

C6

Physics Department  
Univ. of Chicago

ROYAL

# COMPOSITIONS

NAME E. FERMI Univ. of Chicago

Quantum mechanics

VERNON ROYAL LINE

# OFFICIAL PROGRAM

--	--	--

DATE

SECTION	FAMILY NAME				GIVEN NAME					
	MON.	RM.	TUES.	RM.	WED.	RM.	THURS.	RM.	FRI.	RM.
1										
2										
3										
4										
5										
6										
7										
8										
9										
10										
11										
12										

The covers of this book have been treated with a special varnish that protects against moisture and rubbing.

**NOTICE HOW SMOOTH THEY ARE.**

The paper has been specially selected for a smooth writing surface, and uniform quality, which may be identified with the watermark.

*Royal Writing*

**LOOK FOR THE WATERMARK IN THE PAPER.**

VERNON <sup>ROYAL</sup> LINE

MADE IN U. S. A.

## Mechanics

## Optics

Mass point  
 Trajectory  
 Velocity  $v$   
 Variable potential  
 Variation of energy

Wave packet  
 Ray  
 Group velocity  $v$   
 Variable index of refraction  
 Variations of frequency

Trajectory) (1)  $\delta \int \sqrt{W-U} ds = 0$  Maupertuis

Ray) (2)  $\delta \int \frac{ds}{v} = 0$  Fermat

Velocity of the mass point

(3)  $V = \sqrt{\frac{2}{m} (W-U)}$

Velocity of the wave group

(4)  $\frac{1}{V} = \frac{d}{d\nu} \frac{\nu}{v}$

From (1) (2)

(5)  $\frac{1}{v} = f(\nu) \sqrt{W(\nu) - U(x,y,z)}$

From (3) (4) (5)

$$\frac{1}{\sqrt{\frac{2}{m}(W-U)}} = f \sqrt{W-U} + \nu \left\{ f' \sqrt{W-U} + \frac{f W'}{2\sqrt{W-U}} \right\}$$

Hence

$$\left\{ \begin{array}{l} f + \nu f' = 0 \\ \sqrt{2m} = \nu f W' \end{array} \right. \quad \begin{array}{l} f\nu = c_1 \\ W' = \frac{\sqrt{2m}}{c_1} = h \\ W = h\nu + \text{const} \end{array}$$

$$f\nu = \frac{\sqrt{2m}}{h}$$

$$W = h\nu + \text{const}$$

$$W = h\nu$$

$$f = \frac{\sqrt{2m}}{h\nu}$$

$$(6) \quad W = h\nu$$

$$(7) \quad \nu = \frac{h\nu}{\sqrt{2m}} \frac{1}{\sqrt{h\nu - U}}$$

$$(8) \quad V = \sqrt{\frac{2}{m}(h\nu - U)}$$

Wave equation with dispersion law

$$\nu = \nu(\nu, x, y, z)$$

$$\psi = \sum \psi_\nu = \sum u_\nu e^{-2\pi i \nu t}$$

$$\Delta \psi_\nu - \frac{1}{v_\nu^2} \frac{\partial^2 \psi_\nu}{\partial t^2} = 0$$

$$\Delta \psi_\nu + 4\pi^2 \frac{v_\nu^2}{v_\nu^2} \psi_\nu = 0$$

Notation is not clear. Better  $\nu = \sum \psi_\nu = \sum u_\nu(x, y, z) e^{-2\pi i \nu t}$

For our special case (7)

$$\Delta \psi_n + \frac{8\pi^2 m}{h^2} (h\nu - U) \psi_n = 0$$

but since

$$\frac{\partial \psi_n}{\partial t} = -2\pi i \nu \psi_n$$

$$\Delta \psi_n - \frac{8\pi^2 m}{h^2} U \psi_n + \frac{4\pi m i}{h} \frac{\partial \psi_n}{\partial t} = 0$$

or

$$(9) \quad \Delta \psi - \frac{8\pi^2 m}{h^2} U \psi + \frac{4\pi m i}{h} \frac{\partial \psi}{\partial t} = 0$$

a solution of frequency  $\nu$  (Energy  $W = h\nu$ )  
is

$$(10) \quad \psi = u e^{-2\pi i \frac{W}{h} t}$$

With

$$(11) \quad \Delta u + \frac{8\pi^2 m}{h^2} (W - U) u = 0$$

From (7) for  $U=0$   $h\nu = \frac{1}{2} m V^2$  we obtain

$$(12) \quad \lambda = \frac{v}{\nu} = \frac{h}{mV}$$

Davisson & Germer give  $h = \text{Planck's constant}$

4

From (9)

$$\Delta \psi - \frac{8\pi^2 m}{h^2} U \psi + \frac{4\pi m i}{h} \frac{\partial \psi}{\partial t} = 0 \quad \left| \begin{array}{l} \psi^* \\ \psi \end{array} \right.$$

and

$$\Delta \psi^* - \frac{8\pi^2 m}{h^2} U \psi^* - \frac{4\pi m i}{h} \frac{\partial \psi^*}{\partial t} = 0$$

$$-\psi \Delta \psi^* + \psi^* \Delta \psi + \frac{4\pi m i}{h} \frac{\partial (\psi^* \psi)}{\partial t} = 0$$

or

$$(13) \quad 0 = \frac{\partial (\psi^* \psi)}{\partial t} + \text{div} \frac{h \left( \frac{h}{2mi} \right)}{4\pi m i} (\psi^* \text{grad} \psi - \psi \text{grad} \psi^*)$$

Hence

$$(14) \quad \psi^* \psi = \text{density of probability}$$

$$(15) \quad \frac{h}{4\pi m i} (\psi^* \text{grad} \psi - \psi \text{grad} \psi^*) = \text{density of flow}$$

From (14) the normalisation

$$(16) \quad \int \psi^* \psi d\tau = 1$$

Hence in a singular point  $\psi$  must never be ~~more~~ <sup>less</sup> infinite than  $\frac{1}{r^{3/2}}$  and at infinite distance it must ~~vanish~~ <sup>vanish faster than</sup> ~~at least~~ as  $1/r^{3/2}$

Nuclear distance in HCl molecule =  $1.27 \times 10^{-8}$

Generalizations:

Mass point on a line ( $x = abscissa$ )

$$(17) \quad \frac{d^2 \psi}{dx^2} - \frac{8\pi^2 m}{h^2} V(x) \psi + \frac{4\pi m i}{h} \frac{\partial \psi}{\partial t} = 0$$

$$(18) \quad \frac{d^2 u}{dx^2} + \frac{8\pi^2 m}{h^2} (W - V) u = 0$$

Rotator with fixed axis ( $A = \text{mom. of inertia}$ )

$$(19) \quad \frac{\partial^2 \psi(\varphi, t)}{\partial \varphi^2} - \frac{8\pi^2 A}{h^2} V(\varphi) \psi + \frac{4\pi A i}{h} \frac{\partial \psi}{\partial t} = 0$$

$$(20) \quad \frac{d^2 u(\varphi)}{d\varphi^2} + \frac{8\pi^2 A}{h^2} (W - V) u = 0$$

Point on a spherical surface (spherical coordinates  $\theta, \varphi$  operator)

$$(21) \quad \Delta = \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$

$$(22) \quad \frac{1}{r^2} \Delta \psi - \frac{8\pi^2 m}{h^2} V(\theta, \varphi) \psi + \frac{4\pi m i}{h} \frac{\partial \psi}{\partial t} = 0$$

$$(23) \quad \frac{1}{r^2} \Delta u + \frac{8\pi^2 m}{h^2} (W - V) u = 0$$

Dumbbell rotating with fixed center of gravity

$$(24) \quad \Delta \psi - \frac{8\pi^2 A}{h^2} V \psi + \frac{4\pi A i}{h} \frac{\partial \psi}{\partial t} = 0$$

$$(25) \quad \Delta u + \frac{8\pi^2 A}{h^2} (W - V) u = 0$$

This later

6

$$\sum_i \frac{1}{m_i} \Delta_i \psi \sim \Delta \psi$$

general mechanical system with

$$(26) \quad T = \frac{1}{2} \sum m_{ik}(q) \dot{q}_i \dot{q}_k$$

Define

$$(27) \quad ds^2 = \sum m_{ik}(q) dq_i dq_k$$

Let  $\Delta_q$  is Laplace's operator in variety (27)

$$(29) \quad \Delta_q \psi(q_1, \dots, q_f, t) - \frac{8\pi^2}{h^2} U \psi + \frac{4\pi i}{h} \dot{\psi} = 0$$

$$(30) \quad \Delta_q u(q_1, \dots, q_f) + \frac{8\pi^2}{h^2} (W - U) u = 0$$

Examples: one dimensional

a) Point on a closed line (length  $\frac{a}{l}$ ) with  $U=0$

$$(31) \quad u_l(x) = \frac{1}{\sqrt{a}} e^{\frac{2\pi i l}{a} x}$$

$l = \text{any integer}$

$$(32) \quad W_l = \frac{h^2 l^2}{2a^2 m}$$

b) Rotator with fixed axis with  $U=0$

$$(33) \quad u_l(\varphi) = \frac{1}{\sqrt{2\pi}} e^{i l \varphi}$$

$$(34) \quad W_l = \frac{h^2 l^2}{8\pi^2 A}$$

Bitter present here some primary points



c) Limiting condition where the potential becomes infinite

$$\frac{u'}{u} = -\sqrt{\frac{8\pi^2 m V}{h^2}}$$

i.e.

