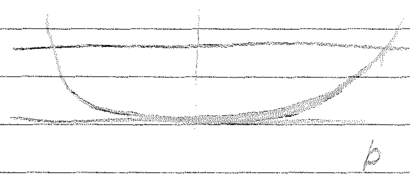
$$= \sin\left[\int_b^x dx'\sqrt{k^2 - \lambda^2/x'^2} + \frac{\pi}{4}\right] \quad ; b = \lambda/k$$

$$= \sin\left[\sqrt{kx^2 - \lambda^2} - \lambda\cos^{-1}\left(\frac{\lambda}{kx}\right) + \frac{\pi}{4}\right]$$

$$\lim_{kx\to\infty} \sin\left[kx - \lambda\cos^{-1}(0) + \frac{\pi}{4}\right]$$

$$\delta_{WKBJ} = \frac{\pi}{4} - \frac{\pi}{2}\lambda$$

5. $\int_{-b}^{b} dx \sqrt{E - Kx^4} = \frac{\hbar}{\sqrt{2m}} \pi \left(n+\frac{1}{2}\right)$



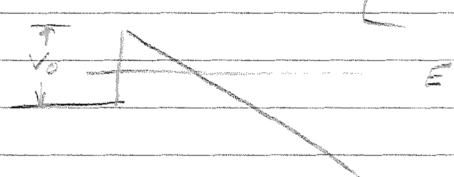
$b = (E/K)^{1/4}$

$\Rightarrow$

THEN $\int_{-b}^{b} dx \sqrt{E - Kx^4} = \sqrt{E}\, b \int_{-1}^{1} dy \left[1 - y^4\right] dy$

$= \frac{E^{3/4}}{K^{1/4}} \int_{-1}^{1} dy \left(1 - y^4\right) dy$

$\therefore E = \left[\frac{\frac{\hbar K^{1/4}}{\sqrt{2m}} \pi \left(n + \frac{1}{2}\right)}{\int_{-1}^{1} dy \sqrt{1 - y^4}} \right]^{4/3}$

6. 

$V(x) = \begin{cases} V_0 - Fx & ; x > 0 \\ 0 & ; x < 0 \end{cases}$

$\psi = e^{-\int_0^b \frac{dx\, p(x)}{\hbar}}$; $b = V_0 - E / F$

$\int_0^b \frac{dx\, p(x)}{\hbar} = \sqrt{\frac{2m}{\hbar^2}} \int_0^b dx \sqrt{V_0 - Fx - E}$

$= \sqrt{\frac{2mF}{\hbar^2}} \int_0^b dx \sqrt{b - x}$

$= -\frac{2}{3} \sqrt{\frac{2mF}{\hbar^2}} \left(b - x\right)^{3/2} \Big|_0^b$

$= \frac{2}{3} b^{3/2}$

$\Rightarrow T = e^{-\frac{2}{3}\sqrt{\frac{2m}{\hbar^2}} \frac{(V_0 - E)^{3/2}}{F}}$

TEST INCLUDES UP TO ONLY WKB.

3 DIMENSIONAL WKBJ

$\psi(r) = Y_l^m R(r)$

$R(r) = \chi(r)/r$

$$\Big[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \underbrace{V(r) + \frac{\hbar^2 \, l(l+1)}{2mr^2}}_{V_{EFF}} - E\Big]\chi(r) = 0$$

LET $\chi = e^{i\sigma/\hbar}$

$$\Rightarrow \chi = \frac{e^{\pm\frac{i}{\hbar}\int dr\, p(r)}}{\sqrt{p}} \quad ; \quad p = \sqrt{2m(E - V_{eff})}$$

BUT IT DON'T WORK TOO HOT. WORKS BETTER WITH $(l+\frac{1}{2})^2$ INSTEAD OF $l(l+1)$. ALSO, χ DOESN'T GO TO ZERO @ $r=0$, (UNLESS WE USE $(l+\frac{1}{2})^2$. THUS, LET

$$V_{EFF} = V(r) + \frac{\hbar^2}{2mr^2}\left(l+\frac{1}{2}\right)^2$$

2-18-75

EXAM SOLUTION

1. $\langle n | e^{\lambda a^+} | m \rangle = \sum_\ell \frac{\lambda^\ell}{\ell!} \langle n | a^{+\ell} | m \rangle$

$$= \frac{1}{(n-m)!} \lambda^{n-m} \sqrt{\frac{n!}{m!}} \quad \text{if } n \geq m$$

$$= 0 \qquad n < m$$

2. $\int_0^b \sqrt{2m(E-Fx)}\, dx = \hbar \pi (n + 3/4)$

$$= \frac{2}{3} \frac{\sqrt{2m}}{F} (E)^{3/2}$$

3. $\psi(r) = R(r)\, Y_\ell^m(\theta, \phi)$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \Rightarrow R = \frac{\chi}{r} \Rightarrow \chi = rR$$

$$\chi = C_1 I_{i k a}(k_0 a e^{-r/a}) + C_2 I_{-ika}(k_0 a e^{-r/a})$$

$\chi(r=0) = 0$ GIVES $\frac{C_2}{C_1} = -\frac{I_{ika}(k_0 a)}{I_{-ika}(k_0 a)}$

GIVES $|C_1| = \frac{|\Gamma(1+ika)|}{\sqrt{2\pi}}$

WKBJ IN 3-DIMENSIONS:

$$\left[\frac{d^2}{dr^2} + \frac{p^2(r)}{\hbar^2}\right]\chi = 0 \qquad \chi = \frac{R}{r}$$

$$p^2(r) = 2m\left[E - V(r)\right] - \frac{\hbar^2 \ell(\ell+1)}{r^2}$$

$$\chi = \frac{C}{p^{1/2}} \sin\left[\frac{1}{\hbar}\int_0^r dr\, p(r) + \frac{\pi}{4}\right] \leftarrow$$

BAD CAUSE:

1. χ DON'T GO TO 0 @ $r = 0$
2. NOT GOOD SOLUTIONS

BETTER:

$$p^2(r) = 2m\left[E - V(r)\right] - \frac{\hbar^2(\ell+\frac{1}{2})^2}{r^2}$$

LET'S HAVE A VARIABLE CHANGE: $x = \ln r$

THEN: $R = e^{-x/2}\, U(x)$

$$\chi = rR = \sqrt{r}\,U = e^{x/2}\,U$$

$$\frac{d\chi}{dr} = \frac{dx}{dr}\frac{d\chi}{dx} = \frac{1}{r}\frac{d\chi}{dx} = \frac{1}{r}\frac{d}{dx}\left(e^{x/2}U\right)$$

$$= e^{-x}\frac{d}{dx}\left(e^{x/2}U\right)$$

$$= e^{-x}\left[e^{x/2}\frac{dU}{dx} + \frac{1}{2}e^{x/2}U\right]$$

$$= e^{-x/2}\left[\frac{1}{2}U + \frac{dU}{dx}\right]$$

$$\frac{d^2\chi}{dr^2} = \frac{dx}{dr}\frac{d}{dx}\frac{d\chi}{dx}$$

$$= e^{x}\left[-\frac{1}{2}e^{-x/2}\left(\frac{U}{2} + \frac{dU}{dx}\right) + e^{-x/2}\left(\frac{1}{2}\frac{dU}{dx} + \frac{d^2U}{dx^2}\right)\right]$$

$$= e^{-3x/2}\left[\frac{d^2U}{dx^2} - \frac{1}{4}U\right]$$

SCHRO'S EQN IS:

$$\left[e^{-3x/2}\left[\frac{d^2}{dx^2} - \frac{1}{4}\right] + \frac{2m}{\hbar^2}\left[E - V(e^x)\right]e^{x/2} - \ell(\ell+1)e^{-2x}\;e^{x/2}\right]U = 0$$

$$\boxed{\text{OR}\quad \frac{d^2U}{dx^2} + \frac{U}{\hbar^2}\left\{2m\left[E - V(x)\right]e^{2x} + (\ell+\tfrac{1}{2})^2\hbar^2\right\} = 0}$$

FOR A NUMBER OF PERTURBATIONS

$W_{kN} = N\, W_k$

FROM IDEAL GAS THEORY

$W = \frac{N}{\Omega} v \sigma$

$\Rightarrow W_{kN} = \frac{N}{\Omega} v_k \sigma \quad , \quad v_k = \frac{\hbar k}{m}$

$$\sigma = \frac{1}{4\pi^2} \frac{m^2}{\hbar^2} \int d\Omega_{k'}\, V(k-k')^2$$

$$\frac{d\sigma}{d\Omega_{k' \to k}} = \frac{1}{4\pi^2} \frac{m^2}{\hbar^2} V(k-k')^2$$

LET $\bar{p} = \sqrt{2m(E - V(e^x))e^{2x} - (\ell + \frac{1}{2})^2 \hbar^2}$

$$U(x) = \begin{cases} \frac{c}{\sqrt{\bar{p}}} \sin\left[\frac{1}{\hbar}\int^x \bar{p}(x')\,dx'\right] \\ \frac{c}{2\sqrt{\bar{p}}} e^{-\frac{1}{\hbar}\int^x dx' |p(x')| dx} \end{cases}$$

$(2m(E - V(e^x))e^x$ MOST IMPORT

as $r \to +\infty$, $x \to +\infty$, $\bar{p} \to e^x\sqrt{2mE}$ (SINE WAV...

as $r \to 0$, $x \to -\infty$, $\bar{p} \to i(\ell + \frac{1}{2})\hbar$ (DEC...

$(\ell + \frac{1}{2})^2 \hbar^2$ MOST IMPORTANT

CONSIDER $V(e^x)e^{2x}$

1. IF $V(x)e^{2x} \to 0$ AS $x \to -\infty$

THEN $(\ell + \frac{1}{2})^2$ IS LARGEST TERM OKAY

2. IF $V(x)e^{2x} \to \infty$ AS $x \to -\infty$ $\bar{p} \to i\infty$

CONSIDER $V(r) = \frac{1}{r^4} = e^{-4x}$ $U \to 0$ ...

$\Rightarrow e^{2x} e^{-4x} = e^{-2x}$ OKAY

3. IF $V(e^x)e^{2x} \to -\infty$ AS $x \to -\infty$

EX $V(r) = -c/r^n$ $n > 2$

THEN $U \neq 0$ & $\chi \neq 0$

$\therefore$ THIS CASE HAS NO SOLUTION

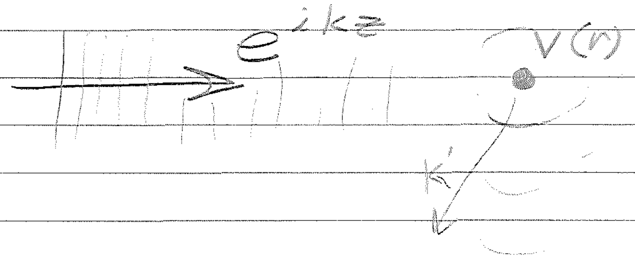
CONVERTING: $x = \ln r$

GIVES:

$$\chi(r) = \frac{c}{\sqrt{p(r)}} \sin \frac{1}{\hbar}\int^r dr'\,p(r')$$

$$p(r) = \sqrt{2m(E - V(r)) - (\ell + \tfrac{1}{2})^2\hbar^2/r^2}$$

EXAMPLE:



MATRIX ELEMENTS.
USE BOX NORMALIZATION:

$$\psi_n^{(0)} = \frac{1}{\sqrt{\Omega}} e^{ik\cdot r} \quad ; \ \Omega = \text{VOLUME}$$

$$V_{KK'} = \frac{1}{\Omega}\int d^3r\, e^{-ik'\cdot r} V(r)\, e^{ik\cdot r}$$

$$= \frac{1}{\Omega} \mathcal{V}(k-k') \quad \leftarrow \text{FOURIER XFRM}$$

$$w_{K\to K'} = \frac{2\pi}{\hbar}\frac{1}{\Omega^2}\mathcal{V}(k-k')^2 \times \delta\left[\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m}\right]$$

W_K = TOTAL P[SCATTER]

$$= \sum_{K'} w_{K\to K'} = \Omega \int \frac{d^3K'}{(2\pi)^3}$$

$$= \frac{2\pi}{\hbar}\frac{1}{\Omega}\int \frac{d^3K}{(2\pi)^3}\mathcal{V}(K-K')^2 \times \delta\left[\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m}\right]$$

$$d^3K' = \int d\Omega_{K'} \cdot K'^2 dK'$$

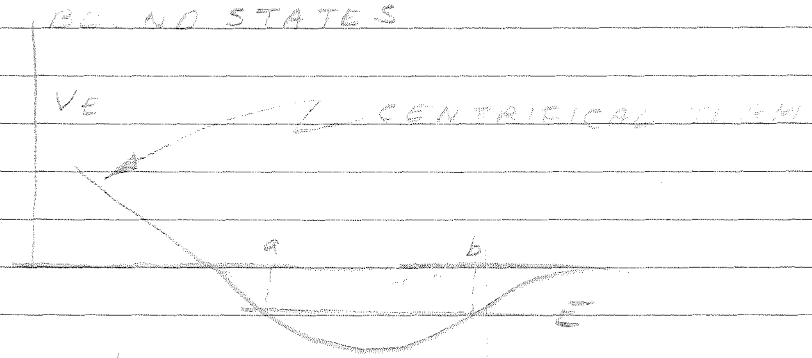
$$\int K'^2 dK' \, \delta\left[\frac{\hbar^2 K^2}{2m} - \frac{\hbar^2 K'^2}{2m}\right] = \frac{Km}{\hbar^2}$$

$$\therefore W_K = \frac{2\pi}{\hbar^2}\frac{1}{(2\pi)^3}\frac{1}{\Omega}\frac{Km}{\hbar^4}\int d\Omega\, \mathcal{V}(K-K')^2 \Big|_{K=K'}$$

EXAMPLE: COULOMB POTENTIAL

$$V(r) = -\frac{Ze^2}{r} \Rightarrow V_{eff}(r) = V(r) + \frac{\hbar^2}{2m}\frac{(\ell+\frac{1}{2})^2}{r^2}$$

BOUND STATES



$$\int_a^b dr\, p(r) = \pi\hbar(n+\tfrac{1}{2})$$

$$\int dr \sqrt{2m\left(E+\frac{Ze^2}{r}\right) - \hbar^2(\ell+\tfrac{1}{2})^2/r^2}$$

LET $\rho = r/a_0 \Rightarrow a_0 = \frac{\hbar^2}{me^2} = 0.529\,Å$

WE GET

$$\int d\rho \sqrt{\frac{E}{E_{ry}} + \frac{2Z}{\rho} - \frac{1}{\rho^2}(\ell+\tfrac{1}{2})^2} = \pi(n+\tfrac{1}{2})$$

$$E_{ry} = 13.6\,eV = \frac{e^2}{2a_0} = \frac{\hbar^2}{2ma_0^2}$$

$$= \int \frac{d\rho}{\rho}\left[\rho^2 \frac{E}{E_{ryd}} + 2Z\rho - (\ell+\tfrac{1}{2})^2\right]^{1/2}$$

$$= \int \frac{d\rho}{\rho}\left[-\alpha^2\rho^2 + 2Z\rho - (\ell+\tfrac{1}{2})^2\right]^{1/2} \quad ; -\alpha^2 = \frac{E}{E_{ryd}}$$

$$= \alpha\int_a^b \frac{d\rho}{\rho}\left[(\rho-a)(\rho-b)\right]^{1/2}$$

$$a+b = \frac{2Z}{\alpha^2}$$

$$-ab = \frac{(\ell+\frac{1}{2})^2}{\alpha^2}$$

$$= \alpha\pi\left[\frac{a+b}{2} - \sqrt{ab}\right] = \alpha\pi\left[\frac{Z}{\alpha^2} - \frac{\ell+\frac{1}{2}}{\alpha}\right] =$$

$$= \pi\left[\frac{Z}{\alpha} - \ell - \frac{1}{2}\right] = \pi(n+\tfrac{1}{2})$$

$$\frac{Z}{\alpha} = n+\ell+1 \Rightarrow \alpha = \frac{Z}{n+\ell+1}$$

$$E = -\frac{E_{ryd}\, Z^2}{(n+\ell+1)^2}$$

NOW SINCE THE P INCREASES WITH TIME, LET

$$P_{M\to e} = |a_e(t)|^2 = t\,\omega_{em}$$

ω_{em} = PROBABILITY / UNIT TIME

THUS, WE REALLY WANNA FIND OUT

$$\omega_{em} = \lim_{t\to\infty} \frac{d}{dt} |a_e(t)|^2$$

LET'S USE BORN APPROX:

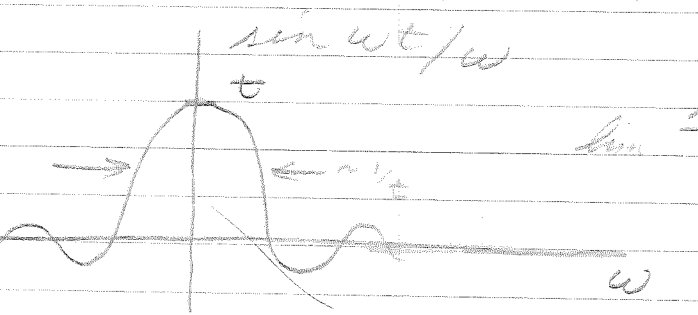
$$a_e(t) = \cancelto{0}{a_e^{(0)}} + a_e^{(1)}$$

$$\Rightarrow \omega_{em} = \lim_{t\to\infty} \frac{d}{dt} \left(\frac{V_{em}}{\hbar}\right)^2 \times \left[\int_0^t dt' e^{it[E_e^{(0)} - E_m^{(0)}]/\hbar}\right]^2$$

$$= \lim_{t\to\infty} V_{em}^2 \frac{d}{dt}\left[\frac{e^{i\Delta Et/\hbar} + e^{-i\Delta Et/\hbar} + 2}{\Delta E^2}\right]$$

$$= \lim_{t\to\infty} \frac{i V_{em}^2}{\Delta E\,\hbar}\left(e^{i\Delta Et/\hbar} - e^{-i\Delta Et/\hbar}\right)$$

$$= \lim_{t\to\infty} \frac{V_{em}^2}{\hbar} 2 \frac{\sin \Delta E t/\hbar}{\Delta E}$$



$$\lim \frac{\sin\omega t}{\omega} = \pi\,\delta(\omega)$$

$$\therefore \omega_{em} = \frac{2\pi}{\hbar} |V_{em}|^2 \delta\left[E_e^{(0)} - E_M^{(0)}\right]$$

1-20-75

ATOMS WITH "HYDROGEN-LIKE" STATES

ALKALI: Li, Na, K, Rb, Cs → CLOSED ATOMIC SHELL + 1 ELEC

ALKALINE: Ba, Ca, Sr, ... } CLOSED SHELL + 2 ELECTRONS
Be, Mg, Cd, Zn, ...

Al, Ga, In, ... } CLOSED SHELL + 3 ELEC

$Li: (1s)^2 \, 2s$ (n, l); n = TOTAL QUANTUM #

$\uparrow \downarrow$ SPIN $l = 0, s$

$1 \; p$
$2 \; d$

$Na: (1s)^2 \, (2s)^2 \, (2p)^6 \, 3s$

$n=1, l=0$ $n=1, l=0$ $n=2, l=1$
$\uparrow \downarrow$ $\uparrow \downarrow$ $m_l = -1, 0, 1$
$\uparrow \downarrow$

$K: (1s)^2 \quad (2s)^2 \quad (2p)^6 \quad (3s)^3 \quad (3p)^6 \quad 4s$

CONSIDER:

$Li \quad (1s)^2 \, 2s$

$E_{1s}^{Li} = 98 \, eV$

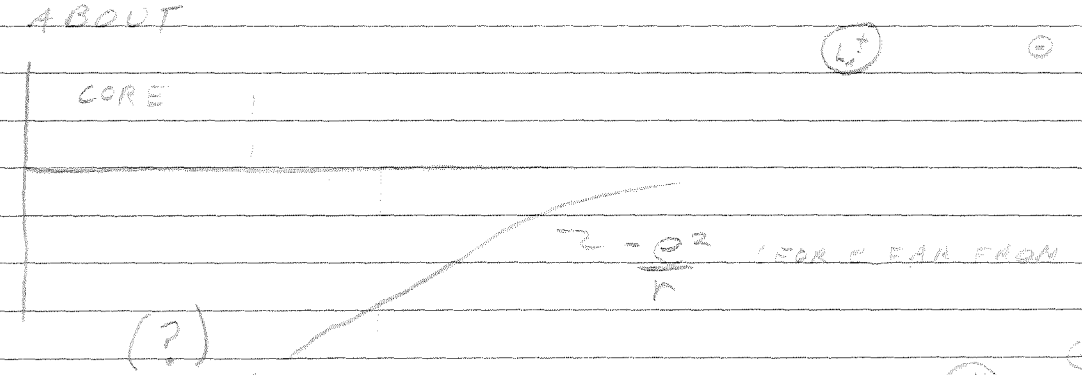
$E_{2s}^{Li} = -5.39 \, eV$ $(b_{1s} = 0.19 \text{Å})$

$\psi_{2s}(r) = ?$

IS THERE $H = \frac{-\hbar^2 \nabla^2}{2m} + V(r)$ TO GIVE

$\psi_{2s}(r) \; \ni \; E_{2s}^{Li}$?

HOW ABOUT



FOR ALKALINE: Mg

$V = -\frac{2e^2}{r}$

FOR BIGGER

$$a_\ell = a_\ell^{(0)} + a_\ell^{(1)} + a_\ell^{(2)} + \ldots$$

$$\Rightarrow i\hbar \dot{a}_\ell^{(0)} = 0$$

$$a_\ell^{(0)}(t) = \text{CONSTANT}$$

NOW $a_M(0) = 1$

$$a_\ell^{(0)}(0) = \delta_{\ell M}$$

FIRST ORDER IS THUS

OMIT

$$i\hbar \dot{a}_\ell^{(1)} = \sum_n a_n^{(0)} V_{\ell n} \theta(t) = V_{\ell M}\theta(t)$$

$$\Rightarrow a_\ell^{(1)}(t) = \frac{1}{i\hbar}\int_0^t dt' \, V_{\ell m}\, \theta(t') + a_\ell^{(1)}(0)$$

FOR $\ell \neq M$, $a_\ell^{(1)} = 0$

$$\Rightarrow a_\ell^{(1)}(t) = \frac{1}{i\hbar}\int_0^t$$

$$i\hbar\, e^{-itE_\ell^{(0)}/\hbar}\, \dot{a}_\ell^{(1)} = \sum_n a_n^{(0)} V_{\ell n}\, \theta(t)$$

$$= V_{\ell M}\,\theta(t)\, e^{-iE_m^{(0)}t/\hbar}$$

$$a_\ell^{(1)} = \frac{1}{i\hbar}\int_0^t dt' \, V_{\ell m}\, e^{it'(E_\ell^{(0)} - E_M^{(0)})/\hbar}$$

$$= \frac{V_{\ell m}}{i\hbar}\int_0^t dt' \, e^{it'(E_\ell^{(0)} - E_M^{(0)})/\hbar}$$

$\therefore$ PROBABILITY OF PARTICLE BEING IN STATE ℓ IS $|a_\ell(t)|^2$

$$= |a_\ell^{(0)} + a_\ell^{(1)} + a_\ell^{(2)} + \ldots|^2$$

$$a_\ell^{(0)} = 0$$

$a_\ell^{(1)}$ IS GIVEN ABOVE

$$E_{n\ell} = -\frac{Z^2 E_{RYD}}{(n^*)^2} \quad ; E_{RYD} = 13.6\ eV$$

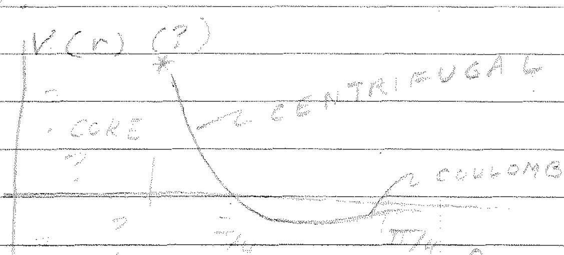
EXPERIMENTAL

E's = E_{n^*s}	$n_* = \sqrt{E_{RYD}/E_{n^*s}}$		E_{n^*p}	n^*
2s -5.390	$1.588 = 2 - .412$	2p		1.966
3s -2.02	$2.596 = 3 - .404$	3p		2.956
4s -1.05	$3.598 = 4 - .402$	4p		
	$\delta_s = .4$			$\delta_p = 0.05$

$$\Rightarrow E_n = \frac{-Z^2 E_{RYD}}{(n-\delta)^2} \quad ; \delta = \text{QUANTUM DEFECT}$$

FOR Na $\delta_s = 0.42$

AGAIN:



FOR WKBJ: $\varphi_T = \pi(n + \ldots) = \varphi_L + \varphi_R$

$$= \frac{\pi}{2} + \frac{1}{\hbar}\int dr\, p(r) \quad (+\pi\gamma)$$

WE CAN'T USE THIS, USE $\frac{\pi}{2} + \pi\gamma$

ADDED γ HAS CORRESPONDING EFFECT

USE $\frac{\pi}{4} + \pi\delta \Rightarrow \delta = \text{QUANTUM DEFECT}$

THE GOLDEN RULE (OR FERMI'S GOLDEN RULE)

W = RATE OF CHANGE FROM ONE STATE TO ANOTHER

$$W_{nm} = \frac{2\pi}{\hbar}\,\delta\left[E_n^{(0)} - E_m^{(0)}\right]\left|\mathcal{T}_{nm}\right|^2$$

$\mathcal{T}_{nm}$ IS A "T" MATRIX

$$\mathcal{T}_{nm} = V_{nm} - \sum_{\ell}\frac{V_{n\ell}V_{\ell m}}{(\quad)} + \ldots$$

$$\mathcal{T}_{nm} \cong V_{nm} \Longleftarrow \text{BORN APPROXIMATION}$$

$$W_{nm} = \frac{2\pi}{\hbar}\,\delta\left(E_n^{(0)} - E_m^{(0)}\right) V_{nm}^2$$

DERIVATION:

$$H_0 \Rightarrow \psi_n^{(0)},\ E_n^{(0)}$$

@ $t=0$, TURN ON POTENTIAL V

WHAT IS P[PARTICLE WILL CHANGE STATES]

SCHRÖEDINGER'S EQ'N WITH TIME DEPENDENCE

$$H\,\psi(r,t) = i\hbar\frac{\delta\psi(r,t)}{\delta t}$$

LET

$$\psi(r,t) = \sum_n a_n(t)\,\psi_n^{(0)}(r)\,e^{-itE_n^{(0)}/\hbar}$$

AT $t=0$ ASSUME PARTICLE IN STATE M.

$$a_m(0) = 1$$

$$\left[H_0 + V\right]\psi(r,t) = \sum_n a_n(t)\,\psi_n^{(0)}(r)\,e^{-itE_n^{(0)}/\hbar}$$

$$\Rightarrow \sum_n a_n(t)\,\psi_n^{(0)}(r)\,e^{-itE_n^{(0)}/\hbar}$$

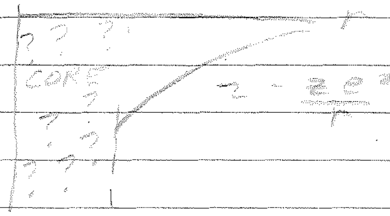
$$\left[E_n^{(0)} + V(r)\,\Theta(t)\right] = E_n^{(0)} + i\hbar\frac{\dot{a}_n(t)}{a_n}$$

MULTIPLY BOTH SIDES BY $\psi_\ell^{(0)}$ & INTEGRATE.

$$e^{-iE_\ell^{(0)}t/\hbar}\,\underline{i\hbar\,\dot{a}_\ell(t) = \sum_n a_n(t)\,V_{\ell n}\,\Theta(t)}\,e^{-iE_n^{(0)}t/\hbar}$$

$\Theta(t)$ = UNIT STEP FUNCTION

EXACT SOLUTION



BEFORE FOR COULOMB:

$\psi(r) = R(r)\, Y_{lm}(\theta,\phi)$

$$\Rightarrow R(r) = r^{l}\, e^{-\frac{r}{a_0 n}}\, F\left(l+1-n,\ 2l+2,\ \frac{2r}{a_0 n}\right)$$

$E = -Z^2/n^2$

BUT NOW:

$E = -Z^2/(n^*)$

$$\Rightarrow R(r) = r^{l}\, e^{-r/a_0 n^*}\, F\left[l+1-n^*,\ 2l+2,\ \frac{2r}{a_0 n^*}\right]$$

BUT THIS DIVERGES! (FOR $n^* \neq$ INTEGER)

THIS Eq. SATISFIES

$$\left[z\frac{d^2}{dz^2} + (b-z)\frac{d}{dz} - a\right] \begin{array}{l} \times F(a,b;z) = 0 \\ \times U(a,b;z) = 0 \end{array}$$

WE THREW OUT $U(a,b;z)$

SINCE $\lim_{z\to 0} U = 1/z^{b-1}$

BUT THAT DON' BUG US NOW

NOW: $U(a,b;z) \xrightarrow[z\to\infty]{} \frac{1}{z^a}$

SO USE:

$$R(r) = \left(\frac{r}{a_0}\right)^{l} e^{-r/a_0 n^*}\, U\left[l+1-n^*;\ 2l+2,\ \frac{2r}{a_0 n^*}\right]$$

R(r) IS A "WHITTAKER'S FUNCTION"

$$\Rightarrow R(r) = W_{n^*,\, l+\frac{1}{2}}\left(\frac{2r}{a_0 n^*}\right)\ ;\ E = \frac{-Z^2(13.6\,eV)}{(n^*)^2}$$

$$U(a,b;z) = \frac{1}{\Gamma(a)}\int_0^\infty dt\, e^{-zt}\, t^{a-1} (1-t)^{b-a-1}$$

n^*: EFFECTIVE QUANTUM NUMBER

NOTE: $\frac{dU(a,b;z)}{dz} = -a\, U(a+1, b+1; z)$

TIME DEPENDENT PERTURBATION THEORY

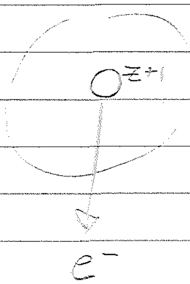
$H_0,\ \psi_n^{(0)},\ E_n^{(0)}$

$V \rightarrow$ TIME DEPENDENT

THREE EASY SOLUTIONS:

1) ADIABATIC LIMIT $\leftarrow$ <u>VERY</u> SLOW
2) SUDDEN APPROX. $\leftarrow$ <u>VERY</u> RAPIDLY
3) PERTURBATION $\leftarrow$ V IS ONLY A SMALL CHANGE

EXAMPLE



FOR $t<0$

$$Z:\ \psi(r,t)=\sum_n a_n \psi_n^{(0)}(r)$$

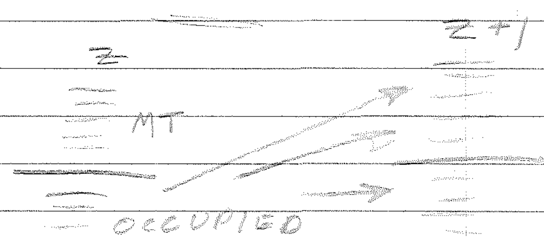
$a_n = 1$ FOR OCCUPIED STATED

FOR $t>0$

$$Z+1:\ \psi(r,t)=\sum_n b_n \phi_n(r)$$

NOW $\displaystyle\sum_n b_n\phi_n(0) = \sum a_n \psi_n^{(0)}(0)$

$$b_n = \sum_m \left[\int \phi_n^*(r)\,\psi_m^{(0)}(r)\right]a_m$$



TERMED "SHAKE-UP"

$$P[\text{SHAKE UP}] = \left[\int \phi_n^*(r)\,\psi_m^{(0)}(r)\,d\vec{r}\right]^2$$

SHAKE OFF $\Rightarrow e^-$ GETS THROWN OUT OF ATOM IN CONTINUUM STATES

ONE CAN SHOW
FOR HYDROGEN:

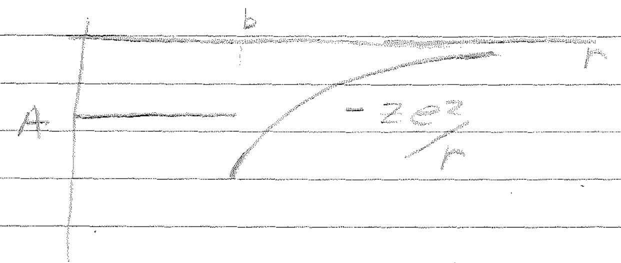
$$\langle n\ell | r^2 | n\ell \rangle_H = \int_0^\infty dr\, r^2 R_{n\ell}^2(r)\, r^2 = \frac{a_0^2}{2} n^2 \left[5n^2 + 1 - 3\ell(\ell+1)\right]$$

$$(d^3r = 4\pi r^2 dr)$$

FOR ALKALI'S:
(& FOR WHITTAKER'S FUNCTIONS):

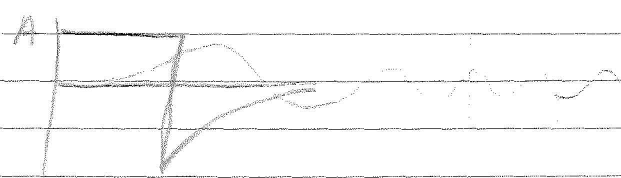
$$\langle r^2 \rangle = \int dr\, r^2\, \psi_{n^*, \ell+\frac{1}{2}}(r)^2\, r^2 = \frac{a_0^2}{2} n^* \left[5n^{*2} + 1 - 3\ell(\ell+1)\right]$$

WHAT DOES CORE LOOK LIKE?
12 YEAR OLD WORK FROM HEINE AND ABARANKOV: "MODEL POTENTIAL"



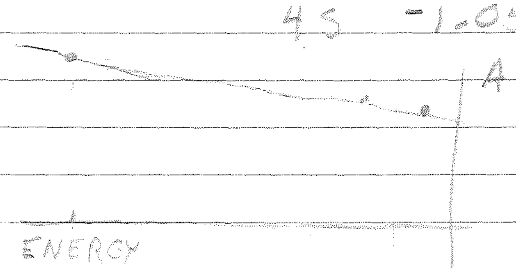
$$V(r) = \begin{cases} A & ; 0 \le r \le b \\ -\frac{Ze^2}{r} & ; r > b \end{cases}$$

CHOOSE b TO BE ION RADIUS FOUND CHEMICALLY (FOUND IN TABLES)
WILL FIND $E(b, Z, A)$
WE WILL FIND $A(b, Z, \ell, E)$
TURNS OUT A IS REPULSIVE



FOR LITHIUM S STATES: Li

	E_{ns} (eV)	A (IN RYDBERGS)
2S	−5.390	8.94
3S	−2.02	8.30
4S	−1.05	8.14

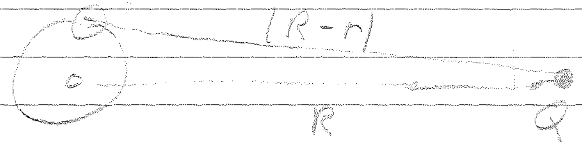


A IS LINEAR FUNCTION OF ENERGY

(EACH ELECTRON ψ IS ORTHOGONAL TO EVERY OTHER'S)

A IS THE PSEUDOPOTENTIAL: THE EFFECTIVE ONE ELECTRON POTENTIAL.

5. $V = Qe/R - \dfrac{Qe}{|R-r|}$



$$V = \frac{Qe}{R} - \frac{Qe}{|R-r|} = \frac{Qe}{R}\sum_{\ell=1}^{\infty}\left(\frac{r}{R}\right)^{\ell} P_\ell(\cos\theta)$$

FIRST ORDER: $\langle 1s | V | 1s \rangle = 0$

SINCE

$$\int_0^{\pi} d\theta \sin\theta \, P_\ell(\cos\theta) = 0$$

SECOND ORDER:

$\langle 1s | V | \lambda \rangle$

LEADING TERM $= \dfrac{Qe}{R^2}\langle 1s | r\cos\theta | \lambda \rangle$

$$\Rightarrow \Delta E = \frac{Q^2}{R^4}\, e^2 \sum_{\lambda} \frac{|\langle 1s | z | \lambda \rangle|^2}{E_{1s} - E_\lambda}$$

$$= -\frac{\alpha}{2}\frac{Q^2}{R^4}$$

WHERE α IS THE POLARIZABILITY

$\alpha = \frac{9}{2} a_0^3$ ← PREVIOUSLY DERIVED

6. $H_0 = -2 E_{RYD} (2)^2 = -8 E_{RYD}$

$\langle V \rangle = \frac{5}{4} Z E_{RYD} = \frac{5}{2} E_{RYD}$

GIVES $-5.50\ E_{RYD}$

EXPERIMENT: $-5.8\ E_{RYD}$

ASSUME:

SOLVE $H = -\frac{\hbar^2 \nabla^2}{2m} + V(r)$

WITH CONSTRAINT THAT WAVE FUNCTION $\psi(r)$ IS ORTHOGONAL TO CORE ELECTRONS $\phi_\alpha(r)$

FIND

$$H\psi = E\psi$$
$$H\phi_\alpha = E_\alpha \phi_\alpha$$

ORTHONANALIZED WAVE FUNCTION:

LET $\psi(r) = \chi(r) - \sum_\alpha \phi_\alpha(r) \langle\alpha|\chi\rangle$

$$\langle\alpha|\chi\rangle = \int d^3r\, \phi_\alpha^*(r)\chi(r)$$

THEN $\langle\alpha'|\psi\rangle = \langle\alpha'|\chi\rangle - \sum_\alpha \underbrace{\langle\alpha'|\alpha\rangle}_{\delta_{\alpha\alpha'}}\langle\alpha|\chi\rangle$
$= 0$

FIND $\chi(r) \to$ PSEUDO WAVE FUNCTION

NOW

$$H\psi = E\psi : H\chi - \sum_\alpha H\phi_\alpha\langle\alpha|\chi\rangle$$
$$= E\chi - \sum_\alpha E\phi_\alpha\langle\alpha|\chi\rangle$$

$$H\chi + \Delta V\chi = E\chi$$

$$\Delta V = \sum_\alpha (E - E_\alpha)|\alpha\rangle\langle\alpha|$$

DIRAC NOTATION: $\Delta V\chi = \sum_\alpha (E - E_\alpha)\phi_\alpha(r)\langle\alpha|\chi\rangle$

EXAMPLE: Li : $(1s)^2\ 2s$

$$\phi_{1s}(r) = \left(\frac{1}{\pi b^3}\right)^{1/2} e^{-r/b}$$

$b = 0.373$ au   1 a.u. OF LENGTH $= a_0 = 0.529$ Å

$\Rightarrow b = 0.197$ Å ; $E_{1s} = -98$ eV

α = CORE STATES WITH SAME SPIN

FOR LITHIUM, $\alpha = 1$

$$\Delta V\chi = (E + 98)\left(\frac{1}{\pi b^3}\right)^{1/2} e^{-rb}\int d^3r' \frac{e^{-r/b}}{(\pi b^3)^{1/2}}\chi(r')$$

LET $\chi(r') = \chi(0)$

$$\Rightarrow \Delta V\chi = \chi(0)(E + 98)\left(\frac{1}{\pi b^3}\right)^{1/2}\int d^3r'\, e^{-r'/b}/(\pi b^3)^{\frac{1}{2}}$$

$$= \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \int_0^\infty r^2 dr\, e^{-r/b} = 4\pi 2b^3$$

$= \chi(0)\, 8\, e^{-r/b}(E + 98\text{eV})$ ← A IS LINEAR WITH E ← > 0

2. $C_m^{(2)}$

FOR STATE M, $C_M^{(2)} = 0$

$$C_m^{(2)} = -\frac{V_{MM}V_{Mm}}{(E_M - E_m)^2} + \sum_l \frac{V_{ml}V_{lm}}{(E_m^{(0)}-E_M^{(0)})(E_l^{(0)}-E_M^{(0)})}$$

WORKED WRONG BY MAHAN

REFLECTIONS:

$$\sum_n |C_n|^2 = 1 = \sum_n \left[C_n^{(0)} + C_n^{(1)} + C_n^{(2)} + \dots\right]^2$$

WE KNOW

$C_M^{(0)} = 1$

$C_m^{(0)} = 0$ IF $m \neq n$

$$\Rightarrow \sum_n \left[C_n^{(0)2} + \cancel{2C_n^{(1)}C_n^{(0)}} + C_n^{(1)2} + 2C_n^{(0)}C_n^{(2)}\right] = 1$$

GIVES

$$C_m^{(2)} = -\frac{1}{2}\, C_m^{(1)2}/C_M^{(0)}$$

3. HARMONIC OSCILLATOR

4. $V' = \lambda\,\delta(r)/r^2$

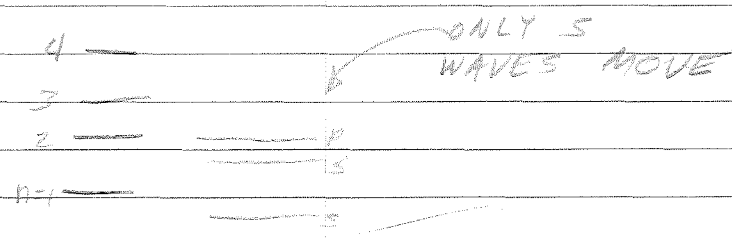
FIRST ORDER: $\langle n|V'|n\rangle = |\psi^2(r=0)|^2$

$= |\psi_s(0)|^2$

$= 0$ FOR ALL NON S WAVES

∴ ONLY S WAVES ARE EFFECTED

FOR H:



RIGHT WAY TO SOLVE IS [illegible]:

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2 + \nabla_3^2\right) - Ze^2\left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3}\right) + e^2\left(\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) \leftarrow \text{TOO HARD}$$

2-24-75

VARIATIONAL THEORY

GOOD FOR FINDING GROUND STATE WAVE FUNCTIONS AND ENERGIES. NOT GOOD FOR EXCITED STATES. (COMPLEMENTS WKBJ)

$$H = -\frac{\hbar^2\nabla^2}{2m} + V(r)$$

SOLVE: $H\psi_\lambda(r) = E_\lambda\psi_\lambda(r)$

THEOREM:

IF E_0 IS THE GROUND STATE ENERGY (LOWEST EIGENVALUES) OF H, THEN FOR ANY FUNCTION $\phi(r)$,

$$\frac{\int d^3r\,\phi^*(r)\,H\,\phi(r)}{\int d^3r\,\phi^*(r)\phi(r)} \geq E_0$$

PROOF:

LET $\psi_\lambda(r)$ AND E_λ BE THE EXACT EIGEN FUNCTIONS (WAVEFUNCTION) AND EIGENVALUE OF H. SINCE $\psi_\lambda(r)$ FORM A COMPLETE SET,

$$\exists \quad \phi(r) = \sum_n a_n\psi_n(r)$$

$$\text{THEN} \quad \int\phi^* H\phi = \sum_{\lambda\lambda'} a_\lambda^* a_{\lambda'}\int\psi_\lambda^* H\psi_{\lambda'}$$

$$= \sum_{\lambda\lambda'} a_\lambda^* a_{\lambda'}\int\psi_\lambda^* E_{\lambda'}\psi_{\lambda'}$$

$$= \sum_\lambda E_\lambda |a_\lambda|^2$$

$$\sum_\lambda |a_\lambda|^2 = \int\phi^*\phi$$

$$\sum_\lambda E_\lambda |a_\lambda|^2 \geq E_0 \sum_\lambda |a_\lambda|^2$$

E_0 IS LOWEST VALUE OF E_λ

$$\sum_\lambda (E_\lambda - E_0)|a_\lambda|^2 \geq 0$$

3/8/75

HOMEWORK

1. $n=3$ — STARK

$m=0$ s p d

$m=1$ p d

$m=-1$ p d

$m=\pm 2$ d → NO CHANGE

$$m=0 \qquad \begin{array}{c} \begin{pmatrix} 0 & V_1 & 0 \\ V_1 & 0 & V_2 \\ 0 & V_2 & 0 \end{pmatrix} \begin{array}{c} s \\ p \\ D \end{array} \end{array}$$

$$V_1 = \langle 1s | eFz | \ell=1, m_\ell=0 \rangle = -3\sqrt{6}\, eFa$$

$$V_2 = \langle \ell=1, m_\ell=0 | eFz | \ell=2, m_\ell=0 \rangle = -3\sqrt{3}\, eFa$$

DIAGONALIZING MATRIX GIVES

$$E = 0, \pm 9eFa$$

$$m=\pm 1 \qquad \begin{pmatrix} 0 & V_3 \\ V_3 & 0 \end{pmatrix}$$

$$V_3 = \langle \ell=1, m_\ell=1 | eFz | \ell=2, m_\ell=1 \rangle$$

$$= \tfrac{9}{2} eFa$$

$$\Rightarrow E = \pm \tfrac{9}{2} eFa$$

SO YOU END UP WITH

$9eFa$

$\underline{2}$ $\tfrac{9}{2} eFa$

$\underline{3}$ 0

$\underline{2}$ $-\tfrac{9}{2} eFa$

$\underline{1}$ $-9eFa$

LET $\phi_{\alpha\beta\gamma}(r)$ ie ϕ IS FUNCTION OF $\alpha\,\gamma\,\beta$ & r

WE GOTTA GUESS A WAVEFUNCTION.

THEN LET

$$\frac{\int d^3r\,\phi^*(r)H\phi(r)}{\int d^3\,\phi^*(r)\phi(r)} = E(\alpha,\beta,\gamma) \geq E_0$$

THEN, MINIMIZE $E(\alpha,\beta,\gamma)$

1. HYDROGEN ATOM (GROUND STATE IS 1S STATE)

$V(r) = e^2/r$

LET $\phi(r) = A e^{-\alpha r}$

PARAMETERS: A; α VARIABLE: r

INTEGRALS:

a. $$\int d^3r\,|\phi(r)|^2 = \int d\Omega \int_0^\infty r^2 dr\,A^2 e^{-2\alpha r}$$

$$= 4\pi \int_0^\infty r^2 dr\,A^2 e^{-2\alpha r}$$

NOW $$\int_0^\infty dx\,x^n e^{-x} = n!$$

$$\Rightarrow \int_0^\infty r^2 dr\,e^{-2\alpha r} = \frac{1}{(2\alpha)^3}\int_0^\infty x^2 dx\,e^{-x} = \frac{1}{4\alpha^3}$$

$$\Longrightarrow \int d^3r\,\phi^2 = \frac{A^2\pi}{\alpha^3}$$

b. $$-\frac{\hbar^2}{2m}\int d^3r\,\phi(r)\,\nabla^2\phi(r) \Rightarrow \text{ALWAYS} > 0$$

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \text{(ANGULAR DERIVATIVES)}$$

$$\Rightarrow -\frac{\hbar^2}{2m}4\pi A^2\int_0^\infty r^2 dr\,e^{-\alpha r}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}e^{-\alpha r}\right)$$

$$= -\frac{\hbar^2}{2m}4\pi A^2\int_0^\infty dr\,e^{-\alpha r}\frac{d}{dr}r^2\frac{d}{dr}e^{-\alpha r}$$

$$= +\frac{\hbar^2}{2m}4\pi A^2\int_0^\infty r^2 dr\left(\frac{\delta}{\delta r}e^{-\alpha r}\right)^2 \qquad > 0$$

$$= \frac{\hbar^2\alpha^2}{2m}4\pi A^2\frac{1}{4\alpha^3} = \frac{\pi A^2}{\alpha}\left[\frac{\hbar^2}{2m}\right]$$

HYPERFINE INTERACTION

$\underset{\sim}{I}$ = NUCLEAR SPIN

$\underset{\sim}{\mu} = g_I \mu_0 \underset{\sim}{I}$ $\qquad \mu_0 = \frac{e\hbar}{2mc}$

$\qquad g_I \sim \frac{1}{2000} \sim \frac{m_e}{m_p}$

$A = m \times \nabla \frac{1}{r}$

$H = \nabla \times A = \nabla \times (m \times \nabla \frac{1}{r}) = \nabla^2 \frac{1}{r} = 4\pi\,\delta(r)$

$H_{int} = -\frac{8\pi}{3} g_I \mu_0^2 \underset{\sim}{I} \cdot (\underset{\sim}{L} + 2\underset{\sim}{S})\,\delta(r)$

NO L TERMS, INTERACT

$H_{INT} = -\frac{8\pi}{3} g_I \mu_0^2 I \cdot L\,\delta(r)$

$\langle H_{INT} \rangle = \frac{8\pi}{3} g_I g_e |\psi_s(0)|^2 I \cdot S$

C. POTENTIAL ENERGY.

$$\int \phi \left(-\frac{e^2}{r}\right) \phi \, d^3r = -4\pi e^2 A^2 \int_0^\infty r\,dr\, e^{-2\alpha r}$$

$$= -\frac{4\pi e^2 A^2}{(2\alpha)^2} \int_0^\infty x\,dx\, e^{-x}$$

$$= -\frac{\pi e^2 A^2}{\alpha^2}$$

THEN

$$E(\alpha) = \frac{\int \phi H \phi}{\int \phi \phi} \qquad \text{(A's DROP OUT)}$$

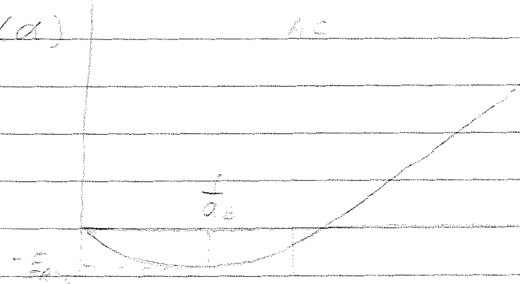
$$= \frac{\dfrac{\pi A^2}{\alpha^3}\dfrac{\hbar^2 \alpha^2}{2m} - \dfrac{\pi A^2}{\alpha^2} e^2 \alpha}{\dfrac{A^2 \pi}{\alpha^3}}$$

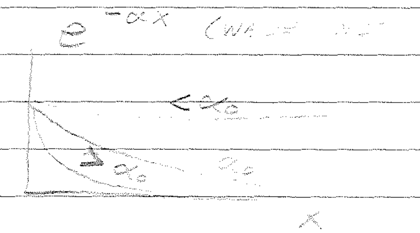
$$= \frac{\hbar^2 \alpha^2}{2m} - e^2 \alpha$$

$$\frac{dE}{d\alpha} = 0 = \frac{\hbar^2 \alpha}{m} - e^2 \Rightarrow \alpha_0 = \frac{e^2 m}{\hbar^2} = \frac{1}{a_B}$$

$$E(\alpha_0) = \frac{\hbar^2}{2m a_B^2} - \frac{e^2}{a_B} = -\frac{e^2}{2a_B} = -E_{ATO} \Leftarrow \text{EXACT ANSWER}$$

CONSIDER $E(\alpha)$

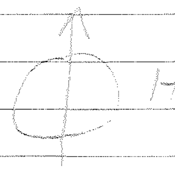




ACTUALLY $\phi = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha x}$

$$\text{ENERGY} = -\tfrac{1}{2}\chi H_0^2 \qquad (\text{FOR } E,\ E = -\tfrac{1}{2}\alpha E^2)$$

χ = SUSCEPTIBILITY



$$M = \chi H_0$$
$$dE = -M \cdot H_0$$

FOR $\chi > 0$, PARAMAGNETIC
$\chi < 0$, DIAMAGNETIC

$\frac{e^2}{8mc^2} H_0^2 (r_\perp)^2$ GIVES

$$E = \sum_i \langle r_{\perp i}^2 \rangle \frac{H_i^2 e^2}{8mc^2} > 0 \Rightarrow \chi < 0$$
$$\Rightarrow \text{DIAMAGNETIC}$$

$\mu_0 H_0 (L + 2S)$ GIVES

$$E = \mu_0^2 \sum_j H_i^2 \frac{|\langle j | L + 2S | g \rangle|^2}{E_g - E_j} < 0 \Rightarrow \chi > 0$$
$$\Rightarrow \text{PARAMAGNETIC}$$

SAME PROBLEM GUESSING THE WRONG ϕ

2. $V(r) = -e^2/r$

TRY: $V(r) = A\, e^{-(r/a_B)^2 \gamma^2}$

γ IS VARIATIONAL PARAMETER

DO THREE INTEGRALS

a. $\int d^3r\, \phi^2 = 4\pi A^2 \int_0^\infty r^2 dr\, e^{-2\gamma^2 r^2/a_B^2}$

$$x = \sqrt{2}\,\gamma\, r/a_B$$

$$\Rightarrow \int d\tau\, \phi^2 = \frac{4\pi A^2 a_B^3}{(\sqrt{2}\gamma)^3} \int_0^\infty x^2 dx\, e^{-x^2}$$

$$= \frac{4\pi A^2 a_B^3}{(\sqrt{2}\gamma)^3} \frac{\sqrt{\pi}}{4}$$

$$= \frac{\pi^{3/2} A^2 a_B^3}{2^{3/2}\gamma^3}$$

b. POTENTIAL ENERGY

$$\int d^3r\, \phi^2\left(-\frac{e^2}{r}\right) = -4\pi A^2 e^2 \int_0^\infty dr\, r\, e^{-2\gamma^2 r^2/a_B^2}$$

$$= \frac{-4\pi A^2 e^2 a_B^2}{2\gamma^2} \int_0^\infty x\, dx\, e^{-x^2}$$

$$= \frac{-4\pi A^2 e^2 a_B^2}{2\gamma^2} \frac{1}{2}$$

$$= \frac{-\pi A^2 e^2 a_B^2}{\gamma^2}$$

c. KINETIC ENERGY

$$\int d^3r \frac{\hbar^2}{2m}\left(\frac{d\phi}{dr}\right)^2 = \frac{4\pi A^2 \hbar^2}{2m}\left(\frac{2\gamma^2}{a_B^2}\right)^2 \int_0^\infty r^2 dr\, e^{-\frac{2\gamma^2}{a_B^2} r^2} r^2$$

$$= \frac{4\pi A^2 \hbar^2}{2m} \frac{4\gamma^4}{a_B^4}\left(\frac{a_B}{\sqrt{2}\gamma}\right)^5 \int_0^\infty x^4 dx\, e^{-x^2}$$

$$= \frac{4\pi A^2 \hbar^2}{2m} \frac{4\gamma^4}{a_B^4}\left(\frac{a_B}{\sqrt{2}\gamma}\right)^5 \frac{3}{8}\sqrt{\pi}$$

$$= \left(\frac{\hbar^2}{2m a_B^2}\right) \frac{\pi^{3/2} A^2 a_B^3}{2^{3/2}\gamma^3} (3\gamma^2)$$

$$E(\gamma) = \left(\frac{\hbar^2}{2m a_B^2}\right)\left[3\gamma^2 - \frac{\gamma\, 2^{5/2}}{\sqrt{\pi}}\right] \xleftrightarrow{\text{SAME FORM}}$$

$$= E_{RYD}\left[3\gamma^2 - \frac{1}{\sqrt{\pi}}\gamma\, 2^{5/2}\right]$$

$$\frac{d}{d\gamma}(E/E_R) = 0 = 6\gamma_0 - \frac{1}{\sqrt{\pi}} 2^{5/2} \Rightarrow \gamma_0 = 2^{3/2}/3\sqrt{\pi}$$

$$E(\gamma_0) = E_R\left[\frac{8}{3\pi} - \frac{16}{3\pi}\right] = \frac{-8}{3\pi} E_R = -0.85\, E_{RYD}$$

MISSES BY ABOUT 15%

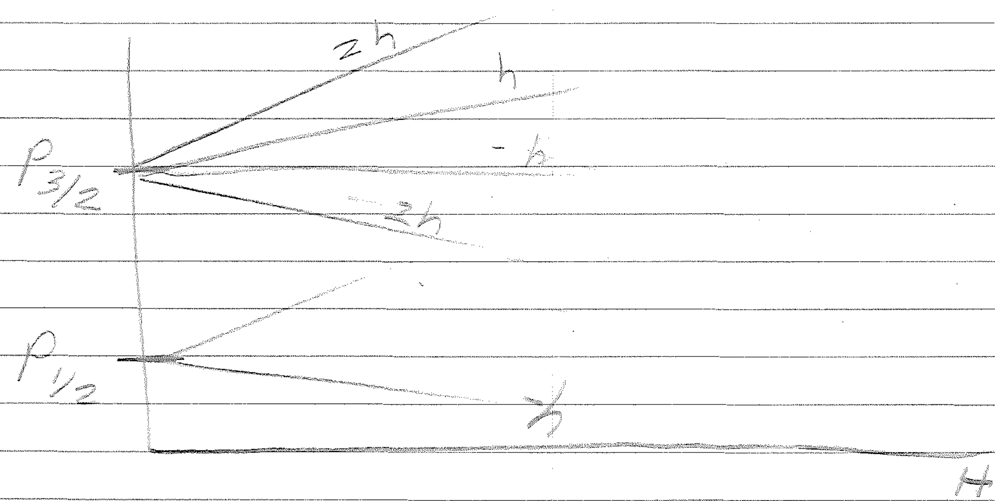
CONSIDER $\quad \xi(\ell\cdot s) = \ell_z s_z + \frac{1}{2}(\ell^+ s^- + \ell^- s^+)$

$$H_{INT} = \xi\, \ell\cdot s + \mu_0 H_0 (\ell_z + 2 s_z)$$

AND DIAGONALIZE $\quad (h = \mu_0 H_0)$

$$\begin{pmatrix} -2h+\frac{\xi}{2} & & & & & \\ & -\frac{\xi}{2} & \frac{\xi}{\sqrt{2}} & & & \\ & \frac{\xi}{\sqrt{2}} & -h & & & \\ & & & h & \frac{\xi}{\sqrt{2}} & \\ & & & \frac{\xi}{\sqrt{2}} & -\frac{\xi}{2} & \\ & & & & & \frac{\xi}{2}+2h \end{pmatrix} \begin{pmatrix} \phi_1^{1}\alpha \\ \phi_1^{1}\beta \\ \phi_1^{0}\alpha \\ \phi_1^{0}\beta \\ \phi_1^{-1}\alpha \\ \phi_1^{-1}\beta \end{pmatrix}$$

$$\rightarrow E = -\frac{1}{2}\left(\frac{\xi}{2}+h\right) \pm \sqrt{\frac{1}{4}\left(h-\frac{\xi}{2}\right)^2 + \frac{\xi^2}{2}}$$



NOTE

$$E = -\frac{1}{2}\left(\frac{\xi}{2}+h\right) \pm \underbrace{\sqrt{\frac{1}{2}\left(h-\frac{\xi}{2}\right)^2 + \frac{\xi^2}{2}}}$$

$$= \underbrace{\frac{\xi}{2} - \frac{2}{3}h - \xi - \frac{1}{3}h}_{\text{SAME AS LANDE } g \text{ VALUES}} - -$$

3. THREE-D HARMONIC OSCILLATOR

CORRECT ANSWER: $\phi(r) = A e^{-\alpha^2 r^2}$ (IN BOOK)

TRY $\phi(r) = A e^{-\alpha r}$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{K}{2} r^2$$

FROM BEFORE:

a. $\int \phi^2 = \pi A^2 / \alpha^2$

b. $-\int \phi \frac{\hbar^2}{2m} \nabla^2 \phi = \frac{\pi A^2}{\alpha^3} \frac{\hbar^2 \alpha^2}{2m}$

NOW

c. $\int \phi^2 \frac{K}{2} r^2 = 4\pi A^2 \frac{K}{2} \int_0^\infty r^2 dr\, r^2 e^{-2\alpha r}$

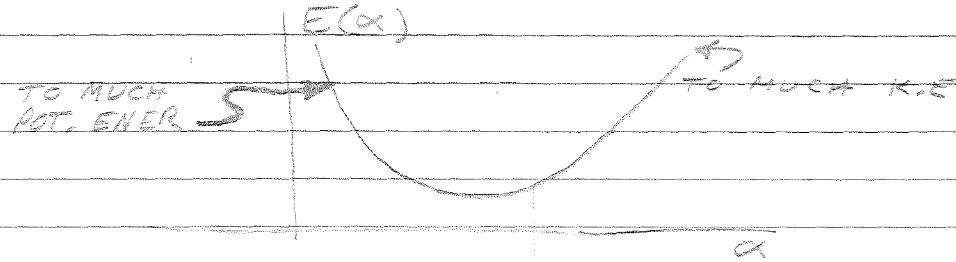
$$= \frac{2\pi A^2 K}{(2\alpha)^5} \int_0^\infty x^4 dx\, e^{-x}$$

$$= \frac{2\pi A^2 K}{(2\alpha)^5} 4!$$

$$= \frac{3}{2} \frac{\pi A^2 K}{\alpha^5}$$

THEN:

$$E(\alpha) = \frac{\hbar^2 \alpha}{2m} + \frac{3K}{2\alpha^2}$$



$$\frac{dE}{d\alpha} = 0 = \frac{\hbar^2}{2m}\alpha_0 - \frac{3K}{\alpha_0^3} \Rightarrow \alpha_0^4 = \frac{2Km}{\hbar^2}$$

$$\Rightarrow E(\alpha_0) = \frac{\hbar^2}{2m}\sqrt{\frac{2Km}{\hbar^2}} + \frac{3}{2}\frac{K}{\sqrt{\frac{3Km}{\hbar^2}}}$$

$$= \frac{\sqrt{3}}{2}\hbar\omega + \frac{\sqrt{3}}{2}\hbar\omega$$

$$= \sqrt{3}\,\hbar\omega$$

RIGHT ANSWER IS $E_0 = \frac{3}{2}\hbar\omega$

$J = L + S$

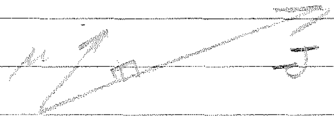
WE WANT TO FIND

$\mu = L + 2S = J + S$

$\langle j\ m | \mu_z | j\ m \rangle$

WE KNOW

$\langle j m | J_z | j m \rangle = m$



$$\langle jm | \mu_z | j m \rangle = \frac{\langle \mu \cdot J \rangle}{\langle J \cdot J \rangle} = \frac{\langle \mu \cdot J \rangle}{j(j+1)}$$

$$= \frac{\langle (J+S) \cdot J \rangle}{j(j+1)} = 1 + \frac{\langle S \cdot J \rangle}{j(j+1)}$$

NOW $J = L + S$

$L = J - S$

$$\Rightarrow \ell(\ell+1) = j(j+1) + s(s+1) - 2S \cdot J$$

$$\therefore \langle jm | \mu_z | jm \rangle = 1 + \frac{1}{2}\left[\frac{j(j+1) + s(s+1) - \ell(\ell+1)}{j(j+1)}\right]$$

$= g$

g	STATE
2	$S_{1/2}$
2/3	$P_{1/2}$
4/3	$P_{3/2}$
⋮	⋮

ETC.

HELIUM ATOM

NUCLEUS: $Z=2$ & 2 ELECTRONS · $\psi(r_1, r_2)$

$$H = \frac{-\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{|r_1 - r_2|}$$

K.E. NUCLEUS ATTRACTION INTERACTION

REMINDER:

$$H = -\frac{\hbar^2 \nabla^2}{2m} - \frac{Ze^2}{r}$$

GIVES $E_n = -E_R Z^2/n^2$

FOR $Z=2$, GRND STATE $\rightarrow -4 E_{RYD}$

HELIUM ATOM WOULD BE THIS IF WE HAD NO LAST TERM, CAUSE

$$\psi(r_1, r_2) = \psi_{hyd}(r_1)\,\psi_{hyd}(r_2)$$

$$(H_1 + H_2)\,\psi_1\psi_2 = (E_1 + E_2)\,\psi_1\psi_2$$
$$= -8 \text{ RYD.}$$

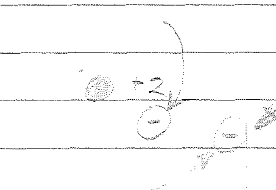
THIS IS ANSWER FOR He^+

ANYWAY, FOR REAL He ATOM, WE TRY

$$\psi(r_1, r_2) = A\,e^{-Z^*(r_1+r_2)/a_B} = \phi_1(r_1)\,\phi_2(r_2)$$

WHERE Z^* IS THE VARIATIONAL PARAMETER

(IF NO ELECT-ELECT. TERM, $Z^* = 2$)



SCREENING; THIS SEES ABOUT A +1 CHARGE

INTEGRALS:

a. NORMALIZATION

$$\int d^3r_1 \int d^3r_2\, \psi(r_1, r_2) = \left(\frac{\pi A^2 a_B^3}{Z^{*3}}\right)^2$$

b.

$$-2\int d^3r_1\, \phi(r_1)^2\, \frac{e^2}{r_1} \int d^3r_2\, \phi(r_2)^2$$

$$= -2\int d^3r_1\, \phi_1(r_1)^2 \left(\frac{\pi A^2 a_B^3}{Z^{*3}}\right)$$

$$= -2\left(\frac{\pi A^2 a_B^3}{Z^{*3}}\right) \frac{e^2 Z^*}{a_B} \left(\frac{\pi A^2 a_B^3}{Z^{*3}}\right)$$

$$H = -\mu_0 H_0 (L + 2S) + \frac{e^2}{8mc^2} H_0^2 r_\perp^2$$

"WEAK" MAGNETIC FIELD: $\mu_0 H_0 < \xi$
YIELDS ZEEMAN EFFECT
"STRONG" $\mu_0 H_0 > \xi$
YIELDS PASCHEN-BACK EFFECT

$$H_0 = \xi\, \ell \cdot s + \underbrace{e F \cdot r}_{E\ \text{FIELD}} \underbrace{- \mu_0 H_0 \cdot (L + 2S)}_{M\ \text{FIELD}}$$

1. JUST MAGNETIC FIELD (NO SPIN ORBIT)

$$H_{INT} = -\mu_0 H (L_z + 2S_z)$$

$$\phi_1^1 \alpha, \ \phi_1^1 \beta, \ \phi_1^0 \alpha, \ \phi_1^0 \beta, \ \phi_1^{-1} \alpha, \ \phi_1^{-1} \beta$$

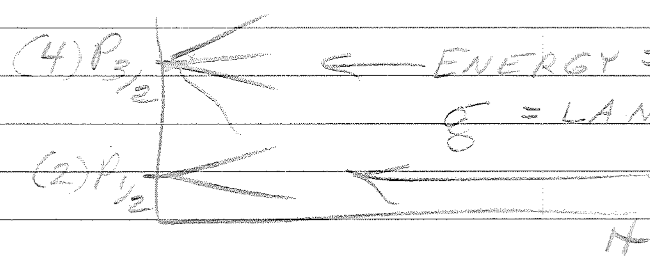
FOR STRONG:

$$-\mu_0 H_0 (2, \ 0, \ 1, \ -1, \ 0, \ -2)$$

$2\ \mu_0 H$
$1\ \mu_0 H$
$0\ \mu_0 H$
$-1\ \mu_0 H$
$-2\ \mu_0 H$

STATES ARE JUST SPREAD

FOR ZEEMAN EFFECT



ENERGY $= m \mu_0 H_0 g$
g = LANDE g FACTOR

ENERGY $= m \mu_0 H_0 g$

WE WILL NOW FIND g

$$I = \int d^3r_1 \int d^3r_2\, \phi_1(r_1)^2 \phi(r_2)^2 \frac{e^2}{|r_1 - r_2|}$$

$$= (4\pi A^2)^2 e^2 \int_0^\infty r_1^2 dr_1\, e^{-2r_1 Z^*/a_B} \int r_2^2 dr_2\, e^{-2r_2 Z^*/a_B}$$

$$\times \int \frac{d\Omega_1}{4\pi} \int \frac{d\Omega}{4\pi} \frac{1}{|r_1 - r_2|}$$

$$\frac{1}{|r_1 - r_2|} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta}}$$

$$= \begin{cases} \sum_{\ell=0}^{\infty} \frac{r_1^\ell}{r_2^{\ell+1}} P_\ell(\cos\theta) & ; r_1 < r_2 \\ \sum_{\ell=0}^{\infty} \frac{r_2^\ell}{r_1^{\ell+1}} P_\ell(\cos\theta) & ; r_2 < r_1 \end{cases}$$

$$\int d\Omega\, P_\ell(\cos\theta) = \begin{cases} 4\pi & ; \ell = 0 \\ 0 & ; \ell \neq 0 \end{cases}$$

$$\therefore \int \frac{d\Omega_1}{4\pi} \int \frac{d\Omega}{4\pi} \frac{1}{|r_1 - r_2|} = \begin{cases} \frac{1}{r_1} & ; r_2 < r_1 \\ \frac{1}{r_2} & ; r_1 < r_2 \end{cases}$$

$$\Rightarrow I = 2(4\pi A^2)^2 e^2 \int_0^\infty r_1^2 dr_1\, e^{-2r_1 Z^*/a_B}$$

$$\times \int_{r_1}^\infty dr_2\, r_2\, e^{-2r_2 Z^*/a_B} e^{-2Z^* r_1/a_B}$$

$$; r_2 > r_1$$

$$= \left(\frac{\pi A^2 a_B^3}{Z^{*3}}\right)^2 \frac{5}{4} Z^* \left(\frac{e^2}{2a_B}\right)$$

THUS GIVING:

$$E[Z^*] = E_R \Big[\underset{\text{K.E.}}{2Z^{*2}} - \underset{\frac{2Ze^2}{r_1} + \frac{2Ze^2}{r_2}}{8Z} + \frac{5}{4} Z^* \Big]$$

$A^2 = \frac{1}{4}(H_0 \times r)^2$

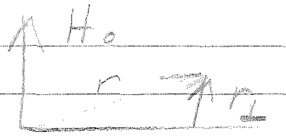
FOR H_0 IN Z DIRECTION

$A_y = \frac{1}{2} H_{0z} X$

$A^2 = \frac{1}{4} H_0^2 (x_i^2 + y_i^2)$

AND

$$\underline{H = -\mu_0 H_0(\underline{L} + 2\underline{S}) + \frac{e^2}{2mc^2} H_0^2 (r_\perp^2)}$$



USUALLY:

$$\frac{e^2}{2mc^2} H_0^2 (r_\perp)^2 << -\mu_0 H_0 (L + 2S)$$

CONSIDER He, A, Ne (CLOSED e SHELLS)

$S = 0$, $L = 0$, $\therefore$ SMALL TERM IS IMPORTANT

2-27-75

REVIEW

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{r_{12}}$$

$$\psi(\underset{\sim}{r_1}, \underset{\sim}{r_2}) = \phi(r_1)\,\phi(r_2)$$ ← ASSUMPTION

$$\phi(r_2) = e^{-\alpha r_2}$$

GIVES $E(\alpha) = \frac{2\hbar^2\alpha^2}{2m} - 2e^2(2\alpha) + \frac{5}{8}e^2\alpha$

$$\alpha = Z^*/a_B \quad ; \quad \frac{\hbar^2}{2ma_B^2} = E_R = \frac{e^2}{2a_B}$$

$$E[Z^*] = E_R[\underbrace{2Z^{*2}}_{K.E.} - \underbrace{8Z^*}_{V} + \underbrace{\tfrac{5}{4}Z^*}_{el\text{-}el}]$$

FOR NO el, el TERM: $E(Z^*) = 2E_R(Z^{*2} - 4Z^*)$

$$Z^*_{MIN} = 2$$

$$\Rightarrow E[Z^*_{MIN}] = -8E_R$$

INCLUDING el-el TERM:

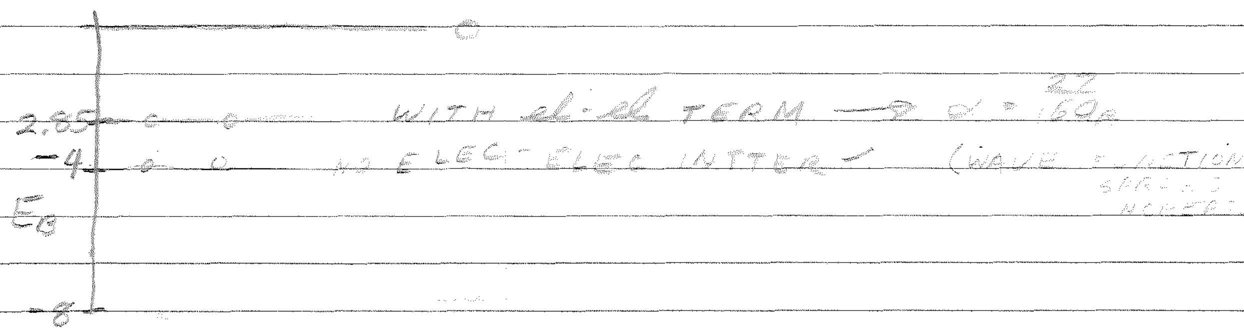
$$\frac{d}{dZ^*}E(Z^*) = 0 = E_R\left[4Z^* - 8 + \frac{5}{4}\right]$$

$$= E_R\left[4Z^* - \frac{27}{4}\right]$$

$$\therefore Z^*_0 = 27/16$$

E OF BOTH ELECTRONS

$$\rightarrow E\left(Z_0 = \frac{27}{16}\right) = -2\left(\frac{27}{16}\right)^2 E_R \approx -5.70\,E_R$$



MAGNETIC FIELDS (STATIC or D.C.)

SPIN: $\mu_0 g_e S \cdot H_0$

μ_0 = BOHR MAGNETRON = $e\hbar/2mc$

$g_e = -2.00$

H_0 = MAGNETIC FIELD

ORBITAL: CONSIDER

$\sum \frac{p_i^2}{2m} \rightarrow [p_i - \frac{e}{c}A(r_i)]^2/2m$

LET $A = \frac{1}{2} H_0 \times r$

$\nabla \times A = H_0$

$$\frac{[p_i - \frac{e}{c}A(r_i)]^2}{2m} = \frac{p_i^2}{2m} - \frac{e}{2mc}[p \cdot A + A \cdot p] + \frac{e^2}{2mc^2}A^2$$

$p_i \notin A_i = 0 \quad i = x, y, z$

$A_x = \frac{1}{2}[H_{0z} Y - H_{0y} Z]$

$$\Rightarrow \frac{p_i^2}{2m} - \underbrace{\frac{2e}{2mc} P \cdot A}_{\text{PARAMAGNETIC}} + \underbrace{\frac{e^2}{2mc^2} A^2}_{\text{DIAMAGNETIC}}$$

$$\frac{e}{mc}\frac{1}{2} P \cdot A = \frac{e}{mc}\frac{1}{2}(H_0 \times r) \cdot p$$

$$= \frac{e}{mc}\frac{1}{2} H_0 \cdot (r \times p)$$

$$= \frac{e}{mc}\frac{1}{2} H_0 \cdot \ell\hbar$$

$$= \mu_0 H_0 \sum_i \ell_i$$

$$L = \sum_i \ell_i$$

$$\Rightarrow \frac{2e}{2mc} p \cdot A = \mu_0 H_0 \cdot L$$

i.e. $H = \mu_0 H_0 (L + 2S)$ + DIAM.

HOW DOES THIS COMPARE WITH EXPERIMENT?

E_{I_1} IONIZATION ENERGY FOR He = 24.5 eV = 1.80 E_{RYD}

$E_I \neq E_B$ = BINDING ENERGY

E_I = MINIMUM ENERGY NEEDED TO REMOVE ~~ONE~~ FIRST ELECTRON

$= E_{N\ \text{PARTICLES}} - E_{N-1\ \text{PARTICLES}}$ $(\neq E_{1\ \text{PART}})$

WHAT HAPPENS WHEN WE TAKE 2 OUT OF He?

WELL, IT TAKES $E = -4E_R$

E_{I_2} MINIMUM E NEEDED TO REMOVE SECOND e = 4.00 RYD

$E_{I_1} + E_{I_2} = 5.80\ E_R$ (EXPERIMENT)

$5.70\ E_R$ (THEORY)

SPIN AND ANGULAR MOMENTUM

ANGULAR MOMENTUM OPERATOR (CLASSICAL):

$$\underline{M} = \vec{r} \times \vec{p} \quad ; \quad M_z = xp_y - yp_x$$
$$M_y = zp_x - xp_z$$
$$M_x = yp_z - zp_y$$

COMMUTATION OPERATOR RELATIONS

$$\begin{aligned}
[M_x, M_y] &= [yp_z - zp_y,\ zp_x - xp_z] \\
&= yp_x[p_z, z] + [z, p_z]p_y x \\
&= yp_x(-i\hbar) + (i\hbar)p_y(x) \\
&= i\hbar(xp_y - yp_x) \\
&= i\hbar M_z
\end{aligned}$$

$$\begin{cases}
[M_y, M_z] = i\hbar M_x \\
[M_z, M_x] = i\hbar M_y \\
[M_x, M_y] = i\hbar M_z
\end{cases}$$

$|\tfrac{3}{2}, \tfrac{3}{2}\rangle = \phi_{\ell=1}^{m_\ell=1}\,\alpha \Rightarrow$ FIRST ROW ALL 0'S

$|\tfrac{3}{2}, \tfrac{1}{2}\rangle = \dfrac{\phi_1^1\beta}{\sqrt{3}} + \sqrt{\tfrac{2}{3}}\,\phi_1^0\alpha$

STATE:

$|\tfrac{1}{2}, \tfrac{1}{2}\rangle = \phi_s(r)\,\alpha$

$|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \phi_s(r)\,\beta$

$eF\langle\phi_1^0|z|\phi_s\rangle = \lambda$

$|\tfrac{3}{2}, -\tfrac{1}{2}\rangle = \sqrt{2/3}\,\phi_1^0\beta - \sqrt{\tfrac{1}{3}}\,\phi_1^{-1}\alpha$

$|\tfrac{3}{2}, -\tfrac{3}{2}\rangle = \phi_1^{-1}\beta$

$|\tfrac{1}{2}, \tfrac{1}{2}\rangle = \sqrt{2/3}\,\phi_1^1\beta - \sqrt{1/3}\,\phi_1^0\alpha$

DIAGONALIZE MATRIX

TAKE OUT TWO $\xi/2$'s LEAVES 6×6

ALL $|--\tfrac{1}{2}\rangle$ MIX & $|--\!-\tfrac{1}{2}\rangle$ MIX

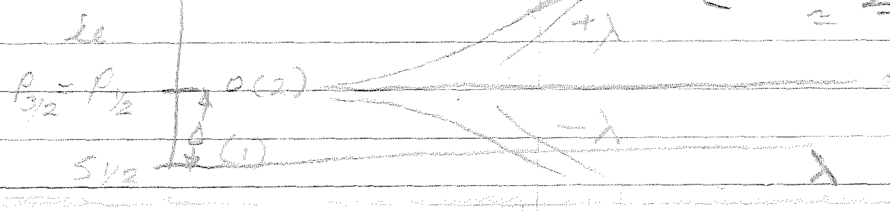
REWRITING MATRIX:

$$
\begin{array}{cccccccc|l}
\xi/2 & & & & & & & & |\tfrac{3}{2},\tfrac{3}{2}\rangle \\
 & \xi/2 & & & & & & & |\tfrac{3}{2},-\tfrac{3}{2}\rangle \\
 & & \xi/2 & 0 & \sqrt{2/3}\,\lambda & & & & |\tfrac{3}{2},\tfrac{1}{2}\rangle\ P_{3/2} \\
 & & 0 & -\xi & -\lambda\sqrt{1/3} & & & & |\tfrac{1}{2},\tfrac{1}{2}\rangle\ P_{1/2} \\
 & & \sqrt{2/3}\,\lambda & -\sqrt{\tfrac{1}{3}}\,\lambda & -\Delta & & & & |\tfrac{1}{2},\tfrac{1}{2}\rangle\ S_{1/2} \\
 & & & & & \xi/2 & 0 & \sqrt{\tfrac{2}{3}}\,\lambda & |\tfrac{3}{2},-\tfrac{1}{2}\rangle\ P_{3/2} \\
 & & & & & 0 & -\xi & \sqrt{\tfrac{1}{3}}\,\lambda & |\tfrac{1}{2},-\tfrac{1}{2}\rangle\ P_{1/2} \\
 & & & & & \sqrt{\tfrac{2}{3}}\,\lambda & \sqrt{\tfrac{1}{3}}\,\lambda & -\Delta & |\tfrac{1}{2},-\tfrac{1}{2}\rangle\ S_{1/2}
\end{array}
$$

$\to$ SUBTRACT E FROM DIAGONAL, & TAKE DET $\Rightarrow$ GIVES

$$0 = E^3 + E^2\left(\Delta - \tfrac{3}{2}\right) + E\left(\tfrac{\Delta\xi}{2} - \tfrac{\xi^2}{2} - \lambda^2\right) - \tfrac{\Delta}{2}\xi^2 - \tfrac{\lambda^2\xi}{2}$$

FOR $\xi = 0$ (NO SPIN-ORBIT) $\rightarrow \begin{cases} E = 0 \\ E = -\dfrac{\Delta}{2} \pm \dfrac{1}{2}\sqrt{\Delta^2 + 9\lambda^2} \\ \quad \simeq -\dfrac{\Delta}{2} \pm \lambda \ \text{(FOR BIG } \lambda\text{)} \end{cases}$



IF $\lambda \gg \Delta$, WE GET STARK EFFECT

IF $\lambda \ll \Delta$ WE GET QUADRATIC

$[M_y, M_z] = i\hbar M_x$
$[M_z, M_x] = i\hbar M_y$ $\qquad M_j^{+} = M_j$
$[M_x, M_y] = i\hbar M_z$

DEFINE

$M^2 = M_x^2 + M_y^2 + M_z^2$
$L^+ = M_x + i M_y$ → RAISING OPERATOR
$L = M_x - i M_y$ → LOWERING OPERATOR

1. $[M^2, M_z] = 0$

PROOF: $[M^2, M_z] = [M_x^2, M_z] + [M_y^2, M_z]$

$$= M_x [M_x, M_z] + [M_x, M_z] M_x + M_y [M_y, M_z] + [M_y, M_z] M_y$$

$$= -i\hbar \{M_x M_y + M_y M_x\} + i\hbar (M_y M_x + M_x M_y)$$
$$= 0$$

SIMILARLY: $[M^2, M_z] = [M^2, M_y] = [M^2, M_x] = 0$

∴ WE CAN FIND THE SIMULTANEOUS EIGENVALUES FOR M^2 & M_z:

$$|j, m\rangle$$

$$\begin{cases} M^2 |j, m\rangle = M_j^2 |j, m\rangle \\ M_z |j\, m\rangle = \hbar m |j\, m\rangle \end{cases}$$

2. $[M^2, L] = 0 = [M^2, L^+]$ PROOF IS TRIVIAL

3. $[L, L^+] = [M_x - iM_y, M_x + iM_y]$

$$= -i [M_y, M_x] + i [M_x, M_y]$$

$$= -i\hbar M_z - i\hbar M_z = -2\hbar M_z$$

4. $[M_z, L] = [M_z, M_x] - i [M_z, M_y]$
$= i\hbar M_y - i(-i\hbar M_x)$

$$= -\hbar L \qquad \text{ALSO } [M_z, L^+] = \hbar L^+$$

5. $M^2 = M_z^2 + \frac{1}{2}(L L^+ + L^+ L)$

4-3-75

SPIN ORBIT INTERACTIONS

$\xi(r)\ \ell\cdot s$

DIAGONALIZED WITH $|j, m_j\rangle$;

EX $\ell\cdot s\,|j,m\rangle = \begin{cases} \ell - \frac{1}{2} \\ -(\ell+1) \end{cases}$

$|j,m\rangle$ EIGENSTATES OF $\xi(r)\ \ell\cdot s$ HAMILTONIAN

FOR ADDED FIELD $eF\cdot r$

MIXES $2S$ & $2P_{\frac{1}{2}}$ MIXES STATES OF SAME m_R

WHAT ABOUT ALL OF EM' TOGETHER ?

ASSUME ALKALIA ATOM IN $\vec{E}$ FIELD

<u>ONLY</u> CONSIDER 2S & 2P STATES (ie Li)

OR 3S & 3P " (ie Na)

(APPROXIMATING FINITE # OF STATES)

TOTAL OF 8 STATES:

	jm_j	
1	$\|3/2, 3/2\rangle$	$P_{3/2}$
2	$\|3/2, 1/2\rangle$	
3	$\|3/2, -1/2\rangle$	
4	$\|3/2, -3/2\rangle$	
5	$\|\frac{1}{2}, \frac{1}{2}\rangle$	$P_{1/2}$
6	$\|\frac{1}{2}, -\frac{1}{2}\rangle$	
7	$\|\frac{1}{2}, 1/2\rangle$	$S_{1/2}$
8	$\|1/2, -1/2\rangle$	

GIVES FOR SPIN ORBIT INTERACTION

	$P_{3/2}$ STATES				$P_{\frac{1}{2}}$		$S_{1/2}$	
1	$\xi/2$	0	$M_{13}=0$	0	0	0	0	0
2	0	$\xi/2$	0	0	0	0	$\sqrt{\frac{2}{3}}\,\lambda$	0
3	0	0	$\xi/2$	0	0	0	0	$\sqrt{\frac{2}{3}}\,\lambda$
4	0	0	0	$\xi/2$				
5	0	0	0	0	$-\xi$	0	$-\sqrt{\frac{1}{3}}\,\lambda$	0
6	0	0	0	0	0	$-\xi$	0	$\sqrt{1/3}\,\lambda$
7	0	$\sqrt{\frac{2}{3}}\,\lambda$	0		$-\sqrt{1/3}\,\lambda$	0	$0-\Delta$	0
8	0	0	$\sqrt{\frac{2}{3}}\,\lambda$		0	$\sqrt{\frac{1}{3}}\,\lambda$	0	$0-\Delta$

$\updownarrow\Delta$ 3P / 3S

$M_{13} = \langle \frac{3}{2}\ \frac{3}{2} | eFz | 3/2\ \frac{-1}{2} \rangle$

ONLY EXISTING ELEMENTS TWIXT 2S, $2P_{\frac{1}{2}}$

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CONTINUE TO FIND EIGEN VALUES:

$$\langle j, m | [M^2, L^+] | j', m' \rangle = 0$$

$$M^2 | j m \rangle = M_j^2 | j m \rangle$$

$$\langle j, m | M^2 = M_j^2 \langle j, m |$$

$$\to (M_j^2 - M_{j'}^2) \langle j m | L^+ | j' m' \rangle = 0$$

IF $M_j \neq M_{j'}$ THEN $\langle j m | L^+ | j' m' \rangle = 0$

ASSUME $j \neq j' \Rightarrow M_j^2 \neq M_{j'}^2$

IF $j = j'$, $\langle j m | L^+ | j m' \rangle = L^+_{j m m'}$

CONSIDER

$$\langle j m | [M_z, L^+] | j m' \rangle = \hbar^2 \langle j m | L | j m' \rangle$$

$M_z | j, m \rangle = \hbar m | j, m \rangle$ $\quad \hbar(m - m') L^+_{j m m'} = \hbar L^+_{j m m'}$

$$\hbar (m - m' - 1) L^+_{j m m'} = 0$$

i.e. EITHER

$m = m' + 1$

OR $L^+_{j m m'} = 0$

i.e.

$L^+_{j m m'} = 0$ UNLESS $m = m' + 1$

i.e. $L^+_{j, m'+1, m'} \neq 0$ ALL OTHERS ARE

SIMILARLY: $L_{j, m-1, m} \neq 0$ ALL OTHERS ARE

$= L_{j, m', m'+1}$

$$\Rightarrow \langle j, m+1 | L^+ | j m \rangle \neq 0$$
$$\langle j m | L | j, m+1 \rangle \neq 0$$

LET $\hbar \lambda_{j m} = \langle j (m+1) | L^+ | j m \rangle$

$\hbar \lambda^*_{j m} = \langle j m | L | j, m+1 \rangle$

NOTE $\langle j m' | L | j m \rangle = (L^+_{j m m'})^*$

$$V = \xi\, \ell\cdot s = \xi\left[\ell_z s_z + \tfrac{1}{2}\underbrace{(\ell^+ s^- + \ell^- s^+)}_{\ell_x s_x + \ell_y s_y}\right]$$

$$\begin{array}{cccccc|c}
\phi_1^1\alpha & \phi_1^1\beta & \phi_1^0\alpha & \phi_1^0\beta & \phi_1^{-1}\alpha & \phi_1^{-1}\beta & \\
\xi/2 & 0 & 0 & 0 & 0 & 0 & \phi_1^1\alpha \\
0 & -\frac{1}{2}\xi & \xi/\sqrt{2} & 0 & 0 & 0 & \phi_1^1\beta \\
0 & \xi/\sqrt{2} & 0 & 0 & 0 & 0 & \phi_1^0\alpha \\
0 & 0 & 0 & 0 & \xi/\sqrt{2} & 0 & \phi_1^0\beta \\
0 & 0 & 0 & \xi/\sqrt{2} & -\xi/2 & 0 & \phi_1^{-1}\alpha \\
0 & 0 & 0 & 0 & 0 & \xi/2 & \phi_1^{-1}\beta
\end{array}$$

$$\ell\cdot s\,|\phi_1^1\alpha\rangle = 1\cdot\tfrac{1}{2}\,\phi_1^1\alpha$$

$$\ell\cdot s\,|\phi_1^1\beta\rangle = 1\left(-\tfrac{1}{2}\right)\phi_1^1\beta + \tfrac{1}{2}\sqrt{2}\,\phi_1^0\alpha$$

$$\ell\cdot s\,|\phi_1^0\alpha\rangle = \tfrac{1}{\sqrt{2}}\,\phi_1^1\beta$$

$$\det\left[\quad\right] \Rightarrow E = \frac{\xi}{2}\ (2)$$

$$\begin{vmatrix} -\frac{\xi}{2} - E & \xi/\sqrt{2} \\ \xi/\sqrt{2} & -E \end{vmatrix} = 0 \Rightarrow E = {}^{(1)}\frac{\xi}{2},\ {}^{(2)}-\xi$$

ALTOGETHER:

$$E = (4)\ \frac{\xi}{2},\ (2)\ -\xi$$

SAME AS CLEBSCH-GORDON COEFFICIENT

$[L, L^+] = 2\hbar M_z$

$\langle jm | LL^+ - L^+L | jm \rangle = -2\hbar \langle jm | \underbrace{M_z | jm}_{\hbar m | jm \rangle} \rangle$

$= -2\hbar^2 m$ FOR $\langle jm | jm \rangle = 1$

? $\rightarrow$ $\langle jm | LL^+ | jm \rangle$

$1 = \sum_{j'\ell'} | j' \ell' \rangle \langle j' m' |$

$\langle jm | LL^+ | jm \rangle = \sum_{j'm'} \langle jm | L | j'm' \rangle \langle j'm' | L^+ | jm \rangle$

WE HAVE SHOWN THIS VANISHES UNLESS

$j = j'$ AND $m' = m+1$

$\Rightarrow \langle jm | LL^+ | jm \rangle = \hbar^2 \lambda^*_{jm} \lambda_{jm}$

? $\rightarrow$ $\langle jm | L^+L | jm \rangle = \sum_{j'm'} \langle jm | L^+ | j'm' \rangle \langle j'm' | L | jm \rangle$

$j' = j \quad m' = m-1$

$\langle jm | L^+L | jm \rangle = \hbar^2 | \lambda_{j,m-1} |^2$

THEN

$\underline{|\lambda_{jm}|^2 - |\lambda_{j,m-1}|^2 = -2m}$

LET $\lambda^2_{jm} = a_0 + a_1 m + a_2 m^2 + a_3 m^3 + \ldots$

$\lambda^2_{j,m-1} = a + a_1(m-1) + a_2(m-1)^2 + a_3(m-1)^3 + \ldots$

$-2m = \lambda^2_{jm} - \lambda^2_{j,m-1} = -a_1 - a_2(1-2m) + a_3(1-3m+3m^2) + \ldots$

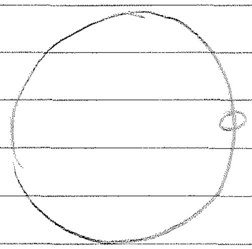
$a_n = 0 \quad \forall \; n \geq 3$

$\lambda^2_{jm} - \lambda^2_{j,m-1} = -a_1 - a_2(1-2m) \Rightarrow$

$\Rightarrow a_2 = +1, \quad a_1 = -1$

$\Rightarrow |\lambda_{jm}|^2 = a - (m + m^2) \geq 0$

$= a - m(m+1) \geq 0$



l, s $\quad \underset{\sim}{j} = \underset{\sim}{l} + \underset{\sim}{s}$

$$j \cdot j = l \cdot l + s \cdot s + 2\, l \cdot s$$

$$j(j+1) = l(l+1) + s(s+1) + 2\langle l \cdot s \rangle$$

$$\langle l \cdot s \rangle = \frac{1}{2}\left[\, j(j+1) - l(l+1) - s(s+1)\right]$$

THEN $\quad \langle \xi(r)\, l \cdot s \rangle = \langle \xi(r) \rangle_r \langle l \cdot s \rangle$

EXAMPLE: $\quad s = \frac{1}{2}$, $\quad j = l + \frac{1}{2}$ OR $j = l - \frac{1}{2}$

$$\langle l \cdot s \rangle = \frac{1}{2} l \qquad ; \; j = l + \frac{1}{2}$$

$$\langle l \cdot s \rangle = -\frac{(l+1)}{2} \qquad ; \; j = l - \frac{1}{2}$$

FOR $l = 1$; $\quad j = 3/2$; $\frac{1}{2}\langle \xi \rangle$; $\quad j = 1/2$; $-\langle \xi \rangle$

$l = 1 \Rightarrow 6$ of EM: $\quad m_l = 1, 0, -1 \quad s = \frac{1}{2}, -\frac{1}{2}$ $\Big\}$ 4 $j = 3/2$; $P_{3/2}$; 2 $j = 1/2$ $\quad P_{1/2}$

$l = 2 \Rightarrow 10$ of EM: $\quad m_l = -2, -1, 0, 1, 2 \quad s = \frac{1}{2}, -\frac{1}{2}$ $\Big\}$ 6 $j = 5/2$ $\quad D_{5/2}$; 4 $\quad j = 3/2$ $\quad D_{3/2}$

———— $3D_{5/2}$

———— $3D_{3/2}$

———— $3P_{3/2}$

———— $3P_{1/2}$

———— $3S$

———— $2P_{3/2}$

———— $2P_{1/2}$

———— $2S$

———— $1S$

$$\phi_{3/2}^{3/2} = \alpha\, \phi_1^1$$

$$\phi_{3/2}^{1/2} = \sqrt{\tfrac{2}{3}}\,\alpha\, \phi_1^0 + \sqrt{\tfrac{1}{3}}\,\beta\, \phi_1^1$$

CONSIDER GOING UP

$$L^+|jm\rangle = \hbar\lambda_{jm}|j,m+1\rangle$$

$$L^+L^+|jm\rangle = (L^+)^2|jm\rangle$$
$$= \hbar^2\lambda_{j,m+1}|j,m+2\rangle$$

$\vdots$

$$(L^+)^\ell|jm\rangle = \hbar^\ell\lambda_{j,m}\cdots\lambda_{j,m+\ell-1}|j,m+\ell\rangle$$

NOW $|\lambda_{jm}|^2 = a_0 - m - m^2 \geq 0$

WHAT IF $a_0 = m_1(1+m_1)$

$\lambda_{j,m} = m_1(1+m_1) - m(1+m)$ IF $m = m_1$

AND $L^+|j,m_1\rangle = \hbar\lambda_{jm}|j,m+1\rangle = 0$

CONSIDER GOING DOWN

$$L|jm\rangle = \hbar\lambda^*_{j,m-1}|j,m-1\rangle$$

TRUNCATES FOR $-(1+m) = m$

m_1 RESTRICTIONS DICTATE THAT

$$\ell = m_1 = \begin{cases} \text{INTEGER} \\ \text{HALF INTEGER} \end{cases}$$

THUS $m = \begin{cases} \text{INT.} \\ \frac{1}{2}\text{ INT.} \end{cases}$

$a_0 = m_1(m_1+1)$; $m_1 = j = \ell$ ANG. MOM.

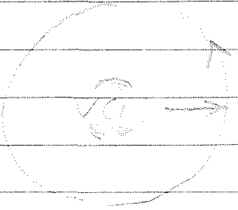
j: TOTAL MOMENTUM

$$L^-|jm_j\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\,|j,m-1\rangle$$

$$L^+|jm_j\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\,|j,m+1\rangle$$

$$-j \leq m \leq j$$

SPIN-ORBIT INTERACTION (RELATIVISTIC)



$\vec{\mu} = g_s \mu_0$

$\mu_0 = \frac{e\hbar}{2mc} = 0.927 \cdot 10^{-20} \frac{\text{ERG}}{\text{GAUSS}}$

$g_s = 2.00$

$\mathcal{H}_{INT} = -\mu \cdot H_{eff}$, H_{eff} : MAGNETIC FIELD
$\mathcal{H}_{INT}$: HAMILTONIAN

$H_{eff} = \frac{v}{c} \times E = \frac{p \times E}{mc}$

$\mathcal{H}_{INT} = -\frac{g_s \mu_0}{mc} \vec{s} \cdot (p \times E)$

$E = \frac{r}{r} \frac{dV}{dr}$

$\mathcal{H}_{INT} = \frac{g_s \hbar}{2m^2c^2} s \cdot (p \times r) \frac{1}{r} \frac{dV}{dr}$

$= \frac{g_s \hbar}{2m^2c^2} s \cdot l \frac{dV}{dr}$; l = ang mom

$= \xi(r)\, s \cdot l$

$\xi(r) = \frac{\hbar^2}{2m^2c^2} \frac{1}{r} \frac{\delta V}{\delta r}$

THIS IS RIGHT ANS. DIFFERS BY FACTOR OF TWO

($\xi(r) > 0$ FOR MOST ATOMS)

FOR SYSTEM OF ELECTRONS

$\sum_i \xi(r_i)\, s_i\, l_i$

$\langle jm | M^2 = M_z^2 + \frac{1}{2}(LL^+ + L^+L) | jm \rangle$

$$M_z^2 = \hbar^2 m^2 + \frac{1}{2}(\lambda_{j,m}^2 + \lambda_{j,m-1}^2)$$

$$= \hbar^2 [m^2 + \frac{1}{2}(j(j+1) - m(m+1) + j(j+1) - (m-1)m)]$$

$$= \hbar^2 j(j+1)$$

$$M^2 |jm\rangle = \hbar^2 j(j+1) |j,m\rangle$$

$j_1 \qquad -j_1 \le m_1 \le j_1$

$j_2 \qquad j_2 \le m_2 \le j_3$

ONE PAR.

$j \; m$

$j = \frac{1}{2} \qquad |\frac{1}{2}, \frac{1}{2}\rangle = \alpha$

$|\frac{1}{2} -\frac{1}{2}\rangle = \beta$

TWO PAR

$(\alpha_1 \beta_1) \quad (\alpha_2, \beta_2)$

$\alpha_1 \alpha_2 \} \; m = 1 \qquad \alpha_2 = \alpha_1 = |\frac{1}{2}, \frac{1}{2}\rangle$

$\beta_1 \beta_2 \} \; m = -1 \qquad \beta_2 = \beta_1 = |\frac{1}{2}, -\frac{1}{2}\rangle$

$\left.\begin{matrix}\alpha_1 \beta_2 \\ \beta_1 \alpha_2\end{matrix}\right\} m = 0$

m's ADD

$J = 1, \quad M = 1, 0, -1$

$J = 0 \quad M = 0$

$j_1 \quad j_2 \qquad J$

$\frac{1}{2} \circledast \frac{1}{2} \qquad 0 \text{ OR } 1 \longrightarrow m = 1, 0, -1$

$\longrightarrow m = 0$

$J = 1 \qquad J \; m$

$|1, 1\rangle \leftarrow$ COMBINED ANG. MOM. STATES

$|1, 0\rangle$

$|1, -1\rangle$

$J = 0 \qquad |0, 0\rangle$

$|1, 1\rangle = \alpha_1 \alpha_2$

$|1, 0\rangle = \frac{1}{\sqrt{2}}(\alpha_1 \beta_2 + \beta_1 \alpha_2)$

$|0, 0\rangle = \frac{1}{\sqrt{2}}(\alpha_1 \beta_2 - \beta_1 \alpha_2)$

$|1, -1\rangle = \beta_1 \beta_2$

$$\psi(r) = \frac{e^{ik\cdot r}}{\sqrt{\Omega}} + \sum_{k'\neq k} \frac{e^{ik'\cdot r}}{\sqrt{\Omega}} \frac{V(k-k')}{\Omega} \Big/ \left(\frac{\hbar^2}{2m}(k^2-k'^2)\right)$$

$$\psi_k^{(0)} + \sum \frac{\psi_{k'}^{(0)} V_{k'k}}{E_k^{(0)} - E_{k'}^{(0)}}$$

IN LIMIT:

$$\psi(r) = \frac{1}{\sqrt{\Omega}}\left[e^{ik\cdot r} + \frac{2m}{\hbar^2}\int \frac{d^3k'}{(2\pi)^3} \frac{e^{ik'\cdot r}\, V(k-k')}{k^2-k'^2}\right]$$

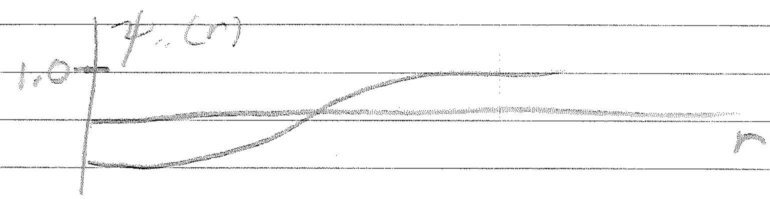
<u>EXAMPLE:</u> $V(r) = \lambda e^{-k_s r}/r$

$$\Rightarrow V(q) = \frac{4\pi\lambda}{q^2+k_s^2}$$

FOR $k=0$

$$\psi_0(r) = \frac{1}{\sqrt{\Omega}}\left[1 + \frac{4\pi\lambda}{(2\pi)^3}\int \frac{d^3k'\, e^{ik'\cdot r}\, 2m}{(k'^2+k_s^2)(-k'^2)\hbar^2}\right]$$

$$= \frac{1}{\sqrt{\Omega}}\left[1 - \frac{4\lambda m}{\hbar^2 k_s^2 r}\left(1 - e^{-k_s r}\right)\right]$$



2-29-75

$M^2|jm\rangle = \hbar^2 j(j+1)|j,m\rangle$

$M_z|jm\rangle = \hbar m|j,m\rangle$

$-j \le m \le j \Rightarrow j$ & m ARE INTEGERS OR HALF INTEGERS

$L|jm\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\;|j,m-1\rangle$; $L^+|jj\rangle = 0$

$L^+|jm\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\;|j,m+1\rangle$; $L|j\,{-j}\rangle = 0$

FOR $j = \ell$ INT $\Rightarrow$ SPHERICICAL HARMONIC

$M_z = \frac{\hbar}{i}\frac{d}{d\phi}$

$Y_{\ell m} = N_{\ell m} P_\ell^m(\theta) e^{im\phi}$

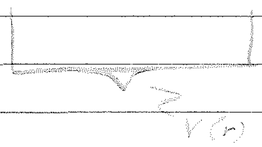
$\Rightarrow \underline{M_z Y_\ell^m = m\hbar Y_\ell^m}$

$M^2 = \nabla^2 - \ell(\ell+1)$

<u>CLEASH-GORDON COEFFICIENTS</u>

CONTINUUM STATES

USE BOX NORMALIZATION



$$\frac{e^{ik\cdot r}}{\sqrt{\Omega}} = \psi_k^{(0)}(r)$$

Ω = BOX'S VOLUME

BOX NORMALIZATION

$H_0 = \frac{p^2}{2m}$

$$\langle k|V|k'\rangle = \int d^3r \, \frac{e^{-ik\cdot r}}{\sqrt{\Omega}} V(r) \frac{e^{ik'\cdot r}}{\sqrt{\Omega}}$$

$$= \frac{1}{\Omega} V(k-k')$$

FOURIER TRANSFORM

$$V(q) = \int d^3r \, e^{iq\cdot r} V(r)$$

ENERGY: $$E(k) = \underbrace{\frac{\hbar^2 k^2}{2m}}_{E_k^{(0)}} + \underbrace{\frac{V(0)}{\Omega}}_{V_k} + \sum_{k' \neq k} \frac{V_{kk'}^2}{E_k^{(0)} - E_{k'}^{(0)}}$$

$$V_{kk'}^2 = \frac{1}{\Omega^2} V(k-k')^2$$

NOW $$\sum_{k'} \rightarrow \frac{\Omega}{(2\pi)^3} \int d^3k'$$

$$E(k) = \frac{\hbar^2 k^2}{2m} + \frac{1}{\Omega}\left[V(0) + \int \frac{d^3k'}{(2\pi)^3} \frac{V(k-k')^2}{k^2 - k'^2} \frac{2m}{\hbar^2}\right]$$

AS $\Omega \to \infty$ $\quad E(k) = \frac{\hbar^2 k^2}{2m}$

ENERGY DOESN'T CHANGE WITH POTENTIAL!!

$\int_0^{2\pi} d\phi = 2\pi$

$\int_0^{\pi} \sin\theta \cos^2\theta \, d\theta = -\frac{1}{3}\cos^3\theta\Big|_0^{\pi} = 2/3$

$\frac{1}{4}\int_0^{\infty} r^2 dr \, r^2 e^{-r/a}(1 - r/2a)$

$\rho = (r/a)$

$\rightarrow a \int_0^{\infty} \rho^4 d\rho \left(1 - \frac{1}{2}\rho\right) e^{-\rho}$

$= a\left[4! - \frac{1}{2}5!\right] = a(24 - 60)$

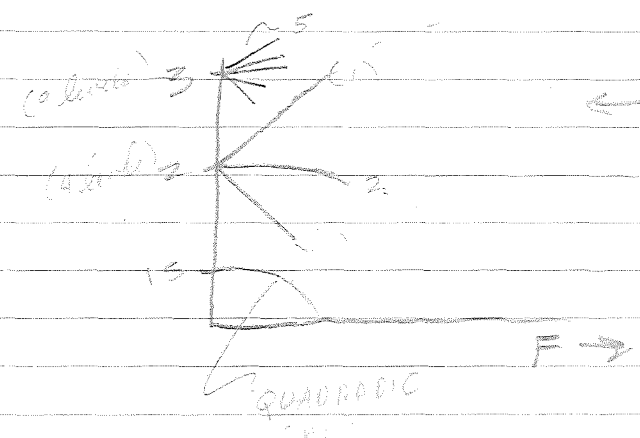
$= -36a$

PUTTING IT ALL TOGETHER:

$\lambda = (eFa)(-36)\,\frac{2}{3}\cdot 2\pi \times \frac{1}{16\pi}$

$= -3aeF$ (UNITS OF ENERGY)

$\Rightarrow E = E_2,\ E_2 \pm 3aeF$



← FIRST ORDER

$\psi_\pm = \psi_2 \pm$ [illegible]

3-7-75

COMPUTOR: RM 064 BASEMENT OF NEW WING

CHARLEY ELLIS RUNS IT

REVIEW

2 ELECTRON WVE FNCTIONS

$$\psi(x_1, x_2) = -\psi(x_2, x_1) \leftarrow \text{ANTISYMMETRIC WAVE FUNCTION}$$

SPIN SINGLET

$$\text{HELIUM } (1s)^2: \quad \psi(x_1, x_2) = \underbrace{\phi_{1s}(r_1)\,\phi_{1s}(r_2)}_{\text{ORBITAL}}\ \underbrace{\frac{1}{\sqrt{2}}(\alpha_1\beta_2 - \alpha_2\beta_1)}_{\text{SPIN}}$$

$\Longrightarrow$ SINGLET $(S=0)$

$\Longrightarrow$ TRIPLET $(S=1)$ $\left\{ \begin{array}{l} \alpha_1\alpha_2 \\ \frac{1}{\sqrt{2}}(\alpha_1\beta_2 + \alpha_2\beta_1) \\ \beta_1\beta_2 \end{array} \right.$

(SIGN ON TRIPLIT DON'T CHANGE UPON INTERCHANGING

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\phi_1(r_1)\,\phi_2(r_2) - \phi_2(r_1)\,\phi_1(r_2)\right] \chi^{M_S}_{S=1}$$

ϕ_j = ORBITAL WAVE FUNCTION OF STATE j

NOTE: HERE, ORBITAL PART CHANGES SIGN AND $\phi_1 \neq \phi_2$

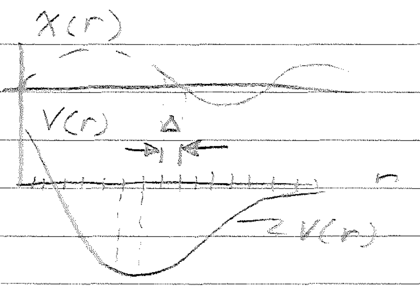
NUMERICAL SOLUTION TO SCHRÖEDINGER'S EQ'N

GIVEN $V(r)$

$$\Rightarrow \psi(r,\theta,\phi) = R(r)\,Y_l^m(\theta,\phi) \quad ; \quad \chi = rR$$

$$\frac{d^2}{dr^2}\chi = A(r)\,\chi(r) \longleftarrow \text{SCHRO'S EQN}$$

$$A(r) = \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}\left[V(r) - E\right]$$



COMPUTOR GIVES $A(r_i) = A_i$

WANT TO SOLVE: $\chi(r_i) = \chi_i$

3-20-75 CANCEL 1 AT '5 CLASS (TUESDAY)

EXAMPLE (CLASSICAL)

STARK EFFECT IN HYDROGEN

$\underline{n=2}$: 4 STATES: $2s$, $2p_z$, $2p_{\pm1}$

$\ell=0$ $\ell=1$ $\ell=1$

$m=0$ $m=0$ $m=\pm1$

APPLY E FIELD IN z DIRECTION

$\Rightarrow V = eFz$

ONLY EXISTING MATRIX ELEMENT IS:

$\langle 2s|V|2p_z\rangle \neq 0$

SINCE $\langle 2s|V|2p_{+}\rangle = \langle 2s|V|2p_{-}\rangle$

$= \langle 2p_z|V|2p_{\pm1}\rangle = \langle 2p_{\pm1}|V|2p_z\rangle = 0$

SINCE $p_{\pm1} \sim e^{\pm i\phi}$, $\int_0^{2\pi} e^{\pm i\phi} = 0$

LOOK AT

$\lambda = \langle 2s|V|2p_z\rangle$

$E_2 = -E_{mc}/2^2$

$$
\begin{array}{cccc}
2s & 2p_z & 2p_{+1} & 2p_{-1} \\
\end{array}
$$

$$
\begin{bmatrix}
E_2 - E & \lambda & 0 & 0 \\
\lambda & E_2 - E & 0 & 0 \\
0 & 0 & E_2 - E & 0 \\
0 & 0 & 0 & E_2 - E
\end{bmatrix}
$$

$\det[\;\;] \Rightarrow E = E_2, E_2, E_2+\lambda, E_2-\lambda$

NOW $\psi_{2s} = \frac{1}{\sqrt{8\pi a^3}} e^{-r/2a}\left(1 - r/2a\right)$

$\psi_{2p_z} = \frac{1}{\sqrt{32\pi a^5}} z\, e^{-r/2a}$

$$\lambda = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} r^2 dr\, \frac{eFr\cos\theta\, e^{-r/a}}{16\pi a^4}$$

$$\times \left(1 - \frac{r}{2a}\right) r\cos\theta$$

42

TAYLOR'S EXPANSION:

$$\chi(r_i+\Delta) = \chi(r) + \Delta \frac{d\chi}{dr} + \frac{1}{2}\Delta^2 \frac{d^2\chi}{dr^2} + \frac{1}{6}\Delta^3 \frac{d^3\chi}{dr^3} + \ldots$$

$$\chi(r_i-\Delta) = \ '' \ - \ '' \ + \ '' \ - \ ''$$

$$\chi(r_i+\Delta) + \chi(r_i-\Delta) = 2\chi_i + \Delta^2 A_i \chi_i + \frac{1}{12}\Delta^4 \frac{d^2}{dr^2}\left(A(r)\chi(r)\right)$$

$$= \chi_{i+1} + \chi_{i-1}$$

WITHOUT $\frac{1}{12}\nabla^4$ TERM $\Rightarrow \chi_{i+1} = \chi_i\left(2+\nabla^2 A_i\right) - \chi_{i-1}$

WITH $\frac{1}{12}\nabla^4$ TERM:

DEFINE: $Y_i = \chi_i - \frac{\Delta^2}{12}\left(\frac{d^2\chi}{dr^2}\right)_{r_i}$

$$= \chi_i - \frac{\Delta^2}{12} A_i \chi_i$$

$$\Rightarrow \chi_i = Y_i \Big/ \left(1 - \frac{\Delta^2 A_i}{12}\right)$$

EMPLOY OPERATOR: $1 - \frac{\Delta^2}{12}\frac{d^2}{dr^2}$ (TURNS χ TO Y)

$$\left(1 - \frac{\Delta^2}{12}\frac{d^2}{dr^2}\right)\chi_i = Y_i$$

$$\left(1 - \frac{\Delta^2}{12}\frac{d^2}{dr^2}\right)\left(\chi_{i+1} + \chi_{i-1}\right) = Y_{i+1} + Y_{i-1}$$

$$= 2Y_i + \Delta^2\left[A_i\chi_i - \frac{\Delta^2}{12}\frac{d^2}{dr^2}(A\chi)\right]$$

$$+ \frac{1}{12}\Delta^4\left[\frac{d^2}{dr^2}(A\chi) - \cancel{\frac{\Delta^2}{12}\frac{d^4}{dr^4}(A\chi)}\right]$$

CANCELS

TOSS OUT

$$\Rightarrow Y_{i+1} + Y_{i-1} = 2Y_i + \Delta^2 A_i \chi_i$$

$$Y_{i+1} = Y_i\left[2 + \frac{A_i\Delta^2}{1 - \frac{A_i\Delta^2}{12}}\right] - Y_{i-1} \Leftarrow$$ GOOD TO ORDER Δ^6

WE KNOW $Y_0 = 0 = \chi_0$ (SINCE $\chi(0) = 0$)

$\Rightarrow$ CHOOSE Y_1 AT RANDOM.
χ WILL BE GENERATED TO A NORMALIZATION FACTOR.

DEGENERATE LEVELS

(PREVIOUSLY ASSUMED NO DEGENERACY)

RECALL

$$a_n\left(E_n^{(0)} - E_n\right) + \sum_m V_{nm}\, a_m = 0$$

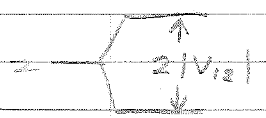
$$\begin{pmatrix} E_1^{(0)} - E_1 + V_{11} & V_{12} & V_{13} & \cdots \\ V_{21} & E_2^{(0)} - E_2 + V_{22} & \cdots & \\ \vdots & & & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = 0$$

$$= \det\left[\left(E_n^{(0)} - E\right)\delta_{nm} + V_{nm}\right] = 0$$

CONSIDER:

$$\det\begin{bmatrix} E_1^{(0)} - E + V_{11} & V_{12} \\ V_{12} & E_1^{(0)} - E_1 + V_{11} \end{bmatrix} = 0$$

$$\Rightarrow E = E_1^{(0)} + V_{11} \pm |V_{12}|$$



$$\psi = a_1\psi_1 + a_2\psi_2$$

$$\psi_\pm = \frac{1}{\sqrt{2}}\left(\psi_1 \pm \psi_2\right)$$

USE

$$\psi_1^{(0)} = \left(\psi_1 + \psi_2\right)\frac{1}{\sqrt{2}}$$

$$\psi_2^{(0)} = \left(\psi_1 - \psi_2\right)\frac{1}{\sqrt{2}}$$

$$\Rightarrow \begin{bmatrix} E_1^{(0)} - E + V_{11} + |V_{12}| & 0 \\ 0 & E_1 - E + V_{11} - |V_{12}| \end{bmatrix}$$

FOR LARGE r: $\chi = D\sqrt{\tfrac{2}{\pi}}\sin(kx+\delta)$

D IS THE SCALING FACTOR SINCE

REALLY: $\chi = \sqrt{\tfrac{2}{\pi}}\sin(kx+\delta)$

ALGORITHM (NOUMEROV METHOD)

```
      R=0
      DR=0.1
      Y0=0
      Y1=0.001
      DO 50 I=1,50
      R=R+DR
      A=F(R)
      B=DR*DR*A
      Y2=Y1*(2.+B/(1.-B/12.))-Y0
      Y0=Y1
      Y1=Y2
50    X(I)=Y0/(1-B/12.)
```

FUNCTION F(X)

$F = C*\left(\frac{1}{X^{2}} - \frac{1}{X^{6}}\right)$

$\frac{2m}{\hbar^2} V$

FOR LARGE r, $\chi_i = D\sin(kr_i+\delta)$

$\chi_m = D\sin(kr_m+\delta)$

$$\frac{\chi_i}{\chi_m} = \frac{\sin kr_i\cos\delta + \cos kr_i\sin\delta}{\sin kr_m\cos\delta + \cos kr_m\sin\delta}$$

$$= \frac{\sin kr_i + \cos kr_i\tan\delta}{\sin kr_m + \cos kr_m\tan\delta}$$

$$\Rightarrow \tan\delta = -\frac{\chi_m\sin kr_i - \chi_i\sin kr_m}{\chi_m\cos kr_i - \chi_i\cos kr_m}$$

AND

FOR $V \ll E$

$$D = \chi_i \Big/ \sin(kr_i+\delta) \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

RUNGE KUTTA OFFERS ALTERNATE METHODS

THEN:

$$C_6 = \tfrac{1}{2} e^2 \alpha_B \sum_{\mu\nu}^{n} \langle n | r_\mu | g \rangle \left[\delta_{\mu\nu} + \frac{3R_\nu R_\mu}{R^2} \right] \langle g | r_\nu | n \rangle$$

$$= \tfrac{1}{2} e^2 \alpha_B \langle g | r^2 + \frac{3(r \cdot R)^2}{R^2} | g \rangle$$

$$= \tfrac{1}{2} e^2 \alpha_B \langle g | r^2 | g \rangle \underbrace{\langle g | 1 + 3\cos^2\theta | g \rangle}_{=2}$$

$$= e^2 \alpha_B \langle r^2 \rangle$$

$$= \frac{e^2}{2} \alpha_B a_B^2 (n^*)^2 [5n^{*2} + 1]$$

FOR Li:

$$C_6 = 0.23 \times 10^{-58} \text{ erg-cm} \quad \text{(Theory)}$$
$$= 0.61 \times 10^{-58} \text{ ''} \quad \text{(Experiment)}$$

$$\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(r_1 - r_2) = \frac{P^2}{2M} + \frac{p^2}{2\mu} + V(r_1 - r_2)$$

$$-\frac{\hbar^2 \nabla_1^2}{2m} - \frac{\hbar^2 \nabla^2}{2m} + V(r_1 - r_2) = \frac{\hbar^2 \nabla_R^2}{2M_T} - \frac{\hbar^2 \nabla_r^2}{2\mu} + V(r)$$

$r = (r_1 - r_2)$

$R = \frac{1}{2}(r_1 + r_2)$

PROBLEM 4: $\left[-\frac{\hbar^2 \nabla_r^2}{2\mu} + V(r)\right]\phi(r)$; $\mu = \frac{1}{2} m$

m = HELIUM MASS

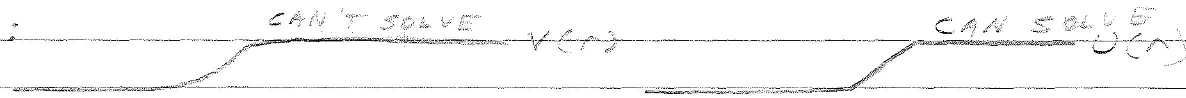
PERTURBATION THEORY

$$H = -\frac{\hbar^2 \nabla^2}{2m} + V(r)$$

LET'S ASSUME THAT A SIMILAR PROBLEM

$H_0 = -\frac{\hbar^2 \nabla^2}{2m} + U(r)$ CAN BE SOLVED EXACTLY.

EXAMPLE:



THEN

$$H_0 = H_0 + V - U$$

$$= H + V' \quad ; \quad V' = V - U \Rightarrow \text{PERTURBATION}$$

H_0 HAS EIGENFUNCTIONS $\psi_n^{(0)}(r)$

AND EIGENVALUES $E_n^{(0)}$

WISH TO SOLVE $H\psi = E\psi$

LET

$$\psi(r) = \sum_n a_n \psi_n^{(0)}(r)$$

$$H = H_0 + V' \quad ; \quad H\psi = E\psi$$

$$\therefore \sum_n a_n (H_0 + V')\psi_n^{(0)} = E \sum_n a_n \psi_n^{(0)}$$

NOW $H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$

$$\sum_n a_n \left[E_n^{(0)} - E + V'(r)\right] \psi_n^{(0)}(r) = 0$$

$$\int \psi_m^{(0)*} \sum_n a_n \left[E_n^{(0)} - E + V'(r)\right] \psi_n^{(0)}(r) = 0$$

$$= a_m \left[E_m^{(0)} + E\right] + \sum_n a_n \underbrace{\int d^3r\, \psi_m^{(0)} V \psi_n^{(0)}}_{\text{MATRIX ELEMENT}} = 0$$

LECTURE

VAN-DER-VAL'S INTERACTION

$$C_6 = e^4 \sum_{n,m} \frac{(r_{nA} \cdot \phi \cdot r_{mB})(r_{mB} \cdot \phi \cdot r_{nA})}{\epsilon_{nA} + \epsilon_{mB}}$$

A $\equiv n$ B $\equiv m$

$$r_{na} = \int d^3r\, \phi_n^*(r)\, r\, \phi_g(r) \quad g \to \text{ground}$$

FOR DISSIMILAR ATOMS

CONTINUUM 5V

He 25eV BOUND 20eV 5.4eV 3eV

$$\frac{1}{\epsilon_{nA} + \epsilon_{Bm}} = \frac{1}{\epsilon_{Bm}\left(1 + \frac{\epsilon_{nA}}{\epsilon_{mB}}\right)} \simeq \frac{1}{\epsilon_{Bm}}$$

GIVES

$$C_6 = e^6 \sum_{nm} \frac{(r_{nA} \cdot \phi \cdot r_{mB})(r_{mB} \cdot \phi \cdot r_{nA})}{\epsilon_{Bm}}$$

POLARLIZABILITY

$$\alpha_{\mu\nu} = 2e^2 \sum_n \frac{\langle g | r_\mu | m \rangle \langle m | r_\nu | g \rangle}{E_m}$$

FOR He: $\alpha_{\upsilon\nu} = \delta_{\upsilon\nu}\alpha$ ← FOR ISOTROPIC

$\Rightarrow$

$$C_6 = \frac{1}{2} e^2 \alpha_B \sum_n r_{nA} \cdot \phi(R) \cdot \phi(R) \cdot r_{nA}$$

$$\phi_{\mu\nu} = \delta_{\mu\nu} - 3R_\mu R_\nu / R^2$$

$$\phi \cdot \phi = \delta_{\mu\nu} + 3R_\mu R_\nu / R^2$$

MATRIX ELEMENT:

$$\langle m|V'|n\rangle = V'_{mn} = \int d^3r\, \psi_m^{(0)}\, V'\, \psi_n^{(0)}$$

THUS:

$$a_m\left[E_m^{(0)} - E\right] + \sum_n a_n V'_{mn} = 0 \quad \Leftarrow \text{EXACT}$$

THIS IS IN FORM OF A DETERMINANT:

SAME

$$\begin{pmatrix} E_1^{(0)} - E + V_{11} & V_{12} & V_{13} \cdots \\ V_{21} & E_2^{(0)} - E + V_{22} & V_{23} \cdots \\ \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = 0$$

OR

$$\det\left|\left(E_i^{(0)} - E\right)\delta_{ij} + V'_{ij}\right| = 0$$

THE MATRIX IS AN INFINATE DIMENSIONAL MATRIX

DIVERSION: USE OF COMPUTOR

SIGMA 5 (FORTRAN) COMPUTOR

OPEN: 2:30 TO 5:30

a. `N FORMAT ('MESSAGE')`

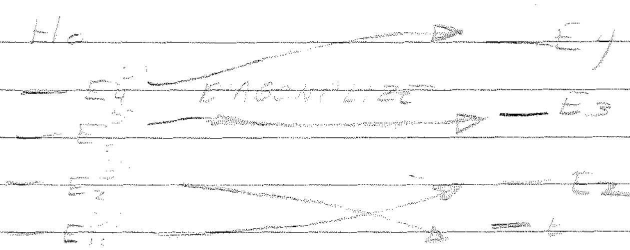
or `N FORMAT ($MESSAGE$)`

b. MULTIPLE EXPRESSIONS:

`X = 1 ; Y = 2`

c. `PRINT 10, X, Y, Z`

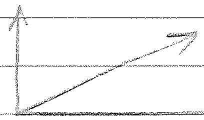
ONE METHOD OF SOLUTION IS A FINITE APPROXIMATION:

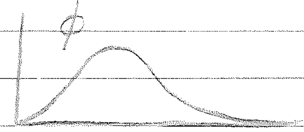


3-18-75

EXAM SOLUTION

(1)





(2)

$$L = \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}$$

$L|3/2\rangle = \sqrt{3}\,|\tfrac{1}{2}\rangle$

$L|1/2\rangle = 2\,|-\tfrac{1}{2}\rangle$

$L|1/2\rangle = \sqrt{3}\,|-3/2\rangle$

$$L^+ = \hbar \begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$L_x = \frac{1}{2}(L^+ + L)$

$L_z|m\rangle = \hbar m|L$

$$= \hbar \begin{bmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{bmatrix}$$

$L^2 = \frac{15}{4} I \hbar^2$

(3) NO. PSEUDOPOTENTIAL IS REPULSIVE.

3-11-75

$H = H_0 + V$

V = PERTURBATION

$H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$

WE WANT: $H\psi = E\psi$

$\psi(r) = \sum_n a_n \psi_n^{(0)}(r)$

THIS GIVES:

$a_n(E_n^{(0)} - E) + \sum_m a_m V_{nm} = 0$

$V_{nm} = \langle n|V|m\rangle = \int d^3r\, \psi_n^{(0)*} V \psi_m^{(0)}$

WE WILL NOW SOLVE, VIA PERTURBATION:

$a_n(E_n^{(0)} - E) + \sum_m a_m V_{nm} = 0$

ASSUME V IS OF ORDER λ $\ni \lambda$ IS A SMALL —

AND: $a_n = a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)} + \ldots$

$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \ldots$

$\Rightarrow (a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)} + \ldots)(E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \ldots - E_n^{(0)})$
$+ \lambda \sum_m V_{nm}(a_m^{(0)} + \lambda a_m^{(1)} + \ldots) = 0$

$\lambda^0: \; a_n^{(0)}(E^{(0)} - E_n^{(0)}) = 0$

$\lambda^1: \; a_n^{(0)} E^{(1)} + a_n^{(1)}(E^{(0)} - E_n^{(0)}) + \sum_m V_{nm} a_m^{(0)} = 0$

$\lambda^2: \; a_n^{(0)} E^{(2)} + a_n^{(1)} E^{(1)} + a_n^{(2)}(E^{(0)} - E_n^{(0)}) + \sum_m V_{nm} a_m^{(1)} = 0$

$\vdots$

WE WILL SOLVE THESE EQN'S

$\lambda^0: \; a_n^{(0)} = 0 \quad \ni \quad n \neq L$

$E^{(0)} = E_n^{(0)}$ IF $n = L$ } ENERGY ...