$$(35) \quad u = 0$$

d) Point moving on a segment (length a) with  $V=0$  from  $x=0$  to  $x=a$

$$(36) \quad u_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$(37) \quad W_n = \frac{h^2 n^2}{8 a^2 m}$$

e) Point on an infinite line with  $V=0$

As a limit from a) or d) we have normalization

$$(38) \quad u_{\omega}(x) \sim e^{i\omega x}$$

$$(39) \quad W = \frac{h^2 \omega^2}{8\pi^2 m}$$

$$\int_{-\infty}^{\infty} e^{i\omega x} dx = \infty \quad \text{but}$$

$$\int_{-\infty}^{\infty} |u_{\Delta\omega}|^2 dx = \text{finite}$$

with  $\omega + \Delta\omega$

$$u_{\Delta\omega} = \int_{\omega}^{\omega + \Delta\omega} e^{i\omega x} dx$$

Hence

$$(40) \quad \lambda = \frac{2\pi}{\omega} = \frac{h}{\sqrt{2mW}} = \frac{h}{mV} \quad \left( \text{With } W = \frac{1}{2} m V^2 \right)$$

$(\frac{1}{2} + i\epsilon) \omega \pm \dots = \omega$

f) Harmonic oscillator

$$(41) \quad U = 2\pi^2 \nu^2 m x^2$$

$$U = \frac{\omega^2}{2} m x^2$$

8

$$(42) \quad \frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2} \left( W - \frac{\omega^2 m}{2} x^2 \right) u = 0$$

With  $\xi = \sqrt{\frac{m\omega}{\hbar}} x$   $\epsilon = \frac{2W}{\hbar\omega}$

$$(43) \quad \xi = 2\pi \sqrt{\frac{mv}{\hbar}} x ; \quad \epsilon = \frac{2W}{\hbar v}$$

$$(44) \quad \frac{d^2 u}{d\xi^2} + (\epsilon - \xi^2) u = 0$$

$$(45) \quad u = v(\xi) e^{-\xi^2/2}$$

$$(46) \quad \frac{d^2 v}{d\xi^2} - 2\xi \frac{dv}{d\xi} + (\epsilon - 1) v = 0$$

Put

$$(47) \quad v = \sum a_r \xi^r$$

recursion formula

$$(48) \quad a_{r+2} = \frac{2r+1-\epsilon}{(r+1)(r+2)} a_r$$

behaves essentially like  $e^{\xi^2}$  if not  $\epsilon = 2n+1$   
eigenvalues

$$\epsilon = 2n+1$$

$$(49) \quad W = \hbar v n + \frac{\hbar v}{2} \quad W = \hbar\omega \left( n + \frac{1}{2} \right)$$

First polynomials of Hermite

$$(50) \quad \begin{cases} H_0 = 1 & H_1 = 2\xi \\ H_2 = -2 + 4\xi^2 & H_3 = -12\xi + 8\xi^3 \end{cases}$$

Eigenfunctions:

$$(51) \quad u_n(\xi) = H_n(\xi) e^{-\xi^2/2}$$

general definition of the Hermite polynomials

$$(52) \quad H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}$$

Proof that:

$$(54) \quad H_n'' - 2\xi H_n' + 2n H_n = 0$$

(54) is equivalent to

$$(55) \quad \frac{d^{n+2}}{d\xi^{n+2}} e^{-\xi^2} + 2\xi \frac{d^{n+1}}{d\xi^{n+1}} e^{-\xi^2} + (2+2n) \frac{d^n}{d\xi^n} e^{-\xi^2} = 0$$

This can be verified for  $n=0$ ; successive derivations yield it for  $n=1, 2, \dots$

Property

$$(56) \quad \frac{d}{d\xi} H_n = 2n H_{n-1}$$

is equivalent to (55) written for  $n-1$  instead of  $n$ .

From (52)(56)

$$(57) \quad \int H_m^2(x) e^{-x^2} dx = \sqrt{\pi} 2^m m!$$

The coeff. of normalizat. of solution (51) (43) is then

$$(58) \quad \left(\frac{4\pi^2 m \nu}{h}\right)^{1/4} \frac{1}{\sqrt{\sqrt{\pi} 2^m m!}} = \left(\frac{m\omega}{h}\right)^{1/4} \frac{1}{\sqrt{\sqrt{\pi} 2^m m!}}$$

Orthog follows also immediately from (51) (56).

For

~~Point in a central field of force  $U(r)$~~ 

$$\Delta \psi + \frac{8\pi^2 m}{h^2} (W - U(r)) \psi = 0$$

~~Develop~~

$$\psi(r, \vartheta, \varphi) = \sum_{\ell m} v_{\ell m} Y_{\ell, m}(\vartheta, \varphi)$$

with

$$Y_{\ell m}(\vartheta, \varphi) =$$

Spherical Harmonics and Legendre polynomials

$$(59) \quad Y_{\ell m}(\vartheta, \varphi) = \frac{1}{N_{\ell m}} e^{im\varphi} \sin^{|m|} \vartheta \frac{d^{|m|} P_{\ell}(\cos \vartheta)}{d(\cos \vartheta)^{|m|}}$$

$$(60) \quad \frac{1}{N_{\ell m}} = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{(\ell - |m|)!}{(\ell + |m|)!} \frac{2^{\ell+1}}{2}}$$

$$(61) \quad P_{\ell}(x) = \frac{1}{2^{\ell} \ell!} \frac{d^{\ell}}{dx^{\ell}} (x^2 - 1)^{\ell}$$

$$(62) \quad (1 - x^2) P'' - 2x P' + \ell(\ell + 1) P = 0$$

$$(63) \quad \int_{-1}^1 P_{\ell}^2(x) dx = \frac{2}{2\ell + 1} \quad \int_{-1}^1 P_{\ell}(x) P_{\ell'}(x) dx = 0 \text{ if } \ell \neq \ell'$$

$$(64) \quad P_{\ell} = \frac{2\ell - 1}{\ell} x P_{\ell-1} - \frac{\ell - 1}{\ell} P_{\ell-2}$$

$$(65) \quad \begin{cases} P_0 = 1 & P_1 = x \\ P_2 = \frac{3}{2}x^2 - \frac{1}{2} & P_3 = \frac{5}{2}x^3 - \frac{3}{2}x \\ P_4 = \frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8} & P_5 = \frac{63}{8}x^5 - \frac{35}{4}x^3 + \frac{15}{8}x \end{cases}$$

Spherical functions satisfy diff. equation

$$(66) \quad \Delta Y_{lm}(\theta, \varphi) = -l(l+1) Y_{lm}(\theta, \varphi)$$

and the orthogonality relation

$$(67) \quad \int_{4\pi} Y_{lm}^* Y_{l'm'} d\omega = \delta_{ll'} \delta_{mm'}$$

Point on spherical surface without forces:  $U=0$   
 Schrödinger equation (23). Put  $\Delta u + \frac{2I}{\hbar^2} W u = 0$

$$(68) \quad u = \sum_{lm} c_{lm} Y_{lm}$$

substitute in (23) [with (66)]

$$(69) \quad \sum_{lm} c_{lm} Y_{lm} \left[ \frac{l(l+1)}{r^2} + \frac{8\pi^2 m}{\hbar^2} W \right] = 0$$

hence non vanishing solution only for

$$(70) \quad W = \frac{\hbar^2 l(l+1)}{8\pi^2 m r^2} = \frac{\hbar^2 l(l+1)}{2m r^2}$$

A dumbbell with no forces (25) has similarly

$$(71) \quad W = \frac{\hbar^2 l(l+1)}{8\pi^2 A} = \frac{\hbar^2 l(l+1)}{2A}$$

$$\nabla^2 u(r, \theta, \varphi) = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \Delta u$$

$$\Delta u = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 u}{\partial \varphi^2}$$

Central forces

$$(72) \quad U = U(r)$$

$$(73) \quad \Delta u + \frac{8\pi^2 m}{h^2} (W - U(r)) u = 0$$

$$(74) \quad \frac{d^2 u}{dr^2} + \frac{2}{r} \frac{du}{dr} + \frac{1}{r^2} \Delta u + \frac{8\pi^2 m}{h^2} (W - U(r)) u = 0$$

$$(75) \quad u = \sum R_{lm}(r) Y_{l,m}(\theta, \varphi)$$

$$(76) \quad \sum_{l,m} Y_{l,m}(\theta, \varphi) \left[ R_{lm}'' + \frac{2}{r} R_{lm}' - \frac{l(l+1)}{r^2} R_{lm} + \frac{8\pi^2 m}{h^2} (W - U(r)) R_{lm} \right] = 0$$

$$(77) \quad R_l'' + \frac{2}{r} R_l' + \frac{8\pi^2 m}{h^2} W R_l - \left\{ \frac{8\pi^2 m}{h^2} U(r) + \frac{l(l+1)}{r^2} \right\} R_l = 0$$

$$(78) \quad y'' + \left[ \frac{8\pi^2 m}{h^2} W - \frac{8\pi^2 m}{h^2} U - \frac{l(l+1)}{r^2} \right] y = 0; \quad y = R_l/r$$

Energy levels are all the e.v. of all the (77)