RECALL: $\int |\psi|^2 = 1 \Rightarrow \sum_n |a_n|^2 = 1$

$\therefore \sum_n |a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)} + \ldots|^2 = 1$

$\lambda^0: \sum_n |a_n^{(0)}|^2 = 1$

$\lambda^1: \sum_n a_n^{(0)} a_n^{(1)} = 0$

$\therefore \; \lambda^0: \; a_n^{(0)} = 0 \quad n \neq L$

$E^{(0)} = E_n^{(0)} \quad n = L$ } ZEROTH ORDER PERTURBATION THEORY

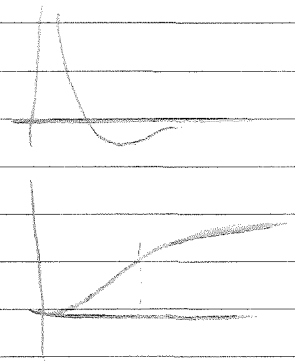
$\sum |a_n^{(0)}| = 1 \Rightarrow n = 1$

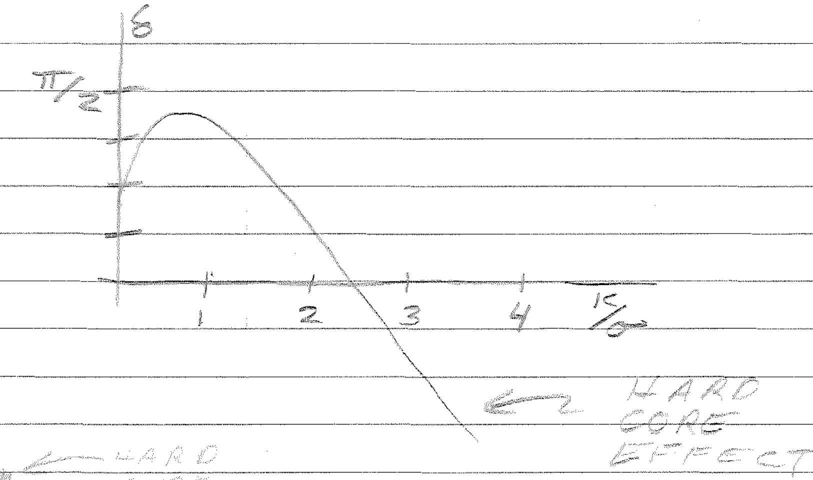
$\psi = \psi_L^{(0)}$

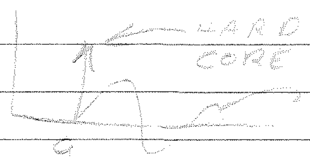
$E_L = E_L^{(0)}$

$a_n^{(0)} = \delta_{nL}$

4.

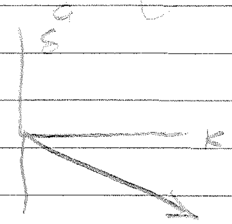






$\sin(k(r-a)) \Rightarrow \underline{\delta = -ka}$

LINEAR



FIRST ORDER

FOR $n = L$

FROM 0^{th} ORDER: $E_n^{(0)} = E^{(0)}$

$$\Rightarrow a_n^{(0)} E^{(1)} - \sum_n V_{nm} a_m^{(0)} = 0$$

FROM 0^{th} ORDER $a_n^{(0)} = \delta_{nL} \Rightarrow E = E_L^{(0)} + V_{LL}$

FROM 1^{ST} ORDER: $\sum_n a_n^{(0)} a_n^{(1)} = 0 \Rightarrow a_L^{(1)} = 0$

FOR $n \neq L$

$$a_n^{(1)} (E_L^{(0)} - E_n^{(0)}) = V_{nL} \Rightarrow a_n^{(1)} = \frac{V_{nL}}{E_L^{(0)} - E_n^{(0)}}$$

$$\psi = \psi_L^{(0)} + \sum_{n \neq L} \frac{V_{nL} \psi_n^{(0)}}{E_L^{(0)} - E_n^{(0)}}$$

$$a_L^{(1)} = 0, \quad a_n^{(1)} = \frac{V_{nL}}{E_L^{(0)} - E_n^{(0)}}$$

SECOND ORDER

$n = L$

$$E^{(2)} = \sum_{m \neq L} \frac{V_{Lm} V_{mL}}{E_L^{(0)} - E_m^{(0)}}$$

$$\boxed{\begin{aligned} E_L &= E_L^{(0)} + V_{LL} + \sum_{m \neq L} \frac{|V_{Lm}|^2}{E_L^{(0)} - E_m^{(0)}} \\ \psi_L &= \psi_L^{(0)} + \sum_{m \neq L} \frac{\psi_m^{(0)}(r) V_{mL}}{E_L^{(0)} - E_m^{(0)}} \end{aligned}}$$

HOMEWORK SOLUTIONS

1. $[a, H] = \hbar\omega a$
$[a^+, H] = -\hbar\omega a$

$\langle n | [a, H] | n' \rangle = \langle n | \hbar\omega a | n' \rangle$
GIVES $\langle n|a|n'\rangle \hbar\omega (n - n' - 1) = 0$
$\Rightarrow$ EITHER $n = n' - 1$
OR $\langle n|a|n'\rangle = 0$

$\langle n | [a^+, H] | n' \rangle = \ldots$
EITHER $n = n' + 1$
OR $\langle n|a^+|n'\rangle = 0$

$\langle n | [aa^+ - a^+a] = 1 | n \rangle = 1$
$= \langle n|a|n+1\rangle\langle n+1|a^+|m\rangle - \langle n|a^+|n-1\rangle\langle n-1|a|n\rangle$
$= \lambda_{n+1}^2 - \lambda_n^2 = 1$

3. $\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2}$ (8 STATES)
$\alpha_1, \beta_1, \alpha_2 \beta_2, \alpha_3 \beta_3$
$\alpha_1 \alpha_2 \alpha_3 = |j = 3/2, m_j = 3/2\rangle$

$|\frac{3}{2}, \frac{1}{2}\rangle = \frac{1}{\sqrt{3}} (\alpha_1 \alpha_2 \beta_3 + \alpha_1 \beta_2 \alpha_3 + \beta_1 \alpha_2 \alpha_3)$

$|\frac{3}{2}, -\frac{1}{2}\rangle = \frac{1}{\sqrt{3}} (\alpha_1 \beta_2 \beta_3 + \beta_1 \alpha_2 \beta_3 + \beta \beta_2 \alpha_3)$

$|\frac{3}{2}, -\frac{3}{2}\rangle = \beta_1 \beta_2 \beta_3$

$$\frac{1}{2} \otimes \frac{1}{2} \left\{ \begin{array}{l} j = 1 \quad 3 \times \frac{1}{2} \\ j = 0 \end{array} \right\} \begin{array}{l} 3/2 \\ 1/2 \\ 1/2 \end{array}$$

$$\frac{1}{2} \otimes \frac{1}{2} : j = 1 \left\{ \begin{array}{l} \alpha_1 \alpha_2 \\ \frac{1}{\sqrt{2}}(\alpha_1 \beta_2 + \alpha_1 \alpha_2 \\ \beta_1 \beta_2 \end{array} \right\} \otimes \frac{1}{2}$$

$\frac{1}{2}\ \frac{1}{2}\rangle - \sqrt{\frac{2}{3}}\,|1\,1\rangle\alpha_3\ \sqrt{\frac{1}{3}}\,|1\,0\rangle\ldots$
$= \frac{\sqrt{2}}{3}(\alpha_1 \alpha_2 \beta_3)$
$- \sqrt{\frac{1}{6}}(\alpha_1 \beta_2 + \alpha_2 \beta_1)\alpha_3$

$|1, \frac{1}{2}\rangle$
$|0, \frac{1}{2}\rangle$

EXAMPLES

1) HARMONIC OSCILLATOR IN ELECTRIC FIELD

$$H = \frac{p^2}{2m} + \frac{K}{2}x^2 + Fx$$

EXACT SOLUTION

$$H = \frac{p^2}{2m} + \frac{K}{2}\left(x + \frac{F}{K}\right)^2 - \frac{F^2}{2K}$$

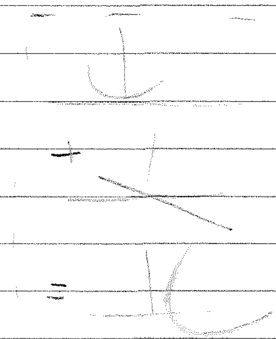
$$x' = x + \frac{F}{K}$$

$$[x, p] = i\hbar \Rightarrow [x', p] = i\hbar$$

$$\Rightarrow H = \frac{p^2}{2m} + \frac{K}{2}x'^2 - F^2/2K$$

$$\omega = K/2$$

$$H = \hbar\omega\left(n + \tfrac{1}{2}\right) - \frac{F^2}{2K}$$



PER. THRY:

$$H = \frac{p^2}{2m} + \frac{K}{2}x^2 + Fx$$

$$H_0 = \frac{p^2}{2m} + \frac{K}{2}x^2$$

$$V = Fx$$

$$E_n^{(0)} = \hbar\omega\left(n + \tfrac{1}{2}\right)$$

$\psi_n^{(0)}$ = HARMONIC OSCILL.

$$E_n = \underbrace{\hbar\omega\left(n + \tfrac{1}{2}\right)}_{E_n^{(0)}} + \underbrace{\langle n|Fx|n\rangle}_{V_{nn}} + \sum_{m\neq n} \frac{|\langle n|Fx|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\langle n|Fx|m\rangle = F\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right]$$

$$|\langle n|Fx|m\rangle|^2 = \frac{F^2\hbar}{2m\omega}\left[n\,\delta_{m,n-1} + (n+1)\,\delta_{m,n+1}\right]$$

$$\frac{|\langle n|Fx|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}} = \frac{F^2\hbar}{2m\omega}\left[\frac{n}{\hbar\omega(n-n+1)} + \frac{n+1}{\hbar\omega(-1)}\right]$$

$$= \frac{F^2}{2m\omega^2}\left[+n - (n+1)\right] = \frac{-F^2}{2m\omega^2} = \frac{-F^2}{2K^2}$$

TO GET A BETTER ANSWER

$$\sum \frac{|\langle \quad \rangle|^2}{2E_0 - E_{m_1} - E_{m_2}}$$ ← ASSUME CONSTANT DENOMINATOR

ASSUME $2E_0 - E_{m_1} - E_{m_2} = 2E_0$

$$\sum_{m_1} |\langle 1s | r_\mu | m_1 \rangle \langle m_1 | r_\nu | 1s \rangle = \langle 1s | r_\mu r_\nu | 1s \rangle =$$

$$= \delta_{\mu\nu} \langle 1s | x^2 | 1s \rangle$$

$$\sum_{m_1} |m_1\rangle\langle m_1| = 1 \qquad = \delta_{\mu\nu}\, a^2$$

$$\sum_{m_1 m_2} \langle 1s | r_{1\mu} | m_1 \rangle \phi_{\mu\nu} \langle 1s | r_{2\nu} | m_2 \rangle \langle m_1 | r_{1\lambda} | 1s \rangle \phi_{\lambda\delta} \langle m_2 | r_{2\delta} | 1s \rangle$$

$$= a^4 \phi_{\mu\nu} \phi_{\lambda\delta} \delta_{\mu\lambda} \delta_{\nu\delta}$$

$$= a^4 T_r(\phi \cdot \phi) =$$

$$= a^4 \frac{6}{R^6}$$

$$\Rightarrow C_6 = \frac{e^4 \frac{6}{R^6} a^4 R^6}{e^2/a} = 6 e^2 a^5$$ ← BETTER ANSWER

NOTATION

$$\langle 1s | x_1 | m \rangle = \int d^3r_1\, \phi_{1s}(r_1)\, x_1\, \phi_{np}(r_1)$$

$$\int d^3r_2\, \phi_{np}(r_2)\, x\, \phi_{1s}(r_2) = \langle m_1 | x | 1s \rangle$$

PRODUCT IS (THRU COMPLETENESS) IS $\langle 1s | x^2 | 1s \rangle$

$$\sum \phi_{\mu p}(r_1)\, \phi_{\mu p}(r_2) = \delta^3(r_1 - r_2)$$

EXAMPLE 2

ATOM IN AN ELECTRIC FIELD

H_0 = ATOM BY ITSELF

$V = eF \sum_i x_i$

$$H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

$$E_n = E_n^{(0)} + \langle n | eF \sum x_i | n \rangle + \sum_m \frac{| \langle \quad \rangle |^2}{}$$

$$\langle n | eF \sum x_i | n \rangle = eF \sum \langle n | x_i | n \rangle$$

DIPOLE MOMENT $= e \sum_i \langle x_i \rangle$

$$e^2 F^2 \sum_m \frac{| \langle n | \sum x_i | m \rangle |^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\alpha_n = 2 e^2 \sum_{m \neq n} \frac{| \langle n | \sum x_i | m \rangle |^2}{E_n^{(0)} - E_m^{(0)}} \leftarrow \text{POLARIZABILITY}$$

FOR HYDROGEN, $\alpha = \frac{9}{2} a^3$

$$\alpha_{s} = 2 e^2 \sum_m \frac{| \langle 1s | z | m, \ell = 1, m_\ell = 0 \rangle |^2}{E_{RYD} + E_{RYD}/m^2}$$

$$\alpha_{1s} = \frac{2 e^2}{\frac{3}{4} E_{RYD}} | \langle 1s | z | 2p_z \rangle |^2 + \dots$$

$$\frac{2^{15}}{3^{10}} a^2 \sim 0.5 a^2 = | \langle \quad \rangle |^2$$

$$\cong 2.7 a^3 \leftarrow \text{FROM FIRST TERM}$$

CONSIDER FOR SIMPLE ATOMS WHERE $\underset{\sim}{d} = 0$

SO WE GOT; TO SLVE:

$$E_n = \sum_{m \neq n} \frac{|\langle n|V|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}} \quad ; q_1 = \text{GROUND STATE}$$

$$= \underbrace{e^4 \sum_{m_1 m_2} \frac{|\langle q_1| \sum_i r_i |m_1\rangle \cdot \phi(R) \cdot \langle q_2| \sum r_j |m_2\rangle|^2}{\underbrace{E_{j1} + E_{j2}}_{E_n^{(0)}} - E_{m_1} - E_{m_2}}}_{\text{LONDON'S FORMULA}} = -\frac{C}{R^6}$$

FOR HYDROGEN : $C_6 \simeq e^2 a^5 (6.47)$

TRY:

$$\langle 1s|\hat{r}|2p\rangle = \hat{x}\langle 1s|x|2p_x\rangle + \hat{y}\langle 1s|y|2p_y\rangle + \hat{z}\langle 1s|z|2p_z\rangle$$

$$\left.\begin{aligned} 2p_z &= z e^{-r/a} \\ 2p_y &= y e^{-r/a} \\ 2p_x &= x e^{-r/a} \end{aligned}\right\} \ell = 1,\ m_\ell = \pm 1$$

$$\langle 1s|r|2p\rangle = \hat{x}\langle 1s|x|2p_x\rangle + \hat{y}\langle 1s|y|2p_y\rangle + z\langle 1s|z|2p_z\rangle$$

$$= \frac{1}{R^3}(x_1 \cdot x_2 + y_1 \cdot y_2 - 2 z_1 \cdot z_2)$$

$$= \frac{1}{R^3}\left[\langle x_1\rangle\langle x_2\rangle + \langle y_1\rangle\langle y_2\rangle - 2\langle z_1\rangle\langle z_2\rangle\right]$$

$$|\langle 1s|r|2p\rangle|^2 = \frac{1}{R^6}\left[\underbrace{\langle x_1\rangle^2}_{\langle 1s|x|{}_{m=\pm1}^{\ell=1}\rangle}\langle x_2\rangle^2 + \langle y_1\rangle^2\langle y_2\rangle^2 + 4\langle z_1\rangle^2\langle z_2\rangle^2\right]$$

$$\therefore C_6 = \frac{6\,|\langle z^2\rangle|^2 e^4}{\frac{3}{2} e^2/2a}$$

RECALL $\langle 1s|z|2p_z\rangle \simeq \frac{1}{2} a_0^2$

$$C_6 = 2e^2 a^5$$

3/15/75

EXAM TUES, 1ST HR.

MATERIAL UP TO PER. THEORY FROM 30 WKBJ

$$E_n = E_n^{(0)} + \langle n|V|n\rangle + \sum_{m\neq n} \frac{|\langle n|V|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\psi_n(r) = \psi_n^{(0)}(r) + \sum_{m\neq n} \frac{\psi_m^{(0)}(r)\,\langle m|V|n\rangle}{E_n^{(0)} - E_m^{(0)}}$$

EXAMPLE 3: LONDON'S FORMULA FOR VAN-DER-WAALS FORCE

ATTRACTION: $-C_6/R^6$

① ②

$V(r) = -C_6/R^6$ C_6 : ERGS × CM^6

ASSUME: ATOM 1, ATOM 2, COULOMB INTERACTION

$H = H_1 + H_2 + V$

RAD. R_i RADIUS r_j

Z_1 $\xleftarrow{R_{12}}$ Z_2

NUCLEUS

$$\Rightarrow V = \frac{Z_1 Z_2 e^2}{R_{12}} - Z_1 e^2 \sum_j \frac{1}{(r_j - R_{12})} - e^2 Z_2 \sum_i \frac{1}{(r_i - R_{12})} + e^2 \sum_{ij} \frac{1}{|r_i - r_j + R_{12}|}$$

ASSUME $R_{12} \gg \langle r_1\rangle, \langle r_2\rangle$

$$\Rightarrow \frac{1}{r_j - R_{12}} = \frac{1}{R_{12}} + \frac{r_j\cdot R_{12}}{R_{12}^3} + \frac{r_j\cdot r_j - \frac{3(r_j\cdot R)^3}{R^2}}{R^3} + \dots$$

UPON PLUGGING AND CHUGGING, $\frac{1}{R_{12}}$ AND $r_j\cdot R_{12}/R_{12}^3$ TERMS CANCEL. USING THREE TERMS GIVES

$$V(r) = \frac{e^2}{R_{12}^3}\left[\sum_i r_i\cdot\sum_j r_j - \frac{3R_{12}\sum_i r_i \cdot R_{12}\cdot\sum r_j}{R_{12}^2}\right]$$

PERTURBATION: $\phi_{\mu\nu} = \frac{1}{R^3}\left[\delta_{\mu\nu} - 3R_\mu R_\nu/R^2\right]$

$$V = e^2\left(\sum_i r_i\right)\cdot\phi\cdot\left(\sum r_j\right)$$

$$\langle n|V|n\rangle = e^2\langle\lambda_1|\sum r_i|\lambda\rangle\cdot\phi(R)\cdot\underbrace{\langle\lambda_2|\sum r_j|\lambda_2\rangle}_{\text{DIPOLE MOMENT}}$$

$$= d_1\cdot\phi\cdot d_2$$

FOR SIMPLE ATOMS, He, Li, ETC, $d_1 = 0$

Phys 611
Due : Jan 23, 1975

#1

1) Evaluate the numerical value of the deBroglie wavelength:

a. For an electron of kinetic energy 100 eV

b. For a neutron of K.E. 300°K

2) Prove that

$$e^{L} a e^{-L} = a + [L, a] + \frac{1}{2!}[L,[L,a]] + \frac{1}{3!}[L,[L,[L,a]]] + \ldots$$

3) If F is any operator which does not explicitly depend upon time, show

$$\frac{\partial}{\partial t}\langle F \rangle =$$

vanishes in a eigenstate with a discrete eigenvalue.

4) Show that the average value of the momentum in a stationary state with a discrete eigenvalue is equal to zero.

5) For the harmonic oscillator problem, evaluate:

a. $\langle n | x^2 | m \rangle$

b. $\langle n | p^2 | m \rangle$

c. $\langle n | \exp(iqx) | m \rangle$ q is a constant

PHYS 611
DUE: JAN 23, 1975
BOB MARKS

50|50

10 a. K = 100 eV, ELECTRON

$\lambda = h/p$

$p = mv \Rightarrow \lambda = \frac{h}{mv}$

$K = \frac{1}{2}mv^2 \Rightarrow v = \sqrt{\frac{2K}{m}}$

$\therefore \lambda = \frac{h}{m}\sqrt{\frac{m}{2K}}$

$= \frac{h}{\sqrt{2KM}}$

$= \frac{6.63 \times 10^{-34} \text{ JOULE-SEC}}{[2 \times (100 \text{ eV}) \times 1.6 \times 10^{-19} \text{ JOULE/eV} \times 9.11 \times 10^{-31} \text{ kg}]^{1/2}}$

$= 1.23 \times 10^{-10} m$

$= 1.23 \text{ Å}$

b. K.E. ~ 300° K, NEUTRON

$K = \frac{n}{2} kT$

WHERE: n = NO. OF NUETRON'S DEGREES OF FREEDOM

k = BOLTZMAN'S CONSTANT

FROM PART a:

$\lambda = \frac{h}{\sqrt{2Km}}$

$= \frac{h}{\sqrt{2(\frac{n}{2})kTm}}$

$= \frac{h}{\sqrt{nkTm}}$

FOR n = 3 (x, y, & z)

$\lambda = \frac{h}{\sqrt{3kTm}}$

$= \frac{6.63 \times 10^{-34} \text{ JOULE-SEC}}{[3 \times (1.38 \times 10^{-23} \text{ JOULE/°K}) \times (300 \text{°K}) \times (1.67 \times 10^{-27} \text{ kg})]^{1/2}}$

$= 1.45 \times 10^{-10}$

$= 1.45 \text{ Å}$

2. SHOW THAT

$$e^{L} a e^{-L} = a + [L, a] + \frac{1}{2!}[L,[L,a]] + \frac{1}{3!}[L,[L,[L,a]]] + \ldots$$

WHERE a AND L ARE NON-COMMUTATIVE OPERATORS

NOW,

$$[L, a] = La - aL$$

$$[L,[L,a]] = (L^2 a - LaL) - (LaL - aL^2)$$

$$= L^2 a - 2LaL + aL^2$$

$$[L,[L,[L,a]]] = (L^3 a - 2L^2 aL + LaL^2) - (L^2 aL - 2LaL^2 + aL^3)$$

$$= L^3 a - 3L^2 aL + 3LaL^2 - aL^3$$

$$[L,[L,[L,[L,a]]]] = (L^4 a - 3L^3 aL + 3L^2 aL^2 - LaL^3)$$

$$- (L^3 aL - 3L^2 aL^2 + 3LaL^3 - aL^4)$$

$$= L^4 a - 4L^3 aL + 6L^2 aL^2 - 4LaL^3 + aL^4$$

OR, IF $\binom{m}{n} = \frac{m!}{n!(m-n)!}$,

$$\underbrace{[L,[L,\ldots[L}_{m\ L\text{'s}},a]\ldots]] = \sum_{n=0}^{m} (-1)^n \binom{m}{n} L^{m-n} a L^n$$

THUS, WE ARE SHOWING THAT

$$e^{L} a e^{-L} = \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{n=0}^{m} (-1)^n \binom{m}{n} L^{m-n} a L^n$$

(CONT.)

ANYWAY, BACK TO THE PROBLEM:

$$e^{L} = \sum_{n=0}^{\infty} \frac{1}{n!} L^n = 1 + L + \frac{1}{2!} L^2 + \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots$$

$$e^{-L} = \sum_{n=0}^{\infty} \frac{1}{n!} L^n (-1)^n = 1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 - \ldots$$

THUS:

$$e^{L} a e^{-L} = (1 + L + \frac{1}{2!} L^2 + \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots) \times a \times (1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots)$$

$$= a(1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots)$$
$$+ La(1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots)$$
$$+ \frac{1}{2!} L^2 a(1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots)$$
$$+ \frac{1}{3!} L^3 a(1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots)$$
$$+ \frac{1}{4!} L^4 a(1 - L + \frac{1}{2!} L^2 - \frac{1}{3!} L^3 + \frac{1}{4!} L^4 + \ldots) + \ldots$$

$$= (a - aL + \frac{1}{2!} aL^2 - \frac{1}{3!} aL^3 + \frac{1}{4!} aL^4 - \ldots)$$
$$+ (La - LaL + \frac{1}{2!} LaL^2 - \frac{1}{3!} LaL^3 + \frac{1}{4!} LaL^4 - \ldots)$$
$$+ \frac{1}{2!}(L^2 a - L^2 aL + \frac{1}{2!} L^2 aL^2 - \frac{1}{3!} L^2 aL^3 + \frac{1}{4!} L^2 aL^4 - \ldots)$$
$$+ \frac{1}{3!}(L^3 a - L^3 aL + \frac{1}{2!} L^3 aL^2 - \frac{1}{3!} L^3 aL^3 + \frac{1}{4!} L^3 aL^4 - \ldots)$$
$$+ \frac{1}{4!}(L^4 a - L^4 aL + \frac{1}{2!} L^4 aL^2 - \frac{1}{3!} L^4 aL^3 + \frac{1}{4!} L^4 aL^4 - \ldots) + \ldots$$

REARANGINGING SUCH THAT SUM OF EXPONENTS ON L IN EACH COLUMN IS THE SAME:

$$e^{L} a e^{-L} = (a - aL + \frac{1}{2!} aL^2 - \frac{1}{3!} aL^3 + \frac{1}{4!} aL^4 - \ldots)$$
$$+ (La - LaL + \frac{1}{2!} LaL^2 - \frac{1}{3!} LaL^3 + \ldots)$$
$$+ \frac{1}{2!}(L^2 a - L^2 aL + \frac{1}{2!} L^2 aL^2 - \ldots)$$
$$+ \frac{1}{3!}(L^3 a - L^3 aL + \ldots)$$
$$+ \frac{1}{4!}(L^4 a - \ldots)$$

(CONT.)

ADDING EACH COLUMN GIVES:

$$e^L a e^{-L} = a + (La - aL) + \left(\frac{1}{2!}L^2 a - LaL + \frac{1}{2!}aL^2\right)$$
$$+ \left(\frac{1}{3!}L^3 a - \frac{1}{2!}L^2 aL + \frac{1}{2!}LaL^2 - \frac{1}{3!}aL^3\right)$$
$$+ \left(\frac{1}{4!}L^4 a - \frac{1}{3!}L^3 aL + \frac{1}{2!2!}L^2 aL^2 - \frac{1}{3!}LaL^3 + \frac{1}{4!}aL^4 + \ldots\right)$$
$$+ \ldots$$

FACTORING OUT DENOMINATOR COEFFICIENTS OF FIRST TERMS:

$$e^L a e^{-L} = a + (La - aL) + \frac{1}{2!}\left[L^2 a - 2!\,LaL + aL^2\right]$$
$$+ \frac{1}{3!}\left[L^3 a - \frac{3!}{2!}L^2 aL + \frac{3!}{2!}LaL^2 - aL^3\right]$$
$$+ \frac{1}{4!}\left[L^4 a - \frac{4!}{3!}L^3 aL + \frac{4!}{2!2!}L^2 aL^2 - \frac{4!}{3!}LaL^3 + aL^4\right] + \ldots$$

OR MORE APPROPRIATELY:

$$e^L a e^{-L} = \binom{0}{0}a + \left[\binom{1}{0}La - \binom{1}{1}aL\right] + \frac{1}{2!}\left[\binom{2}{0}L^2 a - \binom{2}{1}LaL + \binom{2}{2}aL^2\right]$$
$$+ \frac{1}{3!}\left[\binom{3}{0}L^3 a - \binom{3}{1}L^2 aL + \binom{3}{2}LaL^2 - \binom{3}{3}aL^3\right]$$
$$+ \frac{1}{4!}\left[\binom{4}{0}L^4 a - \binom{4}{1}L^3 aL + \binom{4}{2}L^2 aL^2 - \binom{4}{3}LaL^3 + \binom{4}{4}aL^4\right] + \ldots$$
$$= \frac{1}{0!}\sum_{n=0}^{0}(-1)^n\binom{0}{n}L^{0-n}aL^n$$
$$+ \frac{1}{1!}\sum_{n=0}^{1}(-1)^n\binom{1}{n}L^{1-n}aL^n$$
$$+ \frac{1}{2!}\sum_{n=0}^{2}(-1)^n\binom{2}{n}L^{2-n}aL^n$$
$$+ \frac{1}{3!}\sum_{n=0}^{3}(-1)^n\binom{3}{n}L^{3-n}aL^n$$
$$+ \frac{1}{4!}\sum_{n=0}^{4}(-1)^n\binom{4}{n}L^{4-n}aL^n + \ldots$$

PREVIOUSLY, IT WAS SHOWN THAT

$$\underbrace{[L,[L \ldots [L}_{m\ L\text{'s}},a] \ldots]] = \sum_{n=0}^{m}(-1)^n\binom{m}{n}L^{m-n}aL^n$$

THUS

$$e^L a e^{-L} = a + [L,a] + \frac{1}{2!}[L,[L,a]] + \frac{1}{3!}[L,[L,[L,a]]]$$
$$+ \frac{1}{4!}[L,[L,[L,[L,a]]]] + \ldots$$

3. 10/1 SHOW $\frac{\delta}{\delta t}\langle F\rangle = 0$ IN AN EIGENSTATE WITH A DISCRETE EIGENVALUE WHEN THE OPERATOR F DOES NOT EXPLICITLY DEPEND ON TIME.

oh well - i'll give your credit but I suspect whether this was a proof

FOR THE SCHRÖDINGER TREATMENT, IT WAS SHOWN THAT FOR AN OPERATOR O,

$$\frac{\delta}{\delta t}\langle O\rangle = \frac{i}{\hbar}\langle [H,O]\rangle$$

THUS:

$$\frac{\delta}{\delta t}\langle F\rangle = \frac{i}{\hbar}\langle [H,F]\rangle$$

a. CASE 1: IF THE HAMILTONIAN COMMUTES WITH F, THEN $[H,F]=0$, AND $\frac{\delta}{\delta t}\langle F\rangle = \frac{i}{\hbar}\langle 0\rangle = 0$ (TRIVIAL SOL)

b. CASE 2: IF THE HAMILTONIAN DOES NOT COMMUTE WITH F:

$$\frac{\delta}{\delta t}\langle F\rangle = \frac{i}{\hbar}\langle [H,F]\rangle$$
$$= \frac{i}{\hbar}\langle HF - FH\rangle$$
$$= \frac{i}{\hbar}\int \psi^*[HF-FH]\psi\, d\overset{3}{r}$$
$$= \underline{-\frac{1}{i\hbar}\int \psi^* HF\psi\, d\overset{3}{r} + \frac{1}{i\hbar}\int \psi^* FH\psi\, d^3r}$$

if $\left[\frac{d}{dt}, F\right]=0$

then $\left[i\hbar\frac{d}{dt}, F\right]=0$

then $[H, F]=0$

LET THE OPERATOR F HAVE EIGENVALUES SUCH THAT

$$F\psi_m = F_m\psi_m$$

NOTE THAT, SINCE F IS TIME INDEPENDENT (AND LINEAR):

$$\frac{d}{dt}F\psi_m = F\frac{d}{dt}\psi_m \quad \left[\text{ie } \left[\frac{d}{dt}, F\right]=0\right]$$

WE NOW HAVE: $\psi = \sum_m a_m\psi_m$

CONSIDER THE FIRST TERM IN THE ABOVE EXPRESSION FOR $\frac{\delta}{\delta t}\langle F\rangle$:

$$-\frac{1}{i\hbar}\int \psi^* HF\psi\, d\overset{3}{r} = \frac{1}{i\hbar}\int \psi^* HF\left[\sum_m a_m\psi_m\right] d^3r$$
$$= -\frac{1}{i\hbar}\int \psi^* H\left[\sum_m a_m F_m\psi_m\right] d^3r$$

(CONT)

I guess you mean

$$\frac{d}{dt}(F\psi_m) = \left(\frac{d}{dt}F\right)\psi_m + F\left(\frac{d}{dt}\psi_m\right)$$

THE HAMILTONIAN MAY BY EXPRESSED AS

$$H\phi = i\hbar \frac{\delta \phi}{\delta t}$$

THUS, THE FIRST TERM MAY BE WRITTEN:

$$-\frac{1}{i\hbar}\int \psi^* H F \psi \, d^3r = -\int \psi^* \frac{d}{dt}\left[\sum_m a_m F_m \psi_m\right] d^3r$$

$$= -\int \psi^* \left[\sum_m a_m F_m \frac{d}{dt} \psi_m\right] d^3r$$

CONSIDER NOW, THE SECOND TERM OF THE $\frac{\delta}{\delta t}\langle F \rangle$ EXPRESS:

$$\frac{1}{i\hbar}\int \psi^* F H \psi \, d^3r = \frac{1}{i\hbar}\int \psi^* F H \left[\sum_m a_m \psi_m\right] d^3r$$

$$= \int \psi^* F \frac{\delta}{\delta t}\left[\sum_m a_m \psi_m\right] d^3r$$

$$= \int \psi^* F \left[\sum_m a_m \frac{\delta}{\delta t} \psi_m\right] d^3r$$

DUE TO THE TIME INDEPENDENCE OF F:

$$\frac{1}{i\hbar}\int \psi^* F H \psi \, d^3r = \int \psi^* \left[\sum_m a_m \frac{\delta}{\delta t} F \psi_m\right] d^3r$$

$$= \int \psi^* \left[\sum_m a_m F_m \frac{\delta}{\delta t} \psi_m\right] d^3r$$

COMBINING THE TWO MASSAGED TERMS GIVES:

$$\frac{\delta}{\delta t}\langle F \rangle = -\int \psi^* \left[\sum_m a_m F_m \frac{d}{dt} \psi_m\right] d^3r + \int \psi^* \left[\sum_m a_m F_m \psi_m\right] d^3r = 0$$

THUS $\frac{\delta}{\delta t}\langle F \rangle$ VANISHES IN ALL EIGENSTATES OF THE TIME INDEPENDENT OPERATOR F

~~eigenstate of F~~

$$\cancel{\langle F \rangle \equiv \int \psi^* F \psi}$$

$$\cancel{\partial_t \langle F \rangle = \int \partial_t \psi^* (F\psi) + \psi^* F \partial_t \psi}$$

~~if f hermitian then~~

4 IT HAS BEEN SHOWN THAT:

$$\langle p \rangle = m \frac{\delta}{\delta t} \langle r \rangle$$

FOR A STATIONARY STATE, ALL TIMES ARE EQUIVALENT SO FAR AS A GIVEN PHYSICAL SYSTEM IS CONCERNED. THUS, r, VIEWED AS AN OPERATOR, DOES NOT EXPLICITLY DEPEND ON TIME. IN VIEW OF PROBLEM 3:

$$\frac{\delta}{\delta t} \langle r \rangle = 0$$

IT FOLLOWS THEN, THAT

$$\langle p \rangle = 0$$

5a. FIND $\langle n|x^2|\ \rangle$ FOR HARMONIC OSCILLATOR)

$$\langle n|x^2|\ell\rangle \triangleq \int dx\, \phi_n^*(x)\, x^2\, \phi_\ell(x) \quad (\text{BUT } \phi_n = \phi_n^* \text{ FOR } n.o.)$$

$$\phi_n(x) = \frac{1}{\sqrt{x_0}}\, \psi_n\!\left(\frac{x}{x_0}\right) = \psi_n(\xi)$$

$$\Rightarrow \langle n|x^2|\ell\rangle = \frac{1}{x_0}\int dx\, \psi_n\!\left(\frac{x}{x_0}\right) x^2 \psi_\ell\!\left(\frac{x}{x_0}\right)$$

LET $\xi = \frac{x}{x_0} \Rightarrow x^2 = x_0^2 \xi^2$

$$x = x_0\xi \Rightarrow dx = x_0 d\xi$$

$$\Rightarrow \langle n|x^2|\ell\rangle = \frac{1}{x_0}\int (x_0 d\xi)\, \psi_n(\xi)(x_0^2\xi^2)\psi_\ell(\xi)$$

$$= x_0^2 \int d\xi\, \psi_n(\xi)\, \xi^2\, \psi_\ell(\xi)$$

FOR HARMONIC OSCILLATOR:

$$\xi\psi_\ell(\xi) = \sqrt{\frac{\ell}{2}}\,\psi_{\ell-1}(\xi) + \sqrt{\frac{\ell+1}{2}}\,\psi_{\ell+1}$$

$$\xi^2\psi_\ell(\xi) = \sqrt{\frac{\ell}{2}}\,\xi\psi_{\ell-1} + \sqrt{\frac{\ell+1}{2}}\,\xi\psi_{\ell+1}$$

$$= \sqrt{\frac{\ell}{2}}\left[\sqrt{\frac{\ell-1}{2}}\,\psi_{\ell-2} + \sqrt{\frac{\ell}{2}}\,\psi_\ell\right] + \sqrt{\frac{\ell+1}{2}}\left[\sqrt{\frac{\ell+1}{2}}\,\psi_\ell + \sqrt{\frac{\ell+2}{2}}\,\psi_{\ell+2}\right]$$

$$= \frac{\sqrt{\ell(\ell-1)}}{2}\psi_{\ell-2} + \left[\frac{\ell}{2} + \frac{\ell+1}{2}\right]\psi_\ell + \frac{\sqrt{(\ell+1)(\ell+2)}}{2}\psi_{\ell+2}$$

$$= \frac{\sqrt{\ell(\ell-1)}}{2}\psi_{\ell-2} + \frac{2\ell+1}{2}\psi_\ell + \frac{\sqrt{(\ell+1)(\ell+2)}}{2}\psi_{\ell+2}$$

$$\Rightarrow \langle n|x^2|\ell\rangle = \frac{x_0^2}{2}\int d\xi\, \psi_n(\xi)\left[\sqrt{\ell(\ell-1)}\,\psi_{\ell-2} + (2\ell+1)\psi_\ell + \sqrt{(\ell+1)(\ell+2)}\,\psi_{\ell+2}\right]$$

SINCE ψ_m IS A COMPLETE ORTHONORMAL BASIS SET:

$$\langle n|x^2|\ell\rangle = \frac{x_0^2}{2}\left[\sqrt{\ell(\ell-1)}\,\delta_{n,\ell-2} + (2\ell+1)\delta_{n,\ell} + \sqrt{(\ell+1)(\ell+2)}\,\delta_{n,\ell+2}\right]$$

b. FIND $\langle n|p_x^2|\ell\rangle$ FOR THE HARMONIC OSCILLATOR

$$\langle n|p_x^2|\ell\rangle = \frac{1}{x_0}\int d\xi\, \psi_n(\xi)\, p_\xi^2\, \psi_\ell(\xi)$$
$$= -\frac{\hbar^2}{x_0}\int d\xi\, \psi_n(\xi)\frac{d^2}{d\xi^2}\psi_\ell(\xi)$$

FOR THE HARMONIC OSCILLATOR:

$$\frac{d}{d\xi}\psi_\ell(\xi) = \sqrt{\frac{\ell}{2}}\,\psi_{\ell-1}(\xi) - \sqrt{\frac{\ell+1}{2}}\,\psi_{\ell+1}(\xi)$$
$$\frac{d^2}{d\xi^2}\psi_\ell = \sqrt{\frac{\ell}{2}}\frac{d}{d\xi}\psi_{\ell-1}(\xi) - \sqrt{\frac{\ell+1}{2}}\frac{d}{d\xi}\psi_{\ell+1}(\xi)$$
$$= \sqrt{\frac{\ell}{2}}\left[\sqrt{\frac{\ell-1}{2}}\,\psi_{\ell-2} - \sqrt{\frac{\ell}{2}}\,\psi_\ell\right]$$
$$- \sqrt{\frac{\ell+1}{2}}\left[\sqrt{\frac{\ell+1}{2}}\,\psi_\ell - \sqrt{\frac{\ell+2}{2}}\,\psi_{\ell+2}\right]$$
$$= \frac{\sqrt{\ell(\ell-1)}}{2}\psi_{\ell-2} - \left[\frac{\ell}{2}+\frac{\ell+1}{2}\right]\psi_\ell + \frac{\sqrt{(\ell+1)(\ell+2)}}{2}\psi_{\ell+2}]$$
$$= \frac{\sqrt{\ell(\ell-1)}}{2}\psi_{\ell-2} - \left[\frac{2\ell+1}{2}\right]\psi_\ell + \frac{\sqrt{(\ell+1)(\ell+2)}}{2}\psi_{\ell+2}]$$

THUS:

$$\langle n|p_x^2|\ell\rangle = -\frac{\hbar^2}{2x_0}\int d\xi\, \psi_n\left[\sqrt{\ell(\ell-1)}\,\psi_{\ell-2} - (2\ell+1)\psi_\ell + \sqrt{(\ell+1)(\ell+2)}\,\psi_{\ell+2}\right]$$

SINCE ψ_m FORMS ORTHONORMAL SET:

$$\langle n|p_x^2|\ell\rangle = -\frac{\hbar^2}{2x_0}\left[\sqrt{\ell(\ell-1)}\,\delta_{n,\ell-2} - (2\ell+1)\delta_{n,\ell} + \sqrt{(\ell+1)(\ell+2)}\,\delta_{n,\ell+2}\right]$$

Physics 611
Due: Jan 30, 1975
#2

(1) For the harmonic oscillator:

a. Show that the Hamiltonian may be written $H = \hbar\omega(a^\dagger a + \tfrac{1}{2})$

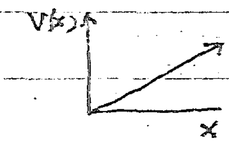
Hint: Start with $H = \frac{P^2}{2m} + \frac{K}{2}x^2$ and define x and p in terms of a and a^+.

b. Evaluate $[a, H] = ?$
$[a^\dagger, H] = ?$

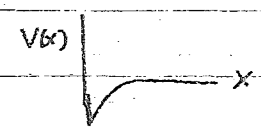
c. Evaluate
$e^{sH} a e^{-sH} = ?$
$e^{sH} a^+ e^{-sH} = ?$ s is a constant

(2) Find the exact eigenvalue equation for the potential

$$V(x) = \infty \quad x<0$$
$$= Fx \quad x>0$$

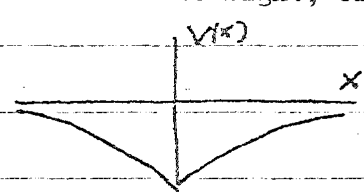


(3) For the potential $V(x) = -|\lambda| \exp(-2x/a)$, $x>0$
$= \infty$ $x<0$
find the phase shift δ_k for states with energy $E = \frac{\hbar^2 k^2}{2m} > 0$.



(4) Find the transmission coefficient, from left to right, of the potential

$$V(x) = -\lambda \, e^{-2|x|/a}$$



(5) Derive the numerical value (in eV) for the bound state energy of an electron in the following potential

$$V(x) = -V_0 \quad |x| \le b$$
$$= 0 \quad x > b$$

$$b = 1.0\ \text{Å} = 1.0 \cdot 10^{-8}\ \text{cm}$$
$$V_0 = 1.0\ \text{eV} = 1.6 \cdot 10^{-12}\ \text{erg}$$

$\sqrt{3}/50$

PHYSICS 611
DUE: JAN 30, 1975
BOB MARKS

9/10

1. a. $H = \frac{p^2}{2m} + \frac{k}{2}x^2$

$= \frac{p^2}{2m} + \left(\frac{m}{2}\right)\left(\frac{k}{m}\right)x^2$

$= \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2$ SINCE $\omega^2 = \frac{k}{m}$

$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2$ SINCE $p^2 = -\hbar^2\frac{d^2}{dx^2}$

$= \frac{\hbar\omega}{2}\left[\frac{m\omega}{\hbar}x^2 - \frac{\hbar}{m\omega}\frac{d^2}{dx^2}\right]$

$= \frac{\hbar\omega}{2}\left[\frac{1}{x_0^2}x^2 - x_0^2\frac{d^2}{dx^2}\right]$ SINCE $x_0^2 = \frac{\hbar}{m\omega}$

$= \frac{\hbar\omega}{2}\left[\left(\frac{x}{x_0}\right)^2 - \frac{d^2}{d(x/x_0)^2}\right]$

$= \frac{\hbar\omega}{2}\left[\xi^2 - \frac{d^2}{d\xi^2}\right]$ SINCE $\xi = \frac{x}{x_0}$

$= \frac{\hbar\omega}{2}\left[\xi^2 + \left\{\left(\xi\frac{d}{d\xi} - \xi\frac{d}{d\xi}\right) + (1-1)\right\} - \frac{d^2}{d\xi^2}\right]$

$= \frac{\hbar\omega}{2}\left[\xi^2 + \xi\frac{d}{d\xi} - \left(1 + \xi\frac{d}{d\xi}\right) - \frac{d^2}{d\xi^2} + 1\right]$

$= \frac{\hbar\omega}{2}\left[\xi^2 + \xi\frac{d}{d\xi} - \frac{d}{d\xi}\xi - \frac{d^2}{d\xi^2} + 1\right]$

$= \frac{\hbar\omega}{2}\left[\left(\xi - \frac{d}{d\xi}\right)\left(\xi + \frac{d}{d\xi}\right) + 1\right]$

$= \hbar\omega\left[\left\{\frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)\right\}\frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right) + \frac{1}{2}\right]$

$= \hbar\omega\left[a^+a + \frac{1}{2}\right]$ ✓ SINCE $a^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)$ & $a = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$

$$\text{b. } [a, H] = aH - Ha$$
$$= a\left[\hbar\omega\left(a^+a + \tfrac{1}{2}\right)\right] - \left[\hbar\omega\left(a^+a + \tfrac{1}{2}\right)\right]a$$
$$= \hbar\omega\left[a\left(a^+a + \tfrac{1}{2}\right)\right] - \hbar\omega\left[a^+a + \tfrac{1}{2}\right]a$$
$$= \hbar\omega\left[\left(aa^+a + \tfrac{1}{2}a\right) - \left(a^+a^2 + \tfrac{1}{2}a\right)\right]$$
$$= \hbar\omega\left[aa^+a - a^+a^2\right]$$
$$= \hbar\omega\left[aa^+ - a^+a\right]a$$
$$= \hbar\omega\left[a, a^+\right]a$$
$$= \hbar\omega a$$

$$[a^+, H] = a^+H - Ha^+$$
$$= a^+\left[\hbar\omega\left(a^+a + \tfrac{1}{2}\right)\right] - \left[\hbar\omega\left(a^+a + \tfrac{1}{2}\right)\right]a^+$$
$$= \hbar\omega\left[a^+\left(a^+a + \tfrac{1}{2}\right) - \left(a^+a + \tfrac{1}{2}\right)a^+\right]$$
$$= \hbar\omega\left[\left((a^+)^2a + \tfrac{1}{2}a^+\right) - \left(a^+aa^+ + \tfrac{1}{2}a^+\right)\right]$$
$$= \hbar\omega\left[a^{+2}a - a^+aa^+\right]$$
$$= \hbar\omega a^+\left[a^+a - aa^+\right]$$
$$= -\hbar\omega a^+\left[aa^+ - a^+a\right]$$
$$= -\hbar\omega a^+\left[a, a^+\right]$$
$$= -\hbar\omega a^+$$

c. $e^{L} a e^{-L} = a + [L,a] + \frac{1}{2!}[L,[L,a]] + \frac{1}{3!}[L,[L,[L,a]]] + \dots$

$$e^{sH} a e^{-sH} = a + [sH,a] + \frac{1}{2!}[sH,[sH,a]] + \frac{1}{3!}[sH,[sH,[sH,a]]] + \dots$$
$$= a + s[H,a] + \frac{1}{2!}[sH, s[H,a]] + \frac{1}{3!}[sH,[sH,s[H,a]]] + \dots$$
$$= a + s[H,a] + \frac{1}{2!} s^2[H,[H,a]] + \frac{1}{3!}[sH, s^2[H,[H,a]]] + \dots$$
$$= a + s[H,a] + \frac{s^2}{2!}[H,[H,a]] + \frac{s^3}{3!}[H,[H,[H,a]]] + \dots$$
$$= a + s(\hbar\omega a) + \frac{s^2}{2!}[H,(\hbar\omega a)] + \frac{s^3}{3!}[H,[H,(\hbar\omega a)]] + \dots$$
$$= a + s\hbar\omega a + \frac{s^2}{2!}\hbar\omega[H,a] + \frac{s^3}{3!}[H,\hbar\omega[H,a]] + \dots$$
$$= a + s\hbar\omega a + \frac{s^2}{2!}\hbar\omega(\hbar\omega a) + \frac{s^3}{3!}\hbar\omega[H,(\hbar\omega a)] + \dots$$
$$= a + s\hbar\omega a + \frac{1}{2!}(s\hbar\omega)^2 a + \frac{s^3}{3!}(\hbar\omega)^2[H,a] + \dots$$
$$= a + s\hbar\omega a + \frac{1}{2!}(s\hbar\omega)^2 a + \frac{1}{3!}(\hbar\omega)^3 a + \dots$$
$$= \left[1 + s\hbar\omega + \frac{1}{2!}(s\hbar\omega)^2 + \frac{1}{3!}(\hbar\omega)^3 + \dots\right] a$$
$$= \left[\sum_{n=0}^{\infty} \frac{1}{n!}(s\hbar\omega)^n\right] a = e^{s\hbar\omega} a$$
$$= a e^{-s\hbar\omega}$$

$$e^{sH} a^+ e^{-sH} = a^+ + [sH,a^+] + \frac{1}{2!}[sH,[sH,a^+]] + \frac{1}{3!}[sH,[sH,[sH,a^+]]] + \dots$$
$$= a^+ + s[H,a^+] + \frac{s^2}{2!}[H,[H,a^+]] + \frac{s^3}{3!}[H,[H,[H,a^+]]] + \dots$$
$$= a^+ + s(-\hbar\omega a^+) + \frac{s^2}{2!}[H,(-\hbar\omega a^+)] + \frac{s^3}{3!}[H,[H,(-\hbar\omega a^+)]] + \dots$$
$$= a^+ + s(-\hbar\omega)a^+ + \frac{s^2}{2!}(-\hbar\omega)[H,a^+] + \frac{s^3}{3!}[H,(-\hbar\omega)[H,a^+]] + \dots$$
$$= a^+ + s(-\hbar\omega)a^+ + \frac{s^2}{2!}(-\hbar\omega)^2 a^+ + \frac{s^3}{3!}(-\hbar\omega)^3 a^+ + \dots$$
$$= \left[1 + s(-\hbar\omega) + \frac{s^2}{2!}(-\hbar\omega)^2 + \frac{s^3}{3!}(-\hbar\omega)^3 + \dots\right] a^+$$
$$= \left[\sum_{n=0}^{\infty} \frac{1}{n!}(-s\hbar\omega)^n\right] a^+$$
$$= e^{-s\hbar\omega} a^+$$
$$= a^+ e^{+s\hbar\omega}$$

oh well

2. $V(x) = \begin{cases} \infty & ; x < 0 \\ Fx & ; x > 0 \end{cases}$

10/10

IT WAS DEMONSTRATED THAT, IF

$$\xi = \left(x - \frac{E}{F}\right)\left(\frac{2mF}{\hbar^2}\right)^{1/3}$$

THEN SCRÖ'S EQ'N IS AIRY'S EQ'N, WHICH IS

$$\left(\frac{d^2}{d\xi^2} - \xi\right)\psi(\xi) = 0$$

THE SOLUTION GIVES

$$\psi(\xi) = a\,A_i(\xi) + b\,B_i(\xi)$$

WHERE

$$A_i(\xi) = \frac{1}{\pi}\int_0^\infty \cos\left(\xi t + \frac{t^3}{3}\right)dt$$

$$B_i(\xi) = \frac{1}{\pi}\int_0^\infty \left[e^{z\xi - z^3/3} + \sin\left(\xi z + \frac{z^3}{3}\right)\right]dz$$

BNDRY CONDITIONS DICTATE

$$\lim_{\xi\to\infty}\psi(\xi) = \lim_{x\to\infty}\psi(x) = 0$$

SINCE

$$\lim_{\xi\to\infty} B_i(\xi) = \infty$$

LET $b = 0$

THIS LEAVES:

$$\psi(\xi) = a\,A_i(\xi)$$

$$= \frac{a}{\pi}\int_0^\infty \cos\left[\xi t + \frac{t^3}{3}\right]dt$$

OR EQUIVALENTLY:

$$\psi(x) = \frac{a}{\pi}\int_0^\infty \cos\left[c\left(x - \frac{E}{F}\right)t + \frac{t^3}{3}\right]dt$$

WHERE

$$c = \left(\frac{2mF}{\hbar^2}\right)^{1/3}$$

THE BOUNDRY CONDITION AT THE ORIGIN DICTATES

$$\psi(0) = 0 = \frac{a}{\pi} \int_0^\infty \cos\left[c\left(x - \frac{E}{F}\right)t + \frac{t^3}{3}\right] dt$$

LET E_n THEN BE ALL ALL REAL VALUES FOR WHICH

$$\int_0^\infty \cos\left[\frac{cE_n t}{F} - \frac{t^3}{3}\right] dt = 0$$

THIS IS THE EIGENVALUE CONDITION. A GENERAL SOLUTION FOR E_n IS IMPOSSIBLE (AT LEAST BY ME) BUT IF NUMERICAL VALUES OF C AND F ARE KNOWN THEN VALUES OF E_n CAN BE GENERATED VIA SOLUTION OF THE ABOVE TRANSENDENTAL MESS.

r h weill

3. 10/10 $V(x) = \begin{cases} -\lambda e^{-2x/a} & ; x > 0 \quad (\lambda > 0) \\ \infty & ; x < 0 \end{cases}$

SOLUTION OF SCHRÖDINGER'S EQ'N FOR $E > 0$ IS

$$\psi(Y) = C_1 J_{ika}(K_0 a Y) + C_2 J_{-ika}(K_0 a Y)$$

WHERE: $Y = e^{-x/a}$

$$K_0^2 = \frac{2m}{\hbar^2}|\lambda|$$

$$K^2 = \frac{2m}{\hbar^2}E$$

@ $x = 0$; $\psi(x) = 0$, $Y = 1$

$$\Rightarrow 0 = C_1 J_{ika}(K_0 a) + C_2 J_{-ika}(K_0 a)$$

$$-C_1 J_{ika}(K_0 a) = C_2 J_{-ika}(K_0 a)$$

$$\therefore C_2 = -C_1 \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)}$$

$$\Rightarrow \psi(Y) = C_1 \left[J_{ika}(K_0 a Y) - \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} J_{-ika}(K_0 a Y) \right]$$

$\lim_{x \to \infty} \psi(x) = 0 \quad \Rightarrow x = \infty, \; Y = (0)$

$$\lim_{z \to 0} J_\gamma(z) = \frac{z^\gamma}{\Gamma(1+\gamma)}$$

$$\therefore \lim_{K_0 a Y \to 0} J_{ika}(K_0 a Y) = \frac{(K_0 a Y)^{ika}}{\Gamma[1 + i K_0 a]}$$

$$\lim_{K_0 a Y \to 0} J_{-ika}(K_0 a Y) = \frac{(K_0 a Y)^{-ika}}{\Gamma[1 - i K_0 a]}$$

$$\Rightarrow \lim_{Y \to 0} \psi(Y) = C_1 \left[\frac{(K_0 a Y)^{ika}}{\Gamma(1 + i K_0 a)} - \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} \frac{(K_0 a Y)^{-ika}}{\Gamma(1 - i K_0 a)} \right]$$

$$= C_1 \left[\frac{(K_0 a e^{-x/a})^{ika}}{\Gamma(1 + i K_0 a)} - \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} \frac{(K_0 a Y)^{-ika}}{\Gamma(1 - i K_0 a)} \right]$$

$$= \frac{C_1 (K_0 a)^{ika}}{\Gamma(1 + i K_0 a)} \left[e^{-ikx} - \frac{\Gamma(1 + i K_0 a)}{\Gamma(1 - i K_0 a)} \frac{(K_0 a)^{-ika}}{(K_0 a)^{ika}} \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} e^{ikx} \right]$$

NOW: $\Gamma[z^*] = \Gamma^*(z)$

AND $J_{\gamma^*}(\xi) = J^*_{\gamma}(\xi)$

FURTHER MORE, LET $C_1' = \dfrac{C_1 (K_0 a)^{ika}}{\Gamma(1 + i K_0 a)}$

THUS:

$$\lim_{x \to \infty} \psi(x) = C_1' \left[e^{-ikx} - \frac{\Gamma(1+ik_0a)}{\Gamma^*(1+ik_0a)} \frac{(K_0a)^{-ika}}{(K_0a)^{ika}} \frac{J_{ika}(K_0a)}{J^*_{ika}(K_0a)} e^{ika} \right]$$

LET $\Gamma(1+ik_0a)(K_0a)^{-ika} J_{ika}(K_0a) = \rho e^{i\delta_K}$

WHERE ρ AND δ_K ARE REAL

$$\Rightarrow \lim_{x \to \infty} \psi(x) = C_1' \left[e^{-ikx} - \frac{\rho e^{i\delta}}{\rho e^{-i\delta}} e^{ikx} \right]$$
$$= C_1' \left[e^{-ikx} - e^{i2\delta} e^{ikx} \right]$$

THUS:

$$e^{i2\delta_K} = \frac{\Gamma(1+ik_0a)(K_0a)^{-i2ka} J_{ika}(K_0a)}{\Gamma(1-ik_0a)\cancel{(K_0a)^{ika}} J_{-ika}(K_0a)}$$

THE PHASE SHIFT, δ_K (IN RADIANS) IS THEN GIVEN BY

$$\delta_K = \frac{1}{i2} \ln \frac{\Gamma(1+ik_0a)(K_0a)^{-i2ka} J_{ika}(K_0a)}{\Gamma(1-ik_0a)\cancel{(K_0a)^{ika}} J_{-ika}(K_0a)}$$

WHERE $K_0^2 = \dfrac{2m\lambda}{\hbar^2}$

$K^2 = \dfrac{2m}{\hbar^2} E$

AND $E = \dfrac{\hbar^2 K^2}{2m} > 0$

$\lambda > 0$

4. $V(x) = -\lambda e^{-2|x|/a}$; $\lambda > 0$

LET:

$$\psi(x) = \begin{cases} \psi_\ell(x) ; & x \le 0 \\ \psi_u(x) ; & x \ge 0 \end{cases}$$

5

a. $\psi_u(x)$ MUST SATISFY:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \lambda e^{-2x/a} - E\right]\psi(x) = 0$$

LET $Y = e^{-x/a}$

$$\frac{d}{dx} = \frac{dY}{dx}\frac{d}{dY} = \left(-\frac{1}{a}\right)e^{-x/a}\frac{d}{dY}$$

$$= -\frac{Y}{a}\frac{d}{dY}$$

$$\frac{d^2}{dx^2} = -\frac{d}{dx}\left(\frac{Y}{a}\frac{d}{dY}\right) = \left(\frac{Y}{a}\frac{d}{dY}\right)\left(\frac{Y}{a}\frac{d}{dY}\right)$$

$$= \frac{Y}{a}\left[\frac{Y}{a}\frac{d^2}{dY^2} + \left(\frac{d}{dY}\right)\times\left[\frac{d}{dY}\left(\frac{Y}{a}\right)\right]\right]$$

$$= \frac{Y}{a}\left[\frac{Y}{a}\frac{d^2}{dY^2} + \frac{1}{a}\frac{d}{dY}\right]$$

$$= \frac{Y^2}{a^2}\frac{d^2}{dY^2} + \frac{Y}{a^2}\frac{d}{dY}$$

THUS:

$$\left[-\frac{\hbar^2}{2m}\frac{Y^2}{a^2}\frac{d^2}{dY^2} - \frac{\hbar^2}{2m}\frac{Y}{a^2}\frac{d}{dY} - \lambda Y^2 - E\right]\psi_u(Y) = 0$$

$$\left[Y^2\frac{d^2}{dY^2} + \frac{\hbar^2 Y}{2ma^2}\left(\frac{2ma^2}{\hbar^2}\right)\frac{d}{dY} + \frac{2ma^2\lambda}{\hbar^2}Y^2 + \frac{2ma^2E}{\hbar^2}\right]\psi(Y) = 0$$

$$\left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} + \frac{2ma^2\lambda}{\hbar^2}Y^2 + \frac{2ma^2E}{\hbar^2}\right]\psi_u(Y) = 0$$

LET $K^2 = \frac{2mE}{\hbar^2}$; $K_0^2 = \frac{2m\lambda}{\hbar^2}$

$$\Rightarrow \left[Y^2\frac{d^2}{dY^2} + Y\frac{d}{dY} + (K_0a)^2Y^2 + (Ka)^2\right]\psi_u(Y) = 0$$

SOL'N OF THIS BESSEL'S EQ'N GIVES FOR $E > 0$

$$\psi_u(Y) = a_u J_{iKa}(K_0aY) + b_u J_{-iKa}(K_0aY)$$

b. $\psi_e(x)$ MUST SATISFY

$$\left[-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2}-\lambda e^{2x/a}-E\right]\psi(x)=0$$

$$\left[\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2}+\lambda e^{2x/a}+E\right]\psi(x)=0$$

LET $z=\frac{1}{Y}=e^{x/a}$

$$\frac{d}{dx}=\frac{dz}{dx}\frac{d}{dz}=\frac{1}{a}e^{x/a}\frac{d}{dz}=\frac{z}{a}\frac{d}{dz}$$

$$\frac{d^2}{dx^2}=\frac{z}{a}\frac{d}{dz}\left(\frac{z}{a}\frac{d}{dz}\right)$$

$$=\frac{z}{a}\left[\frac{z}{a}\frac{d^2}{dz^2}+\frac{d}{dz}\times\left(\frac{d}{dz}\frac{z}{a}\right)\right]$$

$$=\frac{z}{a}\left[\frac{z}{a}\frac{d^2}{dz^2}+\frac{1}{a}\frac{d}{dz}\right]$$

$$=\frac{z^2}{a^2}\frac{d^2}{dz^2}+\frac{z}{a^2}\frac{d}{dz}$$

THUS:

$$\left[\frac{\hbar^2}{2m}\left(\frac{z^2}{a^2}\frac{d^2}{dz^2}+\frac{z}{a^2}\frac{d}{dz}\right)+\lambda z^2+E\right]\psi(z)=0$$

$$\left[\frac{\hbar^2}{2ma^2}\left(z^2\frac{d^2}{dz^2}+z\frac{d}{dz}\right)+\lambda z^2+E\right]\psi(z)=0$$

$$\left[z^2\frac{d^2}{dz^2}+z\frac{d}{dz}+\frac{2m\lambda}{\hbar^2}a^2z^2+\frac{2mE}{\hbar^2}a^2\right]\psi(z)=0$$

$$\left[z^2\frac{d^2}{dz^2}+z\frac{d}{dz}+(K_0a)^2z^2+(Ka)^2\right]\psi(z)=0$$

THIS IS THE SAME D.E. AS BEFORE. THUS, LET

$$\psi_e(z)=a_e J_{ika}(K_0az)+b_e J_{-ika}(K_0az)$$

BUT, SINCE $z=\frac{1}{Y}$:

$$\psi_e(Y)=a_e J_{ika}\left(\frac{K_0a}{Y}\right)+b_e J_{-ika}\left(\frac{K_0a}{Y}\right)$$

NOW: $J_\gamma(w) = w^\gamma \sum_{m=0}^{\infty} \frac{(i w)^m}{2^{2m+\gamma}\, m!\, \Gamma(\gamma+m+1)}$

THUS: $J_{ika}\left(\frac{K_0 a}{Y}\right) = \left(\frac{K_0 a}{Y}\right)^{ika} \sum_{m=0}^{\infty} \frac{(i K_0 a / Y)^m}{2^{2m+ika}\, m!\, \Gamma(ika+m+1)}$

$$= (K_0 a e^{+x/a})^{ika} \sum_{m=0}^{\infty} \frac{(i k a\, e^{x/a})^m}{2^{2m+ika}\, m!\, \Gamma(ika+m+1)}$$

$$= (K_0 a)^{ika} e^{ikx} \sum_{m=0}^{\infty} \frac{(ika)^m e^{mx/a}}{2^{2m+ika}\, m!\, \Gamma(ika+m+1)}$$

LET $f(x) = (K_0 a)^{ika} \sum_{m=0}^{\infty} \frac{(ika)^m e^{mx/a}}{2^{2m+ika}\, m!\, \Gamma(ika+m+1)}$

THEN $J_{ika}\left(\frac{K_0 a}{Y}\right) = f(x)\, e^{ikx}$

ALSO:

$$J_{-ika}\left(\frac{K_0 a}{Y}\right) = J^*_{ika}\left(\frac{K_0 a}{Y}\right) = f^*(x)\, e^{-ikx}$$

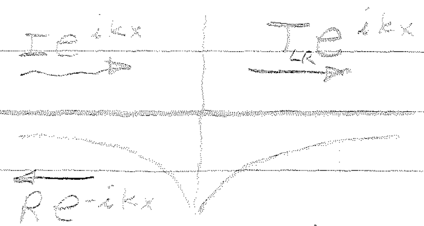
$$J_{ika}(K_0 a Y) = J_{ika}\left(\frac{K_0 a}{Y}\right)\Big|_{x=-x} = f(-x)\, e^{-ikx}$$

$$J_{-ika}(K_0 a Y) = J^*_{ika}(K_0 a Y) = f^*(-x)\, e^{ikx}$$

THE GENERAL SOLUTION MAY THEN BE WRITTEN:

$$\psi_e(x) = a_e f(x) e^{ikx} + b_e f^*(x) e^{-ikx}$$
$$\psi_o(x) = a_o f(-x) e^{-ikx} + b_o f^*(-x) e^{ikx}$$

SINCE WE WANT A SOLUTION OF THE FORM:



WE LET $a_u = 0$ LEAVING

$$\psi_\ell(x) = a_\ell f(x) e^{ikx} + b_\ell f^*(x) e^{-ikx}$$
$$\psi_u(x) = b_u f^*(x) e^{ikx}$$

IF THE PLANE WAVE REACHES THE ORIGIN @ $t = t_0$, WE DEFINE I AS THE INCIDENT PLANE WAVE AMPLITUTE @ $t = t_0^-$ WHILE R AND T_{RL} ARE MEASURED AT $t = t_0^+$. THIS IS NECESSITATED BY THE PLANE WAVE'S AMPLITUDE CHANGE WITH CHANGE IN POSITION. THUS; IF

$$I = a_\ell f(0) = a_\ell (k_0 a)^{ika} \sum_{m=0}^{\infty} \frac{(ika)^{2m}}{2^{2m+ika} m! \Gamma(ika+m+1)}$$

THEN

$$R = b_\ell f^*(0) = b_\ell (k_0 a)^{ika} \sum_{m=0}^{\infty} \frac{(ika)^{2m}}{2^{2m-ika} m! \Gamma(-ika+m+1)}$$

$$T_{LR} = b_u f^*(0) = b_u (k_0 a)^{ika} \sum_{m=0}^{\infty} \frac{(ika)^{2m}}{2^{2m-ika} m! \Gamma(-ika+m+1)}$$

IT REMAINS TO FIND a_e, b_e & b_v

FIRST:

$$\psi_e(x=0) = \psi_v(x=0)$$

$$\Rightarrow a_e J_{ika}(K_0 a) + b_e J_{-ik}(K_0 a) = b_v J_{-ika}(K_0 a)$$

$$\Rightarrow b_v = \frac{a_e J_{ika}(K_0 a) + b_e J_{-ika}(K_0 a)}{J_{-ika}(K_0 a)}$$

$$= a_e \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)} + b_e$$

LET $e^{i2\delta} = \frac{J_{ika}(K_0 a)}{J_{-ika}(K_0 a)}$ NOTE: δ IS <u>REAL</u>

$$\therefore b_v = e^{i2\delta} a_e + b_e$$

SIMILARLY

$$\psi_e'(x=0) = \psi_v'(x=0)$$

NOW:

$$\frac{d\psi_e}{dx} = \frac{d\psi_e(Y)}{dY}\frac{dY}{dx} = \left(-\frac{1}{a}\right) Y \frac{d\psi_e(Y)}{dY}$$

$$= \left(-\frac{Y}{a}\right)\frac{d}{dY}\left[a_e J_{ika}\left(\frac{K_0 a}{Y}\right) + b_e J_{-ika}\left(\frac{K_0 a}{Y}\right)\right]$$

$$W = \frac{K_0 a}{Y} \Rightarrow \frac{dW}{dY} = -\frac{K_0 a}{Y^2}$$

AND $\frac{d\psi_e}{dx} = \left(-\frac{Y}{a}\right)\frac{dW}{dY}\frac{d}{dW}\psi_e(W)$

$$= +\frac{K_0}{Y}\frac{d}{dW}\left[a_e J_{ika}(W) + b_e J_{-ika}(W)\right]$$

NOW: $\frac{d}{dw} J_{\nu}(w) = \frac{1}{2}[J_{\nu-1}(w) - J_{\nu+1}(w)]$

$$\Rightarrow \frac{d\psi_e(x)}{dx} = \frac{k_o}{2Y}\Big[a_e\{J_{ika-1}(w) - J_{ika+1}(w)\} + b_e\{J_{-ika-1}(w) - J_{-ika+1}(w)\}$$

$x \Rightarrow 0,\ Y = 1,\ w = (k_o a)$

$$\therefore \frac{d\psi_e(0)}{\delta x} = \frac{k_o}{2}\Big[a_e\{J_{ika-1}(k_o a) - J_{ika+1}(k_o a)\} + b_e\{J_{-ika-1}(k_o a) - J_{-ika+1}(k_o a)\}\Big]$$

SIMILARLY, FOR $w' = k_o a Y$

$$\frac{d}{dx}\psi_v(x) = \frac{dY}{dx}\cdot\frac{dw'}{dY}\frac{d}{dw'}\psi_v(w)$$
$$= \left(\frac{-Y}{a}\right)(k_o a)\frac{d}{dw'} b_v J_{-ika}(w)$$
$$= \frac{-k_o Y}{2} b_v\left[J_{-ika-1}(k_o a Y) - J_{-ika+1}(k_o a Y)\right]$$
$$\frac{d}{dx}\psi_v(0) = -\frac{k_o}{2} b_v\left[J_{-ika-1}(k_o a) - J_{-ika+1}(k_o a)\right]$$
$$= -\frac{k_o}{2}\left[e^{i2\delta} a_e + b_e\right]\left[J_{-ika-1}(k_o a) - J_{-ika+1}(k_o a)\right]$$

EQUATING $\frac{d}{dx}\psi_v(0)$ & $\frac{d}{dx}\psi_e(0)$ GIVES

$$-\left[e^{i2\delta} a_e + b_e\right]\left[J_{-ika-1}(k_o a) - J_{-ika+1}(k_o a)\right]$$
$$= a_e\left[J_{ika-1}(k_o a) - J_{ika+1}(k_o a)\right]$$
$$+ b_e\left[J_{-ika-1}(k_o a) - J_{-ika+1}(k_o a)\right]$$

$$a_\ell \left[J_{ika-1}(k_0 a) - J_{ika+1}(k_0 a) + e^{i2\delta} J_{-ika-1}(k_0 a) - e^{i2\delta} J_{-ika+1}(k_0 a) \right]$$

$$= -2b_\ell \left[J_{-ika-1}(k_0 a) - J_{-ika+1}(k_0 a) \right]$$

OR

$$a_\ell = \frac{-2b_\ell \left[J_{-ika-1}(k_0 a) - J_{-ika+1}(k_0 a) \right]}{\left[J_{ika-1}(k_0 a) - J_{ika+1}(k_0 a) \right] + e^{i2\delta} \left[J_{-ika-1}(k_0 a) - J_{-ika+1}(k_0 a) \right]}$$

b_ℓ CAN BE SOLVED BY NORMALIZATION OF THE WAVE FUNCTION ($\int \psi \psi^* dx = 1$) WITH KNOWLEDGE OF a_ℓ AS A FUNCTION OF b_ℓ AND b_r A FUNCTION OF b_ℓ & a_ℓ. ~~THIS GIVES~~ THE TRANSMISSION COEFFICIENT HAS A DEFINITE VALUE. DUE TO THE MESSY MATHEMATICS OF THE COMPUTATION, AT THIS POINT, I QUIT FOR $E > 0$

Do it then anyway

FOR $E<0$, K IS IMAGINARY. THUS, LET $K = i\alpha$ WHERE α IS REAL.

THE GENERAL SOL'N FOR SCHRÖDINGER'S EQUATION IS AGAIN

$$\psi_e(x) = a_e J_{ika}\left(\frac{K_0 a}{Y}\right) + b_e J_{-ika}\left(\frac{K_0 a}{Y}\right)$$
$$\psi_v(x) = a_v J_{ika}(K_0 a Y) + b_v J_{-ika}(K_0 a Y)$$

SUBSTSTITUTING $ik = -\alpha$ WE HAVE

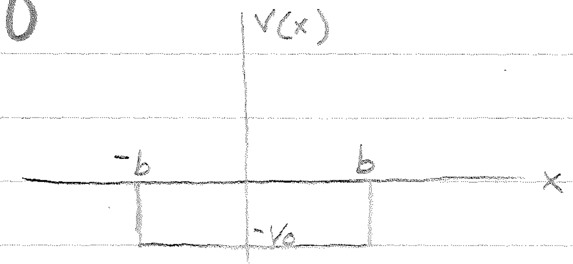
$$\psi_e(x) = a_e J_{-\alpha a}\left(\frac{K_0 a}{Y}\right) + b_e J_{\alpha a}\left(\frac{K_0 a}{Y}\right)$$
$$\psi_v(x) = b_v J_{-\alpha a}\left(\frac{K_0 a}{Y}\right) + b_v J_{\alpha a}\left(\frac{K_0 a}{Y}\right)$$

EVERYTHING (EXCEPT FOR POSSIBIBLY OF THE ARBITRARY CONSTANTS) IS REAL. THUS, ALL DECAYS IN AN EXPONENTIAL MATTER, WE CANNOT GENERATE ANY PLANE WAVES TO COMPUTE TRANSMISSION COEFFICIENTS.

5. 9/10

$$V(x) = \begin{cases} -V_0 & ; \ |x| \le b \\ 0 & ; \ |x| > b \end{cases}$$

This is really a short problem —



LET $\psi(x) = \begin{cases} \psi_\ell(x) & ; \ x \le -b \\ \psi_0(x) & ; \ -b \le x \le b \\ \psi_r(x) & ; \ x \ge b \end{cases}$

$\psi_\ell(x)$ AND $\psi_r(x)$ MUST OBEY:

$$\left[-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} - E\right]\psi(x) = 0$$

$$\left[\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + E\right]\psi(x) = 0$$

$$\left[\frac{\delta^2}{\delta x^2} + \frac{2mE}{\hbar^2}\right]\psi(x) = 0$$

FOR $E < 0$:

$$\left[\frac{\delta^2}{\delta x^2} - \frac{2m|E|}{\hbar^2}\right]\psi(x) = 0$$

LET $K^2 = \dfrac{2m|E|}{\hbar^2}$

$$\Rightarrow \left[\frac{\delta^2}{\delta x^2} - K^2\right]\psi(x) = 0$$

GIVES SOLUTION: $\psi(x) = Ae^{Kx} + Be^{-Kx}$ $\ni K$ IS POS. REAL

THUS: $\psi_\ell(x) = A_\ell e^{Kx} + B_\ell e^{-Kx}$

$\psi_r(x) = A_r e^{Kx} + B_r e^{-Kx}$

FOR $\psi(x)$ TO BE WELL-BEHAVED:

$$\lim_{x\to-\infty} \psi_\ell(x) = \lim_{x\to\infty} \psi_r(x) = 0$$

THUS LET $B_\ell = A_r = 0$

GIVING: $\psi_\ell(x) = A_\ell e^{Kx}$

$\psi_r(x) = B_r e^{-Kx}$

FOR $-b \le x \le b$

$$\left[-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} - (V_0 + E)\right]\psi_c(x) = 0$$

$$\left[\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + (V_0 + E)\right]\psi_c(x) = 0$$

$$\left[\frac{\delta^2}{\delta x^2} + \frac{2m(V_0 + E)}{\hbar^2}\right]\psi_c(x) = 0$$

FOR $E < 0$:

$$\left[\frac{\delta^2}{\delta x^2} + \frac{2m(V_0 - |E|)}{\hbar^2}\right]\psi_c(x) = 0$$

LET $K_0^2 = \frac{2mV_0}{\hbar^2}$

$$\left[\frac{\delta^2}{\delta x^2} + (K_0^2 - K^2)\right]\psi_c(x) = 0$$

GIVES SOLUTION:

$$\psi_c(x) = A_c e^{i\sqrt{K_0^2 - K^2}\,x} + B_c e^{-i\sqrt{K_0^2 - K^2}\,x}$$

$$= A_c e^{i\alpha x} + B_c e^{-i\alpha x} \quad ; \alpha = \sqrt{K_0^2 - K^2}$$

TO ASSURE CONTINUITY @ $-b$

$\Rightarrow \psi_\ell(-b) = \psi_c(-b)$

$$A_\ell e^{-Kb} = A_c e^{-i\alpha b} + B_c e^{+i\alpha b}$$

$$= A_c e^{-i\sqrt{K_0^2 - K^2}\,b} + B_c e^{+i\sqrt{K_0^2 - K^2}}$$

$\Rightarrow \psi_\ell'(-b) = \psi_c'(-b)$

$$A_\ell K e^{-Kb} = A_c(i\alpha)e^{-i\alpha b} + B_c(-i\alpha)e^{i\alpha b}$$

$$= i\alpha A_c e^{-i\alpha b} - i\alpha B_c e^{i\alpha b}$$

$$= KA_c e^{-i\alpha b} + KB_c e^{i\alpha b}$$

$$\therefore KA_c e^{-i\alpha b} + KB_c e^{i\alpha b} = i\alpha A_c e^{-i\alpha b} - i\alpha B_c e^{i\alpha b}$$

$$A_c[K - i\alpha]e^{-i\alpha b} = -B_c[K + i\alpha]e^{i\alpha b}$$

$$\underline{A_c = -\frac{K + i\alpha}{K - i\alpha}e^{i2\alpha b}B_c}$$

$$A_\ell e^{-Kb} = -\left[\frac{K + i\alpha}{K - i\alpha}\right]e^{i2\alpha b}B_c e^{-i\alpha b} + B_c e^{i\alpha b}$$

$$= \left[-\frac{K + i\alpha}{K - i\alpha}e^{i\alpha b} + e^{i\alpha b}\right]B_c$$

$$= \underline{e^{i\alpha b}\left[1 - \frac{K + i\alpha}{K - i\alpha}\right]B_c}$$

TO ASSURE CONTINUITY @ b

$$\Rightarrow \psi_v(b) = \psi_c(b)$$

$$B_v e^{-kb} = A_c e^{i\alpha b} + B_c e^{-i\alpha b}$$

$$\Rightarrow \psi_v'(b) = \psi_c'(b)$$

$$B_v(-k)e^{-kb} = A_c(i\alpha)e^{i\alpha b} + B_c(-i\alpha)e^{-i\alpha b}$$

$$-B_v k e^{-kb} = i\alpha A_c e^{i\alpha b} - i\alpha B_c e^{-i\alpha b}$$

$$= -kA_c e^{i\alpha b} - kB_c e^{-i\alpha b}$$

$$\therefore kA_c e^{i\alpha b} + kB_c e^{-i\alpha b} = -i\alpha A_c e^{i\alpha b} + i\alpha B_c e^{-i\alpha b}$$

$$A_c[k + i\alpha]e^{i\alpha b} = -B_c[k - i\alpha]e^{-i\alpha b}$$

$$\text{OR} \quad \underline{A_c = -\frac{k - i\alpha}{k + i\alpha} e^{-i2\alpha b} B_c}$$

FOR THE $-b$ CONTINUITY CALCULATIONS, WE GOT

$$A_c = -\frac{k + i\alpha}{k - i\alpha} e^{i2\alpha b} B_c$$

THE BOUND ENERGY STATES MAY THEN BE FOUND BY THE EIGEN CONDITION:

$$\frac{k - i\alpha}{k + i\alpha} e^{-i2\alpha b} = \frac{k + i\alpha}{k - i\alpha} e^{i2\alpha b}.$$

SOLVING:

$$\frac{K-i\alpha}{K+i\alpha}\, e^{-i2\alpha b} = \frac{K+i\alpha}{K-i\alpha}\, e^{i2\alpha b}$$

$$(K-i\alpha)^2 e^{-i2\alpha b} = (K+i\alpha)^2 e^{i2\alpha b}$$

$$\Rightarrow (K^2 - i2\alpha K - \alpha^2)(\cos 2\alpha b - i \sin 2\alpha b)$$

$$= (K^2 + i2\alpha K - \alpha^2)(\cos 2\alpha b + i \sin 2\alpha b)$$

$$\Rightarrow [(K^2-\alpha^2) - i2\alpha K][\cos 2\alpha b - i \sin 2\alpha b]$$

$$= [(K^2-\alpha^2) + i2\alpha K][\cos 2\alpha b + i \sin 2\alpha b]$$

$$\Rightarrow [(K^2-\alpha^2)\cos 2\alpha b - 2\alpha K \sin 2\alpha b] - i[(K^2-\alpha^2)\sin 2\alpha b + 2\alpha K \cos 2\alpha b]$$

$$= [(K^2-\alpha^2)\cos 2\alpha b - 2\alpha K \sin 2\alpha b] + i[(K^2-\alpha^2)\sin 2\alpha b + 2\alpha K \cos 2\alpha b]$$

THIS RELATIONSHIP IS TRUE ONLY IF

$$(K^2-\alpha^2)\sin 2\alpha b + 2\alpha K \cos 2\alpha b = 0$$

$$2\alpha K \cos 2\alpha b = (\alpha^2 - K^2)\sin 2\alpha b$$

$$\frac{2\alpha K}{(\alpha^2-K^2)} = \tan 2\alpha b$$

NOW: $K = \frac{\sqrt{2m|E|}}{\hbar} = \frac{\sqrt{2m}}{\hbar}\sqrt{E}$

$$\alpha^2 = K_0^2 - K^2$$

$$\Rightarrow \alpha^2 - K^2 = K_0^2 - 2K^2$$

$$= \frac{2mV_0}{\hbar^2} - 2\,\frac{2m|E|}{\hbar^2}$$

$$= \frac{2m}{\hbar^2}[V_0 - 2\ |E|]$$

$$\alpha K = \sqrt{K_0^2 - K^2}\ K$$

$$= \frac{\sqrt{2m(V_0-|E|)}}{\hbar}\ \frac{\sqrt{2m|E|}}{\hbar}$$

$$= \frac{2m\sqrt{(V_0-|E|)|E|}}{\hbar^2}$$

$$\alpha = \sqrt{\frac{2m(V_0-|E|)}{\hbar^2}}$$

THE EIGEN-RELATIONSHIP IS THEN

$$2\ \frac{4m\sqrt{(V_0-|E|)|E|}}{\hbar^2} \Big/ \frac{2m}{\hbar^2}(V_0 - 2\ |E|) = \tan \frac{2b}{\hbar}\sqrt{2m(V_0-|E|)}$$

$$\frac{2\sqrt{(V_0-|E|)|E|}}{V_0 - 2|E|} = \tan \frac{2b}{\hbar}\sqrt{2m(V_0-|E|)}$$

NOW WE GOTTA SOLVE THIS DUMB TRANSENDENTAL EQUATION WITH

$b = 10^{-10}\ m$

$V_0 = 1.60 \times 10^{-19}$ JOULES $(= 1.0\ eV)$

$h = 2\pi\hbar = 6.63 \times 10^{-34}$ JOULE-SEC

$\Rightarrow \hbar = 1.06 \times 10^{-34}$ JOULE-SEC

$m = 9.11 \times 10^{-31}$ KG

$$C = \frac{2b\sqrt{2m}}{\hbar} = \frac{2\pi \times 2 \times 10^{-10}\left[2 \times 9.11 \times 10^{-31}\right]^{1/2}}{6.63 \times 10^{-34}} = 2.56 \times 10^{9}$$

OUR LITTLE EQ'N BECOMES (WITH $|E| = E$)

$$\frac{2\sqrt{(1.6 \times 10^{-19} - E)E}}{(1.6 \times 10^{-19} - 2E)} = \tan 2.56 \times 10^{9}\sqrt{1.6 \times 10^{-19} - E}$$

ONE SOLUTION IS $|E| = V_0 = 1.0\ eV$.

(CONT)

See Schiff p. 40

LETS TAKE A LOOK @ THE TERMS IN QUESTION

$$T_1(E) = \tan C\sqrt{V_0 - E} \quad ; \quad C = \frac{2b\sqrt{2m}}{\hbar}$$

$$T_1(V_0) = 0$$

$$T_1(0) = \tan C\sqrt{V_0}$$
$$= \tan (2.56\times10^9)\sqrt{1.6\times10^{-19}}$$
$$= \tan (2.56\times10^9)(4\times10^{-10})$$
$$= \tan 1.024$$
$$= 1.643$$

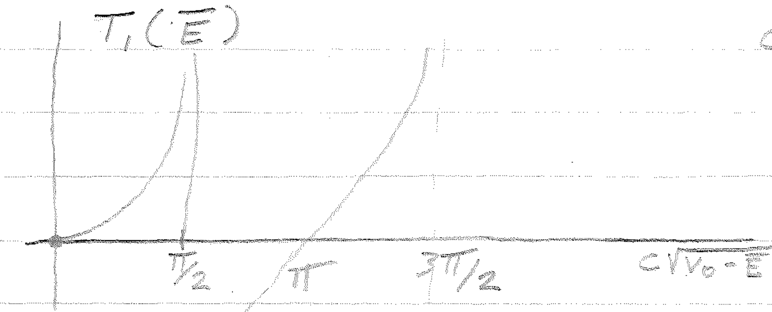
$$\frac{d}{dE}\tan C\sqrt{V_0 - |E|} = \left[\sec^2 C\sqrt{V_0-E}\right]\frac{d}{dE}C\sqrt{V_0-|E|}$$
$$= \left[\sec^2 C\sqrt{V_0-E}\right]\frac{-\frac{1}{2}C}{\sqrt{V_0-E}}$$

$$= \frac{-\frac{1}{2}C\sec^2 C\sqrt{V_0-E}}{\sqrt{V_0-E}} = 0$$

$$\Rightarrow \sec^2 C\sqrt{V_0-E} = \frac{1}{\cos^2 C\sqrt{V_0-E}} = 0$$

∴ THERE ARE NO RELATIVE MAXIMA OR MINIMA FOR $T_1(E)$. WHAT ABOUT DISCONTINUITY?

$$C\sqrt{V_0-E} = \frac{n\pi}{2}$$



∴ DISCONTINUITIES @ $C\sqrt{V_0-E} = \frac{\pm(n+1)\pi}{2}$

$$\Rightarrow E = V_0 - \left[\frac{(n+1)\pi}{2C}\right] < 0 \Rightarrow E > 0$$

∴ $T_1(E)$ IS MONOTONIC ON THE INTERVAL $0 < E < V_0$

$$T_2(\overline{E}) = \frac{2\sqrt{(V_0 - \overline{E})\,\overline{E}}}{V_0 - 2|\overline{E}|}$$

$$T_2(0) = 0, \quad T_2(V_0) = 0, \quad T_2\left(\frac{V_0}{2}\right) = \infty$$

HOW MANY RELATIVE MAXIMA TWIXT 0 & V_0?

$$\frac{dT_2(\overline{E})}{d\overline{E}} = \frac{2(V_0 - 2\overline{E})\frac{d}{d\overline{E}}\sqrt{V_0\overline{E} - \overline{E}^2} - 2\sqrt{V_0\overline{E} - \overline{E}^2}\,(-2)}{(V_0 - 2\overline{E})^2} = 0$$

$$\Rightarrow (V_0 - 2\overline{E})\frac{\frac{1}{2}\left[V_0 - 2\overline{E}\right]}{\sqrt{V_0\overline{E} - \overline{E}^2}} + 2\sqrt{V_0\overline{E} - \overline{E}^2} = 0$$

$$\frac{(V_0 - 2\overline{E})(V_0 - 2\overline{E})}{2\sqrt{V_0\overline{E} - \overline{E}^2}} = -2\sqrt{V_0\overline{E} - \overline{E}^2}$$

$$(V_0 - 2\overline{E})^2 = -4(V_0\overline{E} - \overline{E}^2)$$

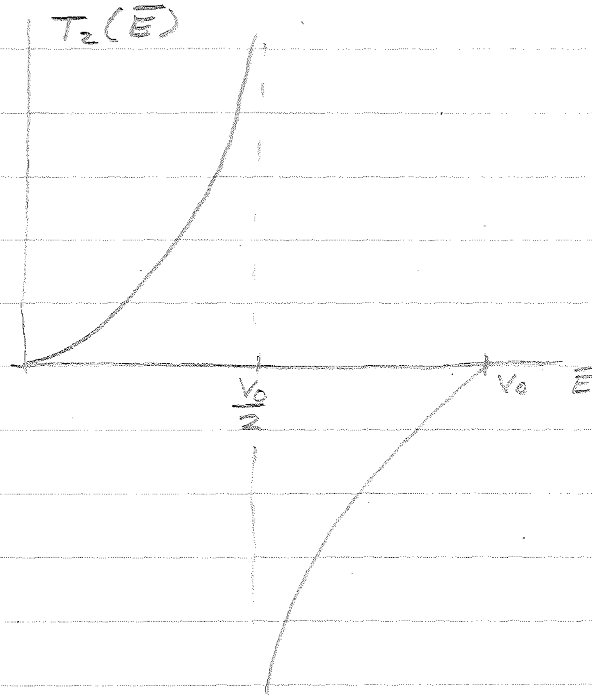
$$V_0^2 - \cancel{4V_0\overline{E}} + \cancel{4\overline{E}^2} = -\cancel{4V_0\overline{E}} + \cancel{4\overline{E}^2}$$

$$V_0^2 = 0 \Leftarrow \text{INCONSISTANT}$$

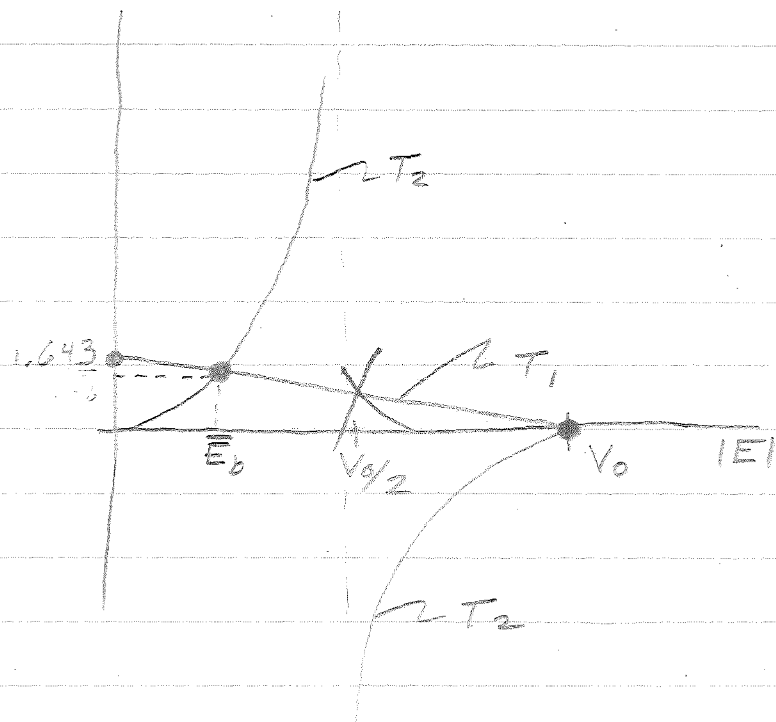
$\therefore$ NO RELATIVE MAXIMA OR MINIMA FOR $T_2(\overline{E})$

NOW $T_2\left(\frac{V_0}{2}-\right) > 0 \quad T_2\left(\frac{V_0}{2}+\right) < 0$

SO ROUGHLY:



SO GRAPHING T_1 & T_2 TOGETHER ROUGHLY GIVES:



THE BOUND STATE ENERGYES ARE GIVEN BY THE INTERSECTIONS OF THE PLOTS. ONE, @ $\bar{E} = V_0$ ($E = -V_0$) HAS ALREADY BEEN IDENTIFIED. THE OTHER, DENOTED BY $\bar{E}_b$ ON THE GRAPH, MAY BE DETERMINED BY THE TRIAL & ERROR METHOD TO FOLLOW.

$\bar{E}$ (JOULES)	$T_1 = \tan 2.56\times10^{9}\sqrt{1.6\times10^{-19}-\bar{E}}$	$T_2 = \frac{2\sqrt{(1.6\times10^{-19}-\bar{E})\bar{E}}}{1.6\times10^{-19}-2\bar{E}}$	LIMITS $0 < \bar{E}_b \leq 0.8\times10^{-19} = \frac{V_0}{2}$
0	1.643	0	$0 < \bar{E}_b < 0.8\times10^{-19}$
0.3×10^{-19}	1.32	1.25	$0.3\times10^{-19} < \bar{E}_b < 0.8\times10^{-19}$
0.35×10^{-19}	1.27	1.47	$0.3\times10^{-19} < \bar{E}_b < 0.35\times10^{-19}$
0.32×10^{-19}	1.302	1.33	$0.30\times10^{-19} \leq \bar{E}_b \leq 0.32\times10^{-19}$
0.31×10^{-19}	1.31	1.29	$0.31\times10^{-19} \leq \bar{E}_b \leq 0.32\times10^{-19}$

THUS, $0.31\times10^{-19} \leq \bar{E}_b \leq 0.32\times10^{-19}$ (JOULES). SINCE 0.31×10^{-19} GIVES THE CLOSEST EQUALITY IN T_1 AND T_2, LET

$$\bar{E}_b = 0.31\times10^{-19} \text{ JOULES}$$

$$\text{OR } E_b = -0.31\times10^{-19} \text{ JOULES} \times \frac{1\,eV}{1.6\times10^{-19}\text{ JOULE}}$$

$$= -0.194\ eV$$

Phys 611
Due: Feb 6, 1975
#3

(1) For the repulsive exponential potential, the wave function had the form

$$\psi(x) = C_1 [\, I_{ika}(k_0 a y) - I_{-ika}(k_0 a y) \,]$$

Find the coefficient C_1 for delta function normalization.

(2) For the Morse potential, find the phase shifts for energy states $E > 0$.

(3) For the Morse potential, make a plot of potential strength $S = \left(\frac{2mA}{\hbar^2 \alpha^2} \right)^{1/2}$ for $0 \leq S \leq 5$ against bound state energy $-E/A$.

(4) From the definition of the confluent hypergeometric function, show that it is the solution to the differential equation

$$\left[z \frac{d^2}{dz^2} + (b - z) \frac{d}{dz} - a \right] F(a, b, z) = 0$$

(5) Consider the one dimensional Schrodinger equation with the delta function potential $V(x) = -\lambda \delta(x)$.

a. For each value of energy $E > 0$, construct two wave functions which are orthogonal to each other, and normalized according to delta function normalization.

b. Show, by explicit integration in x-space, that these wave functions are also orthogonal to the bound state wave function.

c. Show, by explicit integration in k-space, that these wave functions form a complete set.

PHYS. 611
DUE: FEB 6, 1975
BOB MARKS

39/50

1. 9/10 $\psi(x) = C_1 \left[I_{ika}(k_0 a y) - I_{-ika}(k_0 a y) \right]$

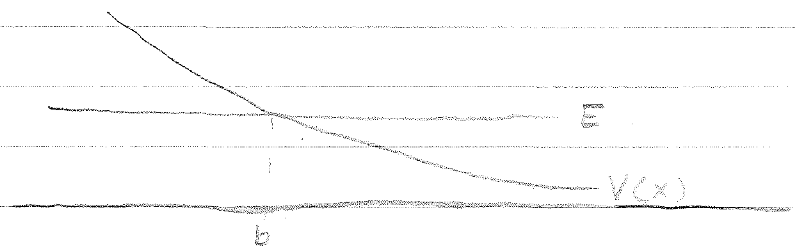
IT WAS SHOWN PREVIOUSLY THAT

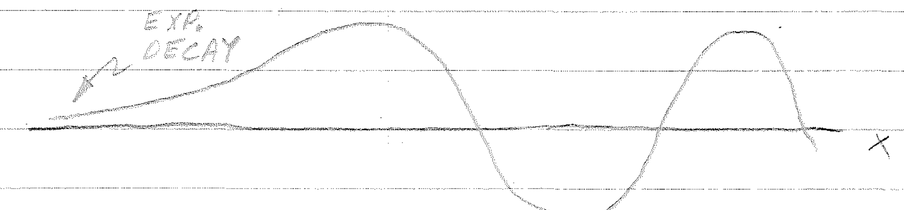
$$\lim_{x\to\infty} \psi(x) = \frac{C_1 (k_0 a)^{ika}}{\Gamma(1+ika)} (i2) e^{i\delta} \sin(kx+\delta)$$

$$= C_2 \sin(kx+\delta)$$

WHERE $e^{i2\delta} = (k_0 a)^{-i2ka} \dfrac{\Gamma(1+ika)}{\Gamma(1-ika)}$

THE POTENTIAL AND WAVE FUNCTION ARE ROUGHLY:





THUS, FOR A POINT $X_0 \gg b \ni V(b) = E$, THE WAVE EQUATION IS AS GIVEN IN THE ABOVE LIMIT.

WE WISH TO FIND C_2 SUCH THAT

$$\int_{-\infty}^{\infty} \psi_k(x)\, \psi_{k'}^*(x)\, dx = \delta(k-k')$$

NOW:

$$\delta(k-k') = \int_{-\infty}^{b} \psi_k(x)\psi_{k'}^*(x)dx + \int_{b}^{\infty} \psi_k \psi_{k'}^*(x)dx$$

$\int_{-\infty}^{b} \psi_k(k)\psi_{k'}^*(x)dx$ IS FINITE

$$\int_{b}^{\infty} \psi_k(x)\psi_{k'}(x)\,dx = |C_2|^2 \int_{b}^{\infty} \sin(kx+\delta)\sin(k'x+\delta)dx$$

IT WAS DEMONSTRATED IN CLASS VIA DELTA FUNCTION NORMALIZATION THAT:

$$|C_2|^2 \int_{b}^{\infty} \sin(kx+\delta)\sin(k'x+\delta)dx = |C_2|^2 \frac{\pi}{2}\delta(k-k')$$

THE VALUE GENERATED BY THE WAVE FUNCTION FROM $-\infty$ TO b IS INCONSEQUENTIAL COMPARED TO THE INFINITE VALUE OF $\delta(k-k')$. THE RESIDUAL VALUE FROM THE b TO ∞ INTEGRATION IS LIKEWISE ASSUMED INSIGNIFICANT. THUS:

$$\int_{-\infty}^{\infty} \psi(x)\psi^*(x)\,dx = |C_2|^2 \frac{\pi}{2}\delta(k-k')$$

$$\Rightarrow |C_2| = \pm\sqrt{2/\pi} \Rightarrow C_2 = \sqrt{2/\pi}\, e^{i\phi'}$$

$\ni \phi$ IS x INDEPENDENDENT AND REAL

NOW

$$-C_2 = \sqrt{\tfrac{2}{\pi}}\, e^{i\phi} = \frac{+C_1 (K_0 a)^{ika}}{\Gamma(1+ika)\,(i2)\,e^{i\delta}}$$

$$\Rightarrow C_1 = \sqrt{\tfrac{2}{\pi}}\, e^{i\phi}\, \frac{\Gamma(1+ika)}{(K_0 a)^{ika}} \left(\frac{i}{2}\right) e^{-i\delta}$$

$$= i\sqrt{\tfrac{1}{2\pi}}\, \Gamma(1+ika)\, (K_0 a)^{-ika}\, e^{-i(\delta-\phi)}$$

NOW, SINCE δ IS REAL AND X INDEPENDENT AND ϕ IS ARBITRARY, REAL AND X INDEPENDENT, THEN $(\delta - \phi)$ CAN TAKE ON ANY REAL X INDEPENDENT VALUE. AS SUCH, LET

$$\theta = \delta - \phi$$

WHERE θ IS AN ARBITRARY REAL X INDEPENDENT VALUE. THEN THE FINAL EXPRESSION FOR C_1 IS

$$C_1 = \cancel{i}\sqrt{\tfrac{1}{\pi}}\, \Gamma(1+ika)\, (K_0 a)^{-ika}\, e^{-i\theta}$$

2. MORSE POTENTIAL SOLUTION IS 10/10

$$\psi(Y) = e^{-sY}\left[c_1 Y^{t} F\left(\tfrac{1}{2}+t-s;\ 1+2t;\ 2sY\right) + c_2 Y^{-t} F\left(\tfrac{1}{2}-t-s,\ 1-2t;\ 2sY\right)\right]$$

$$Y = e^{-\alpha(x-x_0)}$$

$$t^2 = \frac{-2mE}{\hbar^2\alpha^2}$$

$$s^2 = \frac{2mA}{\hbar^2\alpha^2}$$

FOR $E>0$, LET $t = ik$ WHERE k IS REAL

$$\therefore \psi(Y) = e^{-sY}\left[c_1 Y^{ik} F\left(\tfrac{1}{2}+ik-s;\ 1+i2k;\ 2sY\right) + c_2 Y^{-ik} F\left(\tfrac{1}{2}-ik-s;\ 1-i2k;\ 2sY\right)\right]$$

BOUNDARY CONDITIONS DICTATE

$$\lim_{x\to-\infty}\psi(x) = \lim_{Y\to\infty}\psi(Y)$$

SINCE $\lim_{z\to\infty} F(a,b;z) = \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^{z}$

$$\lim_{Y\to\infty}\psi(Y) = \lim_{Y\to\infty} e^{-sY}\left[c_1 Y^{ik}\frac{\Gamma(1+i2k)}{\Gamma(\frac{1}{2}+ik-s)}(2sY)^{-(\frac{1}{2}+ik+s)} e^{2sY} + c_2 Y^{-ik}\frac{\Gamma(1-2ik)}{\Gamma(\frac{1}{2}-ik-s)}(2sY)^{-\frac{1}{2}+ik-s} e^{2sY}\right]$$

$$= \lim_{Y\to\infty} e^{sY}\left[c_1 Y^{ik}(2sY)^{-ik}(2sY)^{-\frac{1}{2}-s}\frac{\Gamma(1+i2k)}{\Gamma(\frac{1}{2}+ik-s)} + c_2 Y^{-ik}(2sY)^{ik}(2sY)^{-\frac{1}{2}-s}\frac{\Gamma(1-2ik)}{\Gamma(\frac{1}{2}-ik-s)}\right]$$

$$= \lim_{Y\to\infty} e^{sY}(2sY)^{-\frac{1}{2}-s}\left[c_1(2s)^{-ik}\frac{\Gamma(1+i2k)}{\Gamma(\frac{1}{2}+ik-s)} + c_2(2s)^{ik}\frac{\Gamma(1-i2k)}{\Gamma(\frac{1}{2}-ik-s)}\right]$$

THIS TERM BLOWS UP UNLESS THE Y INDEPENDENT TERMS VANISH. THUS, LET

$$C_2 (2S)^{ik} \frac{\Gamma(1-i2k)}{\Gamma(\frac{1}{2}-ik-S)} = -C_1 (2S)^{-ik} \frac{\Gamma(1+i2k)}{\Gamma(\frac{1}{2}+ik-S)}$$

$$\therefore C_2 = -C_1 \frac{(2S)^{-ik}}{(2S)^{ik}} \frac{\Gamma(1+i2k)}{\Gamma(1-i2k)} \frac{\Gamma(\frac{1}{2}-ik-S)}{\Gamma(\frac{1}{2}+ik-S)}$$

ALL NUMERATOR DENOMINATOR PAIRS ARE COMPLEX CONJUGATE. THUS, LET

$$e^{i2\delta'} = \frac{(2S)^{-ik}}{(2S)^{ik}} \frac{\Gamma(1+i2k)}{\Gamma(1-i2k)} \frac{\Gamma(\frac{1}{2}-ik-S)}{\Gamma(\frac{1}{2}+ik-S)}$$

[δ' WILL LATER BE SHOWN TO BE IN THE PHASE SHIFT]

SUBSTITUTING INTO WAVE FUNCTION:

$$\psi(Y) = C_1 e^{-SY} \Big[Y^{ik} F(\tfrac{1}{2}+ik-S, 1+i2k; 2SY) - Y^{-ik} e^{i2\delta'} F(\tfrac{1}{2}+ik-S, 1+i2k; 2SY) \Big]$$

WE WISH TO LOOK AT ψ @ $x \Rightarrow \infty$, OR EQUIVALENTLY, AT $Y \Rightarrow 0$. FOR SMALL Y, $e^{-St} \simeq 1$. ALSO, SINCE

$$F(a,b;z) = 1 + \frac{a}{b} z + \frac{a(a+1)}{b(b+1)} \frac{z^2}{2!} + \ldots$$

THEN: $F(a;b;z) \simeq 1$

THUS FOR VERY SMALL Y (VERY LARGE X):

$$\psi(Y) = C_1\left[Y^{ik} - Y^{-ik} e^{i2\delta'}\right]$$

SINCE $Y = e^{-\alpha(x-x_0)}$ THEN, FOR VERY LARGE X

$$\psi(x) = C_1\left[e^{-ik\alpha(x-x_0)} - e^{i2\delta'} e^{ik\alpha(x-x_0)}\right]$$

$$= C_1 e^{+ik\alpha x_0}\left[e^{-ik\alpha x} - e^{i2\delta'} e^{-ik\alpha x_0} e^{-ik\alpha x_0} e^{ik\alpha x}\right]$$

$$= C_1'\left[e^{-ik\alpha x} - e^{i2[\delta' - k\alpha x_0]} e^{ik\alpha x}\right]$$

$$\therefore e^{i2\delta_K} = e^{i2\delta'} e^{-i2k\alpha x_0}$$

$$= (2s)^{-i2k} \frac{\Gamma(1+i2k)}{\Gamma(1-i2k)} \frac{\Gamma(\frac{1}{2}-ik-s)}{\Gamma(\frac{1}{2}+ik-s)} e^{-i2k\alpha x_0}$$

$$= (2s)^{-2t} \frac{\Gamma(1+2t)}{\Gamma(1-2t)} \frac{\Gamma(\frac{1}{2}-t-s)}{\Gamma(\frac{1}{2}+t-s)} e^{-2t\alpha x_0}$$

$\Rightarrow \delta_K$ IS THE PHASE SHIFT ✓

3. $\frac{10}{10}$ $s = \left(\frac{2mA}{\hbar^2\alpha^2}\right)^{1/2}$

THE BOUND ENERGY STATES FOR THE MORSE POTENTIAL WERE SHOWN TO BE

$$E_n = -A\left[1 - \frac{(n+1/2)}{s}\right]^2 \quad \text{UNDER THE CONSTRAINT} \quad n \leq s - \tfrac{1}{2}$$

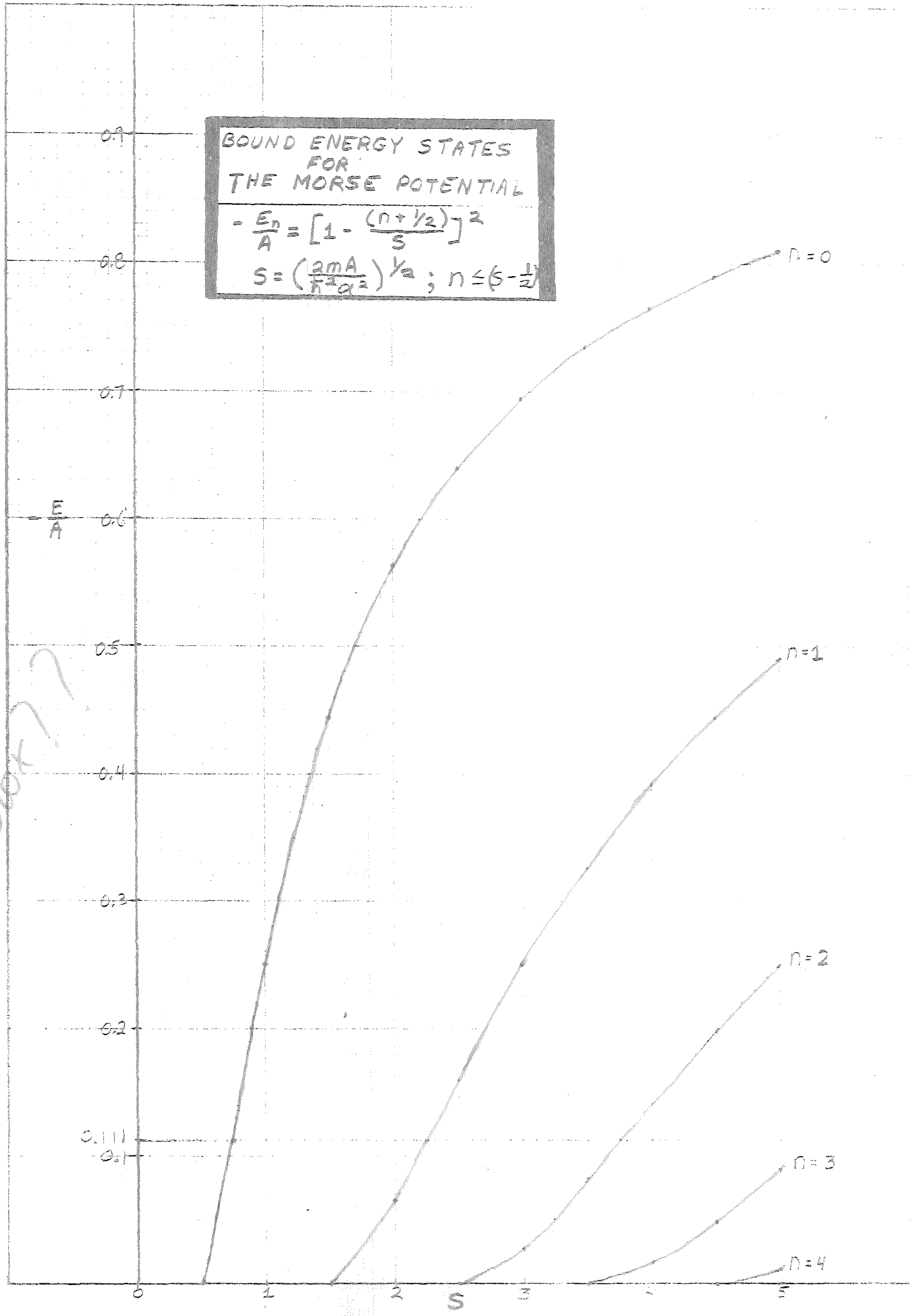
NOW $-\frac{E_n}{A} = \left[1 - \frac{(n+1/2)}{s}\right]^2$

$$\frac{d(-E_n/A)}{dE_n} = 2\left(n+\tfrac{1}{2}\right)\frac{1}{s^2}\left[1 - \frac{(n+1/2)}{s}\right]$$

$$\frac{d^2(-E_n/A)}{dE_n^2} = 0 = \frac{-2}{s^3} - \frac{(-3)(n+1/2)}{s^4} \Rightarrow s = \frac{3}{2}\left(n+\tfrac{1}{2}\right) \Leftarrow \text{INFLECTION POINTS}$$

s	$-E_0/A$	$-E_1/A$	$-E_2/A$	$-E_3/A$	$-E_4/A$	$-E_5/A$
0.5	0.000	—	—	—	—	—
* 0.75	*(0.111)	—	—	—	—	—
1.0	0.250	—	—	—	—	—
1.5	0.444	0.000	—	—	—	—
2.0	0.563	0.063	—	—	—	—
* 2.25		*(0.111)	—	—	—	—
2.5	0.640	0.160	0.000	—	—	—
3.0	0.694	0.250	0.028	—	—	—
3.5	0.735	0.326	0.082	0.000	—	—
* 3.75			*(0.111)			
4.0	0.766	0.391	0.141	0.016	—	—
4.5	0.790	0.444	0.198	0.049	0.000	—
5.0	0.810	0.490	0.250	0.090	0.010	—

* INFLECTION POINTS



BOUND ENERGY STATES
FOR
THE MORSE POTENTIAL
$-\frac{E_n}{A} = \left[1 - \frac{(n+1/2)}{S}\right]^2$
$S = \left(\frac{2mA}{\hbar^2 a^2}\right)^{1/2}$; $n \le (S - \frac{1}{2})$
$-\frac{E}{A}$
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.111
0.1
0
1
2
3
5
S
n = 0
n = 1
n = 2
n = 3
n = 4

Keep??

4. $F(a, b; z) = 1 + \frac{a}{b} z + \frac{a(a+1)}{b(b+1)} \frac{z^2}{2!} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)} \frac{z^3}{3!}$

10

WE WISH TO SHOW

$$\left[z \frac{d^2}{dz^2} + (b-z) \frac{d}{dz} - a \right] F(a, b; z) = 0$$

NOW:

$$F(a, b; z) = 1 + \sum_{n=1}^{\infty} \left[\prod_{j=1}^{n} \frac{a+1-j}{b+1-j} \right] \frac{z^n}{n!}$$

$$\frac{dF(a,b;z)}{dz} = \frac{a}{b} + \frac{a}{b} \frac{(a+1)}{(b+1)} z + \frac{a(a+1)(a+2)}{b(b+1)(b+2)} \frac{z^2}{2!} + \ldots$$

$$= \frac{a}{b} \left[1 + \frac{(a+1)}{(b+1)} z + \frac{(a+1)(a+2)}{(b+1)(b+2)} \frac{z^2}{2!} + \ldots \right]$$

$$= \frac{a}{b} F(a+1, b+1; z)$$

$$\frac{d^2 F(a,b;z)}{dz^2} = \frac{a}{b} \frac{(a+1)}{(b+1)} F(a+2; b+2; z)$$

$$z \frac{d^2}{dz^2} F(a, b; z) = z \frac{a}{b} \frac{(a+1)}{(b+1)} \left[1 + \sum_{n=1}^{\infty} \left(\prod_{j=1}^{n} \frac{a+3-j}{b+3-j} \right) \frac{z^n}{n!} \right]$$

$$= \frac{a(a+1)}{b(b+1)} z + \frac{a(a+1)}{b(b+1)} \sum_{n=1}^{\infty} \left(\prod_{j=1}^{n} \frac{a+3-j}{b+3-j} \right) \frac{z^{n+1}}{n!}$$

$$= \frac{a(a+1)}{b(b+1)} z + \frac{a(a+1)(a+2)}{b(b+1)(b+2)} z^2 + \frac{a(a+1)(a+2)(a+3)}{b(b+1)(b+2)(b+3)} \frac{z^3}{2!} +$$

$$z \frac{d}{dz} F(a, b; z) = \frac{za}{b} F(a+1, b+1; z)$$

$$= \frac{za}{b} \left[1 + \frac{(a+1)}{(b+1)} z + \frac{(a+1)(a+2)}{(b+1)(b+2)} \frac{z^2}{2!} + \frac{(a+1)(a+2)(a+3)}{(b+1)(b+2)(b+3)} \frac{z^3}{3!} + \ldots \right.$$

$$= \frac{a}{b} z + \frac{a(a+1)}{b(b+1)} z^2 + \frac{a(a+1)(a+2)}{b(b+1)(b+2)} \frac{z^3}{2!} + \ldots$$

$$\therefore\ z\left(\frac{d^2}{dz^2}-\frac{d}{dz}\right)F(a,b;z)$$

$$=\left[\frac{a(a+1)}{b(b+1)}-\frac{a}{b}\right]z+\left[\frac{a(a+1)(a+2)}{b(b+1)(b+2)}-\frac{a(a+1)}{b(b+1)}\right]z^2$$

$$+\left[\frac{a(a+1)(a+2)(a+3)}{b(b+1)(b+2)(b+3)}-\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\right]\frac{z^3}{2!}+\ldots$$

$$=\frac{a}{b}\left[\frac{(a+1)}{(b+1)}-1\right]z+\frac{a(a+1)}{b(b+1)}\left[\frac{(a+2)}{(b+2)}-1\right]z^2$$

$$+\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\left[\frac{(a+3)}{(b+3)}-1\right]\frac{z^3}{2!}+\ldots$$

$$=\sum_{n=1}^{\infty}\left(\prod_{j=1}^{n}\frac{a+1-j}{b+1-j}\right)\left(\frac{a+n}{b+n}-1\right)\frac{z^n}{(n-1)!}$$

NOW

$$b\frac{d}{dz}F(a,b;z)=a\,F(a+1,b+1;z)$$

$$=a\left[1+\frac{(a+1)}{(b+1)}z+\frac{(a+1)(a+2)}{(b+1)(b+2)}\frac{z^2}{2!}+\frac{(a+1)(a+2)(a+3)}{(b+1)(b+2)(b+3)}\frac{z^3}{3!}+\ldots\right.$$

$$a\,F(a,b;z)=a\left[1+\frac{a}{b}z+\frac{a(a+1)}{b(b+1)}\frac{z^2}{2!}+\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{z^3}{3!}+\ldots\right]$$

$$\therefore\left[b\frac{d}{dz}-a\right]F(a,b;z)=a\left[\frac{(a+1)}{(b+1)}-\frac{a}{b}\right]z+a\left[\frac{(a+1)(a+2)}{(b+1)(b+2)}-\frac{a(a+1)}{b(b+1)}\right]\frac{z^2}{2!}$$

$$+a\left[\frac{(a+1)(a+2)(a+3)}{(b+1)(b+2)(b+3)}-\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\right]\frac{z^3}{3!}+\ldots$$

$$= a\left[\frac{(a+1)}{(b+1)} - \frac{a}{b}\right] z + \frac{a(a+1)}{(b+1)}\left[\frac{(a+2)}{(b+2)} - \frac{a}{b}\right]\frac{z^2}{2!}$$

$$+ \frac{a(a+1)(a+2)}{(b+1)(b+2)}\left[\frac{(a+3)}{(b+3)} - \frac{a}{b}\right]\frac{z^3}{3!} + \ldots$$

$$= a\left[\frac{(a+1)}{(b+1)} - \frac{a}{b}\right] z + a\sum_{n=2}^{\infty}\left(\prod_{i=2}^{n}\frac{a+2-i}{b+2-i}\right)\left(\frac{(a+n)}{(b+n)} - \frac{a}{b}\right)\frac{z^n}{n!}$$

THUS $\left[z\frac{d^2}{dz^2} + (b-z)\frac{d}{dx} - a\right] F(a, b; z)$

$$= \left[a\left(\frac{(a+1)}{(b+1)} - \frac{a}{b}\right) + \frac{a}{b}\left(\frac{(a+1)}{(b+1)} - 1\right)\right] z$$

$$+ \left[\frac{a(a+1)}{(b+1)}\left(\frac{(a+2)}{(b+2)} - \frac{a}{b}\right) + \frac{2a(a+1)}{b(b+1)}\left(\frac{(a+2)}{(b+2)} - 1\right)\right]\frac{z^2}{2!}$$

$$+ \left[\frac{a(a+1)(a+2)}{(b+1)(b+2)}\left(\frac{(a+3)}{(b+3)} - \frac{a}{b}\right) + \frac{3a(a+1)(a+2)}{b(b+1)(b+2)}\left(\frac{(a+3)}{(b+3)} - 1\right)\right]\frac{z^3}{3!} + \ldots$$

$$= a\left[\frac{(a+1)}{(b+1)} - \frac{a}{b} + \frac{(a+1)}{b(b+1)} - \frac{1}{b}\right] z$$

$$+ a\frac{(a+1)}{(b+1)}\left[\frac{(a+2)}{(b+2)} - \frac{a}{b} + \frac{2(a+2)}{b(b+2)} - \frac{2}{b}\right]\frac{z^2}{2!}$$

$$+ a\frac{(a+1)(a+2)}{(b+1)(b+2)}\left[\frac{(a+3)}{(b+3)} - \frac{a}{b} + \frac{3(a+3)}{b(b+3)} - \frac{3}{b}\right]\frac{z^3}{3} + \ldots$$

$$= \frac{a}{b(b+1)}\left[b(a+1) - a(b+1) + (a+1) - (b+1)\right] z$$

$$+ \frac{a(a+1)}{b(b+1)(b+2)}\left[b(a+2) - a(b+2) + 2(a+2) - 2(b+2)\right]\frac{z^2}{2!}$$

$$+ \frac{a(a+1)(a+2)}{b(b+1)(b+2)(b+3)}\left[b(a+3) - a(b+3) + 3(a+3) - 3(b+3)\right]\frac{z^3}{3!} + \ldots$$

$$= \frac{a}{b(b+1)}\left[ba + b - ab - a + a + 1 - b - 1\right] z$$

$$+ \frac{a(a+1)}{b(b+1)(b+2)}\left[ba + 2b - ab - 2a + 2a + 4 - 2b - 4\right]\frac{z^2}{2!}$$

$$+ \frac{a(a+1)(a+2)}{b(b+1)(b+2)(b+3)}\left[ba + 3b - ab - 3a + 3a + 9 - 3b - 9\right]\frac{z^3}{4!} + \ldots$$

THE n^{TH} TERM WOULD BE:

$$\left[\frac{1}{b}\prod_{i=1}^{n}\frac{a+1-i}{b+2-i}\right]\left[ba + nb - ab - na + na + n^2 - nb - n^2\right]\frac{z^n}{n!} = 0$$

$$\therefore \left[z\frac{d^2}{dz^2} + (b-z)\frac{d}{dz} - a\right]F(a,b;z) = 0$$

D

5. $V(x) = -\lambda\,\delta(x)$

$$\left[\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + \lambda\,\delta(x) + E\right]\psi(x) = 0$$

$$\left[\frac{\delta^2}{\delta x^2} + \frac{2m\lambda}{\hbar^2}\,\delta(x) + \frac{2mE}{\hbar^2}\right]\psi(x) = 0$$

$$\left[\frac{\delta^2}{\delta x^2} + 2\alpha\,\delta(x) - \kappa^2\right]\psi(x) = 0$$

$$\Rightarrow \alpha = \frac{m\lambda}{\hbar^2}\ ; \quad \kappa^2 = -\frac{2mE}{\hbar^2} \Rightarrow \frac{\alpha}{\lambda} = -\frac{\kappa^2}{2E}$$

$$\left[\frac{\delta^2}{\delta x^2} - \kappa^2\right]\psi(x) = -2\alpha\,\psi(0)\,\delta(x)$$

BESIDES SATISFYING THIS DIFFERENTIAL EQUATION

1. $\psi(x)$ MUST BE CONTINUOUS

2. $\psi'(0-) - \psi'(0+) = \frac{2m\lambda}{\hbar^2}\psi(0) = 2\alpha\,\psi(0)$

FOR $E<0$, κ IS REAL AND SOLUTION IS

$$\psi(x) = \begin{cases} A e^{\alpha x} & ; x<0 \\ A e^{-\alpha x} & ; x>0 \end{cases}$$

$$\psi'(0) = \begin{cases} \alpha A & ; x = 0^- \\ -\alpha A & ; x = 0^+ \end{cases}$$

$$\Rightarrow -2\alpha A = -\frac{2m\lambda}{\hbar^2}A \Rightarrow \alpha = \frac{m\lambda}{\hbar^2} \quad ([illegible])$$

$$\int_{-\infty}^{\infty}\psi(x)\psi^*(x)\,dx = |A|^2\int_{-\infty}^{0} e^{2\alpha x}\,dx + |A|^2\int_0^{\infty} e^{-2\alpha x}\,dx$$

$$= 2|A|^2\int_0^{\infty} e^{-2\alpha x}\,dx$$

$$= -\frac{1}{2\alpha}|A|^2\left[e^{-2\alpha x}\right]_0^{\infty}$$

$$= \frac{1}{\alpha}|A|^2$$

$$= 1$$

$$\therefore |A| = \sqrt{\alpha}$$

$$\therefore \psi(x) = \pm\sqrt{\alpha}\,e^{-\alpha|x|}$$

LET $\mu(x) = \begin{cases} 1 & ; x>0 \\ 0 & ; x<0 \end{cases}$

THEN $\psi(x) = \pm\sqrt{\alpha}\left[e^{\alpha x}\mu(-x) + e^{-\alpha x}\mu(x)\right]$

SINCE $\frac{d}{dx}\mu(x) = \delta(x)$ AND $\frac{d}{dx}\mu(-x) = -\delta(x)$:

$$\frac{d\psi(x)}{dx} = \sqrt{\alpha}\left[\alpha e^{\alpha x}\mu(-x) - \delta(x) - \alpha e^{-\alpha x}\mu(x) + \delta(x)\right]$$
$$= \alpha^{3/2}\left[e^{\alpha x}\mu(-x) - e^{-\alpha x}\mu(x)\right]$$
$$\frac{d^2\psi(x)}{dx^2} = \alpha^{3/2}\left[\alpha e^{\alpha x}\mu(-x) - \delta(x) + \alpha e^{-\alpha x}\mu(x) - \delta(x)\right]$$
$$= \alpha^2\left[\sqrt{\alpha}\left\{e^{\alpha x}\mu(-x) + e^{-\alpha x}\mu(x)\right\} - \frac{2}{\sqrt{\alpha}}\delta(x)\right]$$
$$= \alpha^2\left[\psi(x) - \frac{2}{\sqrt{\alpha}}\delta(x)\right]$$

THUS:

$$\left[\frac{\delta^2}{\delta x^2} - \kappa^2\right]\psi(x) = \alpha^2\left[\psi(x) - \frac{2}{\sqrt{\alpha}}\delta(x)\right] - \kappa^2\psi(x)$$
$$= -2\alpha^{3/2}\delta(x)$$

$$\therefore \left[\alpha^2 - \kappa^2\right]\psi(x) = 0$$
$$\Rightarrow \alpha^2 = \kappa^2$$
$$\left(\frac{m\lambda}{\hbar^2}\right)^2 = \frac{-2mE}{\hbar^2}$$
$$\frac{m^2\lambda^2}{\hbar^2} = -2mE \Rightarrow E = \frac{-m\lambda^2}{2\hbar^2} \Leftarrow \text{BOUND STATE}$$

THE BOUND STATE WAVE FUNCTION IS

$$\psi(x) = \sqrt{\alpha}\, e^{i\phi}\left[e^{\alpha x}\mu(-x) + e^{-\alpha x}\mu(x)\right]$$

$\ni \phi$ IS REAL AND x INDEPENDENT

a. A SOLUTION TO THE WAVE EQUATION FOR $E > 0$ AND $x = 0$ IS

$$\psi(x) = A e^{-i\alpha' x} + B e^{i\alpha x}$$

WE MUST HAVE A "CUSP" LIKE RELATIONSHIP AT THE ORIGIN. CONSIDER THEN:

$$\psi(x) = \begin{cases} A e^{i\alpha' x} + B e^{-i\alpha' x} & ; x < 0 \\ C e^{i\alpha' x} + D e^{-i\alpha' x} & ; x > 0 \end{cases}$$

FOR A WAVE COMING FROM THE RIGHT:

$$\psi(x) = \begin{cases} A e^{i\alpha' x} + B e^{-i\alpha' x} & ; x < 0 \\ C e^{i\alpha' x} & ; x > 0 \end{cases}$$

SINCE $\psi(x)$ MUST BE CONTINUOUS AT THE ORIGIN:

$$C = A + B$$

$$\Rightarrow \psi(x) = \begin{cases} A e^{i\alpha' x} + B e^{-i\alpha' x} & ; x < 0 \\ (A+B) e^{i\alpha' x} & ; x > 0 \end{cases}$$

NOW

$$\left.\frac{d\psi(x)}{dx}\right|_{x=0} = \begin{cases} iA\alpha' - iB\alpha' = i\alpha'(A-B) & ; x < 0 \\ i\alpha'(A+B) & ; x > 0 \end{cases}$$

BOUNDRY CONDITIONS DICTATE

$$\psi'(0+) - \psi'(0-) = -2\alpha\,\psi(0)$$

$$\therefore 2i\alpha' B = -2\alpha(A+B) \Rightarrow$$

$$-\frac{i\alpha' B}{\alpha} - B = A$$

$$\text{OR } A = -\left[1 + \frac{i\alpha'}{\alpha}\right] B = \xi B$$

THUS:

$$\psi(x) = \begin{cases} B\left[\xi e^{i\alpha' x} + e^{-i\alpha' x}\right] & ;\ x<0 \\ B(1+\xi)\, e^{i\alpha' x} & ;\ x>0 \end{cases}$$

$$= B\left[\left(\xi e^{i\alpha' x} + e^{-i\alpha' x}\right)\mu(-x) + (1+\xi)\, e^{i\alpha' x}\mu(x)\right]$$

$$\frac{d\psi(x)}{dx} = B\left[\left(i\alpha'\xi e^{i\alpha' x} - i\alpha' e^{-i\alpha' x}\right)\mu(-x) - (\xi+1)\,\delta(x) + i\alpha'(1+\xi)\, e^{i\alpha' x}\mu(x) + (\xi+1)\,\delta(x)\right]$$

$$= Bi\alpha'\left[\left(\xi e^{i\alpha' x} - e^{-i\alpha' x}\right)\mu(-x) + (1+\xi)\, e^{i\alpha' x}\mu(x)\right]$$

$$\frac{d^2\psi(x)}{dx^2} = Bi\alpha'\left[\left(i\alpha\xi e^{i\alpha' x} + i\alpha' e^{-i\alpha' x}\right)\mu(-x) + (1-\xi)\,\delta(x) + i\alpha'(1+\xi)\, e^{i\alpha' x}\mu(x) + (1+\xi)\,\delta(x)\right]$$

$$= -B\alpha'^2\left[\left(\xi e^{i\alpha' x} + e^{-i\alpha' x}\right)\mu(-x) + (1+\xi)\, e^{i\alpha' x}\mu(x) + \frac{2}{i\alpha'}\delta(x)\right]$$

$$= -\alpha'^2\left[B\left(\xi e^{i\alpha' x} + e^{-i\alpha' x}\right)\mu(-x) + B(1+\xi)\, e^{i\alpha' x}\mu(x) + \frac{2B}{i\alpha'}\delta(x)\right]$$

$$= -\alpha'^2\left[\psi(x) + \frac{2B}{i\alpha'}\delta(x)\right]$$

SCHRÖ'S EQ. IS THUS:

$$-\alpha'^2\left[\psi(x) + \frac{2B}{i\alpha'}\delta(x)\right] - \kappa^2\psi(x) = -2\alpha^{3/2}\delta(x)$$

NOW, WE STILL GOTTA FIND α'

$$\int_{-\infty}^{\infty} \psi_{\alpha_1}(x)\, \psi_{\alpha_1}^{*}(x)\, dx = \delta(k-k')$$

NOW $|B|^2 \int_{-\infty}^{0} \left[\xi e^{i\alpha' x} - e^{-i\alpha' x}\right]\left[\xi^{*} e^{-i\alpha' x} - e^{i\alpha' x}\right] dx$

$$= |B|^2 \int_{-\infty}^{0} |\xi|^2 - \xi e^{i(\alpha'+\alpha)x}$$

Physics 611
Due Feb 13, 1975
#4

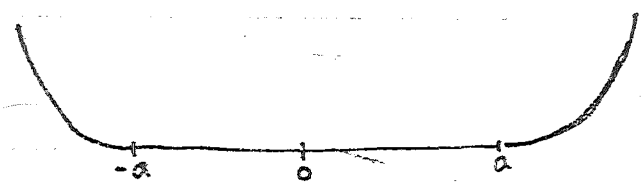
(1) Find the eigenvalues exactly for the half-space harmonic oscillator:

$$V(x) = \tfrac{1}{2}K\,X^2 \qquad x > 0$$
$$= \infty \qquad x < 0$$

(Hint: with a little thought, the answer may be obtained by doing no work whatsoever). Then do the same problem by WKBJ, and compare the two results.