Coulomb forces

$$(79) \quad U(r) = -\frac{Ze^2}{r}$$

$$R_l'' + \frac{2}{r} R_l' + \frac{8\pi^2 m}{h^2} W R_l + \left\{ \frac{8\pi^2 m}{h^2} \frac{Ze^2}{r} - \frac{l(l+1)}{r^2} \right\} R_l = 0$$

$$(80) \quad y'' + \left[ \frac{8\pi^2 m}{h^2} W + \frac{8\pi^2 m Ze^2}{h^2 r} - \frac{l(l+1)}{r^2} \right] y = 0$$

put

$$(81) \quad r_0 = \sqrt{\frac{h^2}{8\pi^2 m |E|}}; \quad x = 2 \frac{r}{r_0}$$

$R_l Y_{l,m}$ 

$R_l = \kappa y(r)$

$\kappa = \frac{2\pi}{\hbar^2}$

$n_0 = \sqrt{\frac{\hbar^2}{2m|E|}}$

13

$$(82) \quad y'' + \left[ \pm \frac{1}{4} + \frac{A}{x} - \frac{l(l+1)}{x^2} \right] y = 0$$

$$(83) \quad A = \frac{Ze^2}{2\epsilon_0 |E|} = \frac{Ze^2}{2|E|} \sqrt{\frac{2m|E|}{\hbar^2}} = \sqrt{\frac{mZ^2 e^4}{2\hbar^2 |E|}}$$

First case:

$\kappa < 0$

$$(84) \quad y'' + \left[ -\frac{1}{4} + \frac{A}{x} - \frac{l(l+1)}{x^2} \right] y = 0$$

$$(85) \quad y = e^{-\frac{x}{2}} v(x)$$

$$(86) \quad v'' - v' + \left( \frac{A}{x} - \frac{l(l+1)}{x^2} \right) v = 0$$

$$(87) \quad v = x^{l+1} \omega(x)$$

$$(88) \quad \omega = \sum_0^{\infty} a_s x^s$$

$$(89) \quad a_{s+1} = a_s \frac{s+l+1-A}{(s+1)(s+2l+2)}$$

$$(90) \quad A = n = n' + l + 1$$

$$(91) \quad W_n = -\frac{2\pi^2 m Z^2 e^4}{\hbar^2 n^2} = -\frac{m Z^2 e^4}{2\hbar^2 n^2}$$

$$n = l+1, l+2, l+3, \dots$$

## Laguerre's polynomials

$$(92) \quad L_n(x) = e^x \frac{d^n}{dx^n} (x^n e^{-x})$$

$$(93) \quad \begin{cases} L_0 = 1 \\ L_1 = 1 - x \\ L_2 = 2 - 4x + x^2 \\ L_3 = 6 - 18x + 9x^2 - x^3 \end{cases}$$

Put

$$(94) \quad f(x) = x^k e^{-x}; \quad L_k = e^x f^{(k)}(x)$$

$$x f' = (k - x) f$$

$$x f^{(k+2)} + (1+x) f^{(k+1)} + (k+1) f^{(k)} = 0$$

$$(95) \quad x L_k'' + (1-x) L_k' + k L_k = 0$$

From (92) follows besides

$$(96) \quad \int_0^\infty L_k(x) L_{k'}(x) e^{-x} dx = \begin{cases} 0 & \text{for } k \neq k' \\ \frac{1}{k!} & \text{for } k = k' \end{cases}$$

Differentiating (95)  $j$  times

$$(97) \quad x L_k^{(j)''} + (j+1-x) L_k^{(j)'} + (k-j) L_k^{(j)} = 0$$

$$(98) \quad L_k^{(j)} = \frac{d^j}{dx^j} \left\{ e^x \frac{d^k}{dx^k} (x^k e^{-x}) \right\}$$

Orthogonality

$$(99) \quad \int_0^\infty L_k^{(j)} L_{k'}^{(j)} x^j e^{-x} dx = \frac{(k!)^3}{(k-j)!} \delta_{kk'}$$



p. 14 $\frac{1}{2}$

$$\text{Potential energy} = -\frac{Ze^2}{r} \left(1 + \frac{\beta}{\epsilon}\right)$$

(82) becomes (for the case  $E < 0$ )

$$(82) \quad y'' + \left[ -\frac{1}{4} + \frac{A}{x} + \frac{2A\beta}{\epsilon_0 x^2} - \frac{l(l+1)}{x^2} \right] y = 0$$

put

$$l'(l'+1) = l(l+1) - \frac{2A\beta}{\epsilon_0}$$

$$(82)'' \quad = l(l+1) - \frac{2\beta}{a}$$

$$a = \frac{\hbar^2}{me^2 Z}$$

Eigenvalues  $n'$

$$A = n' + l' + 1 = n' + l + 1 - (l - l')$$

$$= n - (l - l') = n - l$$

$$(82)''' \quad E = -\frac{me^4 Z^2}{2\hbar^2 [n - l]^2} = (x) \omega$$

Wentzel Kramers Brillouin

$$\psi'' + \frac{2m}{\hbar^2} (E-U) \psi = 0$$

$$\psi'' + g \psi = 0$$

$$\psi = e^{iy} \quad \psi' = iy' e^{iy}$$

$$\psi'' = (-y'^2 + iy'') e^{iy}$$

$$y'^2 - iy'' = g$$

$$y' = \sqrt{g} + \varepsilon$$

$$g + 2\sqrt{g}\varepsilon - \frac{ig'}{2\sqrt{g}} = 0$$

$$\varepsilon = -\frac{ig'}{4g}$$

$$y = \int \sqrt{g} dx - i \log g^{1/4}$$

$$\psi \approx \frac{1}{g^{1/4}} e^{i \int \sqrt{g} dx}$$

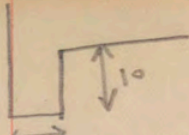
$$\omega(x) = \begin{cases} \frac{1}{x^{1/4}} \cos\left(\frac{2}{3}x^{3/2} - \frac{\pi}{4}\right) \\ \frac{1}{2(-x)^{1/4}} e^{-\frac{2}{3}(-x)^{3/2}} \end{cases}$$

$$\omega'' + x\omega = 0$$

$n = 0, 1, 2, \dots$

$$\int_A^B \sqrt{\frac{2m}{\hbar^2} (E-U)} dx = \pi \left(n + \frac{1}{2}\right)$$

(88)



$$E_0 = 5.4$$

Expression of the e.f. of hydrogenlike systems

$$(100) R_{nl}(r) = \sqrt{\frac{4(n-l-1)!}{a^3 n^4 [(n+l)!]^3}} e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l L_{n+l}^{(2l+1)}\left(\frac{2r}{na}\right)$$

with

$$(101) a = \frac{h^2}{4\pi^2 m Z e^2} = \frac{h^2}{m e^2} \frac{1}{Z}$$

$$(102) u_{n,l,m}(r, \theta, \varphi) = R_{nl}(r) Y_{l,m}(\theta, \varphi)$$

$$\begin{aligned} 1s &= \frac{1}{\sqrt{\pi a^3}} e^{-\sigma} \\ 2s &= \frac{(2-\sigma) e^{-\sigma/2}}{4\sqrt{2\pi a^3}} \\ 2p &= \frac{\sigma e^{-\sigma/2} \cos\theta}{4\sqrt{2\pi a^3}} \\ \sigma &= r/a \end{aligned}$$

Orthogonality of wave functions

$$(103) + \frac{d^2 u_n}{dx^2} + \frac{8\pi^2 m}{h^2} (W_n - U(x)) u_n = 0$$

$$(104) \frac{d^2 u_m}{dx^2} + \frac{8\pi^2 m}{h^2} (W_m - U(x)) u_m = 0$$

$$(105) \frac{d}{dx} (u_m u'_n - u_n u'_m) + \frac{8\pi^2 m}{h^2} (W_n - W_m) u_n u_m = 0$$

With boundary condition  $u(a) = u(b) = 0$

$$(106) u(a) = u(b) = 0$$

follows

$$(107) (W_n - W_m) \int_a^b u_n u_m dx = 0$$

$$u(1s) = \frac{e^{-r/a}}{\sqrt{\pi a^3}}; u(2s) = \frac{1}{4\sqrt{2\pi a^3}} e^{-r/2a} \left(2 - \frac{r}{a}\right); u(2p) \propto r e^{-r/2a} Y_{1m}$$

analogous proof for three dimensions

$$(108) \quad (W_n - W_m) \int u_n^* u_m d\tau = 0$$

Cases of degeneracy (e.g. twofold) by choice of a suitable base

$$(109) \quad \int u_n^* u_m d\tau = \delta_{nm}$$

Coefficients of the expansion

$$(110) \quad u = \sum a_r u_r$$

$$(111) \quad a_r = \int u_r^* u d\tau$$

If the expansion is possible

$$(112) \quad \sum a_r u_r e^{-\frac{2\pi i}{h} W_r t}$$

is the general integral of the time dependent Schrödinger equation (~~discussion of~~)

Determination of the solution of the time dep. Sch. eq. requires knowledge of

$$(113) \quad \psi(x, y, z, 0)$$

Problem on Na atom

# Assumption

$|a_n|^2$   
is (proportional to) the probability that the energy has value  $W_n$

---

## Operators Definitions

~~Linear Operators~~

Linear Operator

a Examples  $( )^2$ ,  $( )^3$ ,  $3$ ,  $\frac{d}{dx}$ ,  $\frac{d^2}{dx^2}$ ,  $(1x^2+1)$

---

## Field in which the functions are defined

b Examples  $x$ ,  $xy z$ , spherical surface, discrete (finite or infinite) set of points, spaces or varieties of any number of dimensions

---

## c Linear operators

d Operators of ~~fields~~ discrete fields, as linear substitution; Matrices

Linear operators as linear vector trans<sub>2</sub>

e formations in the Hilbert space

f Sum, difference, product of operators

h eigenvalues + eigenfunctions of a linear

operator

$$A u_n = a_n u_n$$

Examples

i (114)  $x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} = \frac{\partial}{\partial \varphi}$

(115)  $a_n = n i$

j (116)  $x^2 - \frac{d^2}{dx^2}$

~~(117)~~  $a_n = 2n + 1$

k ~~Hermitian operators~~ Secular equation for the e.v.