(2) Use WKBJ to find the energy of bound states in the one-dimensional potential

$$V(x) = 0\,, \quad |x| < a$$
$$V(x) = \frac{K}{2}\left(|x| - a\right)^2, \quad |x| > a$$



(3) Given that the two dimensional form of the radial Schrodinger equation is

$$\left\{ -\frac{\hbar^2}{2m}\frac{1}{r}\frac{d}{dr}\, r\frac{d}{dr} + V(r) - E \right\} \psi(r) = 0$$

develop the WKBJ form of the radial wavefunction.

(4) Consider the potential in one dimension $V(x) = \lambda^2\hbar^2/(2mx^2)$ where λ^2 is the strength parameter.

a. Find the exact solution to the one dimensional Schrodinger equation. (Hint: they are of the form $\sqrt{x}\; J_\nu(kx)$)

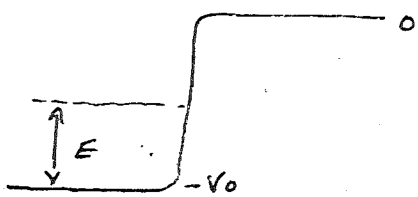
b. As $x \to \infty$ show that $\psi(x) \to \sqrt{\frac{2}{\pi}}\sin(kx+\delta)$ and obtain an explicit expression for the phase shift δ_k.

c. Obtain the wave function for $E > V(x)$ by WKBJ. Calculate the phase shift by this method, and compare with (b).

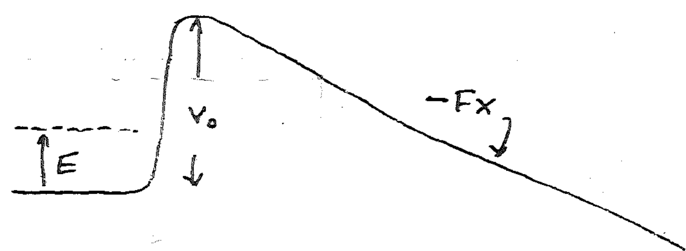
(5) Use WKBJ to find the eigenvalues of the quartic potential $V(x) = K\,x^4$.

Hint: $$\int_0^1 dy\,\sqrt{1-y^4} = \frac{1}{4}\,\frac{\Gamma(1/4)\,\Gamma(3/2)}{\Gamma(7/4)}$$

(6) The potential which keeps electrons within the surface of a metal may be approxim ted by a step potential of height V_0. Application of an electric field F changes the potential toa saw tooth shape. Calculate the tunneling amplitude T through this barrier, as a function of V_0, E, and F. This is called "Fowler-Nordheim" tunneling.



$F=0$



$F\neq 0$

$T = \exp\left[-\frac{2}{\hbar}\int_0^{b}\sqrt{2m(V-E)}\,dx\right]$

PHYSICS 611
DUE FEB. 13, 1975
BOB MARKS

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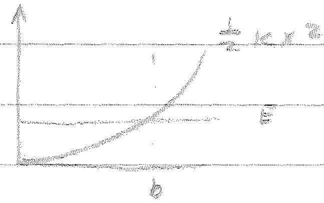
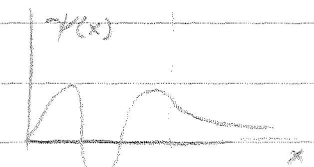
1. $V(x) = \begin{cases} \frac{1}{2}kx^2 & ; x > 0 \\ \infty & ; x < 0 \end{cases}$

0/10



$\frac{1}{2}kb^2 = E \Rightarrow b = \sqrt{\frac{2E}{k}}$



Wrong $(n+1/2)\hbar\omega$
but odd n only

n	n'	2n'+1
	0	
1	1	
3	2	
5		

FOR THE FULL-SPACE HARMONIC OSCILLATOR:

$E_n = \hbar\omega(n+\frac{1}{2}) \quad ; \quad \omega = \sqrt{\frac{k}{m}}$

ONE WOULD EXPECT TWICE THIS EIGEN VALUE IN THE HALF SPACE OSCILLATOR SINCE THE PROBABILITY OF E_n FOR $-\infty < x < \infty$ IS NOW RESTRICTED TO HALF THE INTERVAL $(0 < x < \infty)$. THUS, ONE WOULD EXPECT, FOR THE HALF-SPACE OSCILLATOR:

$E_n = 2\hbar\omega(2n+1)$

NOTE: THE ODD ORDER HERMITE POLYNOMIALS VANISHING AT THE ORIGIN ARE IN SUPPORT OF THIS OBSERVATION, SINCE BOUNDRY CONDITIONS FOR THE HALF SPACE OSCILLATOR DICTATE $\psi(0) = 0$

$\therefore$ get $(2n' + 3/2)\hbar\omega$

b. WKBJ SOLUTION:

$$p(x) = \sqrt{2m(E - V(x))} \quad ; \; x > 0$$

$$= \sqrt{2m}\left[E - \tfrac{1}{2}kx^2\right]^{1/2}$$

$$= \sqrt{2m}\sqrt{\tfrac{1}{2}k}\left[\frac{2E}{k} - x^2\right]^{1/2}$$

$$= \sqrt{mk}\sqrt{b^2 - x^2}$$

USING BOHR-SOMMERFIELD CONDITION:

$$\hbar(n+\tfrac{1}{2})\pi = \int_0^b p(x)\,dx$$

$$= \sqrt{mk}\int_0^b \sqrt{b^2 - x^2}$$

$$= \tfrac{1}{2}\sqrt{mk}\left[x\sqrt{b^2-x^2} + b^2 \sin^{-1}\frac{x}{b}\right]_0^b$$

$$= \tfrac{1}{2}\sqrt{mk}\,b^2 \sin^{-1} 1$$

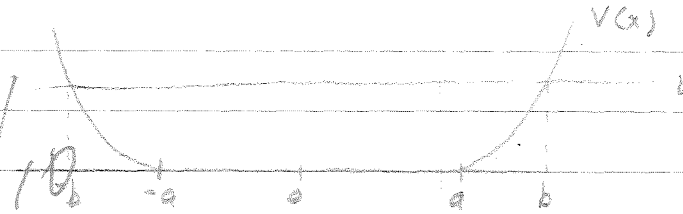
$$= \tfrac{1}{2}b^2\sqrt{mk}\,\frac{\pi}{2}$$

$$\Rightarrow \quad b^2 = 2\frac{2E}{k} = \frac{2}{\pi\sqrt{mk}}\,\hbar(n+\tfrac{1}{2})\pi$$

$$E = 2\sqrt{\frac{k}{m}}\,\hbar(n+\tfrac{1}{2})$$

$$= 2\omega\hbar(n+\tfrac{1}{2})$$

2.



10

$$E = V(b) = \frac{k}{2}(b-a)^2 \Rightarrow b-a = \sqrt{\frac{2E}{k}}$$

$$V(x) = \begin{cases} 0 & ; |x| < a \\ \frac{k}{2}(|x|-a)^2 & ; x > a \end{cases}$$

BOHR-SOMMERFIELD:

$$\int_{-b}^{b} p(x)\,dx = 2\pi\hbar\left(n+\tfrac{1}{2}\right) \quad ; n = 0, 1, 2, \ldots$$

$$p(x) = \sqrt{2m(E - V(x))}$$

$$= \begin{cases} \sqrt{2mE} & ; 0 < x < a \\ \sqrt{2m\left(E - \frac{k}{2}(x-a)^2\right)} & ; x > a \end{cases}$$

$$= \begin{cases} \sqrt{2mE} \\ \sqrt{2m\frac{k}{2}\left[\frac{2E}{k} - (x-a)^2\right]} \end{cases}$$

$$= \begin{cases} \sqrt{2mE} \\ \sqrt{mk\left[(b-a)^2 - (x-a)^2\right]} \end{cases}$$

THEN $\int_{-b}^{b} p(x)\,dx = 2\int_0^b p(x)\,dx$

$$= 2\left[\int_0^a \sqrt{2mE} + \sqrt{mk}\int_a^b \left[(b-a)^2 - (x-a)^2\right]^{1/2} dx\right]$$

$$= 2\sqrt{m}\left[\sqrt{2E}\,a + \sqrt{k}\int_a^b \left[(b-a)^2 - (x-a)^2\right]^{1/2} dx\right]$$

LET $\xi = x - a \Rightarrow d\xi = dx$

$x = a \Rightarrow \xi = 0 \quad ; \quad x = b \Rightarrow \xi = b - a$

$$\Rightarrow \int_{-b}^{b} p(x)\,dx = 2\sqrt{m}\left[\sqrt{2E}\,a + \sqrt{k}\int_0^{b-a}\left[(b-a)^2 - \xi^2\right]^{1/2} dx\right]$$

$$= 2\sqrt{m}\left[\sqrt{2E}\,a + \frac{\sqrt{k}}{2}\left[\xi\sqrt{(b-a)^2-\xi^2} + (b-a)^2 \sin^{-1}\frac{\xi}{b-a}\right]_0^{b-a}\right]$$

$$= 2\sqrt{m}\left[\sqrt{2E}\,a + \frac{\sqrt{k}}{2}\left[(b-a)^2 \sin^{-1} 1\right]\right]$$

$$= 2\sqrt{m}\left[\sqrt{2E}\,a + (b-a)^2\frac{\sqrt{k}}{2}\frac{\pi}{2}\right]$$

$$= 2\sqrt{m}\left[\sqrt{2E}\,a + \frac{2E}{k}\frac{\sqrt{k}\,\pi}{4}\right]$$

$$= 2\sqrt{m}\left[\sqrt{2E}\,a + \frac{\pi E}{2\sqrt{k}}\right]$$

$$\therefore\ 2\sqrt{m}\left[\sqrt{2E}\,a + \frac{\pi E}{2\sqrt{K}}\right] = \pi\hbar\left(n+\tfrac{1}{2}\right)$$

$$\frac{\pi}{2\sqrt{K}}E + \sqrt{2}\,a\sqrt{E} - \frac{\pi\hbar\left(n+\frac{1}{2}\right)}{2\sqrt{m}} = 0$$

USING QUADRADIC FORMULA:

$$\sqrt{E} = \frac{-\sqrt{2}\,a \pm \left[2a^2 + \frac{\pi}{\sqrt{K}}\,\frac{\pi\hbar\left(n+\frac{1}{2}\right)}{\sqrt{m}}\right]^{1/2}}{\pi/\sqrt{K}}$$

$$= \frac{-2a \pm \left[2a^2 + \frac{\pi^2\hbar\left(n+\frac{1}{2}\right)}{\sqrt{mK}}\right]^{1/2}}{\pi/\sqrt{K}}$$

$$= \sqrt{K}\left[\frac{-2a}{\pi} \pm \sqrt{\frac{2a^2}{\pi^2} + \frac{\hbar\left(n+1/2\right)}{\sqrt{mK}}}\right]$$

THE WKBJ BOUND STATE ENERGIES ARE THUS GIVEN BY:

$$E = K\left[\frac{-2a}{\pi} \pm \sqrt{\frac{2a^2}{\pi^2} + \frac{\hbar\left(n+1/2\right)}{\sqrt{mK}}}\right]^2 \; ; \; n = 0, 1, 2, 3, \ldots$$

NOTE: EACH n GIVES TWO ENERGIES

3. $\left[\frac{-\hbar^2}{2m}\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}+V-E\right]\psi(r)=0$

7 | 10 LET $\psi=e^{+i\sigma/\hbar}$

$\frac{d}{dr}e^{i\sigma/\hbar}=\frac{i}{\hbar}\sigma' e^{i\sigma/\hbar}$

$$\frac{d}{dr}r\frac{d}{dr}e^{i\sigma/\hbar}=\frac{i}{\hbar}\left[\frac{d}{dr}(r\sigma')e^{i\sigma/\hbar}+r\sigma'\frac{d}{dr}e^{i\sigma/\hbar}\right]$$
$$=\frac{i}{\hbar}\left[(\sigma'+r\sigma'')e^{i\sigma/\hbar}+r\sigma'\left(\frac{i}{\hbar}\right)\sigma' e^{i\sigma/\hbar}\right]$$
$$=\frac{i}{\hbar}\left[(\sigma'+r\sigma'')+\frac{i}{\hbar}r(\sigma')^2\right]e^{i\sigma/\hbar}$$
$$\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}e^{i\sigma/\hbar}=\frac{i}{\hbar}\left[\left(\frac{\sigma'}{r}+\sigma''\right)+\frac{i}{\hbar}(\sigma')^2\right]e^{i\sigma/\hbar}$$

SCHRÖ'S EQ'N BECOMES

$$\left[-\frac{i\hbar}{2m}\left\{\left(\frac{\sigma'}{r}+\sigma''\right)+\frac{i}{\hbar}(\sigma')^2\right]+(V-E)\right]e^{i\sigma/\hbar}=0$$
$$=\left[\frac{i}{2m}\left\{\frac{\hbar\sigma'}{r}+\hbar\sigma''+i(\sigma')^2\right\}-(V-E)\right]e^{i\sigma/\hbar}=0$$

ASSUME

$$\sigma(r,\hbar)=\sigma_0(r)+\frac{\hbar\sigma_1(r)}{i}+\frac{\hbar^2\sigma_2(r)}{i^2}+\ldots$$

KEEPING ONLY THE FIRST TWO TERMS GIVES

$$\left[\frac{i}{2m}\left\{\frac{\hbar}{r}\left(\sigma_0'+\frac{\hbar}{i}\sigma_1'\right)+\hbar\left(\sigma_0''+\frac{\hbar}{i}\sigma_1''\right)^2+i\left(\sigma_0'+\frac{\hbar}{i}\sigma_1'\right)^2\right\}+(V-E)\right]e^{i\sigma/\hbar}=0$$

$\hbar^0$ SOLUTION IS:

$$\left[\left(\frac{i}{2m}\right)i(\sigma_0')^2+(V-E)\right]e^{i\sigma/\hbar}=0$$
$$\therefore\ \frac{-1}{2m}(\sigma_0')^2=-(V-E)$$
$$\sigma_0'=\pm\sqrt{2m(V-E)}$$
$$\Rightarrow\ \sigma_0=\pm\int^{r}dr\sqrt{2m(V(r)-E)}=\pm\int^{r}dr\,p(r)$$

$\hbar^1$ SOLUTION IS

$$\left[\frac{i}{2m}\left\{\frac{\hbar}{r}\sigma_0'+\hbar(\sigma_0'')^2+i\,2\,\sigma_0'\left(\frac{\hbar}{i}\right)\sigma_1'\right\}+(V-E)\right]e^{i\sigma/\hbar}=0$$
$$\left[\frac{\hbar}{r}\sigma_0'+\hbar(\sigma_0'')^2+2\hbar\sigma_0'\sigma_1'-i2m(V-E)\right]e^{i\sigma/\hbar}=0$$
$$\left[\frac{1}{r}\sigma_0'+(\sigma_0'')^2+2\sigma_0'\sigma_1'-i2m(V-E)/\hbar\right]e^{i\sigma/\hbar}=0$$

$$i \cdot \frac{1}{r} \sigma_0' + (\sigma_0'')^2 + 2\sigma_0' \sigma_1' = \frac{i\,2m(V-E)}{\hbar}$$

$$\sigma_1' = \frac{i\,2m(V-E)}{\hbar} - \frac{\sigma_0'}{2\sigma_0' r} - \frac{(\sigma_0'')^2}{2\sigma_0'}$$

$$= \frac{i\,2m(V-E)}{\hbar} - \frac{1}{2r} - \frac{(\sigma_0'')^2}{2\sigma_0'}$$

Now $\sigma_0' = \pm\sqrt{2m\,(V(r)-E)}$

$$\Rightarrow \sigma_0'' = \frac{\pm\sqrt{2m}\,(\pm)\,V'(r)}{\sqrt{(V(r)-E)}}$$

$$= \pm \frac{m\,V'(r)}{\sqrt{2m\,(V-E)}}$$

$$= \pm \frac{m\,V'(r)}{P(r)}$$

$$\Rightarrow \sigma_1' = -\frac{1}{2r} + \frac{i\,P^2}{\hbar} \pm \frac{m^2 V'^2}{P^2} \cdot \frac{1}{2P}$$

$$= -\frac{1}{2r} + \frac{i\,P^2}{\hbar} \pm \frac{m^2 V'^2}{2P^3}$$

$$\sigma_1 = -\int_b^r \frac{1}{2r}\,dr + \frac{i}{\hbar}\int_b^r P^2\,dr \pm \frac{m^2}{2}\int_b^r \frac{V'^2}{P^3}\,dr$$

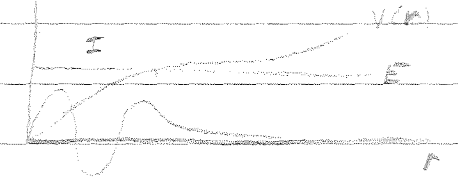
$$= -\frac{1}{2}\ln\left(\frac{r}{b}\right) + \frac{i}{\hbar}\int_b^r P^2\,dr \pm \frac{m^2}{2}\int_b^r \frac{V'^2}{P^3}\,dr$$

You got lost somewhere

NOW

$$\psi(x) = e^{i\sigma/\hbar} = e^{\frac{i}{\hbar}\left[\sigma_0 + \frac{\hbar\sigma_1}{i} + \dots\right]}$$

$$\simeq e^{\frac{i\sigma_0}{\hbar} + \sigma_1}$$



$$e^{\frac{i}{\hbar}\sigma_0} = e^{\pm\frac{i}{\hbar}\int_b^r dr\sqrt{2m[V(r)-E]}}$$

$$e^{\sigma_1} = e^{\frac{1}{2}\ln b/r + \frac{i}{\hbar}\int_b^r p^2 dr \pm \frac{m^2}{2}\int \frac{V'^2}{p^3} dr}$$

$$= \sqrt{\frac{b}{r}}\, e^{\frac{i}{\hbar}\int_b^r p^2 dr \pm \frac{m^2}{2}\int \frac{V'^2}{p^3} dr}$$

$$e^{\frac{i\sigma_0}{\hbar}+\sigma_1} = \sqrt{\frac{b}{r}}\, e^{\pm\frac{m^2}{2}\int_b^r \frac{V'^2}{(2m(V(r)-E))^{3/2}} dr + \frac{i}{\hbar}\int_b^r p^2 dr} \; e^{\pm\frac{i}{\hbar}\int dr\sqrt{2m(V-E)}dr}$$

$$= \sqrt{\frac{b}{r}}\, e^{\frac{i}{\hbar}\int_b^r 2m(V-E)^2 dr}\, e^{\pm\int_b^r\left(\frac{im^2}{2}\frac{V'^2}{[2m(E-V)]^{3/2}} + \frac{i}{\hbar}\sqrt{2m(V-E)}\right)dr}$$

SO THE GENERAL WKBJ SOLUTION IS:

$$\psi(r) = \sqrt{\frac{b}{r}}\, e^{\frac{i}{\hbar}\int_b^r 2m(V-E)^2 dr}\left[C_1 e^{i\int_b^r\left[\frac{m^2}{2}\frac{V'^2}{[2m(E-V)]^{3/2}} + \frac{1}{\hbar}\sqrt{2m(V-E)}\right]dr}\right.$$

$$\left. + C_2 e^{-i\int_b^r\left[\frac{m^2}{2}\frac{V'^2}{[2m(E-V)]^{3/2}} + \frac{1}{\hbar}\sqrt{2m(V-E)}\right]dr}\right]$$

4a. (1) $V(x) = \dfrac{\lambda^2 \hbar^2}{2mx^2}$

SHRÖ'S EQ'N:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda^2 \frac{\hbar^2}{2mx^2} - E\right]\psi(x) = 0$$

$$\left[x^2 \frac{d^2}{dx^2} - \lambda^2 + k^2\right]\psi(x) = 0 \,; \quad k^2 = \frac{2mE}{\hbar^2} > 0$$

EMPLOYING "HINT", WE TRY

$$\psi(x) = A\sqrt{x}\, J_r(kx)$$

THE QUESTION IS: WHAT IS r IN TERMS OF λ?

TO PLUG INTO SCHRÖ'S EQ'N, WE NEED TO KNOW:

$$r J_r(\xi) + \xi J'(\xi) = \xi J_{r-1}(\xi)$$

$$\Rightarrow \frac{dJ_r(kx)}{dx} = k J_{r-1}(kx) - \frac{r}{x} J_r(kx)$$

$$r J_r(\xi) - \xi J_r'(\xi) = \xi J_{r+1}(\xi)$$

$$\therefore (r-1) J_{r-1}(\xi) = \xi J'_{r-1}(\xi) = \xi J_r(\xi)$$

$$\Rightarrow \frac{dJ_{r-1}(kx)}{dk} = \frac{r-1}{x} J_{r-1}(kx) - k J_r(kx)$$

(CONT.)

PLUG AWAY:

$$\psi(x) = \sqrt{x}\; J_\nu(\kappa x)$$

$$\frac{d\psi(x)}{dx} = \frac{1}{2x^{\frac{1}{2}}} J_\nu + x^{\frac{1}{2}}\left[\kappa J_{\nu-1} - \frac{\nu}{x} J_\nu\right]$$

$$= \frac{1}{2x}\psi + x^{\frac{1}{2}}\kappa J_{\nu-1} - \frac{\nu}{x} x^{\frac{1}{2}} J_\nu$$

$$= \left(\frac{1}{2x} - \frac{\nu}{x}\right)\psi + x^{\frac{1}{2}}\kappa J_{\nu-1}$$

$$= \frac{1}{x}\left(\frac{1}{2} - \nu\right)\psi + x^{\frac{1}{2}}\kappa J_{\nu-1}$$

$$= \frac{\alpha}{x}\psi + x^{\frac{1}{2}}\kappa J_{\nu-1} \quad ; \alpha = \frac{1}{2} - \nu$$

$$\frac{d^2\psi}{dx^2} = \frac{-\alpha}{x^2}\psi + \frac{\alpha}{x}\psi' + \frac{1}{2\sqrt{x}}\kappa J_{\nu-1} + \kappa x^{\frac{1}{2}}\left[\frac{\nu-1}{x} J_{\nu-1} - \kappa J_\nu\right]$$

$$= \frac{-\alpha}{x^2}\psi + \frac{\alpha}{x}\psi' + \frac{\kappa}{2x^{\frac{1}{2}}} J_{\nu-1} + \frac{\kappa(\nu-1)}{x^{1/2}} J_{\nu-1} - \kappa^2\psi$$

$$= -\left[\frac{\alpha}{x^2} + \kappa^2\right]\psi + \frac{\alpha}{x}\psi' + \left[\frac{\kappa}{2x^{1/2}} + \frac{\kappa(\nu-1)}{x^{1/2}}\right] J_{\nu-1}$$

$$= -\left[\frac{+\alpha}{x^2} + \kappa^2\right]\psi + \frac{\alpha}{x}\left[\frac{\alpha}{x}\psi + x^{\frac{1}{2}}\kappa J_{\nu-1}\right] + \frac{\kappa}{x^{1/2}}\left(\nu - \frac{1}{2}\right) J_{\nu-1}$$

$$= -\left[\frac{\alpha}{x^2} + \kappa^2\right]\psi + \frac{\alpha^2}{x^2}\psi + \frac{\alpha}{x^{1/2}}\kappa J_{\nu-1} - \frac{\alpha\kappa}{x^{1/2}} J_{\nu-1}$$

$$= \left[\frac{\alpha^2}{x^2} - \frac{\alpha}{x^2} - \kappa^2\right]\psi$$

$$x^2\frac{d^2\psi}{dx^2} = \left[\alpha^2 - \alpha - \kappa^2 x^2\right]\psi$$

SCHRÖ'S EQ'N:

$$(\alpha^2 - \alpha - \kappa^2 x^2) - \lambda^2 + \kappa^2 x^2 = 0$$

$$\alpha^2 - \alpha - \lambda^2 = 0$$

$$\Rightarrow \alpha = \frac{1 \pm \sqrt{1 + 4\lambda^4}}{2} = \frac{1}{2} - \nu$$

$$\nu = \pm\sqrt{1 + 4\lambda^4}/2$$

AND:

$$\psi(x) = \sqrt{x}\left[A J_\nu(\kappa x) + B J_{-\nu}(\kappa x)\right] \quad ; \nu = \sqrt{1 + 4\lambda^4}/2$$

NOW LET'S LOOK @ BOUNDRY CONDITIONS KNOWING

$$J_\gamma(w) = w^\gamma \sum_{n=0}^{\infty} \frac{(w)^{2m}(-1)^m}{2^{2m+\gamma}\, m!\, \Gamma(\gamma+m+1)}$$

FIRST OFF:

$\psi(0) = 0$

SINCE BESSEL FUNCTIONS WITH NEGATIVE REAL INDEX'S BLOW UP @ $x=0$, WE LET $B=0$ LEAVING

$$\psi(x) = A\sqrt{x}\, J_\gamma(kx) \qquad ; \; \gamma = \sqrt{1+4\lambda^4}/2$$

EMPLOYING THE SPHERICAL BESSEL FUNCTION:

$$\mathcal{J}_{\gamma+\frac{1}{2}}(\xi) = \sqrt{\frac{\pi}{2\xi}}\; J_\gamma(\xi)$$

WE KNOW

$$\mathcal{J}_{\gamma+\frac{1}{2}}(kx) = \sqrt{\frac{\pi}{2kx}}\; J_\gamma(kx)$$
$$= \frac{1}{x}\sqrt{\frac{\pi}{2k}}\;\sqrt{x}\; J_\gamma(kx)$$

WE MAY WRITE:

$$\psi(x) = A'\, x\, \mathcal{J}_{\gamma+\frac{1}{2}}(kx)$$

USING DAVYDOV'S HIGH X FORMULA FOR SPHERICAL BESSEL FUNCTIONS (pg 130) GIVES

$$A' = k\sqrt{\frac{2}{\pi}}$$

THUS

$$\psi(x) = k\sqrt{\frac{2}{\pi}}\; x\, \mathcal{J}_{\gamma+\frac{1}{2}}(kx)$$

b. USING AGAIN DAVYDOV'S RECIPE:

$$\lim_{\xi \to \infty} J_\nu(\xi) = \frac{1}{\xi} \cos\left[\xi - \frac{\pi}{2}(\nu + 1)\right]$$
$$= \frac{1}{\xi} \sin\left[\xi - \frac{\pi}{2}(\nu + 2)\right]$$

THUS

$$\lim_{\xi \to \infty} J_{\nu+\frac{1}{2}}(\xi) = \frac{1}{\xi} \sin\left[\xi - \frac{\pi}{2}\left(\nu + \frac{5}{2}\right)\right]$$

ERGO:

$$\lim_{x \to \infty} \psi(x) = K\sqrt{\frac{2}{\pi}} \lim_{x \to \infty} x J_{\nu+\frac{1}{2}}(Kx)$$

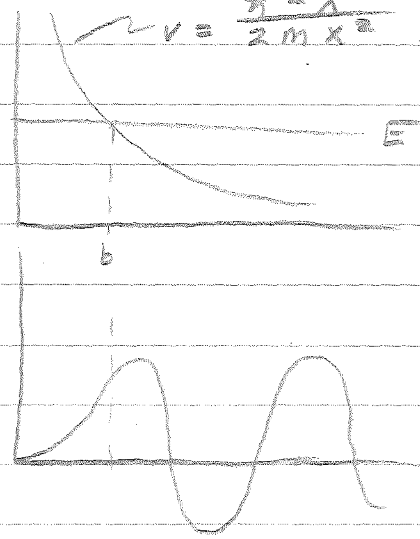
$$= K\sqrt{\frac{2}{\pi}} \frac{x}{(Kx)} \sin\left[Kx - \frac{\pi}{2}\left(\nu + \frac{5}{2}\right)\right]$$

$$= \sqrt{\frac{2}{\pi}} \sin\left[Kx - \left\{\frac{\pi}{2}\left(\sqrt{1 + \lambda^4/2} + \frac{5}{2}\right)\right\}\right]$$

$$\therefore \delta_K = -\frac{\pi}{2}\left[\sqrt{1 + \lambda^4/2} + 5/2\right]$$

$$= -\frac{\pi}{4}\left[\sqrt{1 + \lambda^4} + 5\right]$$

C. WKBJ



$$V(b) = E = \frac{\hbar^2\lambda^2}{2mb^2}$$

$$\Rightarrow b = \frac{\hbar\lambda}{\sqrt{2mE}}$$

$$k^2 = \frac{2mE}{\hbar^2} = \frac{2m}{\hbar^2}\,\frac{\hbar^2\lambda^2}{2mb^2}$$

$$= \frac{\lambda^2}{b^2}$$

$$kx = \frac{\lambda x}{b}$$

FOR $x > b$, WKBJ GIVES

$$\psi(x) = \frac{C}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_b^x dx'\,p(x') + \frac{\pi}{4}\right]$$

$$p(x) = \sqrt{2m(E-V)}$$

$$= \sqrt{2m\left(E - \frac{\hbar^2\lambda^2}{2mx^2}\right)}$$

$$= \left[\frac{2m\hbar^2\lambda^2}{2m}\left(\frac{2Em}{\hbar^2\lambda^2} - \frac{1}{x^2}\right)\right]^{1/2}$$

$$= \hbar\lambda\sqrt{\frac{1}{b^2} - \frac{1}{x^2}}$$

$$= \hbar\lambda\frac{1}{x}\sqrt{\left(\frac{x}{b}\right)^2 - 1}$$

$$\frac{1}{\hbar}\int dx'\,p(x') = \lambda\int_b^x \frac{1}{x}\sqrt{\left(\frac{x}{b}\right)^2 - 1}\,dx$$

LET $\xi = \frac{x}{b} \Rightarrow dx = b\,d\xi$

$x = b \Rightarrow \xi = 1$

$x = x \Rightarrow \xi = x/b$

$$\Rightarrow \frac{1}{\hbar}\int dx'\,p(x') = \lambda\int_1^{x/b}\frac{\sqrt{\xi^2 - 1}}{\xi}\,d\xi$$

$$= \lambda\left[\sqrt{\xi^2 - 1} - \sec^{-1}\xi\right]_1^{x/b}$$

$$= \lambda\left[\sqrt{\left(\frac{x}{b}\right)^2 - 1} - \sec^{-1}\frac{x}{b} + \sec^{-1}1\right]$$

$$= \lambda\left[\sqrt{\left(\frac{x}{b}\right)^2 - 1} - \sec^{-1}\frac{x}{b}\right]$$

$$\therefore \psi(x) = \frac{C\sqrt{x}}{\sqrt{\hbar\lambda}\,\sqrt[4]{\left(\frac{x}{b}\right)^2 - 1}} \sin\left[\lambda\left(\sqrt{\left(\frac{x}{b}\right)^2 - 1} - \sec^{-1}\frac{x}{b} + \frac{\pi}{4}\right)\right]$$

$$\psi(x) = \frac{c}{\sqrt{p}} \sin\left[\lambda\left(\sqrt{\left(\frac{x}{b}\right)^2 - 1} - \sec^{-1}\frac{x}{b}\right) + \frac{\pi}{4}\right]$$

$$\lim_{x \to \infty} p^{\frac{1}{2}} = \sqrt[4]{2mE}$$

$$\lim_{x \to \infty} \sqrt{\left(\frac{x}{b}\right)^2 - 1} = \frac{x}{b}$$

$$\lim_{x \to \infty} \sec^{-1}\frac{x}{b} = \frac{\pi}{2}$$

$$\Rightarrow \lim_{x \to \infty} \psi(x) = \frac{c}{\sqrt[4]{2mE}} \sin\left[\lambda\left(\frac{x}{b} - \frac{\pi}{2}\right) + \frac{\pi}{4}\right]$$

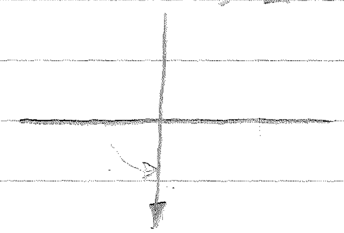
$$= \frac{c}{\sqrt[4]{2mE}} \sin\left[kx - \frac{\pi\lambda}{2} + \frac{\pi}{4}\right]$$

$$= \frac{c}{\sqrt[4]{2mE}} \sin\left[kx + \frac{\pi}{2}\left(\frac{1}{2} - \lambda\right)\right]$$

$$\Rightarrow \delta_{WKBJ} = -\frac{\pi}{2}\left(\lambda - \frac{1}{2}\right)$$

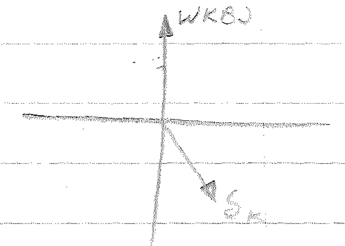
COMPARING

λ	$-\delta_{WKBJ} = \frac{\pi}{2}(2\lambda - \frac{1}{2})$	$-\delta_K = \frac{\pi}{4}\left[\sqrt{1+\lambda^4}+5\right]$
0	$(-\frac{1}{2})\frac{\pi}{2}$	$6\frac{\pi}{4} = 3\frac{\pi}{2}$



GOOD

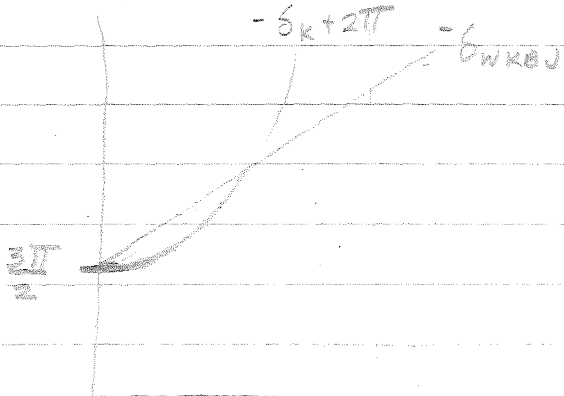
1	$\frac{1}{2}(\frac{\pi}{2})$	$(3.2)\frac{\pi}{2}$



NO GOOD

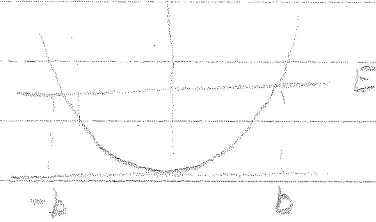
SO (IF ALL IS CORRECT) WKBJ WORKS ONLY FOR $\lambda \ll 1$

A ROUGH GRAPH OF $-\delta_{WKBJ} + 2\pi$ VS $-\delta_K$ GIVES



5. $V(x) = \kappa x^4$

10



$$V(b) = E = \kappa b^4 \Rightarrow b = \sqrt[4]{E/\kappa}$$

$$p(x) = \sqrt{2m\left[E - \kappa x^4\right]}$$

$$\pi\hbar\left(n+\tfrac{1}{2}\right) = \int_{-b}^{b} p(x)\,dx$$

$$= 2\sqrt{2m}\int_0^b \sqrt{E - \kappa x^4}\,dx$$

$$= 2\sqrt{2m}\,\sqrt{E}\int_0^b \sqrt{1 - \tfrac{\kappa}{E}x^4}\,dx$$

$$= 2\sqrt{2mE}\int_0^b \sqrt{1 - (x/b)^4}\,dx$$

$$\xi = x/b \Rightarrow d\xi = \tfrac{1}{b}dx \quad (dx = b\,d\xi)$$

$$x = 0 \Rightarrow \xi = 0$$

$$x = b \Rightarrow \xi = 1$$

$$\therefore \pi\hbar\left(n+\tfrac{1}{2}\right) = 2\sqrt{2mE}\,b\int_0^1 \sqrt{1-\xi^4}\,d\xi$$

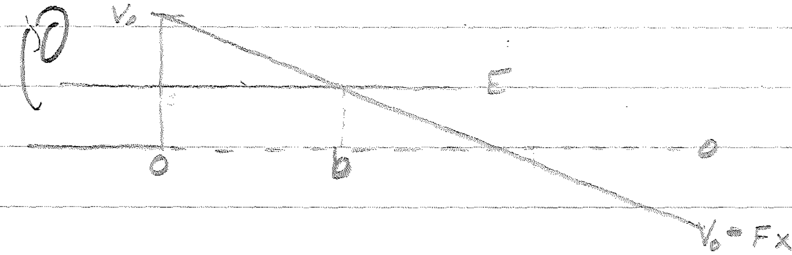
$$= 2\sqrt{2mE}\,b\,\frac{1}{4}\,\frac{\Gamma(1/4)\Gamma(3/2)}{\Gamma(7/4)}$$

$$= \frac{\Gamma(\frac{1}{4})\Gamma(3/2)}{\Gamma(7/4)}\,\frac{\sqrt{2mE}\,b}{2}$$

$$= \frac{\Gamma(\frac{1}{4})\Gamma(3/2)}{\Gamma(7/4)}\,\frac{\sqrt{2mE}}{2}\sqrt[4]{\frac{E}{\kappa}}$$

$$\left[\pi\hbar\left(n+\tfrac{1}{2}\right)\right]^{4/3} = \left[\frac{\Gamma(\frac{1}{4})\Gamma(3/2)}{\Gamma(7/4)}\left(\frac{m}{2}\right)^{1/2}\frac{1}{\kappa^{1/4}}\,E^{3/4}\right]^{4/3}$$

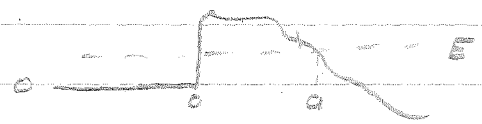
$$\Rightarrow E = \left[\pi\hbar\left(n+\tfrac{1}{2}\right)\frac{\Gamma(7/4)}{\Gamma(\frac{1}{4})\Gamma(3/2)}\right]^{4/3}\left(\frac{2}{m}\right)^{2/3}\kappa^{1/3}$$

6. 

$V_0 - Fb = E$

$\Rightarrow b = \dfrac{V_0 - E}{F}$

DAVYDOV (Pp. 81-84) SHOWS THAT THE TRANSMISSION COEFFICIENT, T, OF A BARRIER AKIN TO



IS APPROXIMATED BY WKBJ TO BE

$$T = e^{-\frac{2}{\hbar}\int_0^a \sqrt{2m(V-E)}\,dx}$$

THUS, FOR OUR PROBLEM:

$$-\frac{2}{\hbar}\int_0^a \sqrt{2m(V-E)}\,dx = -\frac{2\sqrt{2m}}{\hbar}\int_0^b \sqrt{(V_0 - Fx) - E}\;dx$$

$$= -\frac{2\sqrt{2m}}{\hbar}\int_0^b \sqrt{(V_0 - E) - Fx}\;dx$$

$$= -\frac{2\sqrt{2m}}{\hbar}\int_0^b \sqrt{F}\sqrt{b - x}\;dx$$

$$= \frac{-2\sqrt{2mFb}}{\hbar}\int_0^b \sqrt{1 - x/b}\;dx$$

$$\xi = x/b \Rightarrow d\xi = \frac{1}{b}dx \Rightarrow dx = b\,d\xi$$

$$x = 0 \Rightarrow \xi = 0, \quad x = b \Rightarrow \xi = 1$$

$$\Rightarrow -\frac{2}{\hbar}\int_0^a \sqrt{2m(V-E)}\,dx = -\frac{2}{\hbar}\sqrt{2mF}\,b^{3/2}\int_0^1 \sqrt{1-\xi}\;d\xi$$

$$= \frac{2}{\hbar}\sqrt{2mF}\,b^{3/2}\,\frac{2}{3}(1-\xi)^{3/2}\Big|_0^1$$

$$= \frac{-4}{3\hbar}\sqrt{2mF}\,b^{3/2}$$

$$= \frac{-4}{3\hbar}\sqrt{2mF}\left[\frac{V_0 - E}{F}\right]^{3/2}$$

$$= \frac{-4\sqrt{2m}}{3\hbar F}(V_0 - E)^{3/2}$$

$$\therefore\; T = e^{-\frac{4\sqrt{2m}}{3\hbar F}(V_0 - E)^{3/2}}$$

NOTE: EQUAL TO DAVYDOV'S SOL'N: Pg 85 WITH $F = eE$ AND $\varphi = V_0 - E$

Phys 511
Due Feb 27, 1973
#5

(1) Derive the exact eigenvalue equation for the bound states in the three dimensional potential

$$V(r) = -Ze^2/b \qquad r < b$$
$$\qquad = -Ze^2/r \qquad r > b$$

(2) Solve exactly the radial wave equation for the three dimensional harmonic oscillator, and obtain the eigenvalues.

Hint: set $\quad z = (r/x_0)^2 \ , \quad x_0^2 = \hbar/m\omega$

and assume $\quad \chi(r) = z^{\frac{l+1}{2}} e^{-z/2} G(z)$

and $G(z)$ obeys a familiar equation.

(3) Use the three dimensional form of WKBJ to obtain the eigenvalues of the three dimensional harmonic oscillator. What is the lowest eigenvalue?

(4) For the three dimensional harmonic oscillator, what is the degeneracy of each level? That is, how many different states, as a function of N, have the same energy $\quad E_N = \hbar\omega(N + 3/2)$

(5) Using hydrogenic bound state wave functions, show:

a. The 1s state is orthogonal to the $2p_z$ state $\qquad \int d^3r\, \psi_{1s}\, \psi_{2p_z} = 0$

b. Evaluate the matrix element of P_z between the 1s and $2P_z$ state

$$\int d^3r\, \psi_{1s}\, P_z\, \psi_{2p_z}$$

c. Evaluate the matrix element of z between the 1s and $2P_z$ state.

(6) Find the exact eigenvalues of the one dimensional coulomb potential

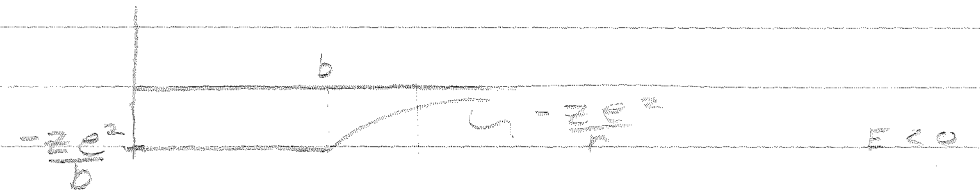
$$V(x) = -Ze^2/x \qquad x > 0$$
$$\qquad = \infty \qquad x \le 0$$

PHYS. 611
DUE FEB 27, 197?
BOB MARKS

60/60

10/10

1. $V(r) = \begin{cases} -\frac{Ze^2}{b} & ; r<b \\ -\frac{Ze^2}{r} & ; r>b \end{cases}$



FOR $0<r<b$

$$V_{EFF} = -\frac{Ze^2}{b^2} + \frac{\hbar^2}{2mr^2}\ell(\ell+1)$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{Ze^2}{b^2} + \frac{\hbar^2}{2mr^2}(\ell+1)\ell - E\right]\chi(r) = 0$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2mr^2}(\ell+1)\ell - \left(E + \frac{Ze^2}{b^2}\right)\right]\chi(r) = 0$$

$$\left[\frac{d^2}{dr^2} - \frac{1}{r^2}(\ell+1)\ell + \frac{2m}{\hbar^2}\left(E + \frac{Ze^2}{b^2}\right)\right]\chi(r) = 0$$

$$\left[\frac{d^2}{dr^2} - \frac{1}{r^2}(\ell+1)\ell + \frac{2m}{\hbar^2}\left(\frac{Ze^2}{b^2} + E\right)\right]\chi(r) = 0$$

$$\left[\frac{d^2}{dr^2} - \frac{1}{r^2}(\ell+1)\ell + (K_0^2 - K^2)\right]\chi(r) = 0$$

$$K_0^2 = \frac{2mZe^2}{\hbar^2 b^2} \qquad K^2 = -\frac{2mE}{\hbar^2} = \frac{2m|E|}{\hbar^2}$$

$$\alpha^2 = K_0^2 - K^2 = \frac{2m}{\hbar^2}\left(\frac{Ze^2}{b^2} + E\right)$$

$$\Rightarrow \left[\frac{d^2}{dr^2} - \frac{1}{r^2}(\ell+1)\ell + \alpha^2\right]\chi(r) = 0$$

GENERAL SOLUTION IS:

$$\chi_\ell(r) = \sqrt{r}\left[A_\ell J_{\ell+\frac{1}{2}}(\alpha r) + B_\ell J_{-\ell-\frac{1}{2}}(\alpha r)\right]$$

NOW

$$\chi_\ell(r) = 0 \quad ; \quad J_\nu(z) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\,\Gamma(k+\nu+1)}\left(\frac{z}{2}\right)^{\nu+2k}$$

$\sqrt{r}\, J_{-\ell-\frac{1}{2}}(\alpha r)$ BLOWS UP @ $r=0 \Rightarrow B_\ell = 0$

LEAVING:

$$\chi_\ell(r) = A_\ell \sqrt{r}\, J_{\ell+\frac{1}{2}}(\alpha r)$$

FOR $r > b$

$$V_{EFF} = -\frac{Ze^2}{r} + \frac{\hbar^2}{2mr^2}\ell(\ell+1)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{Ze^2}{r} + \frac{\hbar^2}{2mr^2}\ell(\ell+1) - E\right]\chi(r) = 0$$

$$\left[\frac{d^2}{dr^2} + \frac{2mZe^2}{\hbar^2 r} - \frac{1}{r^2}\ell(\ell+1) + \frac{2mE}{\hbar^2}\right]\chi(r) = 0$$

$$\left[\frac{d^2}{dr^2} + \frac{(bK_0)^2}{r} - \frac{1}{r^2}\ell(\ell+1) - K^2\right]\chi(r) = 0$$

*SOLUTION IS

$$\chi_U(r) = A_U e^{-kr} r^{\ell+1} F\left[\ell+1 - \frac{(bK_0)^2}{2K}, 2\ell+2, 2kr\right]$$

BUT THIS DIVERGES FOR LARGE r AND

$\ell+1 - \frac{(bK_0)^2}{2K} \neq$ $-$INTEGER. SO WE USE

$$\chi_U(r) = A_U e^{-kr} r^{\ell+1} U\left[\ell+1 - \frac{(bK_0)^2}{2K}, 2\ell+2, 2kr\right]$$

NOW WE GOTTA MATCH χ_U AND χ_ℓ AT $r=b$.

i.e: $\chi_\ell(b) = \chi_U(b)$

$$\therefore A_\ell \sqrt{b}\, J_{\ell+\frac{1}{2}}(\alpha b) = A_U e^{-kb} b^{\ell+1} U\left[\ell+1 - \frac{(bK_0)^2}{2K}, 2\ell+2, 2kb\right]$$

$$\Rightarrow A_\ell = \frac{e^{-kb} b^{\ell+\frac{1}{2}} U\left[\ell+1 - \frac{(bK_0)^2}{2K}, 2\ell+2, 2kb\right]}{J_{\ell+\frac{1}{2}}(\alpha b)} A_U$$

SIMILARLY: $\frac{d\chi_\ell(b)}{dr} = \frac{d\chi_U(b)}{dr}$

*Pg 141 DAVYDOV

$$\frac{d\chi_\ell}{dr} = A_\ell\left[\frac{1}{2\sqrt{r}}\, J_{\ell+\frac{1}{2}}(\alpha r) + \frac{\alpha\sqrt{r}}{2}\left\{J_{\ell-\frac{1}{2}}(\alpha r) - J_{\ell+\frac{3}{2}}(\alpha r)\right\}\right]$$

$$\frac{d\chi_\ell(b)}{dr} = \frac{A_\ell}{2}\left[\frac{1}{\sqrt{b}}\, J_{\ell+\frac{1}{2}}(\alpha b) + \alpha\sqrt{b}\, J_{\ell-\frac{1}{2}}(\alpha b) - \alpha\sqrt{b}\, J_{\ell+3/2}(\alpha b)\right]$$

$$= \frac{A_\ell\sqrt{b}}{2}\left[\frac{1}{b} J_{\ell+\frac{1}{2}}(\alpha b) + \alpha J_{\ell-\frac{1}{2}}(\alpha b) - \alpha J_{\ell+3/2}(\alpha b)\right]$$

NOW $$\frac{d\,U(a,b;z)}{dz} = -a\,U(a+1,b+1;z)$$

$$\therefore \frac{d\chi_u}{dr} = A_u\left[\left(-k + \frac{\ell+1}{r}\right) U\left(\ell+1-\frac{(bk_0)^2}{2k}, 2\ell+2, 2kr\right) + 2k\left(\frac{(bk_0)^2}{2k} - \ell - 1\right) U\left(\ell+2-\frac{(bk_0)^2}{2k}, 2\ell+3, 2kr\right)\right] \times e^{-kr}\, r^{\ell+1}$$

$$\frac{d\chi_u(b)}{dr} = A_u\left[\left(\frac{\ell+1}{b} - k\right) U\left(\ell+1-\frac{(bk_0)^2}{2k}, 2\ell+2, 2kb\right) + \left(b^2k_0^2 - 2k(\ell+1)\right) U\left(\ell+2-\frac{(bk_0)^2}{2k}, 2\ell+3, 2kb\right)\right] \times e^{-kb}\, b^{\ell+1}$$

EQUATING

$$\frac{A_\ell\sqrt{b}}{2}\left[\frac{1}{b} J_{\ell+\frac{1}{2}}(\alpha b) + \alpha J_{\ell-\frac{1}{2}}(\alpha b) - \alpha J_{\ell+3/2}(\alpha b)\right]$$

$$= A_u\left[\left(\frac{\ell+1}{b} - k\right) U\left(\ell+1-\frac{(bk_0)^2}{2k}, 2\ell+2, 2kb\right) + \left(b^2k_0^2 - 2k(\ell+1)\right) U\left(\ell+2-\frac{(bk_0)^2}{2k}, 2\ell+3, 2kb\right)\right] \times e^{-kb}\, b^{\ell+1}$$

$$A_\ell = \frac{\left(\frac{\ell+1}{b} - k\right) U\left(\ell+1-\frac{(kb_0)^2}{2k}, 2\ell+2, 2kb\right) + \left(b^2k_0^2 - 2k(\ell+1)\right) U\left(\ell+2-\frac{(bk_0)^2}{2k}, 2\ell+3, 2kb\right)}{\frac{1}{b} J_{\ell+\frac{1}{2}}(\alpha b) + \alpha J_{\ell-\frac{1}{2}}(\alpha b) - \alpha J_{\ell+3/2}(\alpha b)} \times 2e^{-kb}\, b^{\ell+\frac{1}{2}} A_u$$

EQUATING WITH OTHER BOUNDARY CONDITION GIVES THE TRANSENDENTAL EIGENVALUE EQ'N;

$$\frac{U\left(\ell+1-\frac{(bK_0)^2}{2k}, 2\ell+2, 2kb\right)}{2J_{\ell+\frac{1}{2}}(\alpha b)}$$

$$= \frac{\left(\frac{\ell+1}{b}-k\right)U\left(\ell+1-\frac{(K_0 b)^2}{2k}, 2\ell+2, 2kb\right)+\left(b^2K_0^2-2k(\ell+1)\right)U\left(\ell+2-\frac{(bK_0)^2}{2k}, 2\ell+3, 2kb\right)}{\frac{1}{b}J_{\ell+\frac{1}{2}}(\alpha b)+\alpha J_{\ell-\frac{1}{2}}(\alpha b)-\alpha J_{\ell+3/2}(\alpha b)}$$

INSTEAD OF MESSING WITH THIS HAIRY THING FURTHER LET IT SUFFICE TO SAY THAT, WITH $K_0^2 = \frac{2mZe^2}{\hbar^2 b^2}$, ONE MUST FIND THE VALUES OF $K = \sqrt{-\frac{2mE}{\hbar^2}}$ WITH $\alpha = \sqrt{K_0^2 - K^2}$ SUCH THAT THE ABOVE RELATIONSHIP IS SATISFIED FOR A GIVEN VALUE OF ℓ

THE EIGENVALUES ARE THEN

$$E_{n\ell} = -\hbar^2/2mK_n$$

IN SHORT, $E_{n\ell}$ MUST SATISFY:

$$\left[\frac{\frac{d}{dr}\left[e^{-kr}r^{\ell+1}U\left(\ell+1-\frac{(bK_0)^2}{2k}, 2\ell+2, 2kr\right)\right]}{e^{-kr}r^{\ell+1}U\left(\ell+1-\frac{(bK_0)^2}{2k}, 2\ell+2, 2kr\right)}\right]_{r=b} = \left[\frac{\frac{d}{dr}\sqrt{r}\,J_{\ell+\frac{1}{2}}(\alpha r)}{\sqrt{r}\,J_{\ell+\frac{1}{2}}(\alpha r)}\right]_{r=b}$$

2. $V(r) = \frac{k}{2} r^2$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{k}{2} r^2 + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - E \right] \chi(r) = 0$$

$$\omega = \sqrt{k/m} \Rightarrow k = \omega^2 m$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\omega^2 m}{2} r^2 + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - E \right] \chi(r) = 0$$

$$\left[-\frac{\hbar}{m}\frac{d^2}{dr^2} + \frac{\omega^2 m}{\hbar} r^2 + \frac{\hbar}{m}\frac{\ell(\ell+1)}{r^2} - \frac{2E}{\hbar} \right] \chi(r) = 0$$

$$\left[-\frac{\hbar}{\omega m}\frac{d^2}{dr^2} + \frac{\omega m}{\hbar} r^2 + \frac{\hbar}{\omega m}\frac{\ell(\ell+1)}{r^2} - \frac{2E}{\hbar\omega} \right] \chi(r) = 0$$

$$x_0^2 = \hbar/m\omega$$

$$\left[+ x_0^2 \frac{d^2}{dr^2} - \frac{1}{x_0^2} r^2 - x_0^2 \frac{\ell(\ell+1)}{r^2} + \frac{2E}{\hbar\omega} \right] \chi(r) = 0$$

$$\left[d^2/d(r/x_0)^2 - \left(\frac{r}{x_0}\right)^2 - \frac{\ell(\ell+1)}{(r/x_0)^2} + \frac{2E}{\hbar\omega} \right] \chi(r) = 0$$

$$\xi = r/x_0$$

$$\left[\frac{d^2}{d\xi^2} - \xi^2 - \frac{\ell(\ell+1)}{\xi^2} + \frac{2E}{\hbar\omega} \right] \chi(\xi) = 0$$

$$z = \xi^2 = (r/x_0)^2 \Rightarrow dz = 2\xi\, d\xi$$

$$\frac{d\chi}{d\xi} = \frac{dz}{d\xi}\frac{d\psi}{dz}$$

$$= 2\xi \frac{d\psi}{dz}$$

$$\frac{d^2\chi}{d\xi^2} = \frac{d}{d\xi}\left[2\xi \frac{d\psi}{dz} \right]$$

$$= 2\frac{d\psi}{dz} + 2\xi \frac{d}{d\xi}\frac{d\psi}{dz}$$

$$= 2\frac{d\psi}{dz} + 2\xi \frac{dz}{d\xi}\frac{d}{dz}\frac{d\psi}{dz}$$

$$= 2\frac{d\psi}{dz} + 2\xi (2\xi)\frac{d^2\psi}{dz^2}$$

$$= 2\frac{d\psi}{dz} + 4\xi^2 \frac{d^2\psi}{dz^2}$$

$$= 2\frac{d\psi}{dz} + 4z \frac{d^2\psi}{dz^2}$$

$$\frac{d^2}{d\xi^2} = 2\frac{d}{dz} + 4z\frac{d^2}{dz^2}$$

$$\Rightarrow \left[4z\frac{d^2}{dz^2} + 2\frac{d}{dz} - z - \frac{\ell(\ell+1)}{z} + \frac{2E}{\hbar\omega} \right] \chi(z) = 0$$

LET: $\chi(z) = z^{\frac{\ell+1}{2}} e^{-z/2} G(z)$

$$\frac{d\chi}{dz} = \left[\left(\frac{\ell+1}{2z} - \frac{1}{2}\right)G + \frac{dG}{dz}\right] z^{\frac{\ell+1}{2}} e^{-z/2}$$

$$= z^{\frac{\ell+1}{2}} e^{-z/2}\left[\frac{d}{dz} + \left(\frac{\ell+1}{2z} - \frac{1}{2}\right)\right]G$$

$$\frac{d^2\chi}{dx^2} = \left[-\left(\frac{\ell+1}{2z^2}\right)G + \left(\frac{\ell+1}{2z} - \frac{1}{2}\right)\frac{dG}{dz} + \frac{d^2G}{dz^2} + \left(\frac{\ell+1}{2z} - \frac{1}{2}\right)^2 G + \left(\frac{\ell+1}{2z} - \frac{1}{2}\right)\frac{dG}{dz}\right] z^{\frac{\ell+1}{2}} e^{-z/2}$$

$$= z^{\frac{\ell+1}{2}} e^{-z/2}\left[\frac{d^2}{dz^2} + \left(\frac{\ell+1}{z} - 1\right)\frac{d}{dz} + \left(\frac{\ell+1}{2z} - \frac{1}{2}\right)^2 - \left(\frac{\ell+1}{2z^2}\right)\right]G(z)$$

THUS:

$$\left[4z\left\{\frac{d^2}{dz^2} + \left(\frac{\ell+1}{z} - 1\right)\frac{d}{dz} + \left(\frac{\ell+1-z}{2z}\right)^2 - \frac{\ell+1}{2z^2}\right\} + 2\left\{\frac{d}{dz} + \left(\frac{\ell+1}{2z} - \frac{1}{2}\right)\right\} - z - \frac{\ell(\ell+1)}{z} + \frac{2E}{\hbar\omega}\right]G(z) = 0$$

$$\left[4z\frac{d^2}{dz^2} + 4(\ell+1-z)\frac{d}{dz} + \frac{(\ell+1-z)^2}{z} - \frac{2(\ell+1)}{z} + 2\frac{d}{dz} + \frac{\ell+1}{z} - 1 - z - \frac{\ell(\ell+1)}{z} + \frac{2E}{\hbar\omega}\right]G(z) = 0$$

$$\left[4z\frac{d^2}{dz^2} + 4(\ell+1-z)\frac{d}{dz} + \frac{(\ell+1)^2}{z} - 2(\ell+1) + \cancel{z} - \frac{2(\ell+1)}{z} + 2\frac{d}{dz} + \frac{\ell+1}{z} - 1 - \cancel{z} - \frac{\ell(\ell+1)}{z} + \frac{2E}{\hbar\omega}\right]G(z) = 0$$

$$\left[4z\frac{d^2}{dz^2} + (4\ell+6-4z)\frac{d}{dz} - 2(\ell+1) - 1 + \frac{2E}{\hbar\omega} + \frac{1}{z}\left\{\ell^2 + 2\ell + 1 - 2\ell - 2 + \ell + 1 - \ell^2 - \ell\right\}\right]G(z) = 0$$

$$\left[4z\frac{d^2}{dz^2} + 2(2\ell+3-2z)\frac{d}{dz} - (2\ell+3) + \frac{2E}{\hbar\omega}\right]G(z) = 0$$

$$\left[z\frac{d^2}{dz^2} + \left(\ell+\frac{3}{2} - z\right)\frac{d}{dz} - \left(\frac{\ell}{2} + \frac{3}{4} - \frac{E}{2\hbar\omega}\right)\right]G(z) = 0$$

$$\alpha^2 = \frac{E}{2\hbar\omega}$$

$$\Rightarrow \left[z\frac{d^2}{dz^2} + \left(\ell+\frac{3}{2} - z\right)\frac{d}{dz} - \left(\frac{\ell}{2} + \frac{3}{4} - \alpha^2\right)\right]G(z)$$