Hermitian operators for finite matrices

l (117)  $a_{rs} = a_{sr}^*$

m Hermitian operators have real eigenvalues and orthogonal e.f. (case of field of  $n$  points)

g Sum and product of two operators that can be represented by <sup>finite</sup> matrices

n symmetrised product is Hermitian

Property of Hermitic operators

$$(118) \quad \sum v_r^* (A u)_r = \sum u_r (A v)_r^* \quad (\text{equivalent to definition})$$

or

$$(119) \quad \int v^* (A u) d\tau = \int u (A v)^* d\tau$$

Definition in the latter case, equivalent to definition for <sup>finite</sup> matrixes

From (119) follows: Reality of e.v. and orthogonality of e.f.

Indeed

$$(120) \quad \int v^* A v d\tau = \text{real}$$

Examples:

$$(121) \quad i \frac{\partial}{\partial x} \text{ is hermitian}$$

q' Development in a series of e.f.  
Geometrical discussion

q'' Functions of operators

To each physical magnitude (real)

$$(122) \quad F(x, y, z, p_x, p_y, p_z)$$

there is a corresponding Hermitian operator

$$(123) \quad \hat{F}$$

obtained by

$$(124) \quad p_x = \frac{h}{2\pi i} \frac{\partial}{\partial x}, \dots$$

H

Several physical magnitudes being given it is possible to find for them simultaneously the values

$$(125) \quad \begin{cases} F = a \\ G = b \end{cases}$$

Provided the system

$$(126) \quad \begin{cases} F\psi = a\psi \\ G\psi = b\psi \end{cases}$$

see also  
page 100

has at least one solution

The (125) define the state of the system when the solution of (126) is unique

Δ

⊥

The state of the system at a given time can also be described by giving

ψ



at that time (Measuring of  $F$  shall give them)  
 $F=a$

The time variation of  $\psi$  is according to the time dependent Schrödinger equation

$$(127) \quad H\psi = -\frac{\hbar}{2\pi i} \frac{\partial \psi}{\partial t}$$

If  $\psi$  is an e.f. of  $F$  then

$$(128) \quad F = \text{corresp. e.v.}$$

otherwise develop  $\psi$  in e.f. of  $F$

$$(129) \quad \psi = \sum c_n f_n$$

If everything is normalised

$$(130) \quad |c_n|^2$$

is the probability for the e.v. number  $n$

Jump to after (147)  $\rightarrow$  (167) then insert what follows

Discussion of the system mass point on a straight line

If  $G'$  is a not degenerate e.v. of  $G$  then

$$(131)$$

$$G = G'$$

determines the state as that for which

$$(132)$$

$$G\psi = G'\psi$$

↳ This shift after discussion of the uncertainty relation formula (167)

Vice versa if the state at  $t=0$  is given by

$$(133) \quad \psi(x,0) = \rho(x) e^{i\theta(x)}$$

Put

$$(134) \quad G = \left( p - \frac{\hbar}{2\pi} \frac{d\theta}{dx} \right)^2 + \frac{\hbar^2}{4\pi^2} \frac{1}{\rho} \frac{d^2\rho}{dx^2}$$

Then

$$(135) \quad G\psi = 0$$

or, measure of  $G$  gives result

$$(136) \quad G = 0$$

↓  
 Given  $G(x,p)$  how to measure its value for  $t=t_1$  by a measurement performed at  $t=0$ .

~~The~~ The equation

$$(137) \quad G \psi(x, t_1) = g \psi(x, t_1)$$

determines

$$(138) \quad \psi(x, t_1, g)$$

integrating back time dependent Schrödinger eq find

$$(139) \quad \psi(x, 0, g)$$

With (134) find such an operator  $G_0$  that

$$(140) \quad G_0(x, g) \psi(x, 0, g) = 0$$

Then

$$(141) \quad G = g \quad \text{at } t = t_1$$

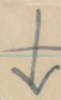
is equivalent to

$$(142) \quad G_0(x, p, g) = 0$$

Solving this with respect to  $g$

$$g = A(x, p)$$

$A(x, p)$  is a magnitude that, measured at  $t=0$  gives as value the same as  $G$  measured at  $t=t_1$ .



Let e.g. put for the case of no forces

$$(143) \quad G = x \quad g = x_1$$

$$(144) \quad \psi(x, t_1) = \delta(x - x_1)$$

$$(145) \quad \frac{\partial^2 \psi}{\partial x^2} = - \frac{4\pi m i}{h} \frac{\partial \psi}{\partial t}$$

corresponding solution

$$(146) \quad \psi(x, t) = \lim_{\alpha \rightarrow t_0} \frac{1}{\sqrt{t_1 - t}} e^{-\frac{(x-x_1)^2}{t_1 - t} \left[ \alpha + \frac{\pi i m}{h} \right]}$$

hence

$$(147) \quad \psi(x, 0) \propto e^{-\frac{\pi i m}{h t_1} (x_1 - x)^2}$$

follows after (167)

24

The uncertainty principle  
 Example: discussion of electronic microscope

~~$$[(A-a)^2 + (B-b)^2] \psi$$

$$(A-a)^2 \psi = -(B-b)^2 \psi$$~~

Wave mechanical interpretation:

↳

$$(148) \quad \psi(x) = \int A(p) e^{\frac{2\pi i}{h} p x} dp$$

$$(149) \quad \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \iiint A^*(p) A(p') e^{\frac{2\pi i}{h} (p'-p)x} dp dp' dx$$

$$(150) \quad \boxed{\int_{-\infty}^{\infty} e^{i\omega x} dx = 2\pi \delta(\omega)}$$

$$(151) \quad N = \int_{-\infty}^{\infty} |\psi|^2 dx = 2\pi \iint A^*(p) A(p') \delta\left[\frac{2\pi}{h} (p'-p)\right] dp' dp$$

$$= h \int_{-\infty}^{\infty} |A(p)|^2 dp$$

$$(152) \quad \bar{x} = \frac{1}{N} \int x |\psi|^2 dx$$

$$(153) \quad \bar{p} = \frac{\hbar}{N} \int p |A(p)|^2 dp$$

$$(154) \quad \Delta x^2 = \frac{1}{N} \int (x - \bar{x})^2 |\psi|^2 dx$$

$$(155) \quad \Delta p^2 = \frac{\hbar}{N} \int (p - \bar{p})^2 |A(p)|^2 dp$$

Take  $\bar{x}$  as origin and put

$$(156) \quad \begin{cases} \varphi(x) = \psi(x) e^{-\frac{2\pi i}{\hbar} \bar{p} x} \\ B(p) = A(\bar{p} + p) \end{cases}$$

then for the new functions

$$(157) \quad \varphi(x) = \int B(p) e^{\frac{2\pi i}{\hbar} p x} dp$$

and

$$(158) \quad \bar{x} = 0 \quad \bar{p} = 0$$

$$(159) \quad \Delta x^2 = \frac{1}{N} \int x^2 |\varphi|^2 dx$$

$$(160) \quad \Delta p^2 = \frac{\hbar}{N} \int p^2 |B|^2 dp$$

$$(161) \quad D = \left| \frac{x}{2\Delta x^2} \varphi + \frac{\partial \varphi}{\partial x} \right|^2 \geq 0$$

$$0 \leq \int D dx = \int \left( \frac{x^2}{4 \Delta x^4} \varphi^* \varphi + \frac{1}{2 \Delta x^2} \frac{\partial}{\partial x} (x \varphi^* \varphi) - \frac{1}{2 \Delta x^2} \varphi^* \varphi + \right. \\ \left. + \frac{\partial}{\partial x} \left( \varphi^* \frac{\partial \varphi}{\partial x} \right) - \varphi^* \frac{\partial^2 \varphi}{\partial x^2} \right) dx$$

$$(162) \quad = -\frac{N}{4 \Delta x^2} - \int \varphi^* \frac{\partial^2 \varphi}{\partial x^2} dx \geq 0$$

$$(163) \quad \left\{ \begin{aligned} \int \varphi^* \frac{\partial^2 \varphi}{\partial x^2} dx &= -\frac{4\pi^2}{h^2} \int p^2 B^*(p') B(p) e^{\frac{2\pi i}{h}(p-p')x} dx dp dp' \\ &= -\frac{4\pi^2}{h} \iint p^2 B^*(p') B(p) \delta(p-p') dp dp' \\ &= -\frac{4\pi^2}{h} \int p^2 |B(p)|^2 dp \\ &= -\frac{4\pi^2 N}{h^2} \int \Delta p^2 \end{aligned} \right.$$

follows

$$(164) \quad -\frac{1}{4 \Delta x^2} + \frac{4\pi^2}{h^2} \Delta p^2 \geq 0$$

$$(165) \quad \Delta x \Delta p \geq \frac{h}{4\pi} \quad \text{back to page 20}$$

Probability distribution of the results of a measurement when state is previously known

A

has e.v.  $a_1, a_2, \dots, a_n, \dots$  & e.f.  $\varphi_1, \varphi_2, \dots, \varphi_n, \dots$

$$(166) \quad \left| \int \varphi_n^* \psi dx \right|^2$$

is proportional to probability of  $A = a_n$

If by actual measurement we find  $A = a_n$  the state of the system is changed to  $\varphi_n(x)$

Time dependent S. e. is description of variation of state. Can be written

$$(167) \quad H\psi = -\frac{\hbar}{2\pi i} \frac{\partial \psi}{\partial t}$$

Insert here what follows (134)

Question:

The state of a mass point is

$$\psi(x) = e^{-i\left(\frac{x^2}{2} - 2x\right)}$$

find

$$(p+x=2) \quad \text{having put } \frac{\hbar}{2\pi} = 1$$

& distributions of  $p+x$

follows after (147)

According to (134) the operator  $G_0$  is

$$(168) \quad p + \frac{2\hbar}{2\pi} \frac{\pi m}{\hbar t_1} (x - x_1)$$

&  $G_0 = 0$  is equivalent to

$$(169) \quad x_1 = x + \frac{t_1 p}{m}$$

28

[Page 66 + commutation rules  
 $xp_x - x_p x = \frac{\hbar}{i}$ ]

Time derivative of an operator

$$(170) \quad H\psi = -\frac{\hbar}{2\pi i} \frac{\partial \psi}{\partial t}$$

$$(171) \quad \begin{aligned} \psi(x, \tau) &= \psi(x, 0) - \frac{2\pi i}{\hbar} \tau H \psi(x, 0) \\ &= \left(1 - \frac{2\pi i \tau}{\hbar} H\right) \psi(x, 0) \end{aligned}$$

notice

$$(172) \quad \begin{cases} \psi(x, t) = e^{-\frac{2\pi i t}{\hbar} H} \psi(x, 0) \\ \psi(x, 0) = e^{\frac{2\pi i t}{\hbar} H} \psi(x, t) \end{cases}$$

$$A(t) = e^{\frac{it}{\hbar} H} A e^{-\frac{it}{\hbar} H}$$

$$(173) \quad \begin{cases} A\psi(x, t) = \psi(x, t) \\ A(\tau)\psi(x, 0) = \psi(x, 0) \end{cases}$$

$$(174) \quad A(\tau) = \left(1 + \frac{2\pi i \tau}{\hbar} H\right) A \left(1 - \frac{2\pi i \tau}{\hbar} H\right)$$

$$(175) \quad \frac{dA}{d\tau} = \frac{2\pi i}{\hbar} (HA - AH)$$

relation with Hamilton equations

$$\psi(x, \tau) = \sum c_n \psi_n$$

$$A(\tau)\psi(x, 0) = \sum c_n$$

$$\psi(x, 0) = \sum c_n \left(1 + \frac{2\pi i \tau}{\hbar} H\right) \psi_n$$

$$A(\tau) \left(1 + \frac{2\pi i \tau}{\hbar} H\right) \psi_n = a_n \left(1 + \frac{2\pi i \tau}{\hbar} H\right) \psi_n$$



## Average of a physical magnitude

$$(177) \quad c_n = \int \psi_n^* A \psi$$

$$(178) \quad \psi = \sum c_n \psi_n$$

$$(179) \quad A \psi = \sum c_n a_n \psi_n$$

$$(180) \quad \int \psi^* A \psi = \sum |c_n|^2 a_n$$

$$\rightarrow A \psi(x, \tau) = \sum c_n \psi_n$$

$$c_n, a_n$$

$$(181) \quad \psi(x, 0) = \sum \left(1 + \frac{2\pi i \tau}{h} H\right) \psi_n c_n$$

$$(182) \quad A(\tau) = \left(1 + \frac{2\pi i \tau}{h} H\right) A \left(1 - \frac{2\pi i \tau}{h} H\right)$$

has the same e.v. as A

a time constant A obeys to

$$(183) \quad AH = HA$$

as example  
 $M_z = x p_y - y p_x$   
 is constant in central  
 field of force.  
~~Hamiltonian equations~~

Physical meaning of the commutation  
 of A + B

Theorem [see page 66]

If  $A$  and  $B$  have the same set of e.f. they commute

$$(184) \quad \begin{pmatrix} \psi_1 & \dots & \psi_n & \dots \\ a_1 & \dots & a_n & \dots \end{pmatrix}$$

$$(185) \quad \begin{pmatrix} b_1 & \dots & b_n & \dots \end{pmatrix}$$

$$(186) \quad \psi = \sum c_n \psi_n$$

$$(187) \quad AB\psi = \sum c_n a_n b_n \psi_n = BA\psi$$

If there is no degeneracy the value of  $A$  determines the value of  $B$  of

$$(188) \quad B = f(A) \quad \left( \begin{array}{l} \text{Provided} \\ AB = BA \end{array} \right)$$

Integration of time dependent S.E.

$$(189) \quad H\psi = -\frac{\hbar}{2\pi i} \frac{\partial \psi}{\partial t}$$

$$(190) \quad \psi = \sum a_n \psi_n$$

$$(191) \quad H\psi_n = \omega_n \psi_n$$

$$(192) \quad -\frac{\hbar}{2\pi i} \dot{a}_n = \omega_n a_n$$

$$(193) \quad a_n = a_{n_0} e^{-\frac{2\pi i}{\hbar} \omega_n t}$$

$$(194) \quad \psi = \sum a_{n_0} e^{-\frac{2\pi i}{\hbar} \omega_n t} \psi_n$$

# Transformation theory

## Unitarian transformations

$$T_{\alpha n}$$

$$(195) \quad \sum_n T_{\alpha n} a_n = a_\alpha$$

$$(196) \quad \sum_n a_n \psi_n = \sum_\alpha a_\alpha \varphi_\alpha = \psi$$

$$(197) \quad a_n = \int \psi_n^* \psi = \sum_\alpha a_\alpha \int \psi_n^* \varphi_\alpha$$

$$(198) \quad a_\alpha = \int \varphi_\alpha^* \psi = \sum_n a_n \int \varphi_\alpha^* \psi_n$$

$$(199) \quad T_{\alpha n} = \int \varphi_\alpha^* \psi_n \quad T_{\alpha n}^* = T_{n\alpha}$$

$$(200) \quad T_{n\alpha} = \int \psi_n^* \varphi_\alpha$$

$$\int \varphi_\alpha^* \varphi_\alpha =$$

$$(201) \quad \delta(x-x_1) = \sum_\alpha \varphi_\alpha^*(x_1) \varphi_\alpha(x)$$

$$(202) \quad \sum_\alpha T_{n\alpha} T_{\alpha m} = \iint \psi_n^*(x_1) \varphi_\alpha(x_1) \varphi_\alpha^*(x_2) \psi_m(x_2)$$

$$= \int \psi_n^*(x_1) \psi_m(x_2) = \delta_{nm}$$

$$T \tilde{T} = 1$$

## Hamilton equations

From

$$(203) \quad pq - qp = \frac{h}{2\pi i}$$

follows

$$(204) \quad F(p, q)q - qF(p, q) = \frac{h}{2\pi i} \frac{\partial F}{\partial p}$$

$$(205) \quad pF(p, q) - F(p, q)p = \frac{h}{2\pi i} \frac{\partial F}{\partial q}$$

proof: If (204) (205) hold for  $p$  &  $q$ ; if they hold for two functions they hold also for sum & product.

From (175) follow Hamilton equations hence (203) as general commutation rules for general coordinates & momenta

Theorem:

If two not degenerate operators  $A$  &  $B$  commute they have equal sets of e.f.

Let

$$(206) \quad \varphi_1 \varphi_2 \dots \varphi_n$$

be the e.f. of  $A$ 

$$(207) \quad A\varphi_n = a_n \varphi_n$$

follows

$$(208) \quad BA\varphi_n = a_n B\varphi_n$$

hence

$$(209) \quad AB = BA$$

$$(210) \quad A(B\varphi_n) = a_n(B\varphi_n)$$

hence

$$(211) \quad B\varphi_n \propto \varphi_n = b_n\varphi_n$$

or  $\varphi_n$  is e.f. of B also

When there is degeneracy  
The e.f. can be chosen in such a way  
as to overlap

Three operators commute  
 $AB = BA \quad AC = CA \quad BC = CB$

See page 66

Angular momentum of a mass point

$$(212) \quad \begin{cases} M_x = y p_z - z p_y \\ M_y = z p_x - x p_z \\ M_z = x p_y - y p_x \end{cases}$$

$$\frac{h}{2\pi i} (z p_y - y p_z)$$

$$(213) \quad M^2 = M_x^2 + M_y^2 + M_z^2$$

Commutation rules

$$(214) \quad M_y M_z - M_z M_y = -\frac{h}{2\pi i} M_x$$

$$(215) \quad \text{or} \quad [\vec{M} \times \vec{M}] = -\frac{h}{2\pi i} \vec{M}$$

$$(216) \quad M^2 M_x - M_x M^2 = 0$$

Eigenvalues of

$$(217) \quad M_z = \text{are } \frac{h}{2\pi} m \quad m = \text{integer}$$

34  $-x(z \frac{\partial}{\partial z} + \frac{h}{2\pi i}) p_x$   $\Lambda + r^2 \frac{\partial^2}{\partial z^2} + 2r \frac{\partial}{\partial z} = r^2 \Delta$   $x p_x x p_x$   
 $x(x p_x + \frac{h}{2\pi i}) p_x$

(218)  $M^2 = (x p_z - z p_x)^2 + (y p_z - x p_y)^2 + (z p_y - y p_z)^2 =$   
 $= x^2 p_z^2 + z^2 p_x^2 + y^2 p_x^2 + x^2 p_y^2 + z^2 p_y^2 + y^2 p_z^2 + x^2 p_x^2 + y^2 p_y^2 + z^2 p_z^2$   
 $- x^2 p_x^2 - y^2 p_y^2 - z^2 p_z^2 - 2xz p_x p_z - 2xy p_x p_y - 2yz p_y p_z$   
 $- \frac{2h}{2\pi i} (x p_x + y p_y + z p_z)$   
 $= (x^2 + y^2 + z^2)(p_x^2 + p_y^2 + p_z^2) - (x p_x + y p_y + z p_z)^2 -$   
 $- \frac{2h}{2\pi i} (x p_x + y p_y + z p_z)$