LOOK LIKE CONFLUENT HYPERGEOMETRIC:

$$\left[z \frac{d^2}{dz^2} + (b-z)\frac{d}{dz} - a\right] F(a,b;z) = 0$$

$$b = \ell + \frac{3}{2}$$

$$a = \frac{\ell}{2} + \frac{3}{4} - \alpha^2 \quad ; \alpha^2 = \frac{E}{2\hbar\omega}$$

SOLUTION WE WANT IS

$$G(z) = F\left(\frac{\ell}{2} + \frac{3}{4} - \alpha^2 ; \ell + \frac{3}{2} ; z\right)$$

THUS:

$$\chi(z) = A z^{\frac{\ell+1}{2}} e^{-z/2} F\left(\frac{\ell}{2} + \frac{3}{4} - \alpha^2 ; \ell + \frac{3}{2} ; z\right)$$

SINCE WE REQUIRE

$$\lim_{z \to \infty} \chi(z) = 0$$

LET

$$a = -n = \frac{\ell}{2} + \frac{3}{4} - \frac{E}{2\hbar\omega}$$

$$\Rightarrow E_n = \left(\frac{\ell}{2} + \frac{3}{4} + n\right) 2\hbar\omega$$

$$= \left(\ell + 2n + \frac{3}{2}\right)\hbar\omega$$

SINCE $z = \left(\frac{r}{x_0}\right)^2$, $x_0^2 = \frac{\hbar}{m\omega}$

$$\chi(r) = A \left(\frac{r}{x_0}\right)^{\ell+1} e^{-\left(\frac{r}{x_0}\right)^2/2} F\left(\frac{\ell}{2} + \frac{3}{4} - \alpha^2 , \ell + \frac{3}{2} , \left(\frac{r}{x_0}\right)^2\right)$$

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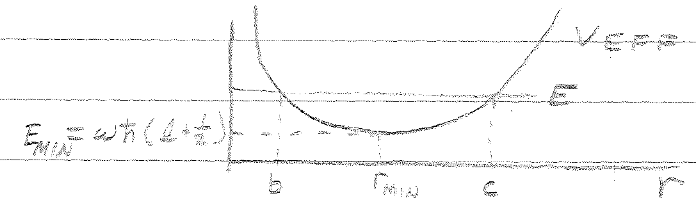
1D

3. $V(r) = \frac{K}{2} r^2$

$$V_{EFF} = \frac{K}{2} r^2 + \frac{\hbar^2}{2m} \frac{(\ell + \frac{1}{2})^2}{r^2}$$



$$\frac{dV_{EFF}}{dr} = Kr - \frac{\hbar^2}{m} \frac{(\ell+\frac{1}{2})^2}{r^3} = 0$$

$$r^4 = \frac{\hbar^2}{mK}(\ell+\tfrac{1}{2})^2 \Rightarrow r^2_{min} = \frac{1}{(mK)^{1/2}} \hbar(\ell+\tfrac{1}{2})$$

$$V_{EFF}(r_{MIN}) = \frac{K}{2}\frac{1}{(mK)^{1/2}}\hbar(\ell+\tfrac{1}{2}) + \frac{\hbar^2}{2m}(\ell+\tfrac{1}{2})^2 \frac{\sqrt{mK}}{\hbar(\ell+\frac{1}{2})}$$

$$= \frac{1}{2}\sqrt{\frac{K}{m}}\hbar(\ell+\tfrac{1}{2}) + \frac{1}{2}\sqrt{\frac{K}{m}}\hbar(\ell+\tfrac{1}{2})$$

$$= \omega\hbar(\ell+\tfrac{1}{2}) = E_{MIN}$$

$$V(d) = E = \frac{K}{2}d^2 + \frac{\hbar^2}{2m}\frac{(\ell+\frac{1}{2})^2}{d^2}$$

$$\Rightarrow \frac{K}{2}d^2 - E + \frac{\hbar^2}{2m}\frac{(\ell+\frac{1}{2})^2}{d^2} = 0$$

$$\frac{K}{2}d^4 - Ed^2 + \frac{\hbar^2}{2m}(\ell+\tfrac{1}{2})^2 = 0$$

$$d^2 = \frac{+E \pm \sqrt{E^2 - \frac{K\hbar^2}{m}(\ell+\frac{1}{2})^2}}{K}$$

$$= \frac{E}{K} \pm \sqrt{\frac{E^2}{K^2} - \frac{\hbar^2}{mK}(\ell+\tfrac{1}{2})^2}$$

$$b^2 = \frac{E}{K} - \sqrt{\frac{E^2}{K^2} - \frac{\hbar^2}{mK}(\ell+\tfrac{1}{2})^2} = \frac{E}{K} - \sqrt{\frac{E^2}{K^2} - \frac{\omega^2\hbar^2}{K^2}(\ell+\tfrac{1}{2})^2}$$

$$c^2 = \frac{E}{K} + \sqrt{\frac{E^2}{K^2} - \frac{\hbar^2}{mK}(\ell+\tfrac{1}{2})^2} = \frac{E}{K} + \sqrt{\frac{E^2}{K^2} - \frac{\omega^2\hbar^2}{K^2}(\ell+\tfrac{1}{2})^2}$$

$$\Rightarrow b^2 = \frac{1}{K}\left[E - \sqrt{E^2 - \omega^2\hbar^2(\ell+\tfrac{1}{2})^2}\right]$$

$$c^2 = \frac{1}{K}\left[E + \sqrt{E^2 - \omega^2\hbar^2(\ell+\tfrac{1}{2})^2}\right]$$

$$b^2 = \frac{1}{K}\left[E - \sqrt{E^2 - E_{MIN}^2}\right]$$

$$c^2 = \frac{1}{K}\left[E + \sqrt{E^2 - E_{MIN}^2}\right]$$

$$p(r) = \left[2m\left(E - \frac{K}{2}r^2\right) - \hbar^2\left(\ell + \tfrac{1}{2}\right)^2 / r^2\right]^{1/2}$$

$$\pi\hbar\left(n + \tfrac{1}{2}\right) = \int_b^c p(r)\,dr$$

$$= \int_b^c \left[2m\left(E - \frac{K}{2}r^2\right) - \hbar^2\left(\ell + \tfrac{1}{2}\right)^2 / r^2\right]^{1/2}$$

$$\pi\left(n + \tfrac{1}{2}\right) = \int_b^c \left[\frac{2m}{\hbar^2}\left(E - \frac{K}{2}r^2\right) - \frac{1}{r^2}\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2}$$

LET $\rho = r^2 \Rightarrow r = \sqrt{\rho} \Rightarrow dr = \frac{+1}{2\sqrt{\rho}}$

$$r = b \Rightarrow \rho = b^2 \; ; \; r = c \Rightarrow \rho = c^2$$

$$\pi\left(n + \tfrac{1}{2}\right) = \int_{b^2}^{c^2} \frac{+1}{2\sqrt{\rho}}\left[\frac{2m}{\hbar^2}\left(E - \frac{K}{2}\rho\right) - \frac{1}{\rho}\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2} d\rho$$

$$+2\pi\left(n + \tfrac{1}{2}\right) = \int_{b^2}^{c^2}\left[\frac{2m}{\rho\hbar^2}\left(E - \frac{K}{2}\rho\right) - \frac{1}{\rho^2}\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2} d\rho$$

$$= \int_{b^2}^{c^2}\left[\frac{2mE}{\rho\hbar^2} - \frac{mK}{\hbar^2} - \frac{1}{\rho^2}\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2} d\rho$$

$$= \int_{b^2}^{c^2} \frac{1}{\rho}\left[-\frac{mK}{\hbar^2}\rho^2 + \frac{2mE}{\hbar^2}\rho - \left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2} d\rho$$

$$= \int_{b^2}^{c^2} \frac{1}{\rho}\left[-\alpha^2\rho^2 + \frac{2mE}{\hbar^2}\rho - \left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2} d\rho \; ; \; \alpha^2 = \frac{mK}{\hbar^2}$$

$$= \alpha\int_{b^2}^{c^2} \frac{1}{\rho}\left[-\rho^2 + \frac{2mE}{\hbar^2\alpha^2}\rho - \frac{1}{\alpha^2}\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2} d\rho \qquad \alpha = \frac{K}{\hbar\omega}$$

ROOTS OF QUADRADIC UNDER RADICAL ARE

$$\rho = \frac{\frac{2mE}{\hbar^2} \pm \left[\frac{4m^2E^2}{\hbar^4} - \frac{4mK}{\hbar^2}\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2}}{+\frac{2mK}{\hbar^2}}$$

$$= \frac{mE \pm \left[m^2E^2 - mK\hbar^2\left(\ell + \tfrac{1}{2}\right)^2\right]^{1/2}}{+mK}$$

$$= \frac{1}{K}\left[+E \pm \left\{E^2 - \frac{K\hbar^2}{m}\left(\ell + \tfrac{1}{2}\right)^2\right\}^{1/2}\right]$$

$$= \frac{1}{K}\left[E \pm \left\{E^2 - \omega^2\hbar^2\left(\ell + \tfrac{1}{2}\right)^2\right\}^{1/2}\right]$$

$$= +\frac{1}{K}\left[E \pm \left\{E^2 - E_{MIN}^2\right\}^{1/2}\right] = b^2, c^2$$

$$\therefore +2\pi\left(n + \tfrac{1}{2}\right) = \alpha\int_{b^2}^{c^2} \frac{1}{\rho}\left[(\rho - b^2)(c^2 - \rho)\right]^{1/2} d\rho$$

$$= \frac{\alpha\pi}{2}\left[b^2 + c^2 - 2ab\right]$$

$$b^2 + c^2 = \frac{2}{K}E$$

$$a^2b^2 = \frac{1}{K^2}\left[E^2 - \left(E^2 - E_{MIN}^2\right)\right] = \frac{E_{MIN}^2}{K^2} \Rightarrow 2ab = \frac{2E_{MIN}}{K}$$

$$+2\left(n + \tfrac{1}{2}\right) = \frac{K}{\hbar\omega}\left[\frac{E}{K} - \frac{E_{MIN}}{K}\right] = \frac{1}{\hbar\omega}\left[E - E_{MIN}\right]$$

$$\therefore E_n = +\hbar\omega 2\left(n + \tfrac{1}{2}\right) + E_{MIN} \quad \ni E_{MIN} = \omega\hbar\left(\ell + \tfrac{1}{2}\right)$$

$$\Rightarrow E_{n\ell} = \hbar\omega\left(2n + \ell + \tfrac{3}{2}\right) \Leftarrow \text{EXACT ANSWER}$$

$$E_{00} = \tfrac{3}{2}\hbar\omega$$

4(D) $E_N = \hbar\omega(N + \frac{3}{2})$

FOR 3D, $N = n_1 + n_2 + n_3$, LET m = DEGENERACY

$N=0$ $(0,0,0) \rightarrow m_0 = 1$

$N=1$ $(0,0,1)(0,1,0)(1,0,0) \rightarrow m_1 = 3$

$N=2$ $(0,0,2)(0,2,0)(2,0,0)(1,0,1)(1,1,0)(0,1,1) \rightarrow m_2 = 6$

$N=3$ $(0,0,3)(0,3,0)(3,0,0)(1,0,2)(1,2,0)(0,1,2)$

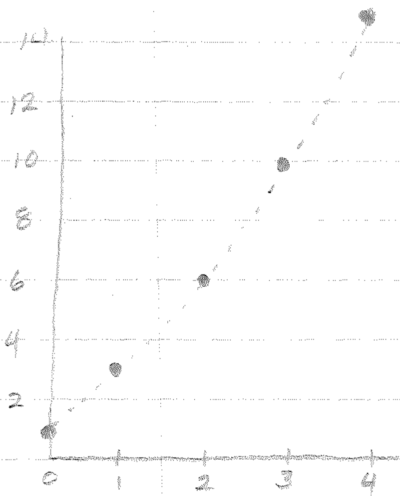
$(0,2,1)(2,1,0)(2,0,1)(1,1,1) \rightarrow m_3 = 10$

$N=4$ $(0,0,4)(0,4,0)(4,0,0)(1,0,3)(1,3,0)(0,1,3)$

$(0,3,1)(3,1,0)(3,0,1)(1,1,2)(1,2,1)(2,1,1)$

$(2,2,0)(0,2,2)(2,0,2) \rightarrow m_4 = 15$

N	m_N
0	1
1	3
2	6
3	10
4	15



THE RELATIONSHIP : $m_N = \frac{1}{2}(N+1)(N+2)$
WORKS FOR $n = 0, 1, 2, 3, 4$. ERGO, BY INDUCTION, WE ACCEPT IT FOR ALL N.
(FOR OUR PURPUSES, $N \geq 0$ ie $N = 0, 1, 2, \ldots$)

5.a. 1s : $(n, l, m) = (1, 0, 0)$

$R_{10}(\rho) = A_1 e^{-\rho}$

10 $Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$

$\Rightarrow \psi_{1s}(\rho) = A_2 e^{-\rho}$; $\rho = r/a$

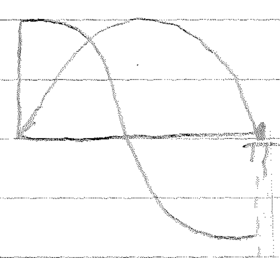
$2p_z$: $(n, l, m) = (2, 1, 0)$

$R_{21}(\rho) = A_3 \rho e^{-\rho Z/2}$

$Y_{10}(\rho) = \sqrt{\frac{3}{4\pi}} \cos\theta$

$\Rightarrow \psi_{2p_z} = A_4 \rho e^{-\rho Z/2} \cos\theta$

$$\therefore \int d^3\rho\, \psi_{1s}\psi_{2p_z} = A_5 \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\cos\theta\, d\theta \int_0^{\infty} \rho e^{-\rho(Z+1)/2} \rho^2 d\rho$$



$\Rightarrow \int_0^{\pi} \sin\theta\cos\theta\, d\theta = 0$

$$\therefore \int d^3\rho\, \psi_{1s}\psi_{2p_z} = \int d^3r\, \psi_{1s}\psi_{2p_z} = 0$$

b. $\int d^3r\, \psi_{1s}\, P_z\, \psi_{2p_z}$

Z : VARIABLE

$\bar{Z}$: ELEMENT #

$P_z = \frac{\hbar}{i}\frac{d}{dz}$

$z = \rho \cos\theta$

$\Rightarrow \int d^3r\, \psi_{1s}\, P_z\, \psi_{2p_z}$

$= A_5 \frac{\hbar}{i} \int d\rho^3\, e^{-\rho} \frac{d}{dz} \rho\, e^{-\rho \bar{Z}/2} \cos\theta$

$= A_5 \frac{\hbar}{i} \int d\rho^3\, e^{-\rho} \frac{d}{dz} \sqrt{x^2+y^2+z^2}\, e^{-\frac{\bar{Z}}{2}\sqrt{x^2+y^2+z^2}} \times \frac{z}{\sqrt{x^2+y^2+z^2}}$

$= A_5 \frac{\hbar}{i} \int d^3\rho\, e^{-\rho} \frac{d}{dz}\, z\, e^{-\frac{\bar{Z}}{2}\sqrt{x^2+y^2+z^2}}$

$= A_5 \frac{\hbar}{i} \int d^3\rho\, e^{-\rho} \Big[e^{-\frac{\bar{Z}}{2}\sqrt{x^2+y^2+z^2}}$

$\quad - \frac{\bar{Z}}{2}(2z)\frac{1}{\sqrt{x^2+y^2+z^2}}\, e^{-\frac{\bar{Z}}{2}\sqrt{x^2+y^2+z^2}} \Big]$

$= A_5 \frac{\hbar}{i} \int d^3\rho\, e^{-\rho} \left[1 - \frac{z\bar{Z}}{r}\right] e^{-\bar{Z}\rho/2}$

$= A_5 \frac{\hbar}{i} \int d^3\rho \left[1 - \bar{Z}\cos\theta\right] e^{-(\bar{Z}+1)\rho/2}$

$= A_5 \frac{\hbar}{i} \left[\int d^3\rho\, e^{-(\bar{Z}+1)\rho/2} - \bar{Z} \int d^3\rho \cos\theta\, e^{-(\bar{Z}+1)\rho/2} \right]$

$$\int d^3\rho\, e^{-(Z+1)\rho/2} = 4\pi \int_0^\infty d\rho\, \rho^2 e^{-(Z+1)\rho/2}$$

$$= 4\pi \frac{2}{\left(\frac{Z+1}{2}\right)^3}$$

$$= \frac{8\pi \times 8}{(Z+1)^3}$$

$$= 64\pi/(Z+1)^3$$

$$\int d^3\rho \cos\theta\, e^{-(Z+1)\rho/2} = 2\pi \int_0^\pi \sin\theta\cos\theta\, d\theta \int_0^\infty d\rho\, \rho^2 e^{-(Z+1)\rho/2}$$
$$= 0$$

$$\Rightarrow \int d^3\rho\, \psi_{1s} P_z \psi_{2p_z} = A_5 \frac{\hbar}{i} \frac{64\pi}{(Z+1)^3}$$

$$A_5 = A_4 A_2$$
$$A_2 = \frac{1}{\sqrt{4\pi}} A_1 \Rightarrow A_5 = \frac{1}{\sqrt{4\pi}} A_4$$

$$A_4 = \sqrt{\frac{3}{4\pi}}\, A_3$$
$$A_3 = \frac{1}{2\sqrt{6}} Z^{7/2} \;*$$
$$A_4 = \frac{1}{2}\sqrt{\frac{3}{\pi}} \frac{1}{2\sqrt{6}} Z^{7/2} = \frac{1}{4\sqrt{2\pi}} Z^{7/2}$$
$$\therefore A_5 = \frac{1}{2\sqrt{\pi}} \frac{1}{4\sqrt{2\pi}} Z^{7/2}$$
$$= \frac{1}{8\pi\sqrt{2}} Z^{7/2}$$

$$\Rightarrow d^3\rho = d^3\left(\frac{r}{a}\right) \Rightarrow a^3 d^3\rho = d^3 r$$

$$\therefore \int d^3 r\, \psi_{1s} P_z \psi_{2p_z} = \frac{-i\hbar\, \overset{8}{\cancel{64}}\pi}{a^3 (Z+1)^3} \frac{1}{8\pi\sqrt{2}} Z^{7/2}$$
$$= \frac{-i\, 8\hbar\, Z^{7/2}}{\sqrt{2}\, a^3 (Z+1)^3}$$

* DAVYDOV, Pg 139

c. $\int dr^3 \psi_{1s}\, z\, \psi_{2ps}$

$$A_5 \int d\rho^3\, e^{-\rho}\, z\, \rho\, e^{-\rho Z/2} \cos\theta$$

$$= A_5 \int d\rho^3\, e^{-\rho} \cos\theta\, \rho\, e^{-\rho Z/2} \cos\theta$$

$$= A_5 \int d\rho^3\, \rho \cos^2\theta\, e^{-\rho(Z+1)/2}$$

$$= A_5\, 2\pi \int_0^{\pi} \cos^2\theta \int_0^{\infty} \rho\, e^{-\rho(Z+1)/2}$$

$$= A_5\, 2\pi \left(\frac{\pi}{2}\right) \frac{1}{\left(\frac{Z+1}{2}\right)^2}$$

$$= A_5\, \pi^2 \frac{4}{(Z+1)^2}$$

$$= \frac{1}{8\pi\sqrt{2}} Z^{7/2}\, \pi^2 \frac{4}{(Z+1)^2}$$

$$= \frac{\pi Z^{7/2}}{2\sqrt{2}(Z+1)^2}$$

$$\therefore \int dr^3 \psi_{1s}\, z\, \psi_{2ps} = \frac{\pi Z^{7/2}}{2\sqrt{2}\, a^4 (Z+1)^2}$$

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6. $V(x) = \begin{cases} -Ze^2/x & ; x > 0 \\ \infty & ; x < 0 \end{cases}$

FOR $x > 0$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{Ze^2}{x} - E\right]\psi(x) = 0$$

LET $\rho = r/a$; $a = \frac{\hbar^2}{me^2}$

$$\left[-\frac{\hbar^2}{2ma^2}\frac{d^2}{d\rho^2} - \frac{Ze^2}{a\rho} - E\right]\psi(\rho) = 0$$

NOW: $\frac{\hbar^2}{2ma^2} = \frac{e^4 m}{\hbar^2}$

$$\left[\frac{d^2}{d\rho^2} + \frac{2Z}{\rho} + \frac{2Ea}{e^2}\right]\psi(\rho) = 0$$

$$\left[\frac{d^2}{d\rho^2} + \frac{2Z}{\rho} - \alpha^2\right]\psi(\rho) = 0 \quad ; \alpha^2 = \frac{-2Ea}{e^2}$$

FOR LARGE ρ

$$\left[\frac{d^2}{d\rho^2} - \alpha^2\right]\psi(\rho) = 0 \Rightarrow \psi(\rho) = Ae^{-\alpha\rho}$$

LET $\psi(\rho) = \rho e^{-\alpha\rho}F(\rho)$

$$\frac{d\psi}{d\rho} = e^{-\alpha\rho}F - \alpha\rho e^{-\alpha\rho}F(\rho) + \rho e^{-\alpha\rho}\frac{dF}{d\rho}$$

$$= e^{-\alpha\rho}\left[(1-\alpha\rho)F(\rho) + \rho\frac{dF}{d\rho}\right]$$

$$= e^{-\alpha\rho}\left[\rho\frac{d}{d\rho} + (1-\alpha\rho)\right]F(\rho)$$

$$\frac{d^2\psi}{d\rho^2} = -\alpha e^{-\alpha\rho}\left[(1-\alpha\rho)F(\rho) + \rho\frac{dF}{d\rho}\right]$$

$$+ e^{-\alpha\rho}\left[-\alpha F(\rho) + (1-\alpha\rho)\frac{dF}{d\rho} + \frac{dF}{d\rho} + \rho\frac{d^2F}{d\rho^2}\right]$$

$$= e^{-\alpha\rho}\left[\rho\frac{d^2F}{d\rho^2} - \alpha\rho\frac{dF}{d\rho} + (2-\alpha\rho)\frac{dF}{d\rho} - \alpha(1-\alpha\rho)F - \alpha F\right]$$

$$= e^{-\alpha\rho}\left[\rho\frac{d^2}{d\rho^2} + (2-2\alpha\rho)\frac{d}{d\rho} - (2\alpha - \alpha^2\rho)\right]F(\rho)$$

$$\therefore \left[\rho\frac{d^2}{d\rho^2} + (2-2\alpha\rho)\frac{d}{d\rho} + (\alpha^2\rho - 2\alpha) + 2Z - \alpha^2\rho\right]F(\rho) = 0$$

$$\left[\rho\frac{d^2}{d\rho^2} + (2-2\alpha\rho)\frac{d}{d\rho} + (2Z - 2\alpha)\right]F(\rho) = 0$$

SOLUTION IS

$$F(\rho) = F\left(1 - \frac{Z}{\alpha}, 2, 2\rho\alpha\right)$$

THUS:

$$\psi(\rho) = A\rho e^{-\alpha\rho} F\left(1-\frac{Z}{\alpha}, 2, 2\rho\alpha\right)$$

IN ORDER NOT TO BLOW UP FOR LARGE ρ:

$$-n = 1 - \frac{Z}{\alpha}$$

$$\Rightarrow \frac{1}{\alpha} = \frac{1}{Z}(1+n) \Rightarrow \alpha^2 = \frac{-2Ea}{e^2} = \frac{Z^2}{(n+1)^2}$$

$$\therefore E_n = -\left(\frac{Ze}{n+1}\right)^2 \frac{1}{2a} \qquad a = \frac{\hbar^2}{me^2}$$

$$= -\left(\frac{Z}{n+1}\right)^2 E_{RYD}$$

Physics 611
Due: March 6, 1975
#6

Each Problem Counts Double (20 points)

(1) Use variational theory to solve the ground state energy of two 1s electrons in a coulomb potential of charge Z. The result for Z = 2 should reproduce the helium result given in lecture.

a. Z = 1: Does the H^- ion exist? If so, what is its binding energy? If not what energy amount does it need to bind?

b. Z = 3: Compare with the Li^+ ion, whose experimental ionization energies are 75.3eV and 121.8eV for the two electrons.

(2) Use variational theory to find the 2s electron binding energy of Li. Compare with the experimental value given in lecture. Use (51.16) of text, but put in electron-electron interactions, and Z^* for the 1s state (which is known from problem (1)).

(3) Solve the Hamiltonian for a hydrogen atom in a constant electric field F

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} + eFr\cos\theta$$

by using the variational wave function for the ground state

$$\psi(r) = A\, e^{-r/a}\left(1 + \lambda \frac{r}{a}\cos\theta\right)$$

where a = bohr radius, and λ is the variational parameter.

a. Find the value of λ which minimizes the energy.

b. Express the energy as a function of F.

c. Expand (b) in a Taylor series about F = 0, $E(F) = E(0) - \alpha F^2/2 + O(F^4)$ Calculate α, which is the polarizability of hydrogen. Compare with the exact result $\alpha = \frac{9}{2}a^3$

PHYSICS 611
DUE: MARCH 6, 1975
BOB MARKS

40/60

MAHAN, Ru. 161

1. ~~T~~20 HIS PROBLEM IS WORKED IN SEC. 88 OF DAVYDOV:

$$H = \frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - Ze^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{|r_1 - r_2|}$$

$$\psi_0 = \frac{1}{\pi}\left(\frac{\beta}{a}\right)^3 e^{-\beta(r_1+r_2)/a}$$

β : VARIATIONAL PARAMETER

SINCE ψ_0 IS ALREADY NORMALIZED, WE NEED TO COMPUTE ONLY:

$$E(\beta) = \int \psi_0 H \psi_0 \, d\tau$$

$$= E_1(\beta) + E_2(\beta) + E_3(\beta)$$

$$E_1(\beta) = \frac{-ae^2}{2}\int \psi_0(\nabla_1^2 + \nabla_2^2)\psi_0 \, d\tau_1 d\tau_2 = \beta^2 \frac{e^2}{a}$$

$$E_2(\beta) = -Ze^2 \int \psi_0\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\psi_0 \, d\tau_1 d\tau_2 = -2Z\beta e^2/a$$

$$E_3(\beta) = e^2 \int \psi_0^2 \frac{1}{|r_1 - r_2|} \, d\tau_1 d\tau_2 = \frac{5}{8}\beta \frac{e^2}{a}$$

$$\Rightarrow E(\beta) = \frac{e^2}{a}\left[\beta^2 - \left(2Z - \frac{5}{8}\right)\beta\right]$$

MINIMIZING:

$$\left.\frac{dE(\beta)}{d\beta}\right|_{\beta_0} = 0 = 2\beta_0 - \left(2Z - \frac{5}{8}\right) \Rightarrow \beta_0 = Z - \frac{5}{16}$$

$$E_0 = E(\beta_0) = -\left(Z^2 - \frac{5}{8}Z + \frac{25}{256}\right)\frac{e^2}{a}$$

$$= -\left(2Z^2 - \frac{5}{4}Z + \frac{25}{128}\right)E_{RYD}$$

$$\left.E_0\right|_{Z=2} = -5.70\, E_{RYD}$$ $\Leftarrow$ AGREES WITH DERIVATION IN CLASS.

(CONT.)

a. $Z = 1 \Rightarrow E_0 = {}^{-}0.95\ E_{RYD}$

THUS, IT TAKES $^{-}0.95\ E_{RYD}$ TO REMOVE THE TWO 1S ELECTRONS FROM THE H^- ION. IT TAKES $-E_{RYD}$ TO REMOVE THE SINGLE 1S ELECTRON FROM THE HYDROGEN ATOM. THUS, $^{+}0.05\ E_{RYD}$ (>0) IS "REQUIRED" TO REMOVE THE FIRST 1S ELECTRON FROM THE H^- ION. ERGO, ALTHOUGH EXISTING, THE H^- ION IS NOT TOO STABLE, IN THAT THE SECOND 1S ELECTRON IS ESSENTIALLY UNWANTED BY THE CONFIGURATION.

b. $^{-}(75.3 + 121.8)\,eV = {}^{-}197.1\ eV \times \frac{1\ E_{RYD}}{13.6\,eV} = {}^{-}14.5\ E_{RYD}$

$E_0\big|_{Z=3} = {}^{-}14.4\ E_{RYD}$ ⟸ VARIATIONAL SOLUTION.

AN ERROR OF LESS THAN 1%

2. c)

3/3

$$\mathcal{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} + eFr\cos\theta$$

$$\nabla^2 = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{d}{d\theta} + \frac{1}{r^2}\frac{d^2}{d\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{d^2}{d\phi^2}$$

$$\psi(r) = Ae^{-r/a}\left(1 + \frac{\lambda r}{a}\cos\theta\right)$$

NOW

$$\frac{d\psi}{dr} = \frac{A}{a}e^{-r/a}\left[\lambda\left(1 - \frac{r}{a}\right)\cos\theta - 1\right]$$

$$\frac{d^2\psi}{dr^2} = -\frac{A}{a^2}e^{-r/a}\left[\lambda\left(2 - \frac{r}{a}\right)\cos\theta - 1\right]$$

$$\frac{d\psi}{d\theta} = -\frac{A\lambda r}{a}e^{-r/a}\sin\theta$$

$$\frac{d^2\psi}{d\theta^2} = -\frac{A\lambda r}{a}e^{-r/a}\cos\theta$$

$$\int_0^\pi \cos\theta\sin\theta\, d\theta = 0$$

$$\int_0^\pi \cos^2\theta\sin\theta\, d\theta = \frac{2}{3}$$

$$\int_0^\infty r^n e^{-2r/a} = n!\left(\frac{a}{2}\right)^{n+1}$$

$$\int d^3r\, \Phi\Theta R = \int_0^\pi \Phi\, d\phi \int_0^{2\pi} \sin\theta\, \Theta\, d\theta \int_0^\infty r^2 R\, dr$$

- NORMALIZATION:

$$\int d^3r\, \psi^2(r)$$

$$= \int d^3r\, A^2 e^{-2r/a}\left(1 + \frac{\lambda r}{a}\cos\theta\right)^2$$

$$= A^2\int d^3r\, e^{-2r/a}\left(1 + \frac{\lambda^2 r^2}{a^2}\cos^2\theta\right)$$

$$= A^2\left[\int d^3r\, e^{-2r/a} + \frac{\lambda^2}{a^2}\int d^3r\, r^2 e^{-2r/a}\cos^2\theta\right]$$

$$= A^2\left[4\pi\int_0^\infty r^2 e^{-2r/a}dr + \frac{\lambda^2}{a^2}2\pi\left(\frac{2}{3}\right)\int_0^\infty r^4 e^{-2r/a}dr\right]$$

$$= A^2 4\pi\left[2\left(\frac{a}{2}\right)^3 + \frac{\lambda^2}{3a^2}24\left(\frac{a}{2}\right)^5\right]$$

$$= A^2 4\pi a^3\left[\frac{1}{4} + \lambda^2 8\frac{1}{32}\right]$$

$$= 4\pi A^2 a^3\left[\frac{1}{4} + \frac{\lambda^2}{4}\right]$$

$$= \pi A^2 a^3\left[1 + \lambda^2\right]$$

• ∇^2 TERMS

1. $\frac{d^2}{dr^2}$

$$\int d\vec{r}^{\,3}\, \psi(r) \frac{d^2}{dr^2} \psi(r)$$

$$= \int d^3r\, A e^{-r/a} \left(1 + \frac{\lambda r}{a} \cos\theta\right) \left(\frac{-A}{a^2}\right) e^{-r/a} \left[\lambda\left(2 - \frac{r}{a}\right)\cos\theta - 1\right]$$

$$= \frac{+A^2}{a^2} \int d\vec{r}^{\,3}\, e^{-2r/a} \left(1 + \frac{\lambda r}{a} \cos\theta\right) \left[(1 - 2\lambda\cos\theta) + \frac{\lambda r}{a}\cos\theta\right]$$

$$= \frac{A^2}{a^2} \int d^3r\, e^{-2r/a} \left[(1 - 2\lambda\cos\theta) + \frac{\lambda^2 r^2}{a^2}\cos^2\theta + (2 - 2\lambda\cos\theta)\frac{\lambda r}{a}\cos\theta\right]$$

$$= \frac{A^2}{a^2} \int d^3r\, e^{-2r/a} \left[1 + \frac{\lambda^2 r^2}{a^2}\cos^2\theta - \frac{2\lambda^2 r}{a}\cos^2\theta\right]$$

$$= \frac{A^2}{a^2} \left[\int d^3r\, e^{-2r/a} + \frac{\lambda^2}{a^2} \int d^3r\, e^{-2r/a}\, r^2 \cos^2\theta \right.$$
$$\left. - \frac{2\lambda^2}{a} \int d^3r\, e^{-2r/a}\, r \cos^2\theta\right]$$

$$= \frac{A^2}{a} \left[4\pi \int_0^\infty dr\, r^2 e^{-2r/a} - 2\pi \frac{2\lambda^2}{a} \times \frac{2}{3} \int_0^\infty r^3 e^{-2r/a}\, dr \right.$$
$$\left. + 2\pi \frac{\lambda^2}{a^2} \frac{2}{3} \int_0^\infty r^4 e^{-2r/a}\, dr\right]$$

$$= \frac{A^2}{a^2} 4\pi \left[2\left(\frac{a}{2}\right)^3 - \frac{2}{3}\frac{\lambda^2}{a} 6 \left(\frac{a}{2}\right)^4 + \frac{1}{3}\frac{\lambda^2}{a^2} 24 \left(\frac{a}{2}\right)^5\right]$$

$$= \frac{A^2}{a^2} 4\pi a^3 \left[\frac{1}{4} - 4\lambda^2 \frac{1}{16} + 8\lambda^2 \frac{1}{32}\right]$$

$$= 4\pi A^2 a \left[\frac{1}{4} - \frac{1}{4}\lambda^2 + \frac{1}{4}\lambda^2\right]$$

$$= \pi A^2 a$$

2. $\frac{2}{r}\frac{d}{dr}$

$$\int d^3r\ \psi(r)\ \frac{2}{r}\frac{d}{dr}\ \psi(r)$$

$$= \int d^3r\ A e^{-r/a}\left(1+\frac{\lambda r}{a}\cos\theta\right)\frac{2A}{ra}e^{-r/a}\left[\lambda\left(1-\frac{r}{a}\right)\cos\theta - 1\right]$$

$$= -\frac{2A^2}{a}\int d^3r\ e^{-2r/a}\ \frac{1}{r}\left(1+\frac{\lambda r}{a}\cos\theta\right)\left[\left(1-\lambda\cos\theta\right)+\frac{\lambda r}{a}\cos\theta\right]$$

$$= -\frac{2A^2}{a}\int d^3r\, e^{-2r/a}\ \frac{1}{r}\left[1+\frac{\lambda^2 r^2}{a^2}\cos^2\theta+\left(2-\lambda\cos\theta\right)\frac{\lambda r}{a}\cos\theta\right]$$

$$= -\frac{2A^2}{a}\int d^3r\, e^{-2r/a}\ \frac{1}{r}\left[1+\frac{\lambda^2 r^2}{a^2}\cos^2\theta-\frac{\lambda^2 r}{a}\cos^2\theta\right]$$

$$= -\frac{2A^2}{a}\int d^3r\, e^{-2r/a}\left[\frac{1}{r}+\frac{\lambda^2 r}{a^2}\cos^2\theta-\frac{\lambda^2}{a}\cos^2\theta\right]$$

$$= -\frac{2A^2}{a}\left[\int d^3r\ \frac{1}{r}e^{-2r/a}+\frac{\lambda^2}{a^2}\int d^3r\ r e^{-2r/a}\cos^2\theta - \frac{\lambda^2}{a}\int d^3r\ e^{-2r/a}\cos^2\theta\right]$$

$$= -\frac{2A^2}{a}\left[4\pi\int_0^\infty r e^{-2r/a}dr+\frac{4\pi}{3}\frac{\lambda^2}{a^2}\int_0^\infty r^3 e^{-2r/a}dr - \frac{4\pi}{3}\frac{\lambda^2}{a}\int_0^\infty r^2 e^{-2r/a}dr\right]$$

$$= -\frac{8\pi A^2}{a}\left[\left(\frac{a}{2}\right)^2+\frac{1}{3}\frac{\lambda^2}{a^2}6\left(\frac{a}{2}\right)^4-\frac{1}{3}\frac{\lambda^2}{a}2\left(\frac{a}{2}\right)^3\right]$$

$$= -8\pi A^2 a\left[\frac{1}{4}+2\lambda^2\frac{1}{16}-\frac{1}{3}\lambda^2\frac{1}{4}\right]$$

$$= -8\pi A^2 a\left[\frac{1}{4}+\left(\frac{1}{8}-\frac{1}{12}\right)\lambda^2\right]$$

$$= -8\pi A^2 a\left[\frac{1}{4}+\frac{1}{24}\lambda^2\right]$$

$$= -\frac{1}{3}\pi A^2 a\left[6+\lambda^2\right]$$

3. $\frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{d}{d\theta}$

$$\int d^3r\,\psi(r)\,\frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{d}{d\theta}\psi(r)$$
$$= \int d^3r\,A e^{-r/a}\left(1+\frac{\lambda r}{a}\cos\theta\right)\frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\left(\frac{-A\lambda r}{a}\right)e^{-r/a}\sin\theta$$
$$= \frac{-A^2\lambda}{a}\int d^3r\,e^{-2r/a}\frac{1}{r}\left(1+\frac{\lambda r}{a}\cos\theta\right)\cos\theta$$
$$= \frac{-A^2\lambda}{a}\int d^3r\,e^{-2r/a}\frac{1}{r}\frac{\lambda r}{a}\cos^2\theta$$
$$= \frac{-A^2\lambda^2}{a^2}\int d^3r\,e^{-2r/a}\cos^2\theta$$
$$= -\frac{2A^2\lambda^2}{3a^2}\int_0^\infty r^2 e^{-2r/a}\times 2\pi$$
$$= -\frac{2A^2\lambda^2}{3a^2}\,2\left(\frac{a}{2}\right)^3\times 2\pi$$
$$= -\frac{4A^2\lambda^2}{3a^2}\frac{a^3}{8}\times 2\pi$$
$$= -\frac{A^2\lambda^2 a}{6}\times 2\pi$$
$$= -\frac{1}{3}A^2\lambda^2 a\pi$$

4. $\frac{1}{r^2}\frac{d^2}{d\theta^2}$

$$\int d^3r\,\psi(r)\,\frac{1}{r^2}\frac{d^2}{d\theta^2}\psi(r)$$
$$= \int d^3r\,A e^{-r/a}\left(1+\frac{\lambda r}{a}\cos\theta\right)\frac{1}{r^2}\left(\frac{-A\lambda r}{a}\right)e^{-r/a}\cos\theta$$
$$= -\frac{A^2\lambda}{a}\int d^3r\,\frac{1}{r}e^{-2r/a}\left(1+\frac{\lambda r}{a}\cos\theta\right)\cos\theta$$
$$= \frac{-A^2\lambda}{a}\int d^3r\,\frac{1}{r}e^{-2r/a}\frac{\lambda r}{a}\cos^2\theta$$
$$= \frac{-A^2\lambda^2}{a^2}\int d^3r\,e^{-2r/a}\cos^2\theta$$
$$= -\frac{2A^2\lambda^2}{3a^2}\int_0^\infty r^2 e^{-2r/a}\,dr\times 2\pi$$
$$= -\frac{2}{3}\frac{A^2\lambda^2}{a^2}\,2\left(\frac{a}{2}\right)^3\times 2\pi$$
$$= -\frac{2}{3}\frac{A^2\lambda^2}{a^2}\frac{a^3}{4}\times 2\pi$$
$$= -\frac{1}{6}A^2\lambda^2 a\times 2\pi$$
$$= -\frac{\pi}{3}A^2\lambda^2 a$$

$$\cancel{-\frac{\hbar^2}{2m}\int \psi(r)\nabla^2\psi(r)\,d^3r}$$
$$\cancel{= -\frac{\hbar^2}{2m}\left[\frac{1}{2}\pi A^2 a(2-\lambda^2) - \frac{1}{4}\pi A^2 a(6+\lambda^2) - \frac{2}{3}\pi A^2\lambda^2 a\right]}$$
$$\cancel{= \frac{\hbar^2}{2m}\pi A^2 a\left[\frac{2}{3}\lambda^2 + \frac{1}{4}(6+\lambda^2) - \frac{1}{2}(2-\lambda^2)\right]}$$
$$\cancel{= \frac{1}{2m}\pi A^2\hbar^2 a\left[\left(\frac{2}{3}+\frac{1}{4}+\frac{1}{2}\right)\lambda^2 + \frac{3}{2} - 1\right]}$$
$$\cancel{= \frac{\hbar^2}{2m}\pi A^2 a\left[\frac{17}{12}\lambda^2 - \frac{1}{2}\right]}$$

• $-\frac{e^2}{r}$ TERM

$$-\int \psi(r)\, \frac{e^2}{r}\, \psi(r)\, d^3r$$

$$= -e^2 \int A^2 e^{-2r/a} \left(1 + \frac{\lambda r}{a}\cos\theta\right)^2 \frac{1}{r}\, d^3r$$

$$= -e^2 A^2 \left[4\pi \int_0^\infty r e^{-2r/a}\, dr + \frac{\lambda^2}{a^2} 2\pi \left(\frac{2}{3}\right) \int_0^\infty r^3 e^{-2r/a}\, dr\right]$$

$$= -e^2 A^2 4\pi \left[\left(\frac{a}{2}\right)^2 + \frac{\lambda^2}{3a^2}\, 6 \left(\frac{a}{2}\right)^4\right]$$

$$= -e^2 A^2 a^2 4\pi \left[\frac{1}{4} + \frac{\lambda^2}{8}\right]$$

$$= -\frac{\pi}{2} e^2 A^2 a^2 \left[2 + \lambda^2\right]$$

• $eFr\cos\theta$ TERM

$$\int d^3r\, \psi(r)\, eFr\cos\theta\, \psi(r)$$

$$= eF \int A^2 e^{-2r/a} \left(1 + \frac{\lambda r}{a}\cos\theta\right)^2 r \cos\theta\, d^3r$$

$$= eFA^2 \int d^3r\, r e^{-2r/a} \left(1 + \frac{\lambda^2 r^2}{a^2}\cos^2\theta + \frac{2\lambda r}{a}\cos\theta\right)\cos\theta$$

$$= eFA^2 \int d^3r\, r e^{-2r/a} \left(\frac{\lambda^2 r^2}{a^2}\cos^3\theta + \frac{2\lambda r}{a}\cos^2\theta\right)$$

$$= \frac{eFA^2\lambda}{a} \int d^3r\, r e^{-2r/a} \left[\frac{\lambda r^2}{a}\cos^3\theta + 2r\cos^2\theta\right]$$

$$= \frac{eFA^2\lambda}{a} \left[\frac{\lambda}{a} \int d^3r\, r^3 e^{-2r/a} \cos^3\theta + 2 \int d^3r\, r^2 e^{-2r/a} \cos^2\theta\right]$$

NOW $\int_0^\pi \cos^3\theta \sin\theta\, d\theta = -\frac{\cos^4\theta}{4}\Big|_0^\pi = 0$

$$\Rightarrow \int d^3r\, \psi(r)\, eFr\cos\theta\, \psi(r)$$

$$= \frac{2eFA^2\lambda}{a} \int d^3r\, r^2 e^{-2r/a} \cos^2\theta$$

$$= \frac{8eFA^2\lambda\pi}{3a} \int_0^\infty r^4 e^{-2r/a}\, dr$$

$$= \frac{8eFA^2\lambda\pi}{3a}\, 24 \left(\frac{a}{2}\right)^5$$

$$= \frac{64\, eFA^2\lambda\pi}{a} \frac{a^5}{32}$$

$$= 2eFA^2\lambda\pi a^4$$

THUS $\int d^3r\, \psi H \psi$

$$= -\frac{\hbar^2}{2m}\left[\pi A^2 a - \frac{1}{3}\pi A^2 a(6+\lambda^2) - \frac{2\pi}{3}A^2 a\lambda^2\right] - \frac{\pi}{2}e^2A^2a^2(2+\lambda^2)$$

$$+ 2eFA^2\lambda\pi a^4$$

$$= \pi a A^2\left[-\frac{\hbar^2}{2m} + \frac{\hbar^2}{6m}(6+\lambda^2) + \frac{\hbar^2}{3m}\lambda^2 - \frac{1}{2}e^2 a(2+\lambda^2) + 2eF\lambda a^3\right]$$

NOW $a = \frac{\hbar^2}{me^2} \Rightarrow \frac{\hbar^2}{m} = e^2 a$

$\therefore \int d^3r\, \psi H\psi$

$$= \pi a A^2\left[-\frac{e^2a}{2} + \frac{e^2a}{6}(6+\lambda^2) + \frac{e^2a}{3}\lambda^2 - \frac{1}{2}e^2a(2+\lambda^2) + 2eF\lambda a^3\right]$$

$$= \pi a A^2\left[\left(\frac{e^2a}{6} + \frac{e^2a}{3} - \frac{e^2a}{2}\right)\lambda^2 + 2eF\lambda a^3 + \left(e^2a - e^2a - \frac{e^2a}{2}\right)\right]$$

$$= \pi a A^2\left[2eFa^3\lambda - \frac{e^2a}{2}\right]$$

$$= \frac{1}{2}\pi a^2A^2 e\left[4Fa^2\lambda - e\right]$$

FROM NORMALIZATION:

$$A^2 = \left[\pi a^3(1+\lambda^2)\right]^{-1} \Rightarrow E(\lambda) = \int \psi H\psi\, d^3r = \frac{4eFa^2\lambda - e^2}{2a(1+\lambda^2)}$$

~~THUS:~~

$$\cancel{E(\lambda) = \int d^3r\, \psi H \psi = \frac{2\pi a^4\, eF\lambda}{\pi a^3(1+\lambda^2)}}$$

$$\cancel{\frac{dE(\lambda)}{d\lambda} = 0 \Rightarrow 2aeF(1+\lambda^2) = 2\lambda(2aeF\lambda)}$$

$$\cancel{= 4aeF\lambda^2}$$

$$\cancel{2+\lambda^2 = 4\lambda^2 \Rightarrow 3\lambda^2 = 2 \Rightarrow \lambda_0 = -\sqrt{\tfrac{2}{3}}}$$

$$\cancel{E(\lambda_0) = -\sqrt{\tfrac{2}{3}}\,\frac{2aeF}{5/3} =}$$

$$\cancel{= -\sqrt{\tfrac{2}{3}}\,\frac{6aeF}{5}}$$

$$\cancel{= \frac{6\sqrt{6}\,aeF}{15}}$$

Do for Li^+: $Z = 3$.

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - Z\left(\frac{e^2}{r_1} + \frac{e^2}{r_2}\right) + \frac{e^2}{|r_1 - r_2|}$$

$$\psi = \frac{Z^{*3}}{\pi a_B^3} e^{-\frac{Z^*(r_1+r_2)}{a_B}}$$

$$E(Z^*, Z) = 2Z^{*2} E_{ryd.} - 4Z^* Z E_{ryd.} + \frac{5}{4} Z^* E_{ry.}$$

$$\boxed{\frac{E}{E_{ryd}} = 2Z^{*2} - 4ZZ^* + 5Z^*/4.}$$

$\cancel{Z = 3}$ $\quad \frac{\partial E}{\partial Z^*} = 0 = 4Z^* - 4Z + 5/4$

$$\boxed{Z^* = Z - 5/16.}$$

$$E/E_{ry} = 2(Z - 5/16)^2 - 4Z(Z - 5/16) + \frac{5}{4}(Z - 5/16)$$
$$= 2Z^2 - \frac{25}{4} + \frac{25}{128} - 4Z^2 + 5/4 Z + \frac{5Z}{4} - \frac{25}{64}.$$

$$E/E_{ry} = -2Z^2 + \frac{5Z}{4} - \frac{25}{128}.$$

Z	$+E/E_{ry}$
1	$-121/128 = -1 + 7/128$ 2nd electron barely unbound!
2	$-749/128 = -5.70 = -4 - (1.70)$.
3	$-\cancel{1??}\,1849/128 = -9.00 - \frac{697}{128} = -9.00 - 5.46$

$$\psi_{1s} = \left(\frac{Z^{*3}}{\pi a_B^3}\right)^{1/2} e^{-Z^* r/a_B}$$

$$\psi_{2s} = \frac{B}{a_B^{3/2}} \left[1 + \gamma\, r/a_B\right] e^{-\alpha r/a_B}$$

---

① <u>Orthogonality</u>

$$\int_0^\infty r^2 dr\, \psi_{1s}\psi_{2s} = 0 = \int_0^\infty \rho^2 d\rho\, e^{-\rho(\alpha+Z^*)}(1+\gamma\rho)$$

$$= \frac{2!}{(\alpha+Z^*)^3} + \frac{\gamma\, 3!}{(\alpha+Z^*)^4} = 0.$$

$$\boxed{\gamma = -\frac{1}{3}(\alpha + Z^*)}$$

② <u>Normalization</u>

$$1 = \int_0^\infty dr\, r^2 \psi_{2s}^2 = B^2 \int_0^\infty \rho^2 d\rho\, e^{-2\alpha\rho}\left[1 + 2\gamma\rho + \gamma^2\rho^2\right].$$

$$1 = B^2\left[\frac{2!}{(2\alpha)^3} + \frac{2\cdot 3!\,\gamma}{(2\alpha)^4} + \frac{\gamma^2\, 4!}{(2\alpha)^5}\right] = \frac{B^2}{4\alpha^3}\left[1 + \frac{3\gamma}{\alpha} + \frac{3\gamma^2}{\alpha^2}\right].$$

$$\frac{B^2}{4\alpha^3} = N(Z^*/\alpha) = \left[1 - (1 + Z^*/\alpha) + \frac{1}{3}(1+Z^*/\alpha)^2\right]^{-1}.$$

$$\boxed{N(\lambda) = 3\left[1 - \lambda + \lambda^2\right]^{-1}}. \qquad \lambda = Z^*/\alpha.$$

③ <u>Potential energy</u>

$$P.E. = -3e^2 \int_0^\infty r^2 dr\, \frac{\psi_{2s}^2}{r} = -\frac{3e^2}{a_B} B^2 \int_0^\infty \rho\, d\rho\, e^{-2\alpha\rho}\left[1 + 2\gamma\rho + \gamma^2\rho^2\right].$$

$$P.E = -\frac{3e^2}{a_B} B^2\left[\frac{1}{4\alpha^2} + \frac{2\gamma\cdot 2!}{(2\alpha)^3} + \frac{\gamma^2 3!}{(2\alpha)^4}\right] = -6\,E_{ryd}\,\frac{B}{4\alpha^2}\left[1 + \frac{2\gamma}{\alpha} + \frac{3}{2}\frac{\gamma^2}{\alpha^2}\right].$$

$$\lambda = Z^*/\alpha$$

$$P.E. = -6E_{ryd}\, N(\lambda)\, \alpha\left[1 - \frac{2}{3}(1+\lambda) + \frac{1}{6}(1+\lambda)^2\right].$$

$$\boxed{P.E. = -E_{ryd}\, N(\lambda)\, \alpha\left[3 - 2\lambda + \lambda^2\right].}$$

④ Kinetic Energy

$$K.E. = \frac{\hbar^2}{2m\,a_B^2} \int_0^\infty \rho^2 d\rho \left(\frac{d\psi_{1s}}{d\rho}\right)^2$$

$$= E_{ryd}\, B^2 \int_0^\infty \rho^2 d\rho \left[e^{-2\alpha\rho}\right]\left[-\alpha(1+\gamma\rho)+\gamma\right]^2$$

$$= \left[(\gamma-\alpha) - \alpha\gamma\rho\right]^2$$

$$K.E. = E_{ryd}\, B^2 \int_0^\infty \rho^2 d\rho\; e^{-2\alpha\rho}\left[(\gamma-\alpha)^2 - 2\alpha\gamma\rho\,(\gamma-\alpha) + \alpha^2\gamma^2\rho^2\right].$$

$$K.E. = \alpha^2 B^2 E_{ryd} \left\{ \left[\frac{(\frac{\gamma}{\alpha}-1)^2\, 2!}{(2\alpha)^3} - \frac{2(\frac{\gamma}{\alpha}-1)\,3!\,\gamma}{(2\alpha)^4} + \frac{\frac{\gamma^2}{\alpha^2}\,4!}{(2\alpha)^5} \right]\right\}.$$

$$K.E. = \alpha^2 N(\lambda) E_{ryd} \left[\left(\frac{\gamma}{\alpha}-1\right)^2 - 3\frac{\gamma}{\alpha}\left(\frac{\gamma}{\alpha}-1\right) + 3\left(\frac{\gamma}{\alpha}\right)^2 \right]$$

$$= \alpha^2 N(\lambda) E_{ryd} \left[\left(-\tfrac{1}{3}(1+\lambda)-1\right)^2 + (1+\lambda)\left(-\tfrac{4}{3}-\tfrac{\lambda}{3}\right) + \tfrac{1}{3}(1+\lambda)^2 \right].$$

$$= \frac{1}{9}\alpha^2 N(\lambda) E_{ryd} \left[(\lambda+4)^2 - 3(1+\lambda)(\lambda+4) + 3(1+\lambda)^2 \right].$$

$$\lambda^2 + 8\lambda + 16 - 3(\cancel{\lambda^2} + 5\lambda + 4) + 3(\cancel{\lambda^2} + 2\lambda + 1)$$

$$(\lambda^2 - \lambda + 7)$$

$$\boxed{K.E. = \frac{1}{9}\alpha^2 N(\lambda) E_{ryd}\,(\lambda^2 - \lambda + 7)}$$

⑤ electron-electron interaction

Do for one core state and multiply by 2.

$$E.E = 2e^2 \int d^3r_1\, \psi_{1s}(r_1)^2 \int d^3r_2\, \psi_{2s}^2(r_2)\, \frac{1}{r_{12}}.$$

$$= \frac{2e^2}{a_B} Z^{*3} B^3 4 \int_0^\infty \rho_1^2 d\rho_1\, e^{-2Z^*\rho_1} \int_0^\infty \rho_2^2 d\rho_2\, e^{-2\alpha\rho_2}(1+\gamma\rho_2)^2 \int \frac{d\Omega}{4\pi}\frac{1}{\rho_{12}}$$

$$\int \frac{d\Omega}{4\pi}\frac{1}{\rho_{12}} = \frac{1}{\rho_2} \text{ if } \rho_2 > \rho_1$$

$$= \frac{1}{\rho_1} \text{ if } \rho_1 > \rho_2.$$

$$= 4^2 E_{ryd} Z^{*3} B^2 \int_0^\infty \rho_2^2 d\rho_2\, e^{-2\alpha\rho_2}(1+\gamma\rho_2)^2 \left[\frac{1}{\rho_2}\underbrace{\int_0^{\rho_2} d\rho_1\, \rho_1^2 e^{-2Z^*\rho_1}}_{\rho_2>\rho_1} + \underbrace{\int_{\rho_2} d\rho_1\, \rho_1\, e^{-2Z^*\rho_1}}_{\rho_1>\rho_2} \right].$$

$$\text{and} \int_{\rho_2}^{\infty} d\rho_1\, \rho_1\, e^{-2Z^*\rho_1} = \frac{1}{4Z^{*2}} \int_{2Z^*\rho_2}^{\infty} dx\, x\, e^{-x} = -\frac{1}{4Z^{*2}} \left[x+1\right] e^{-x} \Big/_{2Z^*\rho_2}^{\infty} = \frac{1}{4Z^{*2}} \left[2Z^*\rho_2+1\right] e^{-2Z^*\rho_2}$$

$$\frac{1}{\rho_2} \int_0^{\rho_2} d\rho_1\, \rho_1^2\, e^{-2Z^*\rho_1} = \frac{1}{(2Z^*)^3\rho_2} \int_0^{2\rho_2 Z^*} x^2 dx\, e^{-x} = -\frac{1}{\rho_2 (2Z^*)^3}\, e^{-x}\left[x^2+2x+2\right]_0^{2\rho_2 Z^*}$$

$$= \frac{1}{\rho_2 (2Z^*)^3} \left[2 - e^{-2\rho_2 Z^*}\left((2\rho_2 Z^*)^2 + 4\rho_2 Z^* + 2\right)\right].$$

Get

$$E.E. = 4 E_{ryd}\, B^2 \int_0^{\infty} \rho_2\, d\rho_2\, e^{-2\alpha\rho_2}(1+\gamma\rho_2)^2 \Big\{ 1 - e^{-2\rho_2 Z^*}\left(\cancel{2\rho_2^2 Z^{*2}} + 2\rho_2 Z^* + 1\right)$$

$$+ Z^*\rho_2\left[\cancel{2Z^*\rho_2} + 1\right] e^{-2Z^*\rho_2} \Big\}.$$

$$\underset{\substack{\uparrow \\ -2/3\ P.E.}}{\{1} - e^{-2\rho_2 Z^*}\left[1 + \rho_2 Z^*\right]\}.$$

$$(1 + \rho_2 Z^*)(1 + 2\gamma\rho_2 + \gamma^2\rho_2^2).$$

$$E.E. = +\frac{2}{3}|P.E.| - 4 E_{ryd}\, B^2 \Big\{ \frac{1!}{[2(\alpha+Z^*)]^2} + \frac{(Z^*+2\gamma)\,2!}{[2(\alpha+Z^*)]^3} + \frac{(\gamma^2+2\gamma Z^*)\,3!}{[\quad]^4}$$

$$+ \frac{Z^*\gamma^2\, 4!}{[\quad]^5} \Big\}.$$

$$E.E. = 2/3\, |P.E.| - 4 E_{ryd}\, \alpha\, N(\lambda) \Big\{ \frac{1}{(1+\lambda)^2} + \frac{\left(\lambda - \frac{2}{3}(4\lambda)\right)}{(1+\lambda)^3} + \frac{1}{2}\, \frac{\left[(1+\lambda)\right]\left[2\lambda - \frac{1}{3}(1+\lambda)\right]}{(1+\lambda)^4}$$

$$+ \frac{1}{3}\, \frac{\lambda(1+\lambda)^2}{(1+\lambda)^5} \Big\}.$$

$$E.E. = 2/3\, |P.E.| - \frac{2}{3}\, \frac{E_{ryd}\, \alpha\, N(\lambda)}{(1+\lambda)^3} \Big\{ \underset{(5\lambda+3)}{6(1+\lambda]} + \cancel{6\lambda} - 4(1+\lambda) - (\cancel{6\lambda} - 1 - \lambda) + 2\lambda \Big].$$

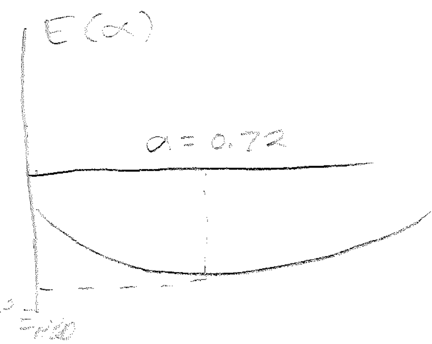
$$\frac{E(\alpha)}{E_{ryd}} = N(\lambda)\left\{ \frac{\alpha^2}{9}(\lambda^2 - \lambda + 7) - \frac{1}{3}\alpha(\lambda^2 - 2\lambda + 3) - \frac{2}{3}\frac{\alpha}{(1+\lambda)^3}(5\lambda + 3)\right\}.$$

$$\lambda = Z^*/\alpha$$

$$N(\lambda) = \frac{3}{\lambda^2 - \lambda + 1}$$

From Problem #1, $\underline{Z^* = 3 - 5/16 = 43/16}$.

Vary α to find minimum $E(\alpha)$.



EXPERMENTAL ~ -5.4 eV

#3). $H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} + eFr\cos\theta.$

$$\psi = \frac{A}{a^{3/2}} e^{-r/a}\left(1 + \lambda\frac{r}{a}\cos\theta\right).$$

1) <u>normalization</u>

$$1 = A^2 \int_0^\infty \rho^2 d\rho\, e^{-2\rho} \underbrace{\int_{-1}^{1} \frac{d\nu}{2}\left(1 + 2\lambda\rho\nu + \lambda^2\rho^2\nu^2\right)}_{\left(1 + \frac{\lambda^2\rho^2}{3}\right)}. \qquad \nu = \cos\theta$$

$$1 = A^2\left[\frac{2}{8} + \frac{\lambda^2 4!}{3\cdot 2^5}\right] = A^2\left[\frac{1}{4} + \lambda^2/4\right] \therefore A^2$$

$$\boxed{A^2 = \frac{4}{1+\lambda^2}}.$$

2) <u>Potential Energy</u>

$$P.E. = -\frac{e^2}{a_B}A^2\int_0^\infty \rho\, d\rho\, e^{-2\rho}\left(1 + \frac{\lambda^2\rho^2}{3}\right).$$

$$= -2E_{ryd}A^2\left[\frac{1}{4} + \frac{\lambda^2}{3}\cdot\frac{6}{16}\right] = -2E_{ryd}\frac{4}{1+\lambda^2}\frac{1}{4}\left(1 + \frac{\lambda^2}{2}\right).$$

$$P.E. = -E_{ryd}\left(\frac{2+\lambda^2}{1+\lambda^2}\right).$$

3). <u>Electric field</u>

$$E.F. = eFaA^2\int_0^\infty \rho^3 d\rho\, e^{-2\rho}\underbrace{\int_{-1}^{1}\frac{d\nu}{2}\,\nu\left(1 + 2\lambda\rho\nu + \lambda^2\rho^2\nu^2\right)}_{\frac{2\lambda\rho}{3}}$$

$$= \frac{2}{3}eF\lambda\underbrace{\int_0^\infty \rho^4 d\rho\, e^{-2\rho}}_{\frac{4!}{2^5} = \frac{3\cdot 8}{32} = \frac{3}{4}}$$

$$= \frac{1}{2}\,\frac{2eFa\lambda}{1+\lambda^2}.$$

4). <u>Kinetic Energy</u>:

Kinetic Energy

$$\nabla^2 = \frac{1}{r}\frac{d}{dr} r^2 \frac{d}{dr} + \frac{1}{r^2 \sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}.$$

$$-\frac{\hbar^2}{2m}\int \psi\,\nabla^2\psi = \frac{\hbar^2}{2m a_B{}^2}A^2\left\{\int_0^\infty \rho^2 d\rho \int_{-1}^{1}\frac{d\nu}{2}\left[\frac{d}{d\rho}\,e^{-\rho}(1+\lambda\rho\nu)\right]^2 + \int_0^\infty d\rho\, e^{-2\rho}\int_{-1}^{1}\frac{d\nu}{2}\underbrace{\left(\frac{d}{d\theta}(1+\lambda\rho\cos\theta)\right)^2}_{\rho^2\lambda^2(1-\nu^2)}\right.$$

$$e^{-\rho}[\lambda\nu - 1 - \lambda\rho\nu].$$

$$K.E. = E_{ryd}\,A^2\left\{\int_0^\infty \rho^2 d\rho\, e^{-2\rho}\left[1+\frac{\lambda^2}{3}(1-\rho)^2\right] + \frac{2\lambda^2}{3}\int_0^\infty \rho^2 d\rho\, e^{-2\rho}\right\}.$$

$$= E_{ryd}\,A^2\left\{\frac{2}{8} + \frac{\lambda^2}{3}\left(\frac{2}{8} - \frac{2\cdot\cancel{6}}{16} + \frac{24}{32}\right) + \frac{2}{3}\frac{\lambda^2 2}{2^3}\right\}.$$

$$= E_{ryd}\,\frac{A^2}{4}\left[1 + \lambda^2\left(\frac{1}{3}+\frac{1}{3}\right) + \cancel{\beta}\right]$$

$$\boxed{K.E. = E_{ryd}}.$$

$$E(\lambda) = E_{ryd}.\left\{1 - \frac{2+\lambda^2}{1+\lambda^2}\right\} + \frac{2eFa\lambda}{1+\lambda^2}.$$

$$= -E_{ryd}.\frac{1}{1+\lambda^2} + \frac{2eFa\lambda}{1+\lambda^2}$$

$$\left(\frac{\partial E}{\partial\lambda}\right) = 0: \quad 0 = +E_{ryd}\frac{2\lambda}{(1+\lambda^2)^2} + \frac{2eFa}{(1+\lambda^2)} - \frac{(2eFa)\lambda^2 2}{(1+\lambda^2)^2}$$

$$0 = E_{ryd}\cdot 2\lambda + (2eFa)(1+\lambda^2 - 2\lambda^2).$$

$$\boxed{b = \frac{2eFa}{E_{ryd}}}. \qquad 0 = \lambda^2 - \frac{2\lambda}{b} - 1.$$

$$0 = (\lambda - \tfrac{1}{b})^2 - (1 + 1/b^2)$$

$$\lambda_0 = \frac{1}{b} - \sqrt{\frac{1}{b^2}+1} \qquad b = \frac{2eFa}{e^2/2a} = \frac{4Fa^2}{e}.$$

$$E(\lambda_0) = -E_{ryd}\left[\frac{1}{1+\lambda_0^2} - \frac{b\lambda_0}{1+\lambda_0^2}\right].$$

$$\lambda_0^2 = \frac{1}{b^2} + \frac{1}{b^2} + 1 - \frac{2}{b}\sqrt{\frac{1}{b^2}+1} =$$

$$\lambda_0^2 + 1 = 2\left[1 + \frac{1}{b^2} - \frac{1}{b}\sqrt{\frac{1}{b^2}+1}\right] = 2\sqrt{\frac{1}{b^2}+1}\left[\sqrt{\frac{1}{b^2}+1} - 1/b\right].$$

$$E(\lambda_0) = -\frac{E_{ryd.}}{2\sqrt{\frac{1}{b^2}+1}}\left[\frac{1 - 1 + \sqrt{1+b^2}}{\sqrt{\frac{1}{b^2}+1} - 2/b.}\right]$$

$$E(\lambda_0) = -\frac{E_{ryd}\, b^2}{2\left(\sqrt{b^2+1} - 1\right).}\left[\frac{\sqrt{b^2+1}+1}{\sqrt{b^2+1}+1}\right].$$

$$\boxed{E(b) = -\frac{E_{ryd}}{2}\left[\sqrt{b^2+1} + 1\right]}.$$

$$\sqrt{1+b^2} = 1 + \frac{1}{2}b^2 + \cdots$$

$$E(b) = -E_{ryd}\left[1 + \frac{1}{4}b^2\right]. \qquad b^2 = \frac{16F^2a^4}{e^2} = \frac{8F^2a^3}{E_{ryd.}}$$

$$E(F) = -E_{ryd} - 2F^2a^3 + O(F^4).$$

$$\boxed{\alpha = 4a^3}.$$

Not bad agreement with exact answer $\frac{9}{2}a^3$!