$r^2 \frac{\partial^2}{\partial z^2} + 2r \frac{\partial}{\partial z}$   
 $r^2(x \frac{\partial^2}{\partial x^2} + 1) \frac{\partial}{\partial z}$

(219)  $M^2 = -\frac{h^2}{4\pi^2} \left[ r^2 \Delta - r^2 \frac{\partial^2}{\partial z^2} - 2r \frac{\partial}{\partial z} \right]$

(220)  $r^2 \Delta = \Lambda + r^2 \frac{\partial^2}{\partial z^2} + 2r \frac{\partial}{\partial z}$

(221)  $M^2 = -\frac{h^2}{4\pi^2} \Lambda$   
 Since e.v. of  $\Lambda$  are  $-l(l+1)$ , e.v. of  $M$  are  $\frac{h^2}{4\pi^2} l(l+1)$

Eigenfun for

(222)  $\begin{cases} M_z = \frac{h}{2\pi} m \\ M^2 = \left(\frac{h}{2\pi}\right)^2 l(l+1) \end{cases}$

(223) are  $f(r) Y_{l,m}(\theta, \phi)$

# Perturbation theory

~~Perturbation theory~~

~~Transformation theory~~

Instead of

~~$\Psi$~~

Use the coefficients

$$(224) \quad (H_0 + \mathcal{H}b) u = w u$$

$$(225) \quad H_0 u_n^0 = w_n^0 u_n$$

$$(226) \quad (H_0 + \lambda \mathcal{H}b) (u_i^{(0)} + \lambda u_i^{(1)} + \lambda^2 u_i^{(2)} + \dots) = (w_i^{(0)} + \lambda w_i^{(1)} + \dots) (u_i^{(0)} + \lambda u_i^{(1)} + \dots)$$

$$(227) \quad \left\{ \begin{aligned} H_0 u_i^{(0)} &= w_i^{(0)} u_i^{(0)} \\ H_0 u_i^{(1)} - w_i^{(0)} u_i^{(1)} - w_i^{(1)} u_i^{(0)} &= -\mathcal{H}b u_i^{(0)} \\ H_0 u_i^{(2)} - w_i^{(0)} u_i^{(2)} - w_i^{(1)} u_i^{(1)} - w_i^{(2)} u_i^{(0)} &= -\mathcal{H}b u_i^{(1)} + w_i^{(1)} u_i^{(1)} \end{aligned} \right.$$

$$(228) \quad u_i^{(1)} = \sum_j' c_{ij}^{(1)} u_j^{(0)} ; \quad u_i^{(2)} = \sum_j' c_{ij}^{(2)} u_j^{(0)} ; \dots$$

$$(229) \quad \left\{ \begin{aligned} \sum_j' c_{ij}^{(1)} (w_j^{(0)} - w_i^{(0)}) u_j^{(0)} - w_i^{(1)} u_i^{(0)} &= -\mathcal{H}b u_i^{(0)} \\ \sum_j' c_{ij}^{(2)} (w_j^{(0)} - w_i^{(0)}) u_j^{(0)} - w_i^{(2)} u_i^{(0)} &= -\mathcal{H}b u_i^{(1)} + w_i^{(1)} u_i^{(1)} \end{aligned} \right.$$

Put

$$(230) \quad \mathcal{H}b_{rs} = \int u_r^{(0)*} \mathcal{H}b u_s^{(0)} d\tau$$

36

$$c_{ij}^{(2)} = \sum_l \frac{\mathcal{H}_{jl} \mathcal{H}_{li}}{(w_i - w_l)(w_i - w_j)} - \frac{\mathcal{H}_{ji} \mathcal{H}_{ii}}{(w_i - w_j)^2}$$

(231)

$$w_i^{(1)} = \mathcal{H}_{ii}$$

(232)

$$c_{ij}^{(1)} = \frac{\mathcal{H}_{ji}}{w_i^{(0)} - w_j^{(0)}}$$

(233)

$$w_i^{(2)} = \sum_j \frac{\mathcal{H}_{ij} \mathcal{H}_{ji}}{w_i^{(0)} - w_j^{(0)}} = \sum_j \frac{|\mathcal{H}_{ij}|^2}{w_i^{(0)} - w_j^{(0)}}$$

Example

Oscillator perturbed by constant force  $F$ 

$$\mathcal{H} = -Fx$$

First order perturbation vanishes

$$w_0^{(2)} = -\frac{|\mathcal{H}_{01}|^2}{h\nu}$$

$$u_0^{(0)}(\xi) = N_0 e^{-\xi^2/2}$$

$$u_1^{(0)}(\xi) = 2\xi N_1 e^{-\xi^2/2}$$

$$\xi = 2\pi \sqrt{\frac{m\nu}{h}} x$$

$$N_0 = \left(\frac{4\pi m\nu}{h}\right)^{1/4} = \left(\frac{m\omega}{\pi h}\right)^{1/4}$$

$$N_1 = \left(\frac{4\pi m\nu}{h}\right)^{1/4} \frac{1}{\sqrt{2}}$$

$$x_{01} = \int_{-\infty}^{\infty} N_0 N_1 2\xi e^{-\xi^2/2} x dx = \sqrt{\frac{h}{8\pi^2 m\nu}} = \sqrt{\frac{h}{2m\omega}}$$

$$x_{02} = x_{03} = \dots = 0$$



# Zeeman effect without spin

36½

$$H = \frac{1}{2M} \left( p - \frac{e}{c} A \right)^2 + V(r)$$

$$= \frac{p^2}{2M} + V(r) - \frac{e}{Mc} p \cdot A + \text{quadratic term}$$

$$A_x = -\frac{H}{2} y$$

$$A_y = \frac{H}{2} x$$

$$A_z = 0$$

$$\text{Hamiltonian} = \frac{p^2}{2M} + V(r) + \frac{eH}{2Mc} (x p_y - y p_x) =$$

Unperturbed

$$u_{n,l,m} = R_{nl}(r) Y_{l,m}(\theta, \varphi)$$

$$\left( \frac{p^2}{2m} + V(r) \right) u_{nlm} = E_{nl} u_{nlm}$$

$$\text{Ham } u_{nlm} \oplus = E_{nl} u_{nlm} + \frac{e \hbar H m}{2Mc} u_{nlm}$$

Discussion: Selection rule

$$\Delta m \rightarrow \begin{matrix} m+1 \\ m \\ m-1 \end{matrix}$$

Correspondence principle

Dimensional analysis

$$H = \frac{1}{2} m (v - \frac{1}{2} A)^2 + U(x)$$

$$= \frac{1}{2} m v^2 - m v A + \frac{1}{2} m A^2 + U(x)$$

$$A_1 = \frac{h}{m \lambda}$$
$$A_2 = \frac{h}{m \lambda}$$
$$A_3 = \frac{h}{m \lambda}$$

$$H = \frac{1}{2} m v^2 - m v A + \frac{1}{2} m A^2 + U(x)$$

Substituted

$$U(x) = \frac{1}{2} m \omega^2 x^2$$

$$\left( \frac{1}{2} m v^2 - m v A + \frac{1}{2} m A^2 \right) + U(x)$$

$$H = \frac{1}{2} m v^2 - m v A + \frac{1}{2} m A^2 + U(x)$$

Dimensional analysis

$$h \rightarrow m \cdot \lambda$$

Correspondence principle

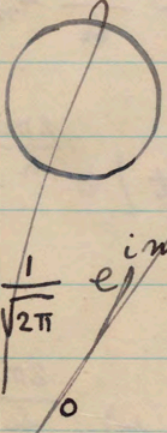
$$w_0^{(2)} = - \frac{F^2 \hbar}{8\pi^2 m \nu \cdot \hbar \nu} = - \frac{F^2}{8\pi^2 m \nu^2}$$

Direct proof:

$$H = \frac{p^2}{2m} + 2\pi^2 m \nu^2 x^2 - Fx$$

$$= \frac{p^2}{2m} + 2\pi^2 m \nu^2 (x - \alpha)^2 - \frac{F^2}{4\pi^2 m \nu^2}$$

$$= \frac{p^2}{2m} + 2\pi^2 m \nu^2 \left(x - \frac{F}{4\pi^2 m \nu^2}\right)^2 - \frac{F^2}{8\pi^2 m \nu^2}$$



$$\frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

$$\frac{1}{\sqrt{2\pi}} e^{-im\varphi}$$

$$\frac{A}{2\pi} e^{-2im\varphi} \cos\varphi$$

$A \cos\varphi$

Hydrogen perturbed by constant field  $F$   
 For perturbations with degeneracy  
 see page 106

## Time dependent perturbations

$$(H_0 + \mathcal{H}_1) \psi = - \frac{\hbar}{2\pi i} \frac{\partial \psi}{\partial t}$$

~~$$H_0 \psi^{(0)} \quad H_0 u_n^{(0)} = W_n^{(0)} u_n^{(0)}$$~~

~~$$\psi = \sum c_n(t) u_n^{(0)}$$~~

~~$$c_n(t) W_n^{(0)}$$~~

~~$$\psi_n^{(0)} = u_n^{(0)} e^{-\frac{2\pi i}{\hbar} W_n^{(0)} t}$$~~

$$\psi = \sum a_n(t) u_n^{(0)} e^{-\frac{2\pi i}{\hbar} W_n^{(0)} t}$$

$$\dot{a}_m = -\frac{2\pi i}{\hbar} \sum_n \mathcal{H}_{nm}(t) a_n(t) e^{\frac{2\pi i}{\hbar} (W_n^{(0)} - W_m^{(0)}) t}$$

First approximation

$$a_m = a_m^{(0)} - \frac{2\pi i}{\hbar} \sum_n a_n^{(0)} \int_0^t \mathcal{H}_{nm}(t) e^{\frac{2\pi i}{\hbar} (W_n^{(0)} - W_m^{(0)}) t} dt$$