Physics 611
Due: March 13, 1975
#7

(1) For the harmonic oscillator, we had
$$H = \hbar\omega(a^+a + 1/2)$$
$$[a,a] = 0$$
$$[a,a^+] = 1$$
$$[a^+,a^+] = 0$$

Starting from just these statements, derive the eigenvalue spectrum of the harmonic oscillator. Hint: Assume an eigenstate $|n\rangle$ of a^+a, $a^+a|n\rangle = n|n\rangle$ and give arguements that show n must be a non-negative integer.

(2) Derive a table of Clebsch-Gordon coefficients for $\frac{1}{2} \otimes 3/2$

(3) Write down the spin states obtained by combining three spin ½ states.

COMPUTER (HF)

(4) Two helium atoms interact with a potential which is often described by a Lennard-Jones form

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$\varepsilon = 1.41\ 10^{-16} \text{ ergs} \quad (-15)$$
$$\sigma = 2.56\ \text{Å}$$
$$m_{He} = 6.65\ 10^{-24} \text{ gms}$$

Numerically solve Schrodingers equation for E = 0. and obtain the relative wave function of the two atoms. Remember: the reduced mass is used in relative coordinates.

COMPUTER

(5) Use the same potential for two heliums to compute the relative s-wave phase shift as a function of k for $0 \leq k\sigma \leq 4$

PHYSICS 6111
DUE: MARCH 13, 1975
BOB MARKS

10/50

1. $[H, aa^+] = \hbar\omega\left[(a^+a+\tfrac{1}{2})a^+a - a^+a(a^+a+\tfrac{1}{2})\right] = 0$

SIMULTANEOUS EIGEN-VALUES:

1 – 10 $H|n\rangle = E_n|n\rangle$

$aa^+|n\rangle = A_n|n\rangle$

2 – 0 NOW:

3 – 0 $[H, a] = \hbar\omega\left[(a^+a+\tfrac{1}{2})a - a(a^+a+\tfrac{1}{2})\right]$

$= \hbar\omega\left[a^+a^2 - aa^+a\right]$

$= \hbar\omega\left[a^+a - aa^+\right]a$

4 – 0 $= \hbar\omega[a^+, a]a$

5 – 0 $= -\hbar\omega a$

$[H, a^+] = \hbar\omega\left[(a^+a+\tfrac{1}{2})a^+ - a^+(a^+a+\tfrac{1}{2})\right]$

$= \hbar\omega\left[a^+aa^+ - a^{+2}a\right]$

$= \hbar\omega a^+[a, a^+]$

$= \hbar\omega a^+$

Bwell

$$H|n\rangle = \hbar\omega\left[aa^{+} + \tfrac{1}{2}|n\rangle\right]$$
$$= \hbar\omega\left[aa^{+}|n\rangle + \tfrac{1}{2}|n\rangle\right]$$
$$= \hbar\omega\left[A_n + \tfrac{1}{2}|n\rangle = E_n|n\rangle\right.$$
$$\Rightarrow E_n = \hbar\omega(A_n + \tfrac{1}{2})$$
$$\langle n'|[H, a^{+}]|n\rangle = \hbar\omega\langle n'|a^{+}|n\rangle$$
$$= \langle n'|Ha^{+}|n\rangle - \langle n'|a^{+}H|n\rangle$$
$$= (E_{n'} - E_n)\langle n'|a^{+}|n\rangle$$
$$\therefore E_{n'} - E_n = \hbar\omega \quad \text{OR} \quad \langle n'|a^{+}|n\rangle = 0 \qquad (1)$$
$$\langle n'|[H, a]|n\rangle = -\hbar\omega\langle n'|a|n\rangle$$
$$= \left[\langle n'|Ha|n\rangle - \langle n'|aH|n\rangle\right]\hbar\omega$$
$$= -\hbar\omega\left[(E_{n'} - E_n)\langle n'|a|n\rangle\right]$$
$$\therefore E_n - E_{n'} = \hbar\omega \quad \text{OR} \quad \langle n'|a|n\rangle = 0 \qquad (2)$$

(1) AND (2) DICTATE BOUND STATE ENERGIES SEPARATED BY $\hbar\omega$

FOR (1): $\quad n' = n+1$

$$\hbar\omega = E_{n+1} - E_n$$
$$= \hbar\omega\left[A_{n+1} - A_n\right] \Rightarrow A_{n+1} - A_n = 1$$

FOR (2): $\quad n' = n-1$

$$\hbar\omega = E_n - E_{n-1}$$
$$= \hbar\omega\left[A_n - A_{n-1}\right] \Rightarrow A_n - A_{n-1} = 1$$ (SAME THING)

EQUIVALENTLY

$$[H, a^+]|n\rangle = \hbar\omega a^+|n\rangle$$

$$= Ha^+|n\rangle - a^+H|n\rangle = Ha^+|n\rangle - E_n a^+|n\rangle$$

$$\Rightarrow Ha^+|n\rangle = [E_n + \hbar\omega]a^+|n\rangle$$

$$[H, a]|n\rangle = -\hbar\omega a|n\rangle$$

$$= Ha|n\rangle - aH|n\rangle = Ha|n\rangle - E_n a|n\rangle$$

$$\Rightarrow Ha|n\rangle = [E_n - \hbar\omega]a|n\rangle$$

NOW, FROM (1)

$$\langle n'| a^+|n\rangle = 0 \quad \forall \quad n' \neq n+1$$

FROM (2)

$$\langle n''|a|n\rangle = 0 \quad \forall \quad n'' \neq n-1$$

NOW:

$$\langle m|aa^+|m\rangle = \sum_{m'} \langle m|a|m'\rangle\langle m'|a^+|m\rangle$$

$$= \langle m|a|m+1\rangle\langle m+1|a^+|m\rangle = A_m$$

$$\langle m|a^+a|m\rangle = \sum_{m'} \langle m|a^+|m'\rangle\langle m'|a|m\rangle$$

$$= \langle m|a^+|m-1\rangle\langle m-1|a|m\rangle$$

LET $m = k+1$ $(k = m-1)$

$$\langle k+1|a^+a|k+1\rangle = \langle k|a|k+1\rangle\langle k+1|a^+|k\rangle = A_k$$

$$\Rightarrow \langle m|a^+a|m\rangle = \langle m-1|a|m\rangle\langle m|a^+|m-1\rangle$$

$$= A_{m-1}$$

$$\therefore \langle m|[a, a^+]|m\rangle = 1 = A_m - A_{m-1} \quad \text{(SAME THING)}$$

$$\Rightarrow A_m = m + C \ni C = \text{CONSTANT}, \ m \text{ AN INTEGER}$$

WE HAVE THUS ESTABLISHED THAT E_n IS SEPARATED BY INTEGRAL MULTIPLES OF $\hbar\omega$:

$$E_n = \hbar\omega(n + C + \tfrac{1}{2})$$

NOW

$$A_m = \langle m+1 | a^+ a | m+1 \rangle = \langle m | a a^+ | m \rangle$$

THIS CONDITION IS SATISFIED FOR

$$a|m\rangle = \sqrt{k}\,|k-1\rangle$$

$$a^+|m\rangle = \sqrt{k+1}\,|k+1\rangle$$

LET k BE THE SMALLEST EIGEN VALUE. FROM BEFORE:

$$1 = \langle k | [a, a^+] | k \rangle = \langle k | a a^+ | k \rangle - \langle k | a^+ a | k \rangle$$

$\langle k | a^+ a | k \rangle = 0$ SINCE STATE $k-1$ DOESN'T EXIST.

$$\therefore \langle k | [a, a^+] | k \rangle = 1 = \langle k | a a^+ | k \rangle$$

$$= (k+1) \langle k | k \rangle$$

$$= k+1 \Rightarrow k = 0$$

THUS, $C = 0$ AND,

$$E_n = \hbar \omega \left(n + \frac{1}{2}\right)$$

2. $j_1 = \frac{1}{2}$ $\qquad -j_1 \le m_1 \le j_1 \Rightarrow m_1 = -\frac{1}{2}, \frac{1}{2}$

$j_2 = \frac{3}{2}$ $\qquad -j_2 \le m_2 \le j_2 \Rightarrow m_2 = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

$\alpha_1 : |\frac{1}{2}, \frac{1}{2}\rangle \qquad \alpha_2 = |\frac{3}{2}, -\frac{3}{2}\rangle$

$\beta_1 : |\frac{1}{2}, -\frac{1}{2}\rangle \qquad \beta_2 = |\frac{3}{2}, -\frac{1}{2}\rangle$

$\gamma_2 = |\frac{3}{2}, \frac{1}{2}\rangle$

$\delta_2 = |\frac{3}{2}, \frac{3}{2}\rangle$

$\alpha_1\alpha_2 = -\frac{1}{2} \qquad \beta_1\alpha_2 = -2$

$\alpha_1\beta_2 = 0 \qquad \beta_1\beta_2 = -1$

$\alpha_1\gamma_2 = 1 \qquad \beta_1\gamma_2 = 0$

$\alpha_1\delta_2 = 2 \qquad \beta_1\delta_2 = \frac{1}{2}$

$J = 2 \qquad |2, -2\rangle \qquad \beta_1\alpha_1$

$|2, -1\rangle \qquad \beta_1\beta_2$

$|2, 0\rangle \qquad \alpha_1\beta_2 + \beta_1\gamma_2$

$|2, +1\rangle \qquad \alpha_1\gamma_2$

$|2, +2\rangle \qquad \alpha_1\delta_2$

$J = 1 \qquad |1, -1\rangle \qquad \beta_1\beta_2$

$|1, 0\rangle \qquad \beta_1\gamma_2 - \alpha_1\beta_2$

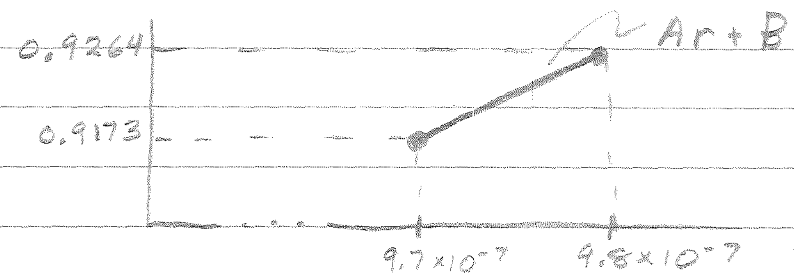
$|1, 1\rangle \qquad \alpha_1\gamma_2$

4. FOR LARGE r:

$$\frac{d^2}{dr^2}\chi = 0 \Rightarrow \chi = Ar + B$$

FROM DATA:

$$\chi(9.7\times10^{-7}) = 0.09173$$
$$\chi(9.8\times10^{-7}) = 0.09264$$

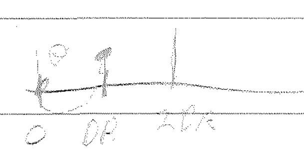


$$A(9.7\times10^{-7}) + B = 0.09173$$
$$A(9.8\times10^{-7}) + B = 0.09264$$
$$\Rightarrow A = \frac{0.00091}{0.1\times10^{-7}} = 0.000091\times10^{7} = 9.1\times10^{4}$$

$$B = 0.092 - 9.1\times10^{4}(9.7\times10^{-7}) = -0.091$$

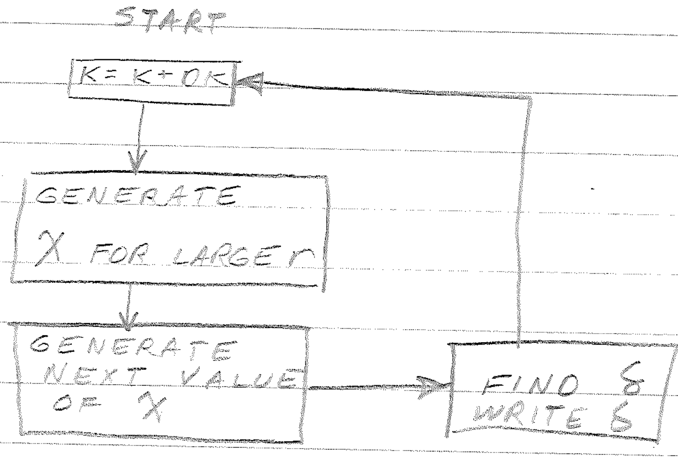
```
      HBR2=(1.054/(10.**27.))**2.
      EE=2.56/(10.**8.)
      XM=6.65/(10.**24.)
      R=0.1/(10.**8.)
      DR=.1/(10.**8.)
      Y0=0.
      Y1=0.0001
      DØ 50 N=2,1000
      R=R+DR
      SØR=S/R
      V=4.*EE*((SØR**12.)-(SØR**6.))
      A=2.*XM*V/HBR2
      B=A*DR*DR
      Y2=Y1*(2.+B/(1.-B/12.))-Y0
      X2=Y2/(1.-B/12.)
      PRINT 51,N,R,X2
      Y0=Y1
   50 Y1=Y2
   51 FØRMAT(2X,I4,2X,F15.8,2X,F15.8)
WARNING: END STATEMENT PRØVIDED BY CØMPILER.
```

Y2



158	.00000016	.01579497
159	.00000016	.01589493
160	.00000016	.01599489
161	.00000016	.01609485
162	.00000016	.01619481
163	.00000016	.01629477
164	.00000016	.01639473
165	.00000016	.01649469
166	.00000017	.01659465
167	.00000017	.01669461
168	.00000017	.01679457
169	.00000017	.01689453
170	.00000017	.01699449
171	.00000017	.01709446
172	.00000017	.01719442
173	.00000017	.01729438
174	.00000017	.01739434
175	.00000017	.01749430
176	.00000018	.01759426
177	.00000018	.01769422
178	.00000018	.01779418
179	.00000018	.01789414
180	.00000018	.01799410
181	.00000018	.01809406
182	.00000018	.01819402
183	.00000018	.01829398
184	.00000018	.01839394
185	.00000018	.01849391
186	.00000019	.01859387
187	.00000019	.01869383
188	.00000019	.01879379
189	.00000019	.01889375
190	.00000019	.01899371
191	.00000019	.01909367
192	.00000019	.01919363
193	.00000019	.01929359
194	.00000019	.01939355
195	.00000019	.01949351
196	.00000020	.01959347
197	.00000020	.01969343
198	.00000020	.01979339
199	.00000020	.01989336
200	.00000020	.01999332
201	.00000020	.02009328
202	.00000020	.02019324
203	.00000020	.02029320
204	.00000020	.02039316
205	.00000020	.02049312
206	.00000021	.02059308
207	.00000021	.02069304
208	.00000021	.02079300
209	.00000021	.02089296
210	.00000021	.02099292

5/10



(IT DIDN'T WORK)

```
      HBR2=(1.054/(10.**27.))**2.
      EE=1.41/(10.**15.)
      S=2.56/(10.**8.)
      XM=6.65/(10.**24.)
      XK=0.
      DK=0.1*(10.**8.)
      DØ 14 K=1,17
      DR=.1/(10.**8.)
      R=0.1/(10.**8.)
      YØ=0.
      Y1=0.0001
      E=XK*XK*HBR2/(2.*XM)
      DØ 11 N=2,1000
      IF (N-1000)9,12,12
    9 R=R+DR
      SØR=S/R
      V=4.*EE*((SØR**12.)-(SØR**6.))
      IF (V/E-1000.)10,12,12
   10 A=2.*XM*(V-E)/HBR2
      B=A*DR*DR
      Y2=Y1*(2.+B/(1.-B/12.))-YØ
      YØ=Y1
   11 Y1=Y2
      GØ TØ 13
   12 PRINT 50,K
   13 X2=Y2/(1.-B/12.)
      R=R+DR
      SØR=S/R
      V=4.*EE*((SØR**12.)-(SØR**6.))
      A=2.*XM*(V-E)/HBR2
      B=A*DR*DR
      Y3=Y2*(2.+B/(1.-B/12.))-Y1
      X3=Y3/(1.-B/12.)
      RI=R-DR
      XNUM=X3*SIN(XK*RI)-X2*SIN(XK*R)
      DEN=X3*CØS(XK*RI)-X2*CØS(XK*R)
      DEL=ATAN((-1.)*XNUM/DEN)
      PRINT 90,K,XK,DEL
   14 XK=XK+DX
   50 FØRMAT(15X,I8)
   90 FØRMAT(2X,I9,2X,F15.8,2X,F15.8)
WARNING: END STATEMENT PROVIDED BY COMPILER.
```

Physics 611
Due April 3, 1975
8

1) Work out the first order Stark effect for the $n = 3$ states of hydrogen.

2) In the perturbation theory solution, obtain $a_m^{(2)}$ and hence the second order correction to the wave function.

3) The exact eigenvalue spectrum for $H = p^2/2m + \frac{1}{2}m(\omega^2+\delta^2)x^2$ is

$E_n = \hbar\sqrt{\omega^2+\delta^2}\,(n+\frac{1}{2})$ Take $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$, $V = \frac{1}{2}m\delta^2x^2$

Treat V as a perturbation to H_0, and determine its contribution to the energy by first and second order perturbation theory. Successive terms should correspond to expanding the exact result: $E_n = \hbar\omega(n+\frac{1}{2})\sqrt{1+\delta^2/\omega^2} = \hbar\omega(n+\frac{1}{2})(1 + \frac{1}{2}\frac{\delta^2}{\omega^2} + \cdots)$

4) Consider a hydrogen atom which has an added delta function potential $V' = \frac{\lambda\delta(r)}{r^2}$
If λ is small, how does this perturb the levels of the atom? Are states with different ℓ values affected differently?

5) A small charge Q ($Q << e$) is placed at a long distance R ($R >>$ bohr radius) from a hydrogen atom. What is the leading term, in powers of $1/R$, of the energy change in the system?

6) For the helium atom, write $H = H_0 + V$. Estimate the ground state energy by (a) Obtain the ground state energy of H_0, and (b) Include V by first order perturbation theory.

$$H_0 = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - Ze^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right)$$

$$V = \frac{e^2}{|\underset{\sim}{r_1} - \underset{\sim}{r_2}|}$$

PHYS. 611
DUE APRIL 3, 1975
BOB MARKS

10/

$\lambda^3 / 6$

1. $n = 3$

ℓ	m	STATE	Y_ℓ^m	$R_\ell^n(r)$
0	0	$3s_0$	$\frac{1}{\sqrt{4\pi}}$	$C_s\left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2}\right)e^{-r/3a}$
1	-1	$3P_{-1}$	$\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\phi}$	
1	0	$3P_0$	$\sqrt{\frac{3}{4\pi}} \cos\theta$	$C_p r \, e^{-r/3a}\left(1 - \frac{r}{6a}\right)$
1	$+1$	$3P_1$	$-\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\phi}$	
2	-2	$3d_{-2}$	$\sqrt{\frac{15}{32\pi}} \sin^2\theta \, e^{-i2\phi}$	
2	-1	$3d_{-1}$	$+\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta \, e^{-i\phi}$	
2	0	$3d_0$	$\sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$	$C_d r^2 e^{-r/3a}$
2	1	$3d_1$	$-\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta \, e^{i\phi}$	
2	2	$3d_2$	$\sqrt{\frac{15}{32\pi}} \sin^2\theta \, e^{i2\phi}$	

$V = eFr\cos\theta$

ONLY NON-ZERO ELEMENTS ARE

$\langle 3s_0 | V | 3P_0 \rangle = \lambda_1$

$\langle 3P_0 | V | 3d_0 \rangle = \lambda_3$

$\langle 3P_1 | V | 3d_1 \rangle = \lambda_2$

$\langle 2P_{-1} | V | 3d_{-1} \rangle = \lambda_4$

GROUPING WITH SAME m GIVES $\langle V \rangle$:

	$3s_0$	$3p_0$	$3d_0$	$3p_1$	$3d_1$	$3p_{-1}$	$3d_{-1}$	$3d_2$	$3d_{-2}$
$3s_0$	$-E$	λ_1	0	0	0	0	0	0	0
$3p_0$	λ_1	$-E$	λ_3	0	0	0	0	0	0
$3d_0$	0	λ_3	$-E$	0	0	0	0	0	0
$3p_1$	0	0	0	$-E$	λ_2	0	0	0	0
$3d_1$	0	0	0	λ_2	$-E$	0	0	0	0
$3p_{-1}$	0	0	0	0	0	$-E$	λ_4	0	0
$3d_{-1}$	0	0	0	0	0	λ_4	$-E$	0	0
$3d_2$	0	0	0	0	0	0	0	$-E$	0
$3d_{-2}$	0	0	0	0	0	0	0	0	$-E$

GIVES:

$$+E^3 = (\lambda_1^2 + \lambda_3^2)E \Rightarrow E = \pm\sqrt{\lambda_1^2 + \lambda_3^2},\ 0$$

$$E = \pm \lambda_2$$

$$E = \pm \lambda_4$$

$$E = 0$$

- $\int_0^\infty r^2 R_s^2(r)\,dr = 1 \Rightarrow R_s(r) = C_s\left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2}\right)e^{-r/3a}$

DAVYDOV: $R_{3s}(\rho) = \frac{2}{3\sqrt{3}}\left(1 - \frac{2}{3}\rho + \frac{2}{27}\rho^2\right)e^{-\rho/3}$

$$\int_0^\infty \rho^2 R_{3s}^2(\rho)\,d\rho = 1$$

$$= \frac{4}{27}\int_0^\infty \rho^2\left(1 - \frac{2}{3}\rho + \frac{2}{27}\rho^2\right)^2 e^{-2\rho/3}\,d\rho$$

$\rho = r/a$

$$\Rightarrow 1 = \frac{4}{27a^3}\int_0^\infty r^2\left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2}\right)e^{-2r/3a}\,dr$$

$$\therefore C_s^2 = \frac{4}{27a^3} \Rightarrow C_s = \frac{2}{3\sqrt{3a^3}}$$

- $\int_0^\infty r^2 R_{3p}^2(r)\,dr = 1$

DAVYDOV: $R_{3p}(\rho) = \frac{8}{27\sqrt{6}}\left(1 - \frac{1}{6}\rho\right)\rho\, e^{-\rho/3}$

$$1 = \left(\frac{8}{27\sqrt{6}}\right)^2 \int_0^\infty \rho^4\left(1 - \frac{1}{6}\rho\right)^2 e^{-2\rho/3}\,d\rho$$

$\rho = r/a$

$$\therefore 1 = \frac{1}{a^5}\left(\frac{8}{27\sqrt{6}}\right)^2 \int_0^\infty r^4\left(1 - \frac{r}{6a}\right)^2 e^{-2r/3a}\,dr$$

$$\Rightarrow c^2 = \frac{1}{a^5}\left(\frac{8}{27\sqrt{6}}\right)^2 \Rightarrow c = \frac{8}{27\sqrt{6a^5}}$$

- $\int_0^\infty r^2 R_{3d}^2(r)\,dr = 1$

DAVYDOV: $R_{3d}(\rho) = \frac{4}{81\sqrt{30}}\rho^2 e^{-\rho/3}$

$$1 = \left(\frac{4}{81\sqrt{30}}\right)^2 \int_0^\infty \rho^6 e^{-2\rho/3}\,d\rho$$

$\rho = r/a$

$$\therefore 1 = \left(\frac{4}{81\sqrt{30}}\right)^2 \frac{1}{a^7}\int_0^\infty r^6 e^{-2r/3a}\,dr$$

$$C_{3d} = \frac{4}{81\sqrt{30a^7}}$$

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

$$R_{3p}(r) = \frac{8}{27\sqrt{6a^5}}\, r\left(1 - \frac{r}{6a}\right)e^{-r/3a}$$

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

$$\lambda_1 = \langle 3S_0 | V | 3P_0 \rangle$$

$$= eF \langle 3S_0 | r\cos\theta | 3P_0 \rangle$$

$$= eF \int d^3r \frac{1}{\sqrt{4\pi}} \frac{2}{3\sqrt{3a^3}} \left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2}\right) e^{-r/3a}$$

$$\times r\cos\theta \times \sqrt{\frac{3}{4\pi}}\cos\theta \times \frac{2^3}{3^3\sqrt{6a^5}} r\left(1 - \frac{r}{6a}\right) e^{-r/3a}$$

$$= eF \frac{\sqrt{3}}{4\pi} \frac{2^4}{3^4 \cdot 3\sqrt{2}} \frac{1}{a^4}$$

$$\times \int \cos^2\theta \, r^2 \left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2}\right)\left(1 - \frac{r}{6a}\right) e^{-2r/3a} d^3r$$

$$= eF \frac{2^2\sqrt{3}}{\pi 3^5 \sqrt{2}} \frac{1}{a^4} \times 2\pi$$

$$\int_0^\pi \cos^2\theta \sin\theta \, d\theta$$

$$\int_0^\infty r^4 \left(1 - \frac{2r}{3a} + \frac{2r^2}{3^3a^2}\right)\left(1 - \frac{r}{6a}\right) e^{-2r/3a} d^3r$$

$$= eF \frac{2^3}{3^5}\sqrt{\frac{3}{2}}\, a \left(\frac{2}{3}\right) \int_0^\infty \rho^4 \left(1 - \frac{2}{3}\rho + \frac{2}{3^3}\rho\right)\left(1 - \frac{1}{6}\rho\right) e^{-\frac{2}{3}\rho} d\rho$$

$$= eF \frac{2^4}{3^6}\sqrt{\frac{3}{2}}\, a$$

$$\times \int_0^\infty \rho^4 \left[1 - \left(\frac{2}{3} + \frac{1}{6}\right)\rho + \left(\frac{1}{3^2} + \frac{2}{3^3}\right)\rho^2 - \frac{1}{3^4}\rho^3\right] e^{-\frac{2}{3}\rho} d\rho$$

$$= eF \frac{2^3\sqrt{6}}{3^6} a \int_0^\infty \rho^4 \left[1 - \frac{5}{6}\rho + \frac{5}{3^3}\rho^2 - \frac{1}{3^4}\rho^3\right] e^{-\frac{2}{3}\rho} d\rho$$

$$= eFa \frac{2^3\sqrt{6}}{3^6} \left[4!\left(\frac{3}{2}\right)^5 - \frac{5}{6}5!\left(\frac{3}{2}\right)^6 + \frac{5}{3^3}6!\left(\frac{3}{2}\right)^7 - \frac{1}{3^4}7!\left(\frac{3}{2}\right)^8\right]$$

$$= eFa \frac{2^3\sqrt{6}}{3^6} 4!\left(\frac{3}{2}\right)^5 \left[1 - \frac{5^2}{2\cdot 2}\cdot\frac{3}{2} + \frac{5\cdot 2\cdot 2\cdot 5\cdot 3^2}{3^3\, 2^2} - \frac{7\cdot 3\cdot 2\cdot 5\cdot 3^3}{3^4\, 2^{3}}\right]$$

$$= eFa\sqrt{6} \frac{4\cdot 3\cdot 2}{3\cdot 2^2} \left[1 - \frac{5^2}{2^2} + \frac{5^2}{2} - \frac{35}{2^2}\right]$$

$$= eFa\sqrt{6} \frac{1}{2} \left[4 - 25 + 50 - 35\right]$$

$$= eFa\sqrt{6} \frac{1}{2} \left[-6\right]$$

$$= -3\sqrt{6}\, eFa$$

$$\lambda_2 = \langle 3p_1 | V | 3d_1 \rangle$$

$$= eF \langle 3p_1 | r\cos\theta | 3d_1 \rangle$$

$$= eF \int {}^{*}\sqrt{\tfrac{3}{8\pi}} \sin\theta \, e^{-i\phi} \frac{8}{3^3\sqrt{6a^5}} r\left(1-\frac{r}{6a}\right) e^{-r/3a}$$

$$\times r\cos\theta \times \sqrt{\tfrac{15}{8\pi}} \sin\theta\cos\theta \, e^{i\phi} \times \frac{4}{3^4\sqrt{30a^7}} r^2 e^{-r/3a} \, d^3r$$

$$= eF \, \frac{\sqrt{2^3 5}}{8\pi} \, \frac{2^5}{3^7 a^6 \sqrt{2^3 5 2^2}}$$

$$\times \int \sin^2\theta \cos^2\theta \, r^4 \left(1-\frac{r}{6a}\right) e^{-2r/3a} \, d^3r$$

$$= \frac{2^4 eF}{2^3\pi \, 3^7 a^6} 2\pi \int_0^\pi \sin^3\theta \cos^2\theta \, d\theta$$

$$\times \int_0^\infty r^6 \left(1-\frac{r}{6a}\right) e^{-2r/3a} \, dr$$

$$\int_0^\pi \sin^3\theta \cos^2\theta \, d\theta$$

$$= -\frac{1}{5} \sin^2\theta \cos^3\theta \Big|_0^\pi + \frac{2}{5} \int \cos^2\theta \sin\theta \, d\theta$$

$$= -\frac{1}{5}\left[0\right] + \frac{2}{5}\cdot\frac{2}{3}$$

$$= \frac{4}{15}$$

$$\lambda_2 = \frac{2^2 eF}{3^7 a^6} \times \frac{2^2}{3\cdot 5} \int_0^\infty r^6 \left(1-\frac{r}{6a}\right) e^{-2r/3a} \, dr$$

$$= \frac{2^4 eF}{3^8\cdot 5 \cdot a^6} a^7 \int_0^\infty \rho^6 \left(1-\frac{1}{6}\rho\right) e^{-2/3\,\rho} \, d\rho$$

$$= \frac{2^4 eF}{3^8\cdot 5} a \left[6!\left(\frac{3}{2}\right)^7 - \frac{1}{6}\, 7!\left(\frac{3}{2}\right)^8\right]$$

$$= \frac{2^4 eFa}{3^8\cdot 5} \, 6! \left[\left(\frac{3}{2}\right)^7 - \frac{7}{6}\left(\frac{3}{2}\right)^8\right]$$

$$= \frac{2^4 eFa}{3^8\cdot 5} \, 6! \left(\frac{3}{2}\right)^7 \left[1 - \frac{7\cdot 3}{6\cdot 2}\right]$$

$$= \frac{eFa}{2\cdot 2^3\cdot 5} \, 6\cdot 5\cdot 4\cdot 3\cdot 2 \left[1 - \frac{7}{4}\right]$$

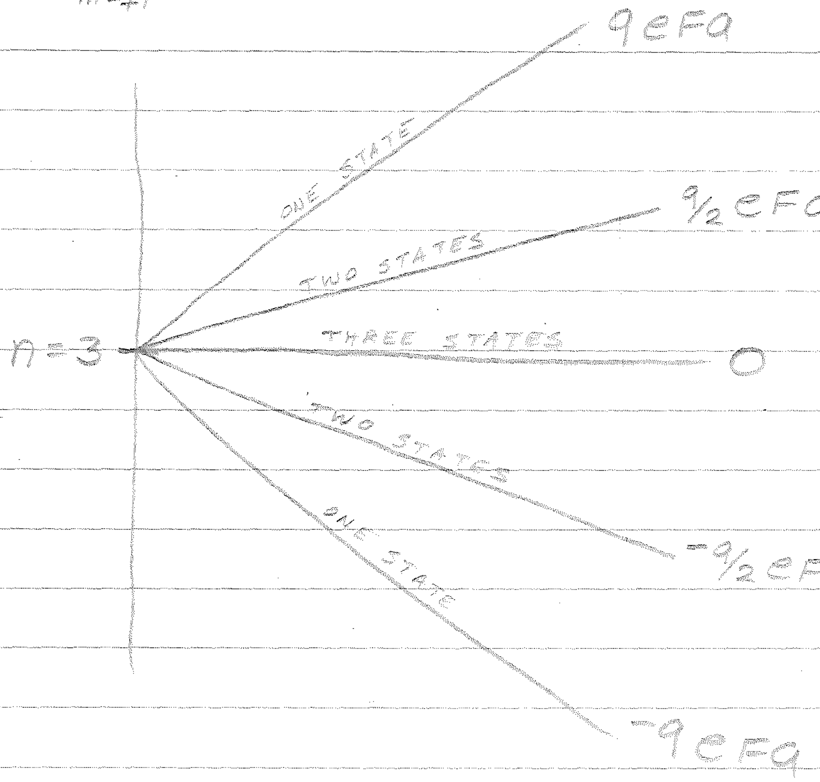
$$= 6 eFa \left[-\frac{3}{4}\right]$$

$$= -\frac{9}{2} eFa$$

NOTE: $\lambda_2 = \lambda_4$

$$\lambda_3 = \langle 3p_0|V|3d_0\rangle$$
$$= eF\langle 3p_0|r\cos\theta|3d_0\rangle$$
$$= eF\int d^3r\, \sqrt{\tfrac{3}{4\pi}}\cos\theta\, \frac{2^2}{3^3\sqrt{6a^5}}\, r\left(1-\frac{r}{6a}\right)e^{-r/3a}\cdot r\cos\theta$$
$$\times \sqrt{\tfrac{5}{16\pi}}\,(3\cos^2\theta - 1)\,\frac{2^2}{3^4\sqrt{30a^7}}\, r^2 e^{-r/3a}$$
$$= eF\,\frac{\sqrt{15}}{2^3\pi}\,\frac{2^5}{3^7 6\cdot\sqrt{5}}\,\frac{1}{a^6}$$
$$\times\int \cos^2\theta(3\cos^2\theta - 1)\, r^4\left(1-\frac{r}{6a}\right)e^{-2r/3a}\, d^3r$$
$$= eF\,\frac{2\sqrt{3}}{3^8\pi}\,\frac{1}{a^6}\times 2\pi$$
$$\times\int_0^\pi \cos^2\theta(3\cos^2\theta - 1)\sin\theta\, d\theta$$
$$\int_0^\infty r^6\left(1-\frac{r}{6a}\right)e^{-2r/3a}\, dr$$
Now $3\int_0^\pi \cos^4\theta\sin\theta = -\frac{3}{5}\cos^5\theta\Big|_0^\pi$
$$= \frac{6}{5}$$
$$\int_0^\pi \cos^2\theta\sin\theta\, d\theta = -\frac{1}{3}\cos^3\theta\Big|_0^\pi =$$
$$= \frac{2}{3}$$
$$\frac{6}{5} - \frac{2}{3} = \frac{18-10}{15} = \frac{8}{15}$$
$$\Rightarrow \lambda_3 = eF\,\frac{2^2\sqrt{3}}{3^8 a^6}\times\frac{2^3}{3\cdot 5}\int_0^\infty r^6\left(1-\frac{r}{6a}\right)e^{-2r/3a}\, dr$$
$$= eF\,\frac{\sqrt{3}\,2^5}{3^9\, 5}\, a\int_0^\infty \rho^6\left(1-\frac{1}{6}\rho\right)e^{-2/3\rho}\, d\rho$$
$$= eF\,\frac{\sqrt{3}\,2^5}{3^9\, 5}\, a\left[6!\left(\frac{3}{2}\right)^7 - \frac{1}{6}\,7!\left(\frac{3}{2}\right)^8\right]$$
$$= eF\,\frac{\sqrt{3}\,2^5}{3^9\, 5}\, a\, 6!\left(\frac{3}{2}\right)^7\left[1 - \frac{7}{6}\cdot\frac{3}{2}\right]$$
$$= aeF\,\frac{\sqrt{3}}{\cancel{5}\,2^2\,3^2}\times 6\times\cancel{5}\times 4\times 3\times 2\left[1-\frac{7}{4}\right]$$
$$= aeF\, 4\sqrt{3}\left(\frac{-3}{4}\right)$$
$$= -3a\, eF\sqrt{3}$$

$$E_{m=0} = \pm\sqrt{\lambda_1^2 + \lambda_3^2}$$
$$= \pm\left[2\cdot 3^3 + 3^3\right]^{1/2} eFa$$
$$= \pm\sqrt{3^4}\, eFa$$
$$= \pm 9 eFa \quad \text{or } 0$$
$$E_{m=\pm 1} = \pm \frac{9}{2} eFa$$



3. 10

$$H = \frac{p^2}{2m} + \frac{1}{2} m(\omega^2 + \delta^2)x^2$$

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

$$V = \frac{1}{2} m \delta^2 x^2$$

H_0 IS HARMONIC OSCILLATOR

$$\psi_n^{(0)}(\xi) = N_n e^{-\xi^2/2} H_n(\xi)$$

$$\xi = x/x_0 \qquad N_n = \left[2^n n! \sqrt{\pi}\right]^{-1/2} \; ; \; x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

$$E_n^{(0)} = \hbar\omega(n + \tfrac{1}{2})$$

$$E_\ell = E_\ell^{(0)} + V_{\ell\ell} + \sum_{m \neq \ell} \frac{|V_{\ell m}|^2}{E_\ell^{(0)} - E_m^{(0)}}$$

FROM SOME OLD HOMEWORK:

$$\langle n|x^2|\ell\rangle = \frac{x_0^2}{2}\left[\sqrt{\ell(\ell-1)}\,\delta_{n,\ell-2} + (2\ell+1)\,\delta_{n,\ell} + \sqrt{(\ell+1)(\ell+2)}\,\delta_{n,\ell+2}\right]$$

$$\begin{aligned} V_{\ell\ell} &= \langle \ell|\tfrac{1}{2}m\delta^2 x^2|\ell\rangle \\ &= \tfrac{1}{2} m \delta^2 \langle \ell|x^2|\ell\rangle \\ &= \frac{x_0^2}{4} m\delta^2 (2\ell+1) \\ &= \frac{\hbar\delta^2}{4\omega}(2\ell+1) = \frac{\hbar\delta^2}{2\omega}(\ell + \tfrac{1}{2}) \end{aligned}$$

SO FIRST ORDER APPROXIMATION IS

$$\begin{aligned} E_\ell &= \hbar\omega(\ell+\tfrac{1}{2}) + \frac{\hbar\delta^2}{2\omega}(\ell+\tfrac{1}{2}) \\ &= \hbar\omega(\ell+\tfrac{1}{2})\left(1 + \frac{\delta^2}{2\omega^2}\right) \end{aligned}$$

$$\sum_{m\neq l} \frac{|V_{lm}|^2}{E_l^{(0)}-E_m^{(0)}} = \sum_{m\neq l} \frac{|V_{lm}|^2}{\hbar\omega(l+\frac{1}{2}) - \hbar\omega(m+\frac{1}{2})}$$

$$= \frac{1}{\hbar\omega}\sum_{m\neq} \frac{|V_{lm}|^2}{l-m}$$

$$V_{ml} = \langle m | \tfrac{1}{2} m\delta^2 x^2 | l \rangle$$
$$= \tfrac{1}{2} m\delta^2 \langle m | x^2 | l \rangle$$
$$= \frac{m\delta^2 x_0^2}{4}\left[\sqrt{l(l-1)}\,\delta_{m,l-2} + (2l+1)\,\delta_{ml} + \sqrt{(l+1)(l+2)}\,\delta_{m,l+2}\right]$$
$$= \frac{\delta^2\hbar}{4\omega}\left[\sqrt{l(l-1)}\,\delta_{m,l-2} + (2l+1)\,\delta_{ml} + \sqrt{(l+1)(l+2)}\,\delta_{m,l+2}\right]$$
$$|V_{ml}|^2 = \frac{\delta^4\hbar^2}{16\omega^2}\left[l(l-1)\,\delta_{m,l-2} + (2l+1)^2\,\delta_{ml} + (l+1)(l+2)\,\delta_{m,l+2}\right]$$

$$\sum_{m\neq l} \frac{|V_{ml}|^2}{E_l^{(0)}-E_m^{(0)}} = \frac{\delta^4\hbar}{16\omega^3}\sum_{m\neq l} \frac{l(l-1)\,\delta_{m,l-2}}{l-m} + \frac{(l+1)(l+2)\,\delta_{m,l+2}}{l-m}$$

$$= \frac{\delta^4\hbar}{16\omega^3}\sum_{m\neq l} \frac{l(l-1)\,\delta_{m,l-2}}{2} - \frac{(l+1)(l+2)\,\delta_{m,l+2}}{2}$$

$$= \frac{\delta^4\hbar}{32\omega^3}\left[l(l-1) - (l+1)(l+2)\right]$$
$$= \frac{\delta^4\hbar}{32\omega^3}\left[l^2 - l - (l^2+3l+2)\right]$$
$$= \frac{\delta^4\hbar}{32\omega^3}\left[-4l-2\right]$$
$$= \frac{\delta^4\hbar}{8\omega^3}\left[l+\tfrac{1}{2}\right]$$

SO SECOND ORDER APPROXIMATION IS

$$E_l = \hbar\omega(l+\tfrac{1}{2})\left(1+\frac{\delta^2}{2\omega^2}\right) - \frac{\delta^4\hbar\omega}{8\omega^4}(l+\tfrac{1}{2})$$
$$= \hbar\omega(l+\tfrac{1}{2})\left(1+\frac{\delta^2}{2\omega^2} - \frac{\delta^4}{8\omega^4}\right)$$

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4. FOR HYROGEN

$$E_n = \frac{-E_{RYD}}{(n+\ell+1)^2}$$

$$R(\rho) = N_{n\ell} \left(\frac{2\rho}{n}\right)^{\ell} F[-n+\ell+1, 2\ell+2, 2\rho/n]\, e^{-\rho/n}$$

$$N_{n\ell} = \frac{1}{(2\ell+1)!} \left[\frac{(n+\ell)!}{2n(n-\ell-1)!}\right]^{1/2} \left(\frac{2}{n}\right)^{3/2}$$

$$V = \frac{\lambda}{r^2}\,\delta(r) = \lambda\,\delta(\vec{r})$$

$$V_{\ell\ell} = \int d^3r\, \psi_\ell^2(r) \left[\frac{\lambda}{r^2}\,\delta(r)\right]$$

$$= \lambda \int_0^{\pi}\int_0^{2\pi} (Y_\ell^m)^2\, d\phi\, d\theta \int_0^{\infty} R^2(r)\,\delta(r)$$

$$= \lambda R^2(0) \int_0^{\pi}\int_0^{2\pi} (Y_\ell^m)^2\, d\phi\, d\theta$$

NOW $R^2(0) = 0 \quad \forall\ \ell \neq 0$

$$\int_0^{\pi}\int_0^{2\pi} (Y_0^0)^2\, d\phi\, d\theta = 1 \qquad \left(\text{ie } Y_0^0 = \frac{1}{\sqrt{4\pi}}\right)$$

$$\Rightarrow V_{\ell\ell} = \lambda R_{n0}^2(0)\, \delta_{\ell 0}$$

$$R(0) = N_{n\ell}$$

$$N_{n0} = \frac{1}{1!}\left[\frac{n!}{2n(n-1)!}\right]^{1/2} \left(\frac{2}{n}\right)^{3/2}$$

$$= \frac{1}{\sqrt{2}\,n}\,\frac{\sqrt{2}\,2}{n^{3/2}} = \frac{2}{n^3} \quad (\text{FOR } \rho)$$

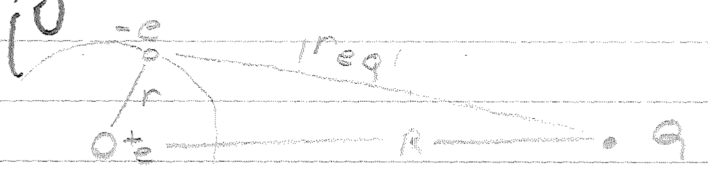
$$N_{n0} = \frac{4}{n^3 a^3} \quad (\text{FOR } r = \rho a)$$

PERTURBATION E:

$$\Rightarrow \Delta E_{n\ell m} = \begin{cases} \dfrac{4\lambda}{n^3 a^3}; & \ell = 0 \\ 0; & \ell \neq 0 \end{cases}$$

ONLY S STATES ARE EFFECTED. A GIVEN S STATE'S ENERGY CHANGE IS PROPORTIONAL TO THE DIRAC DELTA'S "STRENGTH" λ.

5. 5 (a)



$$r_{eq} = \sqrt{R^2 + r^2 - 2Rr\cos\theta}$$

FROM NUCLEUS: $\frac{Qe}{r}$

FROM ELECTRON: $\frac{-Qe}{\sqrt{R^2+r^2-2Rr\cos\theta}}$

THE PERTURBATION IS

$$V = \frac{Qe}{r} - \frac{Qe}{\sqrt{R^2+r^2-2rR\cos\theta}}$$

$$= \frac{Qe}{r}\sum_{\ell=1}^{\infty}\left(\frac{r}{R}\right)^{\ell} P_{\ell}(\cos\theta)$$

SCHIFF* EXPLORES THE SOLUTION OF THIS PROBLEM AND SHOWS THE PERTURBED E IS

$$-Q^2\sum_{\ell=1}^{\infty}\frac{(\ell+2)(2\ell+1)!}{\ell\, 2^{2\ell+1}}\, a^{2\ell+1}/R^{2\ell+2}$$

WE'LL LEAVE IT HERE IN LIEU OFF COPYING SHIFF'S SOLUTION.

Whatever $2\ell+2 = ?$

*SHIFF, "QUANTUM MECHANICS" Pp. 267-8

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6. $H_0 = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right)$

$V = e^2/|r_1 - r_2|$

a. $H = -\frac{\hbar^2}{2m}\nabla^2 - 2\frac{e^2}{r}$

GIVES $E_n = -4E_{RYD}/n^2$

GROUND STATE IS

$E_0 = -4E_{RYD}$

THUS, FOR H_0, GROUND STATE IS $E_0 = -8E_{RYD}$

(CONT.)

FOR He, GROUND STATE WAVE FUNCTION IS

$\psi_{1s}(r) = Ce^{-r/a}$

$\int \psi_{1s}^2(r)\,dr = 1 = C^2 4\pi \int_0^\infty r^2 e^{-2r/a}\,dr$

$= 4\pi C^2\, 2!\left(\frac{a}{2}\right)^3$

$= 4\pi C^2 \frac{a^3}{4}$

$= \pi C^2 a^3 \Rightarrow C = \frac{1}{\sqrt{\pi a^3}}$

$\therefore \psi_{1s} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$

THUS, FOR H_0

$\psi(r_1, r_2) = \frac{1}{\pi a^3} e^{-(r_1+r_2)/a}$

FIRST ORDER P THEORY:

$E = E_\ell^{(0)} + V_{\ell\ell}$

$V_{\ell\ell} = \langle 1s | \frac{e^2}{|r_1 - r_2|} | 1s \rangle$

$= \langle 1s | \sum_{\ell=0}^{\infty} e^2 \frac{r_1^\ell}{r_2^{\ell+1}} P_\ell(\cos\theta) | 1s \rangle \quad ; r_1 < r_2$

$\cancel{= \frac{1}{\pi a^6} \int d^3r\, e^{-2(r_1+r_2)/a} \sum_{\ell=0}^{\infty} \frac{r_1^\ell}{r_2^{\ell+1}} P_\ell(\cos\theta)}$

NOW

$\int d\Omega\, P_\ell(\cos\theta) = \begin{cases} 4\pi & ; \ell = 0 \\ 0 & ; \ell \neq 0 \end{cases}$

$\int \frac{d\Omega_1}{4\pi} \int \frac{d\Omega_2}{4\pi} \frac{1}{|r_1 - r_2|} = \frac{1}{r_2} \quad ; r_1 < r_2$

$$V_{LL} = e^2\frac{(4\pi)^2}{\pi^2 a^6}\int_0^\infty r_1^2\,dr_1\,e^{-r_1/a}\int_0^\infty r_2^2\,dr_2\,e^{-r_2/a} \times \int\frac{d\Omega_1}{4\pi}\int\frac{d\Omega_2}{4\pi}\frac{1}{|r_1-r_2|}$$

$$= e^2\frac{16}{a^6}\int_0^\infty r_1^2\,dr_1\,e^{-r_1/a}\int_{r_1}^\infty r_2\,dr_2\,e^{-r_2/a}$$
$$= e^2\frac{16}{a^6}\int_0^\infty r_1^2\,dr_1\,e^{-r_1/a}\,a^2 e^{-r_2/a}\left(\frac{r_2}{a}-1\right)\Big|_{r_1}^\infty$$
$$= e^2\frac{16}{a^4}\int_0^\infty r_1^2\,dr_1\,e^{-r_1/a}\,e^{-r_1/a}\left(\frac{r_1}{a}-1\right)$$
$$= e^2\frac{16}{a^4}\int_0^\infty r_1^2\left(\frac{r_1}{a}-1\right)e^{-2r_1/a}\,dr_1$$

$$= e^2\frac{16}{a^4}\left[\frac{1}{a}\,3!\left(\frac{a}{2}\right)^4 - 2!\left(\frac{a}{2}\right)^3\right]$$
$$= e^2\frac{16}{a^4}\left[3\,\frac{a^3}{8}-\frac{a^3}{8}\right]$$
$$= \frac{32}{8a}e^2$$
$$= 4/a\,e^2$$
$$= 8\left(\frac{e^2}{2a}\right)$$
$$= 8E_{RYD}$$

THIS ANSWER IS OBVIOUSLY INCORRECT IN THAT IT GIVES A GROUND STATE E OF $-16\,E_{RYD}$ FOR THE He ATOM ON SECOND APPROXIMATION. THE EXPERIMENTAL VALUE IS $-5.8\,E_{RYD}$. ONE WOULD EXPECT THE TRUE YIELD OF FIRST ORDER PERT. TO GIVE ABOUT $2\,E_{RYD}$.

Physics 611
Due April 15, 1975
#9 pg 149

✓1) Consider an electron in free space which is under the influence of a constant electric field F in the x direction and a constant magnetic field H_0 in the z direction. Describe the motion of the electron by solving the classical equations

$$m\frac{d\underset{\sim}{v}}{dt} = -e\left[\underset{\sim}{F} + \frac{1}{c}\underset{\sim}{v}\times\underset{\sim}{H_0}\right]$$

2) Show that the Hamiltonian of problem (1) may be written as:

$$\mathcal{H} = \frac{1}{2m}\left[P_x^2 + P_z^2 + \left(P_y - \frac{e}{c}xH_0\right)^2\right] + eFx$$

Solve this Hamiltonian, and show that the energy and eigenstates are

$$E = \frac{\hbar^2 k_z^2}{2m} + (n+\tfrac{1}{2})\hbar\omega_c + \frac{m}{2}v_d^2 + eFX_0\,;\quad \psi = \psi_n(x-X_0)\,e^{i(k_y y + k_z z)}$$

where $\omega_c = \frac{eH_0}{mc}$, $v_d = \frac{cF}{H_0}$. Determine X_0, and discuss physically how the electron is moving. Hint: to solve $\mathcal{H}$, make the variable change $X = x - p_y/(m\omega_c)$, $Y = y - p_x/(m\omega_c)$, $P_y = p_y$, $P_x = p_x$.

3) Consider a spinless (S = 0) particle in the in the n = 2 state of a hydrogen atom. Assume that a magnetic and electric field are both perturbing the atom.

$$\mathcal{H}_{int} = -\mu_0\,\underset{\sim}{L}\cdot\underset{\sim}{H_0} + e\,\underset{\sim}{F}\cdot\underset{\sim}{r}$$

Find the new energy levels for the cases (a) H_0 parallel F, (b) H_0 perpendicular F Only consider terms linear in H_0 and F.

✓4) Calculate the Golden Rule in the second Born Approximation. That is, calculate $a_m^{(2)}(t)$ and find the transition rate

$$w = \lim_{t\to\infty}\frac{d}{dt}\left|a_m^{(1)} + a_m^{(2)}\right|^2$$

✓5) For the Yukawa potential $V(r) = \lambda e^{-k_0 r}/r$

a. Write down the differential cross section $\frac{d\sigma}{d\Omega}$ in the Born Approx.

b. Obtain the total cross section σ by integrating (a) over solid angle $d\Omega$.

PHYSICS 611
DUE 4/15/75
BOB MARKS

37/50

1. $m\frac{d\underset{\sim}{V}}{dt} = -e\left[\underset{\sim}{E} + \frac{1}{c}\underset{\sim}{V}\times\underset{\sim}{H}\right]$ 10

$$\frac{d\underset{\sim}{V}}{dt} = \frac{-e\underset{\sim}{E}}{m} + \frac{e}{cm}\underset{\sim}{V}\times\underset{\sim}{H}$$

$$\underset{\sim}{V} = V_x\underset{\sim}{a}_x + V_y\underset{\sim}{a}_y + V_z\underset{\sim}{a}_z$$

$$\underset{\sim}{E} = F\underset{\sim}{a}_x$$

$$\underset{\sim}{H}_0 = H_0\underset{\sim}{a}_z$$

$$\underset{\sim}{V}\times\underset{\sim}{H}_0 = \begin{vmatrix} \underset{\sim}{a}_x & \underset{\sim}{a}_y & \underset{\sim}{a}_z \\ V_x & V_y & V_z \\ 0 & 0 & H_0 \end{vmatrix} = H_0V_y\underset{\sim}{a}_x - H_0V_x\underset{\sim}{a}_y$$

IN X DIRECTION:

$$\frac{dV_x}{dt} = \frac{-eF}{m} - \frac{H_0e}{cm}V_y$$

IN Y DIRECTION:

$$\frac{dV_y}{dt} = \frac{eH_0}{cm}V_x$$

NOW: $\frac{d^2V_x}{dt^2} = -\frac{H_0e}{cm}\frac{dV_y}{dt}$ —

$$\Rightarrow \frac{dV_y}{dt} = -\frac{cm}{H_0e}\frac{d^2V_x}{dt^2} = \frac{eH_0}{cm}V_x$$

$$\therefore \frac{d^2V_x}{dt^2} = -\left(\frac{eH_0}{cm}\right)^2V_x$$

LET $\omega = \frac{eH_0}{cm}$

$$\frac{d^2V_x}{dt^2} = -\omega^2V_x \Longrightarrow V_x = V_x(0)e^{-j\omega t}$$

$$\frac{dV_x}{dt} = -j\omega V_x(0)e^{-j\omega t}$$

$$= \frac{-eF}{m} - \omega V_y$$

$$\therefore V_y = \frac{1}{\omega}\left[\frac{-eF}{m} + j\omega V_x(0)e^{-j\omega t}\right]$$

$$= \frac{-eF}{\omega m} + jV_x(0)e^{-j\omega t}$$

IN Z DIRECTION:

$$\frac{dV_z}{dt} = 0 \Rightarrow V_z(t) = V_z(0)$$

NOW $\frac{-eF}{\omega m} = \frac{-eF}{m}\frac{cm}{eH_0} = \frac{-cF}{H_0}$

IN SUMMARY:

$$V_x(t) = V_x(0)e^{-j\omega t}$$
$$V_y(t) = -\frac{cE}{H_0} + jV_x(0)e^{-j\omega t}$$
$$V_z(t) = V_z(0)$$

ELECTRON'S Z VELOCITY UNALTERED

Y DIRECTION CONSTANT VELOCITY COMPONENT INVERSE WITH MAGNETIC FIELD STRENGTH.

IF INITIAL X VELOCITY COMPONENT, e^- OSCILLATES WITH FREQUENCY $\omega = \frac{eH_0}{cm}$ AND AMPLITUDE $V_x(0)$ AS VIEWED ON X & Y.

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3. $\mathcal{H}_{INT} = -\mu_0 \underset{\sim}{\ell_0} H_0 + e\underset{\sim}{F} \cdot \underset{\sim}{r}$

a. H_0 PARALLEL TO F

LET: $e\underset{\sim}{F} \cdot \underset{\sim}{r} = eFr\cos\theta$

$-\mu_0 \underset{\sim}{\ell_0} \underset{\sim}{H_0} = -\mu_0 L_z H_0$

$$
\begin{array}{c|cccc}
 & 2S & 2P_0 & 2P_{+1} & 2P_{-1} \\
\hline
2S & 0 & \lambda_1 & 0 & 0 \\
2P_0 & \lambda_1 & 0 & 0 & 0 \\
2P_{+1} & 0 & 0 & \lambda_2 & 0 \\
2P_{-1} & 0 & 0 & 0 & \lambda_3
\end{array}
$$

$\lambda_1 = \langle 200 | eFr\cos\theta | 210 \rangle$

$= eF\langle 200 | r | 210 \rangle$

$= -3aeF$

$\lambda_2 = -\mu_0 H_0 \langle 211 | L_z | 2,1,1 \rangle$

$= -\mu_0 H_0 (1)$

$= -\mu_0 H$

$\lambda_3 = -\mu_0 H_0 \langle 2,1,-1 | L_z | 2,1,-1 \rangle = \mu_0 H_0$

DIAGONALIZING:

$\Delta E = \pm\lambda_1, \lambda_2, \lambda_3$

$= \pm 3aeF, -\mu_0 H_0, \mu_0 H_0$

$= \pm 3aeF, \pm\mu_0 H_0$

b. H_0 PERPENDICULAR TO F

LET: $-\mu_0 \underset{\sim}{L} \cdot \underset{\sim}{H}_0 = \mu_0 L_x H_0$

$e\underset{\sim}{F} \cdot \underset{\sim}{r} = eFr\cos\theta$

$$\begin{array}{c|cccc} & 2S & 2P & 2P_{+1} & 2P_{-1} \\ \hline 2S & 0 & \lambda_1 & 0 & 0 \\ 2P & \lambda_1 & 0 & \lambda_2 & \lambda_3 \\ 2P_{+1} & 0 & \lambda_2 & 0 & 0 \\ 2P_{-1} & 0 & \lambda_3 & 0 & 0 \end{array}$$

$$\lambda_1 = \langle 200 | eFr\cos\theta | 210 \rangle = -3aeF$$

$$\lambda_2 = -\langle 210 | \mu_0 L_x H_0 | 211 \rangle$$

$$= -\frac{\mu_0 H_0}{2} \langle 210 | 2L_x | 211 \rangle$$

$$= -\frac{\mu_0 H}{2} \langle 210 | L^- | 211 \rangle$$

$$= -\frac{\mu_0 H_0}{2} (\sqrt{2}) = -\frac{\mu_0 H_0}{\sqrt{2}}$$

$$\lambda_3 = \lambda_2 = -\mu_0 H_0 / \sqrt{2}$$

DIAGONALIZING GIVES

$$\Delta E = 0, \pm \sqrt{\lambda_2^2 + \lambda_1^2}$$

$$= 0, \pm \sqrt{\tfrac{1}{2}\mu_0^2 H_0^2 + (3aeF)^2}$$

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4. IN GENERAL

$$i\hbar\, \dot{a}_e(t) = \sum_n a_n(t) V_{en} \Theta(t) e^{i\omega_{en}t}$$

$$\omega_{en} = [E_e^{(0)} - E_n^{(0)}]/\hbar$$

$$a_e = a_e^{(0)} + a_e^{(1)} + a_e^{(2)} + \ldots$$

$$a_e^{(0)} = \delta_{eM}$$

$$a_M^{(0)} = 1$$

$$i\hbar \dot{a}_e^{(2)} = \sum_n a_e^{(0)} V_{en} \Theta(t) e^{i\omega_{en}t}$$

$$= V_{eM}\, e^{i\omega_{eM}(t)}$$

$$a_e^{(2)} = \frac{1}{i\hbar} V_{em} \int_0^t e^{i\omega_{em}(t)} dt$$

$$= \frac{1}{i\hbar} V_{em} \frac{1}{i\omega_{em}} e^{i\omega_{em}t}\Big|_0^t$$

$$= \frac{V_{em}}{i\hbar\, i\omega_{em}} [e^{i\omega_{em}t} - 1]$$

SUBSTITUTING INTO FIRST EQUATION

$$i\hbar \dot{a}_e^{(2)} = \sum_n \frac{V_{nm} V_{en}}{i\hbar} \frac{1}{i\omega_{nm}} [e^{i\omega_{em}t} - 1]$$

$$\dot{a}_e^{(2)} = \frac{1}{(i\hbar)^2} \sum_n V_{nm} V_{en} \frac{1}{i\omega_{nm}} [e^{i\omega_{em}t} - 1]$$

$$a_e^{(2)} = \frac{1}{(i\hbar)^2} \sum_n \int_0^t V_{nm} V_{en} \frac{1}{i\omega_{nm}} [e^{i\omega_{em}t} - 1] dt$$

$$= \frac{1}{(i\hbar)^2} \sum_n V_{nm} V_{en} \int_0^t \frac{1}{i\omega_{nm}} [e^{i\omega_{nm}t} - 1] dt$$

$$= \frac{1}{(i\hbar)^2} \sum_n V_{nm} V_{em} \frac{1}{i\omega_{nM}} \Big[\frac{1}{i\omega_{eM}} (e^{i\omega_{em}t} - 1) - \frac{1}{i\omega_{en}} (e^{i\omega_{en}t} - 1)\Big]$$

$$\approx \frac{1}{(i\hbar)^2} \sum_n V_{nm} V_{en} \frac{1}{i\omega_{nM}} \Big[\frac{1}{i\omega_{eM}} (e^{i\omega_{em}t} - 1)\Big]$$

$$|a_e^{(1)} - a_e^{(2)}|^2 = \frac{1}{\hbar^2} \Big| \frac{e^{i\omega_{eM}t} - 1}{\omega_{em}} \Big(V_{eM} - \sum_n \frac{V_{en} V_{nM}}{E_n - E_M}\Big)\Big|^2$$

$$\lim_{t\to\infty} |a_e^{(1)} - a_e^{(2)}|^2 = \frac{2\pi}{\hbar} \delta[E_e - E_M] \Big| V_{KM} - \sum_{n \neq M} \frac{V_{en} V_{nM}}{E_n - E_M}\Big|^2$$

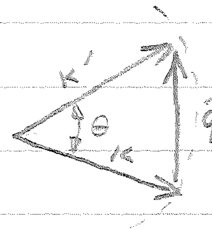
ok well

5. $V(r) = \frac{\lambda}{r} e^{-K_s r}$ A

FROM CLASS NOTES

$$V(q) = \frac{4\pi\lambda}{q^2 + K_s^2}$$

$$\underline{q} = \underline{k} - \underline{k}'$$



$$q = 2k\sin\frac{\theta}{2}$$

$$\therefore V(k-k') = \frac{4\pi\lambda}{4k^2\sin^2\frac{\theta}{2} + K_s^2}$$

$$\frac{d\sigma}{d\Omega}_{k\to k'} = \frac{m^2}{4\pi^2\hbar^2} V^2(k-k')$$

$$= \frac{m^2}{4\pi^2\hbar^2} \frac{16\pi^2\lambda^2}{(4k^2\sin^2\theta/2 + K_s^2)^2}$$

$$= \frac{4m^2\lambda^2}{\hbar^2} \frac{1}{(4k^2\sin^2\theta/2 + K_s^2)^2}$$

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega}$$

$$= \left(\frac{2m\lambda}{\hbar}\right)^2 \int_0^{2\pi} d\phi \int_0^{\pi} \frac{d\theta}{(4k^2\sin^2\frac{\theta}{2} + K_s^2)^2}$$

$$= 2\pi \left(\frac{2m\lambda}{\hbar}\right)^2 \int_0^{\pi} \frac{d\theta}{(4k^2\sin^2\theta/2 + K_s^2)^2}$$

$$= 2\pi \left(\frac{2m\lambda}{\hbar}\right)^2 \int_0^{\pi} \frac{d\theta}{[2k^2(1-\cos\theta) + K_s^2]^2}$$

$$= 2\pi \left(\frac{2m\lambda}{\hbar}\right)^2 \int_0^{\pi} \frac{d\theta}{[K_s^2 + 2k^2 - 2k^2\cos\theta]^2}$$

$$= 2\pi \left(\frac{2m\lambda}{\hbar}\right)^2 \left[\frac{2}{K_s^2(K_s^2 + 4k^2)}\right]$$

$$= \left(\frac{4m\lambda}{\hbar K_s}\right)^2 \frac{\pi}{K_s^2 + 4k^2}$$

Physics 611
Due April 25
#10

1) Derive the differential cross section in the Born Approximation for elastic scattering from a fixed potential $V(r)$. Assume the incident particle is going relativistic energies. What is the result for Rayleigh scattering (elastic scattering of photons)?.

2) What is the differential cross section in the Born approximation for electron scattering from a coulomb potential of charge Z? Compare with the Rutherford formula.

3) Consider a hypothetical nuclear reaction N^* $N + e^+ + e^-$ (electron plus positron). Calculate the distribution of final energies of the electron. Use relativistic kinematics for the electron and positron. Assume a constant matrix element, and also that the final kinetic energy of the nucleon is small.

4) Calculate the oscillator strength f, analytically and numerically, for the transition between the ground and the first excited state of the following potentials:

a. hydrogen atom
b. three dimensional harmonic oscillator
c. One dimensional box of length L and infinite walls.

PHYSICS 611
DUE APRIL 25
BOB MARKS

$\boxed{\dfrac{40}{40}}$

1. $w_{\ell m} = \frac{2\pi}{\hbar} |V|^2_{\ell m} \delta[E_\ell^{(0)} - E_m^{(0)}]$

INCIDENT WAVE

$E_m^{(0)} = \sqrt{p^2c^2 + m^2c^4}$; $p = \hbar k$

$|k\rangle = \frac{1}{\sqrt{\Omega}} e^{ik\cdot r}$

SCATTERED WAVE

$E_\ell^{(0)} = \sqrt{p'^2c^2 + m^2c^4}$

$|k'\rangle = \frac{1}{\sqrt{\Omega}} e^{ik'\cdot r}$

THEN

$$V_{kk'} = \frac{1}{\Omega} \int d^3r\, e^{-ik\cdot r} V(r) e^{+ik'\cdot r}$$

$$= \frac{1}{\Omega} \mathcal{V}(k-k') \quad \leftarrow \text{FOURIER XFORM}$$

$$\Rightarrow w_{k\to k'} = \frac{2\pi}{\hbar\Omega^2} \mathcal{V}^2(k-k') \delta\left[\sqrt{p'^2c^2+m^2c^4} - \sqrt{p^2c^2+m^2c^4}\right]$$

NOW

$$w_k = \sum_{k'} w_{k\to k'}$$

$$= \Omega \int dk'^3 \frac{1}{(2\pi)^3} w_{k\to k'}$$

$$= \frac{1}{\hbar\Omega(2\pi)^2} \int d^3k'\, \mathcal{V}^2(k-k') \delta\left[\sqrt{p'^2c^2+m^2c^4} - \sqrt{p^2c^2+m^2c^4}\right]$$

$$= \frac{1}{\hbar\Omega(2\pi)^2} \int d\Omega_k\, \mathcal{V}^2(k-k') \int dk'\, k'^2 \delta\left[\sqrt{p'^2c^2+m^2c^4} - \sqrt{p^2c^2+m^2c^4}\right]$$

LET

$$I = \int_0^\infty dk'\, k'^2 \delta\left[\sqrt{p'^2c^2+m^2c^4} - \sqrt{p^2c^2+m^2c^4}\right]$$

SINCE $p' = \hbar k'$

$$I = \frac{1}{\hbar^3} \int_0^\infty dp'\, p'^2 \delta\left[\sqrt{p'^2c^2+m^2c^4} - \sqrt{p^2c^2+m^2c^4}\right]$$

$$= \frac{1}{\hbar^3} \int_0^\infty dp'\, p'^2 \frac{\delta(p-p')}{\frac{d}{dp}\sqrt{p^2c^2+m^2c^4}}$$

$$= \frac{1}{\hbar^3} \int_0^\infty dp'\, p'^2 \frac{1}{p'c^2} \sqrt{p^2c^2+m^2c^4}\, \delta(p-p')$$

$$= \frac{1}{\hbar^3 c^2} p \sqrt{p^2c^2+m^2c^4} = \frac{1}{\hbar^3c^2} E_m p$$

$$\Rightarrow w_K = \frac{1}{\hbar \Omega (2\pi)^2} \frac{1}{\hbar^3 c^2} E m p \int d\Omega_K \, V^2(K-K')$$

$$= \frac{E m p}{\hbar^4 c^2 \Omega (2\pi)^2} \int d\Omega_K \, V^2(K-K')$$

FOR N PARTICLES (IDEAL GAS THEORY)

$$w_{NK} = \frac{N}{\Omega} \frac{\hbar K}{m} \sigma = \frac{E m p N}{\hbar^4 c^2 \Omega (2\pi)^2} \int d\Omega_K \, V^2(K-K')$$

$$= \frac{N}{\Omega} \frac{p}{m} \sigma$$

$$\Rightarrow \sigma = \frac{m E m}{\hbar^4 c^2 (2\pi)^2} \int d\Omega_K \, V^2(K-K')$$

AND THE DIFFERENTIAL CROSS SECTION IS:

$$\frac{d\sigma}{d\Omega} = \frac{m E}{\hbar^4 c^2 (2\pi)^2} V^2(K-K')$$

FOR RALEIGH SCATTERING:

FOR THE PHOTON: $p = mc \Rightarrow m = \frac{p}{c}$

$$\Rightarrow \sigma = \frac{E}{\hbar^4 \, 4\pi^2 \, c^2} \left(\frac{p}{c}\right) \int d\Omega_K \, V^2(K-K')$$

$$= \frac{E p}{4\pi^2 \hbar^2 c^3} \int d\Omega_K \, V^2(K-K')$$

$$\frac{d\sigma}{d\Omega} = \frac{E p}{4\pi^2 \hbar^2 c^3} V^2(K-K')$$

$$E = pc$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{p^2}{4\pi^2 \hbar^2 c^2} V^2(K-K')$$

(i)

2. $V(r) = \frac{-Ze^2}{r}$

$$\frac{d\sigma}{d\Omega}_{k\to k'} = \frac{1}{4\pi^2}\frac{m^2}{\hbar^2}V^2(k-k')$$

$$V(q) = -Ze^2\int d^3r\,\frac{1}{r}e^{iq\cdot r}$$
$$= -4\pi Ze^2\int_0^\infty dr\, r e^{iq\cdot r}$$

FROM LAPLACE TRANSFORMS: $\int_0^\infty t e^{-st} = \frac{1}{s^2}$

$$\Rightarrow V(q) = 4\pi Ze^2\frac{1}{q^2}$$

$$\Rightarrow \frac{d\sigma}{d\Omega}_{k\to k'} = \frac{16\pi^2 Z^2 e^4 m^2}{4\pi^2\hbar^2|q|^4} \quad ; q = k-k'$$
$$= \frac{4Z^2e^4m^2}{\hbar^2}\frac{1}{|q|^4}$$

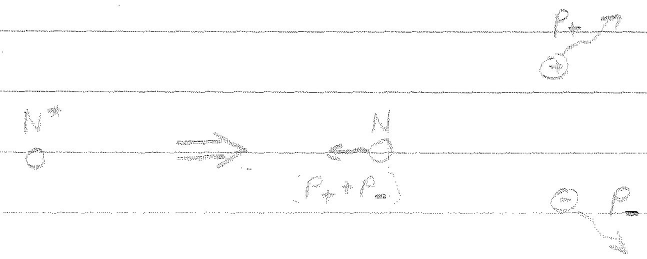
$$|q|^2 = |k-k'|^2 = k^2 + k'^2 - 2kk'\cos\theta$$

FOR $|k|=|k'|$; $|q|^2 = 2k^2 - 2k^2\cos\theta$
$$= 2k^2(1-\cos\theta)$$
$$\Rightarrow |q|^4 = 4k^4(1-\cos\theta)$$

$$\therefore \frac{d\sigma}{d\Omega} = \left(\frac{2mZe^2}{\hbar}\right)^2\frac{1}{4k^4(1-\cos\theta)^2}$$

$$= \left[\frac{mZe^2}{\hbar k^2(1-\cos\theta)}\right]^2 \Leftarrow$$ RUTHERFORD'S FORMULA

3.



LET Δ = EXCESS KINETIC ENERGY

$+ \rightarrow$ POSITRON, $- \rightarrow$ ELECTRON, $N \rightarrow$ NUCLEUS

$E_+ = \sqrt{P_+^2 c^2 + m^2 c^4}$ $\quad m = m_+ = m_-$

$E_- = \sqrt{P_-^2 c^2 + m^2 c^4}$

$E_N = \sqrt{(P_+ + P_-)^2 c^2 + m_N^2 c^4}$

$\Delta \simeq E_+ + E_-$

FROM FERMI

$$w_{i \to f} = \frac{2\pi}{\hbar} |M|^2 \delta[\Delta - E_+ - E_-]$$

$\Rightarrow E_f - E_i = \Delta - E_+ - E_-$

$$w = \sum_{P_+ P_-} w_{i \to f}$$

ASSUMING M CONSTANT:

$$= \frac{2\pi}{\hbar^2} |M|^2 \frac{1}{(2\pi)^6} \int d^3P_+ \, d^3P_- \, \delta[\Delta - E_+ - E_-]$$

$$= \frac{|M^2|}{\hbar^2 (2\pi)^5} (4\pi)^2 \int dP_+ P_+^2 \int dP_- P_-^2 \, \delta(\Delta - E_+ - E_-)$$

NOW

$$E_+^2 = P_+^2 c^2 + m^2 c^4$$

$$E_+ dE_+ = P_+ c^2 dP_+ \qquad P_+ = \frac{1}{c} \sqrt{[E_+^2 - m^2 c^4]}$$

$$P_+^2 dP_+ = \frac{1}{c^2} P_+ E_+ dE_+ =$$

$$= \frac{1}{c^3} \sqrt{E_+^2 - m^2 c^4} \, E_+ dE_+$$

$$\Rightarrow \omega = \frac{4|M|^2}{\hbar^2(2\pi)^3}\int dP_+ P_+^2 \int \frac{1}{c^3}\sqrt{E_-^2 - m^2c^4}\, E_- dE_- \,\delta(\Delta - E_- - E_+)$$

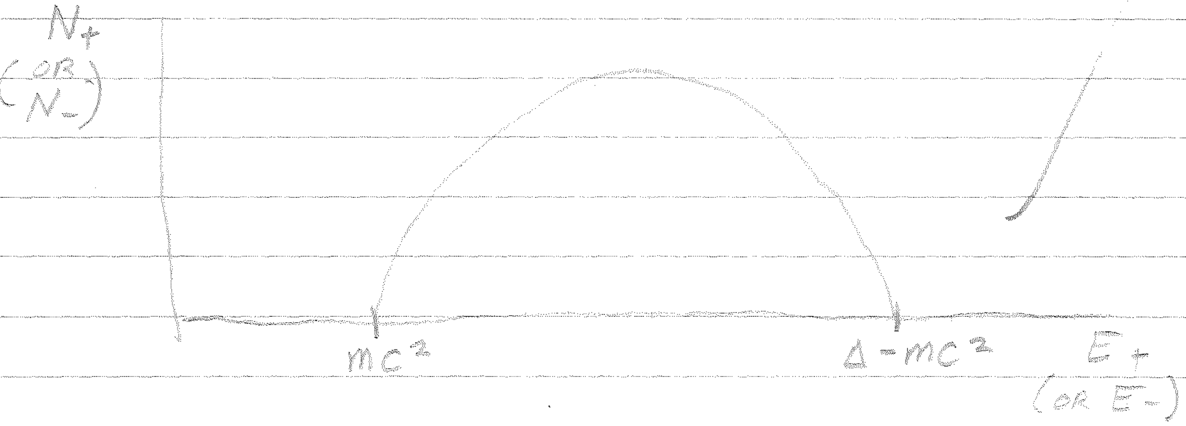
$$= \frac{4|M|^2}{c^3\hbar^2(2\pi)^3}\int dP_+ P_+^2 \left[(\Delta - E_+)^2 - m^2c^4\right]^{1/2}(\Delta - E_+)$$

$$= \frac{|M|^2}{2c^3\hbar^2\pi^3}\int \frac{dE_+}{c^3}\sqrt{(E_+^2 - m^2c^4)\left[(\Delta - E_+)^2 - m^2c^4\right]}\,(\Delta - E_+)E_+$$

$$N_+ = \frac{d\omega}{dE_+} = ¢\,\sqrt{(E_+^2 - m^2c^4)\left[(\Delta - E_+)^2 - m^2c^4\right]}\,(\Delta - E_+)E_+$$

$$¢ = \text{CONSTANT} = \frac{|M|^2}{2c^6\hbar^2\pi^3}$$

DUE TO SYMMETRY OF THE PROBLEM SAME ANSWER FOR $\frac{d\omega}{dE_-} = N_-$



40. GROUND STATE IS 1S

1^{ST} EXCITED STATE IS $2P_z$

$$f_{if} = \frac{2(\hat{n}\cdot \vec{x}_{if})^2 m\,\omega_{fi}}{\hbar}$$

CHOOSE $\hat{n}$ IN z DIRECTION

$$\Rightarrow f_{if} = \frac{1}{\hbar}\,|\langle i|z|f\rangle|^2 m\,\omega_{fi}$$

IT WAS SHOWN THAT

$$\langle 1S|z|2P_z\rangle = \frac{\sqrt{2}\,2^7}{3^5}\,a$$

ALSO: $E_{1S} = -E_{RYD}$

$E_{2P} = -\frac{1}{4}E_{RYD}$

$$\Rightarrow \omega_{fi} = \frac{3}{4\hbar}E_{RYD}$$

PUTTING IT ALL TOGETHER:

$$f_{if} = \frac{2}{\hbar^2}\left(\frac{\sqrt{2}\,2^7}{3^5}\right)^2 a^2 m\,\frac{3}{4}E_{RYD}$$

$$= \frac{3}{2}\,\frac{2^{15}}{3^{10}}\,\frac{a^2 m E_{RYD}}{\hbar^2}$$

$$= \frac{2^{14}}{3^9}\,\frac{a^2 m}{\hbar^2}\,\frac{e^2}{2a}$$

$$= \frac{2^{13}}{3^9}$$

$= 0.416$

4b. ASSUME INITIAL STATE

$$\psi_i(r) = \phi_0(x)\,\phi_0(Y)\,\phi_0(z)$$

AND FINAL STATE

$$\psi_f(r) = \phi_0(x)\,\phi_0(Y)\,\phi_1(z)$$

AND $\hat{n}$ IN z DIRECTION

THEN

$$\langle i|z|f\rangle = \langle\phi_0(x)|\phi_0(x)\rangle\langle\phi_0(Y)|\phi_0(Y)\rangle$$
$$\langle\phi_0(z)|z|\phi_0(z)\rangle$$
$$= (1)(1)\frac{1}{\sqrt{2}\,\alpha} \ni \alpha^2 = \frac{m\omega}{\hbar}$$

AND $\omega = \sqrt{K/m}$

FOR HARMONIC OSCILL. IN ONE-DIMENSION:

$$E_n = (n+\tfrac{1}{2})\hbar\omega$$
$$\Rightarrow \omega_{fi} = \omega$$

PUTTING IT ALL TOGETHER:

$$f_{ij} = \frac{2|\langle i|z|f\rangle|^2 m\omega}{\hbar}$$

$$= \frac{2}{\hbar}\,\frac{1}{2\alpha^2}\,m\omega$$

$$= \frac{1}{\hbar}\left(\frac{\hbar}{m\omega}\right)m\omega$$

$$= 1$$

4c. $f_{if} = \frac{2}{\hbar} (\hat{n} \cdot \underset{\sim}{x})^2 m \omega_{fi}$

FOR BOX POTENTIAL

$\psi_n(x) = \sqrt{2/L}\, \sin \frac{n \pi x}{L}$; $E_n = \left(\frac{n\pi}{L}\right)^2 \frac{\hbar^2}{2m}$

ERGO

$\psi_1(x) = \sqrt{\frac{2}{L}}\, \sin \frac{\pi x}{L}$; $\psi_2(x) = \sqrt{\frac{2}{L}}\, \sin \frac{2\pi x}{L}$

$\hat{n}$, OF COURSE IN X DIRECTION:

$$\langle 1 | x | 2 \rangle = \frac{2}{L} \int_0^L x \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L}\, dx$$

$$= \frac{4}{L} \int_0^L x \sin^2 \frac{\pi x}{L} \cos \frac{\pi x}{L}\, dx$$

$$= -\frac{16}{9} \frac{L}{\pi^2}$$

$$\omega_{fi} = \frac{1}{\hbar}\left[4 \left(\frac{\pi}{L}\right)^2 \frac{\hbar^2}{2m} - \left(\frac{\pi}{L}\right)^2 \frac{\hbar^2}{2m}\right]$$

$$= 3 \left(\frac{\pi}{L}\right)^2 \frac{\hbar}{2m}$$

PUTTING IT ALLOGETHER

$$f_{if} = \frac{2}{\cancel{\hbar}} \left(\frac{16}{9}\right)^2 \frac{\cancel{L^2}}{\pi^4}\, \cancel{m}\, 3 \left(\frac{\pi}{\cancel{L}}\right)^2 \frac{\cancel{\hbar}}{\cancel{2m}}$$

$$= \left(\frac{16}{9}\right)^2 \frac{3}{\pi^2} = 0.961$$

$p = \hbar k$

1. $|k\rangle = \frac{1}{\sqrt{\Omega}} e^{i k \cdot r}$ $\leftarrow$ INIT

$|k'\rangle = \frac{1}{\sqrt{\Omega}} e^{i k' \cdot r}$

$$w_{k \to k'} = \frac{2\pi}{\hbar} \frac{1}{\Omega^2} V^2(k-k') \, \delta\left[\sqrt{p^2c^2+m^2c^4} - \sqrt{p'^2c^2+m^2c^4}\right]$$

$$w_k = \sum_{k'} w_{k \to k'}$$

$$\to \Omega \int \frac{d^3k'}{(2\pi)^3} w_{k \to k'}$$

$$= \frac{2\pi}{\hbar} \frac{1}{\Omega} \int \frac{d^3k}{(2\pi)^3} V^2(k-k') \, \delta\left[\sqrt{\quad} - \sqrt{\quad}\right]$$

$$= \frac{2\pi}{\hbar} \frac{1}{\Omega} \int d\Omega_{k'} V^2(k-k') \int_0^\infty k'^2 dk' \, \delta\left[\sqrt{\quad} - \sqrt{\quad}\right]$$

$$\int_0^\infty dk \, k'^2 \delta\left(\sqrt{\quad} - \sqrt{\quad}\right)$$

$$= \frac{1}{\hbar^3} dp' p'^2 \delta\left(\sqrt{\quad} - \sqrt{\quad}\right)$$

$$= \frac{1}{\hbar^3} \int_0^\infty dp' p'^2 \frac{\delta(p'-p)}{\frac{d}{dp'}\sqrt{p'^2c^2+m^2c^4}}\Bigg|_{p'=p}$$

$$= \frac{1}{\hbar^3 c^2} p \sqrt{p^2c^2+m^2c^4}$$

$$= \frac{1}{\hbar^3 c^2} E p \quad ; \; E = \sqrt{p^2c^2+m^2c^4}$$

$$\int d^3r\, V(r) e^{iq\cdot r} = \int dr\, r^2 V(r) \int d\theta\, d\phi \sin\theta\, e^{iqr\cos\theta}$$
$$= \frac{4\pi}{q^2}$$

2. $V(r) = \frac{-Ze^2}{r}$

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2}\frac{m^2}{\hbar^2} \mathcal{V}(k-k')^2$$

$$\mathcal{V}(q) = -z^2e^2 \int d^3r \frac{1}{r} e^{iq\cdot r}$$
$$= -4\pi z^2 e^2 \int_0^\infty r e^{iqr} dr$$
$$u = r \qquad dv = e^{iqr}dr$$
$$du = dr \qquad v = \frac{1}{iq} e^{iqr}$$
$$\mathcal{V}(q) = -4\pi z^2 e^2 \left[\frac{r}{iq} e^{iqr} - \frac{1}{iq}\int e^{iqr} dr\right]$$
$$= -4\pi z^2 e^2 \frac{1}{iq}\left[r e^{iqr} - \frac{1}{iq} e^{iqr}\Big|_0^\infty\right]$$

YECH!

NOW: $\int_0^\infty t e^{-st} dt = \frac{1}{s^2}$
$$\Rightarrow \int_0^\infty r e^{iqr} = \frac{-1}{q^2}$$
$$\Rightarrow \mathcal{V}(q) = \frac{4\pi Z e^2}{q^2}$$

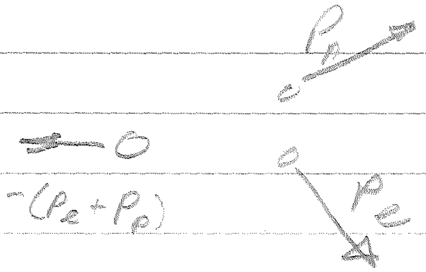
$$\mathcal{V}^2(k-k') = (4\pi Z)^2 \left|\frac{e}{k-k'}\right|^4$$

$$\frac{d\sigma}{d\Omega}_{k\to k'} = \frac{1}{\cancel{4\pi^2}}\frac{m^2}{\hbar^2}\, 4\cdot\cancel{4\pi^2}\, z^2 e^4 \frac{1}{|k-k'|^4}$$
$$= \left(\frac{2mZe^2}{\hbar}\right)^2 \frac{1}{|k-k'|^4}$$

$$q^2 = |\vec{k}-\vec{k}'|^2 = k^2 + k'^2 - 2kk'\cos\theta$$
$$= 2k^2 - 2k^2\cos\theta$$
$$= 2k^2(1-\cos\theta)$$

$$\frac{d\sigma}{d\Omega} = \left(\frac{2mZe^2}{\hbar}\right)^2 \frac{1}{4k^4(1-\cos\theta)^2}$$ RUTHERFORD FORMULA

3.



$$E_p = \sqrt{p_p^2 c^2 + m^2 c^4}$$
$$E_e = \sqrt{p_e^2 c^2 + m^2 c^4}$$

Δ = EXCITATION E

$$\Delta = \underbrace{\cancel{\frac{\hbar^2}{2M}(p_e+p_p)^2}}_{\text{NEGLIGIBLE}} + E_p + E_e$$

$$w_{i\to f} = \frac{2\pi}{\hbar}|M_{if}|^2 \delta(E_f - E_i)$$
$$= \frac{2\pi}{\hbar}|M_{if}|^2 \delta(\Delta - E_p - E_e)$$

$$w = \sum_f w_{i\to f}$$
$$= \frac{2\pi}{\hbar}(4\pi)^2 \frac{M^2}{(2\pi)^6}\int p_p^2\,dp_p \int p_e^2\,dp_e\,\delta(\Delta - E_p - E_e)$$

$$E_p^2 = p_p^2 c^2 + m^2 c^4$$
$$E_p\,dE_p = p_p\,dp_p\,c^2$$
$$\frac{1}{c^2}E_p\,dE_p\,p_p = p_p^2\,dp_p$$
$$p_p^2\,dp_p = \frac{1}{c^2}dE_p\,E_p\,\frac{1}{c}\sqrt{E_p^2 - m^2c^4}$$
$$= \frac{1}{c^3}E_p\,dE_p\sqrt{}$$

ALSO
$$p_e^2\,dp_e = \frac{1}{c^3}dE_e\,E_e\sqrt{E_e^2 - m^2c^4}$$

$$w_{fi} = \frac{E_f - E_i}{\hbar}$$

$4a_0$ 1s $\quad e^{-r/a} \quad Y$

2p $\quad r e^{-r/a} \quad Y$ $\quad a = \frac{\hbar^2}{me^2}$

$$\langle 1s | \cancel{z} | 2p_z \rangle = a_B \frac{2^7 \sqrt{2}}{3^5}$$

$$E_i = -E_{RYD}$$

$$E_f = -\frac{E_{RYD}}{4}$$

$E_{RYD} = \frac{e^2}{2a}$

$$\hat{n} \sim \hat{z}$$

$$f_{ij} = \frac{2\left[a_B \frac{2^7\sqrt{2}}{3^5}\right]^2 \frac{3}{4} E_{RYD}}{\hbar^2}$$

$$f_{ij} = \frac{2(\hat{n} \cdot x_{ij})^2 \, m\omega_{fi}}{\hbar}$$

4b. $\psi_i = \phi_0(x)\,\phi_0(y)\,\phi_0(z)$

$$f_{if} = \frac{2\,|\langle i|x|f\rangle|^2 m}{\hbar}\,\omega_{fi}$$

$\psi_f = \phi_1(x)\,\phi_0(y)\,\phi_0(z)$

$\omega_{fi} = \omega$

$$\langle i|x|f\rangle = \langle \phi_0(x)|x|\phi_1(x)\rangle \times \langle \phi_0(y)|\phi_0(y)\rangle \times \langle \phi_0(z)|\phi_0(z)\rangle$$

$$= \frac{1}{\alpha\sqrt{2}}$$

$$f_{if} = \frac{2m\omega}{2\hbar\alpha^2} = \frac{2m\omega}{2\hbar m\omega} \qquad \alpha^2 = \frac{m\omega}{\hbar}$$

$$f_{if} = 1$$

$$\phi_n(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}\,2^n n!}}\;H_n(\alpha x)\,e^{-\frac{1}{2}\alpha^2 x^2}$$

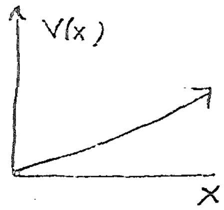
$$\alpha^2 = \frac{m\omega}{\hbar}$$

Examination
Physics 611
Quantum Mechanics
Feb. 18, 1975

DO ALL THREE PROBLEMS. ALL COUNT EQUALLY.

(1) Use WKBJ to find the bound states of the one dimensional potential

$$V(x) = Fx \qquad x>0$$
$$= \infty \qquad x<0$$



(2) If $|n\rangle$ and $|m\rangle$ are harmonic oscillator wave functions in one dimension, evaluate

$$\langle n| e^{\lambda a^+} |m\rangle = ? \qquad \lambda = \text{constant}$$

(3) In three dimensions, the potential is

$$V(r) = \lambda \exp(-2r/a) \;; \qquad \lambda > 0$$

For the case $\ell = 0$, write down the exact wavefunction, with delta function normalization, for states with $E > 0$.

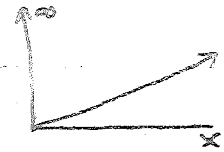
Physics 611

Examination
March 18, 1975

DO ALL THREE PROBLEMS

(1) Do a variational calculational to find the lowest bound state of the one dimensional potential

$$V(x) = Fx \qquad x > 0$$
$$= \infty \qquad x < 0$$



(2) Consider the angular momentum state J = 3/2. Denote the four m-states (3/2, ½, -½, -3/2) by the four vectors $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$ $\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$ $\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ $\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

a. What are the 4 by 4 matrices L and L^+ in this representation?

b. What are the 4 by 4 matrices L_x and L_y in this representation?

c. What are the 4 by 4 matrices L_z and L^2 in this representation?

(3) Would you expect a Helium ion (Z=2) to bind three electrons at once? Explain your answer. Describe how you might do a theoretical calculation to ascertain the answer to this question.

Physics 611
Final Examination
May 1, 1975

DO ALL THREE PROBLEMS

(1) An alkali valence electron in a d-orbital (ℓ =2) is perturbed by a strong magnetic field (Paschen-Back effect). Find the energy levels. Include the spin orbit interaction. $H_{int} = -\mu_0 (\underset{\sim}{\ell} + 2\underset{\sim}{s}) \cdot \underset{\sim}{H_0} - .3\, \underset{\sim}{\ell} \cdot \underset{\sim}{s}$

(2) Calculate the differential cross section $\frac{d\sigma}{d\Omega}$ of a charged particle of mass M scattering from an atom <u>in</u>elastically. Assume the atom is fixed (no recoil), and the scattering particle is nonrelativistic. Assume a matrix element $M_{pp'}$ exists which describes the rate of inelastic scattering $p \rightarrow p'$ where the atom is excited a discrete amount of energy Δ . $\mathcal{E}_{p'} < \mathcal{E}_p$.

(3) Derive the matrix element $M_{pp'}$ for problem (2) for a particle (μ^- meson) scattering from an hydrogen atom , and exciting it from the 1s to the 2s state. Carefully state which integrals need to be done in order to evaluate the matrix element , but do not take the time to do these integrals.

From the structure of Eq. (33.14), we expect that the coordinate representation of the ket $|1\rangle$ can be written in the form

$$\langle \mathbf{r}|1\rangle = \sum_{l=1}^{\infty} f_l(r)P_l(\cos\theta) \tag{33.19}$$

Substitution of (33.19) into (33.14) leads to the following differential equation for $f_l(r)$:

$$\frac{d^2f_l}{dr^2} + \frac{2}{r}\frac{df_l}{dr} - \frac{l(l+1)}{r^2}f_l + \frac{2}{a_0r}f_l - \frac{1}{a_0^2}f_l = -\frac{2Z}{a_0R^{l+1}(\pi a_0^3)^{\frac{1}{2}}}\,r^le^{-r/a_0} \tag{33.20}$$

As expected, this agrees with Eq. (33.14) when we put $l = 1$ and $\mathsf{E} = -Ze/R^2$.

A solution of Eq. (33.20) is easily found in analogy with (33.5) and again contains only two terms. Substitution into (33.19) gives

$$\langle \mathbf{r}|1\rangle = \sum_{l=1}^{\infty} \frac{Z}{R^{l+1}(\pi a_0^3)^{\frac{1}{2}}}\left(\frac{a_0r^l}{l} + \frac{r^{l+1}}{l+1}\right)e^{-r/a_0}P_l(\cos\theta) \tag{33.21}$$

which, in accordance with (33.16), is equal to $\psi_1(\mathbf{r})$. Similarly, Eq. (33.15) shows that W_2 is given by

$$W_2 = \langle 0|H'|1\rangle = -Z^2e^2\sum_{l=1}^{\infty}\frac{(l+2)(2l+1)!}{l2^{2l+1}}\frac{a_0^{2l+1}}{R^{2l+2}} \tag{33.22}$$

Again, the leading term ($l = 1$) agrees with (33.7) when $\mathsf{E} = -Ze/R^2$.

It should be noted that, although Eq. (33.22) gives the first two terms of an asymptotic series in $1/R$ correctly, the third term, which is proportional to $1/R^8$, is dominated by the leading term of W_3. Equation (33.17) shows that $W_3 = \langle 1|H'|1\rangle$ in this case and that the leading term for large R is proportional to $1/R^7$ (see Prob. 15).[1]

34 THE WKB APPROXIMATION

In the development of quantum mechanics, the Bohr-Sommerfeld quantization rules of the old quantum theory (Sec. 2) occupy a position intermediate between classical and quantum mechanics. It is interesting that there is a method for the approximate treatment of the Schrödinger wave

[1] A. Dalgarno and A. L. Stewart, *Proc. Roy. Soc. (London)* **A238**, 276 (1956). It should be noted that, unlike the situation with the van der Waals interaction discussed in the preceding section, there is no correction arising from retardation in the present problem. This is because the only motion is that of a single electron in the electrostatic potential of two fixed charges.

equation that shows its connection with the quantization rules. It is based on an expansion of the wave function in powers of $\hbar$, which, although of a semiconvergent or asymptotic character, is nevertheless also useful for the approximate solution of quantum-mechanical problems in appropriate cases. This method is called the *Wentzel-Kramers-Brillouin* or *WKB approximation*, although the general mathematical technique had been used earlier by Liouville, Rayleigh, and Jeffreys.[1] It is applicable to situations in which the wave equation can be separated into one or more total differential equations, each of which involves a single independent variable.

CLASSICAL LIMIT

A solution $\psi(\mathbf{r},t)$ of the Schrödinger wave equation (6.16)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2\mu}\nabla^2\psi + V(\mathbf{r})\psi$$

can be written in the form

$$\psi(\mathbf{r},t) = A\exp\frac{iW(\mathbf{r},t)}{\hbar}$$

in which case W satisfies the equation

$$\frac{\partial W}{\partial t} + \frac{1}{2\mu}(\nabla W)^2 + V - \frac{i\hbar}{2\mu}\nabla^2W = 0 \tag{34.1}$$

In the classical limit ($\hbar \to 0$), Eq. (34.1) is the same as Hamilton's partial differential equation for the principal function W:[2]

$$\frac{\partial W}{\partial t} + H(\mathbf{r},\mathbf{p}) = 0 \qquad \mathbf{p} = \nabla W$$

Since the momentum of the particle is the gradient of W, the possible trajectories are orthogonal to the surfaces of constant W and hence, in the classical limit, to the surfaces of constant phase of the wave function ψ.

[1] It is sometimes called the *BWK method*, the *classical approximation*, or the *phase integral method*. For the original work, see J. Liouville, *J. de Math.* **2**, 16, 418 (1837); Lord Rayleigh, *Proc. Roy. Soc. (London)* **A86**, 207 (1912); H. Jeffreys, *Proc. London Math. Soc.* (2)**23**, 428 (1923); G. Wentzel, *Z. Physik.* **38**, 518 (1926); H. A. Kramers, *Z. Physik.* **39**, 828 (1926); L. Brillouin, *Compt. Rend.* **183**, 24 (1926). For more recent developments, see E. C. Kemble, "The Fundamental Principles of Quantum Mechanics," sec. 21 (McGraw-Hill, New York, 1937); R. E. Langer, *Phys. Rev.* **51**, 669 (1937); W. H. Furry, *Phys. Rev.* **71**, 360 (1947); S. C. Miller, Jr., and R. H. Good, Jr., *Phys. Rev.* **91**, 174 (1953). The treatment of this section resembles most closely those of Kramers and Langer.

[2] E. T. Whittaker, "Analytical Dynamics," 3d ed., sec. 142 (Cambridge, London, 1927); H. Goldstein, "Classical Mechanics," sec. 9-4 (Addison-Wesley, Reading, Mass., 1950).

METHOD OF DALGARNO AND LEWIS

The foregoing procedure can be generalized in the following way.[1] We start with Eq. (31.11), which is applicable to the ground state of any system since in all known cases this state is nondegenerate:

$$W_2 = S'_n \frac{\langle 0|H'|n\rangle\langle n|H'|0\rangle}{E_0 - E_n} \tag{33.10}$$

Suppose now that an operator F can be found such that

$$\frac{\langle n|H'|0\rangle}{E_0 - E_n} = \langle n|F|0\rangle \tag{33.11}$$

for all states n other than the ground state. Substitution into (33.10) then gives

$$W_2 = S'_n\langle 0|H'|n\rangle\langle n|F|0\rangle = \langle 0|H'F|0\rangle - \langle 0|H'|0\rangle\langle 0|F|0\rangle \tag{33.12}$$

where the term $n = 0$ has first been added in to make the summation complete and then subtracted out. Thus, if F can be found, the evaluation of W_2 is greatly simplified, since only integrals over the unperturbed ground-state wave function need be evaluated.

Equation (33.11) can be written as

$$\langle n|H'|0\rangle = (E_0 - E_n)\langle n|F|0\rangle = \langle n|[F,H_0]|0\rangle$$

which is evidently valid if F satisfies the operator equation

$$[F,H_0] = H' + C$$

where C is any constant. However, this last equation is unnecessarily general; it is enough that F satisfy the much simpler equation

$$[F,H_0]|0\rangle = H'|0\rangle + C|0\rangle \tag{33.13}$$

from which it follows that $C = -\langle 0|H'|0\rangle$.

We now define a new ket $|1\rangle$, which is the result of operating on $|0\rangle$ with F. Then Eq. (33.13) may be written

$$(E_0 - H_0)|1\rangle = H'|0\rangle - \langle 0|H'|0\rangle|0\rangle \qquad \text{where} \qquad |1\rangle \equiv F|0\rangle \tag{33.14}$$

The ket $|1\rangle$ can evidently have an arbitrary multiple of $|0\rangle$ added to it; we choose this multiple so that $\langle 0|1\rangle = 0$. If now Eq. (33.14), which is an inhomogeneous differential equation, can be solved for $|1\rangle$, the second-order perturbed energy (33.12) can be written in terms of it as

$$W_2 = \langle 0|H'|1\rangle \tag{33.15}$$

[1] A. Dalgarno and J. T. Lewis, *Proc. Roy. Soc.* (*London*) **A233**, 70 (1955); C. Schwartz, *Ann. Phys.* (*N.Y.*) **6**, 156 (1959).

In similar fashion the series (31.9) for ψ_1 can be written in closed form:

$$\psi_1 = S'_n \frac{|n\rangle\langle n|H'|0\rangle}{E_0 - E_n} = S'_n|n\rangle\langle n|F|0\rangle$$
$$= F|0\rangle - |0\rangle\langle 0|F|0\rangle = |1\rangle \tag{33.16}$$

It is apparent that Eqs. (33.15) and (33.16) are consistent with Eq. (31.7), as of course they must be.

The Dalgarno-Lewis method thus replaces the evaluation of the infinite summation (31.9) by the solution of the inhomogeneous differential equation (33.14). The latter procedure may be much simpler even when it cannot be done in closed form, as with (33.4).

THIRD-ORDER PERTURBED ENERGY

The ket $|1\rangle = F|0\rangle$ is all that is needed to find the third-order perturbed energy W_3. We make use of Eqs. (31.7), (31.12), (31.13), and the complex conjugate of (33.11) to write

$$\begin{aligned} W_3 &= (u_0, H'\psi_2) \\ &= S'_k \frac{\langle 0|H'|k\rangle}{E_0 - E_k}\left(S'_n \frac{\langle k|H'|n\rangle\langle n|H'|0\rangle}{E_0 - E_n} - \frac{\langle k|H'|0\rangle\langle 0|H'|0\rangle}{E_0 - E_k}\right) \\ &= S'_k\langle 0|F^\dagger|k\rangle(S'_n\langle k|H'|n\rangle\langle n|F|0\rangle - \langle k|F|0\rangle\langle 0|H'|0\rangle) \\ &= \langle 0|F^\dagger H'F|0\rangle - \langle 0|F^\dagger|0\rangle\langle 0|H'F|0\rangle - \langle 0|F^\dagger H'|0\rangle\langle 0|F|0\rangle \\ &\qquad - \langle 0|F^\dagger F|0\rangle\langle 0|H'|0\rangle + 2\langle 0|F^\dagger|0\rangle\langle 0|H'|0\rangle\langle 0|F|0\rangle \\ &= \langle 1|H'|1\rangle - \langle 1|1\rangle\langle 0|H'|0\rangle \end{aligned} \tag{33.17}$$

since $\langle 0|1\rangle = 0$. We thus obtain a closed expression for W_3 as well.[1]

INTERACTION OF A HYDROGEN ATOM AND A POINT CHARGE

As an example of this method, we now calculate the change in energy of a hydrogen atom in its ground state when a point charge Ze is placed at a fixed distance R. The perturbation is

$$\begin{aligned} H' &= \frac{Ze^2}{R} - \frac{Ze^2}{(R^2 + r^2 - 2Rr\cos\theta)^{\frac{1}{2}}} \\ &= -\frac{Ze^2}{R}\sum_{l=1}^{\infty}\left(\frac{r}{R}\right)^l P_l(\cos\theta) \end{aligned} \tag{33.18}$$

provided that $R > r$ or, equivalently, that R is much greater than a_0.

[1] This result can also be obtained directly from Eqs. (31.4) and (31.6) as a special case of the formula derived in Prob. 14.

Exam #1

~~Problem Set~~

1. Let $\Psi_n(x)$ denote the ortho-normal stationary states of a system corresponding to the energies E_n. At time $t = o$, the normalized state function of the system is

$$\Psi(x,o) = \sum_n a_n \Psi_n(x).$$

Assuming the Ψ_n and a_n to be given,

a) Write the wavefunction of the system for $t > o$.
b) What is the probability that a measurement of the energy at time t will yield the value E_n?
c) What is the expectation value of the energy at any time t?

2. Prove that the eigenfunctions of the parity operator P, defined by $P\Psi(x) = \Psi(-x)$, form a complete orthogonal set of functions.

3. Let x_o and p_o denote the expectation values of x and p for the state $\Psi_o(x)$. Consider the state $\Psi(x)$ defined by

$$\Psi(x) = e^{-ip_o x/h}\Psi_o(x_o+x)$$

Show that both $\langle x\rangle$ and $\langle p\rangle$ vanish for this state. Does this violate the uncertainty principle? Explain.
Give another example of a case where both $\langle x\rangle$ and $\langle p\rangle$ vanish.

4. For a classical particle in periodic motion, it is possible to show that $2\overline{T} = \overline{\vec{r}\cdot\vec{\nabla}V}$ where $\overline{T}$ is the kinetic energy averaged over one period. Prove an equivalent quantum-mechanical relation for the one dimensional case by finding an expression for the quantity $\frac{d}{dt}\langle\Psi|px|\Psi\rangle$ and then considering the special case when Ψ is a stationary state. If V is proportional to x^n, show that

$$2\langle T\rangle = n\langle V\rangle.$$

P453 EXAM

ANSWERS

1. a) $\psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t/\hbar}$

b) $a_n^* a_n$

c) $\langle E \rangle = \sum_n E_n a_n^* a_n$

2. We showed in class that the eigenfunction of P are either even or odd.

$$P\psi_{even}(x) = \psi_{even}(-x) = \psi_{even}(x)$$

$$P\psi_{odd}(x) = \psi_{odd}(-x) = -\psi_{odd}(x)$$

a) Completeness: any function can be expanded in terms of an even and an odd part: $\psi(x) = \underbrace{\tfrac{1}{2}(\psi(x)+\psi(-x))}_{even} + \underbrace{\tfrac{1}{2}(\psi(x)-\psi(-x))}_{odd}$

b) Orthogonal: ψ_1 orthogonal to ψ_2 if $\int_{-\infty}^{\infty} \psi_1^* \psi_2 \, dx = 0$

$\int_{-\infty}^{\infty} \psi_{even}^* \psi_{odd} \, dx = 0$ because the product of $\psi_{even}^* \psi_{odd}$ is odd

[Note: Any even function (or odd function) is a eigenfunction of P with eigenvalue $+1$ (-1). One can choose a complete set of orthogonal even functions and expand any other function in terms of these.]

3. Given $x_0 = \int \psi_0^* x \psi_0 \, dx$ $\quad p_0 = \int \psi_0^* p \psi_0 \, dx$ $\quad \psi(x) = e^{-\frac{ip_0 x}{\hbar}} \psi_0(x+x_0)$

$$\langle x \rangle = \int \psi^* x \psi \, dx = \int e^{\frac{ip_0 x}{\hbar}} \psi_0^*(x+x_0)\, x\, e^{-\frac{ip_0 x}{\hbar}} \psi_0(x+x_0)\, dx$$

let $x' = x + x_0$ $\quad \langle x \rangle = \int \psi_0^*(x')(x'-x_0)\psi_0(x')\, dx' = x_0 - x_0 = 0$

$$\langle p \rangle = \int \psi^* p \psi \, dx = -i\hbar \int e^{\frac{ip_0 x}{\hbar}} \psi_0^*(x+x_0) \frac{\partial}{\partial x} e^{-\frac{ip_0 x}{\hbar}} \psi_0(x+x_0)\, dx$$

$$= \int \psi_0^*(x+x_0)(p-p_0)\psi_0(x+x_0)\, dx = -p_0 + \int \psi_0^*(x')\, p\, \psi_0(x')\, dx' = 0$$

4. Consider $\frac{d}{dt}\langle \Psi | px | \Psi \rangle$

The theorem is clear that $\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar}\langle [H, A] \rangle + \langle \frac{\partial A}{\partial t} \rangle$

$\therefore \frac{d}{dt}\langle px \rangle = \frac{i}{\hbar}\langle [H, px] \rangle + \langle \frac{\partial}{\partial t} px \rangle$

Neither the operator p nor x depends explicitly on time

$\therefore \langle \frac{\partial}{\partial t} px \rangle = 0$

Need to calculate $[H, px] = \left[\frac{p^2}{2m} + V(x), px\right]$

Now $[p^2, px] f(x) = (p^3 x - px\,p^2) f(x) = (-i\hbar)^3 \left(\frac{d^3}{dx^3} x f(x) - \frac{d}{dx} x \frac{d^2 f}{dx^2}\right)$

$= (-i\hbar)^3 \left(3\frac{d^2 f}{dx^2} + x\frac{d^3 f}{dx^3} - \frac{d^2 f}{dx^2} - x\frac{d^3 f}{dx^3}\right)$

$= -i\hbar\, 2p^2 f$

and $[V(x), px] f(x) = (V(x)\,px - px\,V(x)) f(x) = V(x)(-i\hbar)\left(f(x) + x\frac{df}{dx}\right) -$

$- (-i\hbar)\left(V(x) f(x) + x \frac{dV}{dx} f(x) + x V(x) \frac{df}{dx}\right) = +i\hbar\, x \frac{dV}{dx}$

$\therefore [H, px] = -i\hbar\left(\frac{2p^2}{2m} - x\frac{dV}{dx}\right)$

and $\frac{d}{dt}\langle px \rangle = \frac{i}{\hbar}\langle [H, px] \rangle = 2\langle T \rangle - \langle x \frac{dV}{dx} \rangle$

But for a stationary state $\frac{d}{dt}\langle A \rangle = 0 \Rightarrow \boxed{2\langle T \rangle = \langle x \frac{dV}{dx} \rangle}$

If $V \propto x^n$ $\quad x\frac{dV}{dx} = nV \quad$ so $2\langle T \rangle = \langle nV \rangle = n\langle V \rangle$

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16 PAGE BLUE BOOK

NAME BOB MARKS

COURSE QUANTUM MECHANICS I

PROFESSOR DR. MAHAN HOUR

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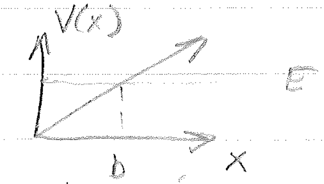


SOLUTION IS

$$\psi(x) = \frac{1}{\pi}\int_0^\infty dt \cos\left(\xi t + \frac{t^3}{3}\right)$$

$$= A_i(\xi) \quad ; \xi = \left(x - \frac{E}{F}\right)\left(\frac{2meF}{\hbar^2}\right)^{\frac{1}{3}}$$

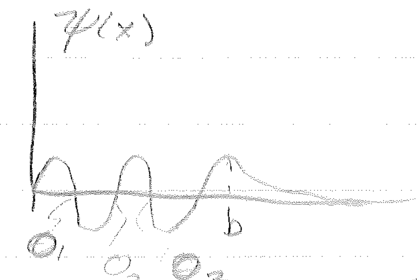
EIGENVALUE CONDITION IS

$$A(\xi_0) = A(x=0) = 0$$

ie

$$A\left[-\frac{E}{F}\left(\frac{2meF}{\hbar^2}\right)^{1/3}\right] = 0$$

~~LET~~

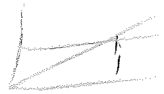


LET THE O'S OF $\psi(x)$ (ie $A(\xi_0)$)
BE $O_0, O_1, O_2, O_3, O_4,$ NOTE $0 < O_n < b$

THEN

$$-\frac{E}{F}\left(\frac{2meF}{\hbar^2}\right)^{1/3} = O_n$$

$$\Rightarrow E_n = -FO_n\left(\frac{\hbar^2}{2meF}\right)^{1/3}$$

BY WKBJ  E $\quad Fb = E \Rightarrow b = \frac{E}{F}$

$$\int_0^b dx\, p(x) = \hbar\left(n+\tfrac{3}{4}\right)\pi \Leftarrow$$ BOHR-SOMMERFELD FOR ABRUPT POTENTIAL

$$\sqrt{2m}\int_0^b dx\sqrt{E-Fx}$$

$$\sqrt{2mF}\int_0^b dx\sqrt{\tfrac{E}{F}-x}$$

$$\sqrt{2mF}\int_0^b dx\sqrt{b-x}$$

$$\frac{d}{dx}(b-x)^{3/2} \qquad -\tfrac{3}{2}(b-x)$$

$$= -\tfrac{2}{3}\sqrt{2mF}\,(b-x)^{3/2} \qquad \int b-x = -\tfrac{2}{3}(b-x)^{3/2}$$

$$= \sqrt{2mF}\left(\tfrac{2}{3}\right) b^{3/2} = \hbar\left(n+\tfrac{3}{4}\right)\pi$$

$$b^{3/2} = \left(\frac{E}{F}\right)^{3/2} = \frac{3\hbar\left(n+\frac{3}{4}\right)\pi}{2\sqrt{2mF}} \checkmark$$

$$E^{3/2} = \frac{3}{2}\,\frac{\hbar\left(n+3/4\right)\pi}{\sqrt{2mF}}\,F^{3/2}$$

$$\rightarrow \boxed{E_n = \left[\frac{3}{2}\,\frac{\hbar\left(n+3/4\right)\pi F}{\sqrt{2m}}\right]^{2/3}}$$

WE CAN NORMALIZE $\chi(r)$:

~~$\lim R(r) = \lim \frac{\chi(r)}{r}$~~

$$\lim \chi(r) = \lim \sqrt{4\pi}\, r\, \psi(r)$$

$$= c_1 \left(\frac{k_0 a}{2}\right)^{ika} \frac{1}{\Gamma(1+ika)}\, i2e^{i\delta}$$
$$\times \sin(kr+\delta)$$

THEN:

$$\left| c_1 \left(\frac{k_0 a}{2}\right)^{ika} \frac{1}{\Gamma(1+ika)}\, i2e^{i\delta} \right|$$

$$= \left| \frac{2c_1}{\Gamma(1+ika)} \right| = \sqrt{\frac{2}{\pi}}$$

$$\Rightarrow |c_1| = \sqrt{\frac{2}{\pi}}\, \frac{|\Gamma(1+ika)|}{2}$$

$$= \frac{|\Gamma(1+ika)|}{\sqrt{2\pi}}$$

2. EVALUATE

$$\langle n| e^{\lambda a^+} |m\rangle$$

$$[a, a^+] = aa^+ + a^+a = 1$$

$$= \langle n| \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (a^+)^n |m\rangle$$

$$= \int_{-\infty}^{\infty} \psi_n^* \left[\sum_{k=0} \frac{\lambda^k}{k!} (a^+)^k\right] \psi_m \, dx$$

$$a^+ \psi_m = \sqrt{m+1}\, \psi_{m+1}$$

$$(a^+)^2 \psi_m = \sqrt{(m+1)(m+2)}\, \psi_{m+2}$$

$$\vdots$$

$$(a^+)^k \psi_m = \sqrt{\frac{(m+k)!}{m!}}\, \psi_{m+k}$$

$$\Rightarrow \langle n| e^{\lambda a^+} |m\rangle$$

$$= \int_{-\infty}^{\infty} \psi_n^* \sum_{h=0}^{\infty} \frac{\lambda^k}{h!} \sqrt{\frac{(m+k)!}{m!}}\, \psi_{m+k}$$

$$= \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \sqrt{\frac{(m+k)!}{m!}}\, \delta_{n, m+k}$$

$$\psi(r) = \frac{c_1}{\sqrt{4\pi}\, r}\left[I_{ika}(k_0 a Y) - \frac{I_{ika}(ak_0)}{I_{-ika}(ak_0)} I_{-ika}(k_0 a Y) \right]$$

$$\lim_{\substack{r\to\infty \\ Y\to 0}} \psi(r) = \frac{c_1}{\sqrt{4\pi}\, r}\left[\frac{1}{\Gamma(1+ika)}\left(\frac{k_0 a Y}{2}\right)^{ika} - \frac{I_{ika}}{I_{-ika}} \frac{1}{\Gamma(1-ika)} \left(\frac{k_0 a Y}{2}\right)^{-ika} \right]$$

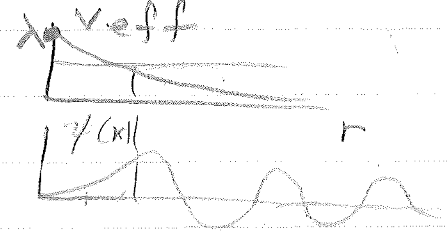
LET $$e^{i2\delta} = \frac{I_{ika}(k_0 a)}{I_{-ika}(k_0 a)} \frac{\Gamma(1+ika)}{\Gamma(1-ika)} \frac{\left(\frac{k_0 a}{2}\right)^{-ika}}{\left(\frac{k_0 a}{2}\right)^{ika}}$$

$$\Rightarrow \lim \psi(r) = \frac{c_1}{\sqrt{4\pi}\, r}\left(\frac{k_0 a}{2}\right)^{ika} \frac{1}{\Gamma(1+ika)} \left[e^{-ikr} - e^{i2\delta} e^{ikr} \right]$$

$$= \frac{-c_1}{\sqrt{4\pi}\, r}\left(\frac{k_0 a}{2}\right)^{ika} \frac{1}{\Gamma(1+ika)} e^{i\delta} \times i2 \times \sin[kr+\delta]$$

$$= \frac{c_1}{\sqrt{4\pi}}\left(\frac{k_0 a}{2}\right)^{ika} \frac{1}{\Gamma(1+ika)}\, i2 e^{i\delta} \times \frac{\sin(kr+\delta)}{r}$$

$\boxed{\cancel{\lim_{z \to 0} I_r(z)}}$



$r \to \infty \Rightarrow Y \to 0$

$$\lim_{z \to 0} I_r(z) = \frac{1}{\Gamma(1+v)} \left(\frac{z}{2}\right)^r$$

$\boxed{\cancel{\lim_{r \to 0} \chi(r)}}$

$$\chi(r) = r R(r)$$

$$\begin{aligned} \psi(r) &= R(r) Y_\ell^m \\ &= \frac{1}{r} \chi(r) Y_\ell^m \quad ; \ \ell = m = 0 \\ &= \frac{1}{r} \chi(r) Y_0^0 \\ &= \frac{1}{\sqrt{4\pi}} \frac{1}{r} \chi(r) \end{aligned}$$

3, $V(r) = \lambda e^{-2r/a}$ $\lambda > 0$

$$V_{EFF} = V(r) + \frac{\hbar^2}{2mr^2} \ell(\ell+1)$$

FOR $\ell = 0$

$$V_{EFF} = V(r)$$

WAVE EQ'N:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) - E\right]\chi(r) = 0$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \lambda e^{-2r/a} - E\right]\chi(r) = 0$$

FOR $Y = e^{-r/a}$

$K^2 = 2mE/\hbar^2$; $K_0^2 = \frac{2m\lambda}{\hbar^2}$

SOLUTION IS

$$\chi(Y) = c_1 I_{ika}(ak_0 Y) + c_2 I_{-ika}(ak_0 Y)$$

BOUNDRY CONDITIONS:

$$\chi(r=0) = \chi(Y=1) = 0$$

$\therefore$ $c_1 I_{ika}(ak_0) = -c_2 I_{-ika}(ak_0)$

$$\frac{c_2}{c_1} = -\frac{I_{ika}(ak_0)}{I_{-ika}(ak_0)}$$

$$\Rightarrow \chi(Y) = c_1\left[I_{ika}(ak_0 Y) - \frac{I_{ika}(ak_0)}{I_{-ika}(ak_0)} I_{-ika}(ak_0 Y)\right]$$

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PROF. ____________

HOUR ____________

DATE ____________

SEAT ____________

1	5
2	3
3	4
4	12
5	
6	
7	
8	
9	
10	
11	
12	
13	
14	
15	
TOTAL	
GRADE	

wrong BC

-5

1. ASSUME $\phi(x) = A e^{-\alpha x}$

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E$$

$$\int_0^\infty \phi^2(x)\,dx = A^2 \int_0^\infty e^{-2\alpha x}$$

$$= A^2 \frac{1}{2\alpha}$$

$$\frac{d^2}{dx^2} A e^{-\alpha x} = A\alpha^2 e^{-\alpha x}$$

$$\frac{\hbar^2}{2m}\int_0^\infty \phi(x)\frac{d^2}{dx^2}\phi(x)\,dx$$

$$= \frac{-\hbar^2}{2m} A^2 \alpha^2 \, 1/2\alpha$$

$$= \frac{-\hbar^2}{4m} A^2 \alpha$$

$$F\int_0^\infty \phi(x)\, x\, \phi(x)\,dx$$

$$= A^2 F \int_0^\infty x e^{-2\alpha x}\,dx$$

$$= A^2 F \left(\frac{1}{2\alpha}\right)^2$$

$(\alpha = \frac{1}{2\alpha})$

$$E(\alpha) = \frac{\frac{F}{4\alpha^2} - \frac{\hbar^2}{4m}\alpha}{1/2\alpha}$$

$$= \frac{F}{2\alpha} - \frac{\hbar^2}{2m}\alpha^2$$

$$\frac{dE(\alpha)}{d\alpha} = \frac{-F}{2}\frac{1}{\alpha^2} - \frac{\hbar^2}{m}\alpha = 0$$

no minimum

$$\frac{-F}{2}\frac{1}{\alpha^2} = \frac{\hbar^2}{m}\alpha$$

$$\cancel{\alpha^3 = \frac{-2m}{F\hbar} \Rightarrow \alpha = -\sqrt[3]{\frac{2m}{F\hbar^2}}}$$

$$\alpha^3 = \frac{-Fm}{2\hbar^2} \Rightarrow \alpha = -\sqrt[3]{\frac{Fm}{2\hbar^2}}$$

$\cancel{E_0}$ $\alpha_0 = -\sqrt[3]{\frac{Em}{2\hbar^2}}$

$$E(\alpha) = \frac{E}{2\alpha} - \frac{\hbar^2}{2m\alpha^2}$$

$$E_0 = E(\alpha_0) = \frac{\hbar^2}{2m}\left(\frac{Em}{2\hbar^2}\right)^{2/3} - \frac{E}{2}\left[\frac{Em}{2\hbar^2}\right]^{-1/3}$$

3. NO.

TO FIND OUT HOW THEORETICALLY, ONE would employ the "Hydrogen-like atom" approach for the a helium nucleus with two core electrons and a ~~the~~ third electron acted upon by the resulting pseudo-potential.

~~Binding energy in ...~~

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$L_x = L_x^2 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$L_y^2 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

Test time up

~~$-2L_z = LL^{+}$~~

~~$L = M_z L \, L M_z$~~

This is right — but you erred in doing multiplication?

$LL^{+} - LL^{+} = -2L_z$

$$\underset{L}{\begin{bmatrix} 0&0&0&0\\ 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0 \end{bmatrix}} \underset{L^{+}}{\begin{bmatrix} 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1\\ 0&0&0&0 \end{bmatrix}} \stackrel{?}{=} \underset{L}{\cancel{\begin{bmatrix} 0&0&0&0\\ 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0 \end{bmatrix}}}$$

$$\underset{L^{+}}{\begin{bmatrix} 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1\\ 0&0&0&0 \end{bmatrix}} \underset{L}{\begin{bmatrix} 0&0&0&0\\ 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0 \end{bmatrix}} = \underset{L^{+}}{\begin{bmatrix} 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1\\ 0&0&0&0 \end{bmatrix}}$$

$LL^{+} - LL^{+} = 2L_z$

$L - L^{+} = 2L_z$

$$\Rightarrow L_z = \frac{1}{2}\begin{bmatrix} 0&-1&0&0\\ 1&0&-1&0\\ 0&1&0&-1\\ 0&0&1&0 \end{bmatrix}$$

2. $m_1 = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$ $m_2 = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$

$m_3 = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ $m_4 = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

a. $L m_1 = m_2$

$L m_2 = m_3$

$L m_3 = m_4$

$L m_4 = 0$

no ~~$L = \hbar\sqrt{j(j+1) - m(m-1)}$~~

$$L m_1 = \begin{bmatrix} 0&0&0&0\\ 1&0&0&0\\ 0&0&0&0\\ 0&0&0&0 \end{bmatrix}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} \Rightarrow \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$L m_2 = \begin{bmatrix} 0&0&0&0\\ 0&0&0&0\\ 0&1&0&0\\ 0&0&0&0 \end{bmatrix}\begin{bmatrix}0\\1\\0\\0\end{bmatrix} \Rightarrow \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$$

~~$m_z = \begin{bmatrix}0\\0\\m_1 m_1^T\\0\end{bmatrix}$~~ ~~$L|m_i\rangle = \begin{bmatrix}\delta_{ijk} & \delta_{ijl} & \delta_{ijk}\\ \delta_{ijl} & \delta_{ijk}\end{bmatrix}$~~

$$L m_3 = \begin{bmatrix} 0&0&0&0\\ 0&0&0&0\\ 0&0&0&0\\ 0&0&1&0 \end{bmatrix}\begin{bmatrix}0\\0\\1\\0\end{bmatrix} \Rightarrow \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

$$\begin{pmatrix} 0 & & & 0 \\ \sqrt{3} & 0 & & \\ 0 & 2 & 0 & \\ 0 & & \sqrt{3} & 0 \end{pmatrix}$$

$$L = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$L^+ m_3 = m_2$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\Rightarrow L^+ = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

b. L_x AND L_y

$L^+ = (L_x + L_y)$

$L = L_x - \underbrace{L_y}_{2i}$

$$L_x = \frac{1}{2}\left[L + L^+\right]$$

$$= \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & \end{bmatrix}$$

2. $L_y = L^+ - L$

$$L_y = \frac{1}{2}\left[L^+ - L\right]$$

$$= \frac{1}{2}\begin{bmatrix} 0 & +1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$