Probability of transition proportional to

$$|\mathcal{H}_{nm}|^2$$

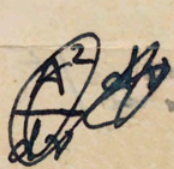
$$\mathcal{H} = e A z \cos \omega t$$

$$\mathcal{H}_{nm} = e A z_{nm} \cos \omega t$$

$$\dot{a}_n \approx -\frac{ie}{2\hbar} A z_{nm} e^{i(\omega_{nm} - \omega)t}$$

$$a_m = +\frac{e}{2\hbar} A z_{nm} \frac{e^{i(\omega_{nm} - \omega)t} - 1}{\omega - \omega_{nm}}$$

$$|a_m|^2 = \frac{e^2 A^2 |z_{nm}|^2}{\hbar^2} \frac{\sin^2(\omega - \omega_{nm}) \frac{t}{2}}{(\omega - \omega_{nm})^2}$$



$$\boxed{\frac{A^2}{d\omega}} d\omega$$

$$\frac{c A^2}{8\pi} = dI$$

$$A^2 = \frac{8\pi c dI}{d\omega}$$

$$|a_m|^2 = \frac{e^2}{\hbar^2} |z_{nm}|^2 \frac{8\pi}{c} \frac{dI}{d\omega} \frac{\pi t}{2}$$

$$\text{prob. of transition} = \frac{4\pi^2 e^2}{c \hbar^2} |z_{nm}|^2 \frac{dI}{d\omega}$$

Prob of transition in isotropic radiation of volume density  $u(\omega) d\omega$

$$\frac{4}{3} \frac{\pi^2 e^2}{\hbar^2} |r_{nm}|^2 u(\omega)$$

Einstein's A, B

$$n_2 (A + B u) = n_1 B u$$

$$\frac{A}{B u} + 1 = \frac{n_1}{n_2} = e^{\frac{\hbar \omega}{kT}}$$

$$\frac{A}{B} = u \times \left( e^{\frac{\hbar \omega}{kT}} - 1 \right)$$

$$d\omega u = \frac{\omega^2 d\omega}{\pi^2 c^3} \frac{\hbar \omega}{e^{\frac{\hbar \omega}{kT}} - 1}$$

$$\frac{A}{B} = \frac{\hbar \omega^3}{\pi^2 c^3} \quad B = \frac{4\pi^2}{3} \frac{e^2}{\hbar^2} \left| \frac{e}{m c} \right|^2$$

$$A = \frac{4}{3} \frac{e^2 \omega^3}{\hbar c^3} \left| \frac{e}{m c} \right|^2 = \frac{1}{\tau}$$

Sinusoidal perturbation

$$H = L \cos 2\pi \nu t$$

Resonance

Perturbations produced by the radiation field

$$\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \pi$$

Absorption and forced emission  
Einstein's A's & B's

$$\frac{A}{B} = \frac{8\pi h \nu^3}{c^3} = \frac{A_{21} \nu_{21}^3}{A_{10} \nu_{10}^3}$$

Example Stark effect on Hydrogen

$$n=2 \quad l=0$$

~~$$R_{20} = \frac{1}{2\sqrt{2\pi}} \left(1 - \frac{r}{2a}\right) e^{-\frac{r}{2a}}$$~~

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

$$R_{21} = \frac{1}{2\sqrt{6}} a^{-3/2} e^{-\frac{r}{2a}} \frac{r}{a}$$

taking unity of length  $a = \frac{h^2}{4\pi^2 m e^2}$

Normalized

$$\left( \begin{array}{l} \psi_{20} = \frac{1}{2\sqrt{2\pi}} \left(1 - \frac{r}{2}\right) e^{-\frac{r}{2}} \\ \psi_{21} = \frac{1}{2\sqrt{6}} e^{-\frac{r}{2}} \left\{ \begin{array}{l} \sqrt{\frac{3}{8\pi}} \sin \vartheta e^{i\varphi} \\ \sqrt{\frac{3}{4\pi}} \cos \vartheta \\ \sqrt{\frac{3}{8\pi}} \sin \vartheta e^{-i\varphi} \end{array} \right. \\ \psi_{10} = \frac{1}{\sqrt{\pi}} e^{-r} \end{array} \right.$$

Einstein's  $A'$ 's &  $B'$ 's

$$\frac{n_2}{n_1} = e^{-\frac{h\nu}{kT}}$$

$$\text{also } n_1 B u_\nu = n_2 (A + B' u_\nu)$$

$$u_\nu \left[ B e^{\frac{h\nu}{kT}} - B' \right] = A$$

$$u_\nu = \frac{A}{B \left\{ e^{\frac{h\nu}{kT}} - \frac{B'}{B} \right\}} = \frac{8\pi \cdot h\nu^3 / c^3}{e^{\frac{h\nu}{kT}} - 1}$$

$$\begin{cases} B' = B \\ \frac{A}{B} = \frac{8\pi h\nu^3}{c^3} \end{cases}$$

Absorption of radiation  
~~Field~~ Perturbing potential

$$e x \sum_{n=0}^{\infty} A_n \cos\left(\frac{2\pi n}{T} t + \beta_n\right)$$

$$\dot{a}_2 = -\frac{2\pi i}{h} e x_{12} \sum_n A_n \cos\left(\frac{2\pi n}{T} t + \beta_n\right) e^{2\pi i \nu t}$$

$$w_2 - w_1 = h\nu$$

$$\dot{a}_2 = -\frac{2\pi i}{h} e x_{12} \sum_n \frac{A_n}{2} e^{-i\beta_n} e^{+2\pi i \left(\nu - \frac{n}{T}\right) t}$$



41

$$a_2 = - \frac{e x_{12}}{2h} \sum_n A_n e^{-i\beta_n} \frac{e^{2\pi i (\nu - \frac{n}{T})t} - 1}{\nu - \frac{n}{T}}$$

$$|a_2|^2 = \frac{e^2 |x_{12}|^2}{h^2} \sum_n A_n^2 \frac{\sin^2 \pi t (\frac{n}{T} - \nu)}{(\frac{n}{T} - \nu)^2} + \sum_{nm} \dots$$

$$\overline{|a_2|^2} = \frac{e^2 |x_{12}|^2}{h^2} \overline{A_\nu^2} \int_{-\infty}^{\infty} \frac{\sin^2 \pi t (\frac{n}{T} - \nu)}{(\frac{n}{T} - \nu)^2} dn$$

$$u_\nu d\nu = \frac{1}{8\pi} \left( \overline{E_x^2} + \overline{E_y^2} + \overline{E_z^2} + \overline{H_x^2} + \overline{H_y^2} + \overline{H_z^2} \right) (d\nu)$$

$$= \frac{3}{4\pi} \overline{E_x^2} (d\nu) = \frac{3}{4\pi} \frac{\overline{A_\nu^2}}{2} T d\nu$$

$$u_n = \frac{3}{8\pi} \overline{A_\nu^2} T$$

$$\overline{|a_2|^2} = \frac{e^2 |x_{12}|^2}{h^2} \pi^2 t T \overline{A_\nu^2}$$

$$= \frac{8\pi^3}{3} \frac{e^2 |x_{12}|^2}{h^2} u_\nu t$$

$$B = \frac{8\pi^3}{3} \frac{e^2}{h^2} \left\{ |x_{12}|^2 + |y_{12}|^2 + |z_{12}|^2 \right\}$$

$$A = \frac{1}{T} = \frac{64\pi^3 e^2 \nu^3}{3c^3 h^2} \left[ |x_{12}|^2 + |y_{12}|^2 + |z_{12}|^2 \right]$$

42

Application to point in central field  
of force

eigenfunctions

$$R(r) Y_{lm}(\theta, \varphi) = u_{nlm}$$

Interpretation of q.n. m & l

$$M_z = \frac{\hbar}{2\pi i} \frac{\partial}{\partial \varphi}$$

$$M^2 = -\frac{\hbar^2}{4\pi^2} \Delta$$

$$\begin{aligned} M^2 u_{nlm} &= -\frac{\hbar^2}{4\pi^2} R_n(r) \Delta Y_{lm} = \\ &= \frac{\hbar^2}{4\pi^2} l(l+1) u_{nlm} \end{aligned}$$

thus

$$M^2 = \left(\frac{\hbar}{2\pi}\right)^2 l(l+1)$$

or total momentum is  $\sqrt{l(l+1)}$  in  
units  $\hbar$ .

$$M_z u_{nlm} = m u_{nlm}$$

or

z component of ang momentum is m  
in units  $\hbar$ .

$$Y_{l+1, m-1} Y_{l, m} = \sqrt{\frac{3}{8\pi}} \sqrt{\frac{(l+m)(l+1+m)}{(2l+1)(2l+3)}} Y_{l+1, m} - \sqrt{\frac{3}{8\pi}} \sqrt{\frac{(l-m)(l+1-m)}{(2l+1)(2l-1)}} Y_{l-1, m}$$

$$Y_{l+1, 0} Y_{l, m} = \sqrt{\frac{3}{4\pi}} \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}} Y_{l+1, m} + \sqrt{\frac{3}{4\pi}} \sqrt{\frac{l^2 - m^2}{(2l+1)(2l-1)}} Y_{l-1, m}$$

$$Y_{l-1, -1} Y_{l, m+1} = \sqrt{\frac{3}{8\pi}} \sqrt{\frac{(l-m)(l+1-m)}{(2l+1)(2l+3)}} Y_{l+1, m} - \sqrt{\frac{3}{8\pi}} \sqrt{\frac{(l+m)(l+1+m)}{(2l+1)(2l-1)}} Y_{l-1, m}$$

$$Y_{l, 0} = \sqrt{\frac{3}{4\pi}} \cos \vartheta \quad Y_{l, 1} = -\sqrt{\frac{3}{8\pi}} \sin \vartheta e^{i\varphi}$$

$$Y_{l, -1} = \sqrt{\frac{3}{8\pi}} \sin \vartheta e^{-i\varphi}$$


---

$$\int \cos \vartheta Y_{l, m} Y_{l+1, m}^* d\omega = \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}}$$

$$\int \cos \vartheta Y_{l, m} Y_{l-1, m}^* d\omega = \sqrt{\frac{l^2 - m^2}{(2l+1)(2l-1)}}$$

$$\int \sin \vartheta e^{\pm i\varphi} Y_{l, m \mp 1} Y_{l+1, m}^* d\omega = \mp \sqrt{\frac{(l \pm m)(l+1 \pm m)}{(2l+1)(2l+3)}}$$

$$\int \sin \vartheta e^{\pm i\varphi} Y_{l, m \mp 1} Y_{l-1, m}^* d\omega = \pm \sqrt{\frac{(l \mp m)(l+1 \mp m)}{(2l+1)(2l-1)}}$$

$$Y_{1-1} = \sqrt{\frac{2}{10}} \frac{(m-1)(m+1)}{(s+1)(s-1)} - Y_{1+1} = \sqrt{\frac{2}{10}} \frac{(m-1)(m+1)}{(s+1)(s-1)}$$

$$Y_{1+1} = \sqrt{\frac{2}{10}} \frac{(m^2-1)}{(s+1)(s-1)} + Y_{1-1} = \sqrt{\frac{2}{10}} \frac{(m^2-1)}{(s+1)(s-1)}$$

$$Y_{1-1} = \sqrt{\frac{2}{10}} \frac{(m-1)(m+1)}{(s+1)(s-1)} - Y_{1+1} = \sqrt{\frac{2}{10}} \frac{(m-1)(m+1)}{(s+1)(s-1)}$$

$$Y_{10} = \sqrt{\frac{2}{10}} \cos \theta \quad Y_{1-1} = -\sqrt{\frac{2}{10}} \sin \theta$$

$$Y_{1-1} = \sqrt{\frac{2}{10}} \sin \theta$$

$$Y_{10} = \sqrt{\frac{2}{10}} \cos \theta = \frac{(m-1)(m+1)}{(s+1)(s-1)}$$

$$Y_{10} = \sqrt{\frac{2}{10}} \cos \theta = \frac{(m^2-1)}{(s+1)(s-1)}$$

$$Y_{10} = \sqrt{\frac{2}{10}} \cos \theta = \frac{(m-1)(m+1)}{(s+1)(s-1)}$$

$$Y_{10} = \sqrt{\frac{2}{10}} \cos \theta = \frac{(m-1)(m+1)}{(s+1)(s-1)}$$

selection rules

states

$$u_{nlm} = R_n(r) P_{lm}(\cos\theta) e^{im\varphi}$$

$$u_{n'l'm'} = R_{n'}(r) P_{l'm'}(\cos\theta) e^{im'\varphi}$$

$$x = r \sin\theta \cos\varphi$$

$$y = r \sin\theta \sin\varphi$$

$$z = r \cos\theta$$

$$x_{nlm, n'l'm'} = \int_0^\infty r^3 R_{n'}(r) R_n(r) dr \times$$

y

$$\times \int_0^\infty \sin^2\theta P_{l'm'}(\cos\theta) P_{lm}(\cos\theta) d\theta \times$$

$$\times \int_0^\infty \cos\varphi e^{i(m-m')\varphi} d\varphi$$

$$z_{nlm, n'l'm'} = \int_0^\infty r^3 R_{n'} R_n dr \times \int_0^\infty \sin\theta \cos\theta P_{l'm'} P_{lm} d\theta \times$$

$$\times \int_0^\infty e^{i(m-m')\varphi} d\varphi$$

$$\Delta m = 0, \pm 1$$

$$\Delta l = \pm 1$$

Lifetime of  $u_{210}$  of Hydrogen

$$z_{100,210} = \frac{2^7 \sqrt{2}}{3^5} a = 0.75 a$$

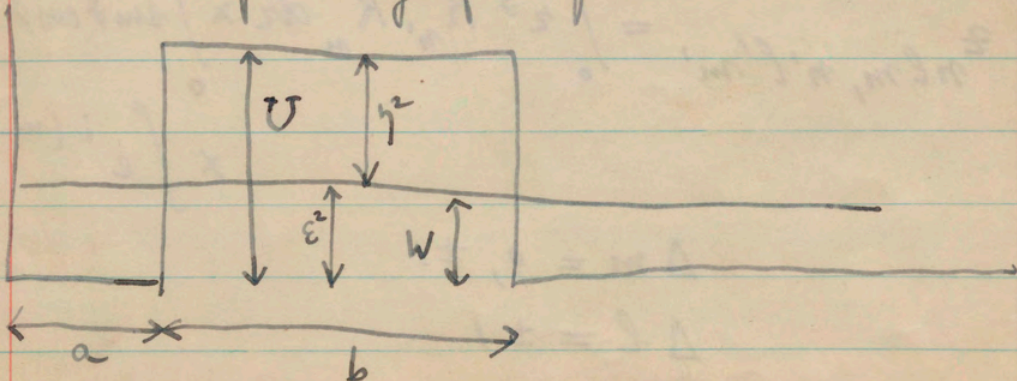
Theorem

be a homog polynomial of  $x y z$   
degree  $l$

Then

~~$$v_l = r^l \sum_{n=0}^l \sum_{m=-l+2n}^{l-2n} c_{l-2n,m} Y_{l-2n,m}$$~~

Transparency of a potential wall



$$\psi'' + \frac{8\pi^2 m}{h^2} (E - U) \psi = 0$$

$$4A^2 = e^{2by} \left( \sin \epsilon a + \frac{\epsilon}{\eta} \cos \epsilon a \right)^2 \left( 1 + \frac{\eta^2}{\epsilon^2} \right) +$$

$$+ 2 \left( \sin^2 \epsilon a - \frac{\epsilon^2}{\eta^2} \cos^2 \epsilon a \right) \left( 1 - \frac{\eta^2}{\epsilon^2} \right)$$

$$+ e^{-2by} \left( \sin \epsilon a - \frac{\epsilon}{\eta} \cos \epsilon a \right)^2 \left( 1 + \frac{\eta^2}{\epsilon^2} \right)$$

~~$$= \frac{p^2}{h^2} e^{2by} + 2P_0$$

$$e^{2by} \left( \frac{U - U_0}{\epsilon} \right)^2 + e^{-2by}$$~~

Gamow theory of  $\alpha$  particle emission

Life time  $\tau$

$$\frac{1}{\tau} \sim \frac{v}{a} e^{-2 \sqrt{\frac{8\pi^2 m}{h^2} (U - E)} b}$$

Gamow Pot barrier

~~$$P = \frac{16\pi^2}{h} \frac{2Ze^2}{\sigma} \left( \arccos \frac{1}{\sigma} - \sqrt{\frac{1}{\sigma} - \frac{1}{\sigma^2}} \right)$$~~

U	4.09	$4.410^9 \frac{1}{a}$
Ra	4.79	1550a
Rn	5.49	382d
RaC'	7.68	$10^{-5}$ sec

$$\sigma = \frac{2Ze^2}{E_0 \rho}$$

U 4.09 Mev  
~~P~~ S

## Spin of the electron (Pauli)

$$\begin{matrix} M_x \\ M_y \\ M_z \end{matrix}$$

$$M_y M_z - M_z M_y = -\frac{h}{2\pi i} M_x$$

$$\mu_x = \frac{h}{4\pi} \sigma_x$$

$$\mu_y = \frac{h}{4\pi} \sigma_y$$

$$\mu_z = \frac{h}{4\pi} \sigma_z$$

$$\sigma_y \sigma_z - \sigma_z \sigma_y = 2i \sigma_x$$

$$\sigma_x \sigma_y = -\sigma_y \sigma_x$$

$$\sigma_y \sigma_z = i \sigma_x$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi \\ 0 \end{pmatrix} = \begin{pmatrix} a\psi \\ b\psi \end{pmatrix} = \begin{pmatrix} \psi \\ 0 \end{pmatrix}$$

$$\begin{matrix} a=1 & d=-1 \\ c=0 & b=0 \end{matrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & e^{i\alpha} \\ e^{-i\alpha} & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & e^{i\beta} \\ e^{-i\beta} & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\alpha - \beta = \frac{\pi}{2} + n\pi$$

$$e^{i\alpha} \cos \theta - i e^{i\alpha} \sin \theta$$



Generalities on electron spin

Fourth coordinate  $\xi$

$$\psi(x, y, z, \xi)$$

$\xi$  is two valued (take  $\xi = \pm 1$ )

$$\psi(x, y, z, \xi) = \begin{cases} \psi_+(x, y, z) \\ \psi_-(x, y, z) \end{cases}$$

Spin operators  $\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$

Search for three operators

$$\sigma_x, \sigma_y, \sigma_z$$

to represent the 3 components of the spin vector  
Normalize them so that e.v. are  $\pm 1$ . Hence

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$$

Also with  $\alpha, \beta, \gamma$  arbitrary direction cosines

$$(\alpha \sigma_x + \beta \sigma_y + \gamma \sigma_z)^2 = 1$$

From this: anticommutation

$$\sigma_y \sigma_z + \sigma_z \sigma_y = 0, \dots$$

By proper choice of the base one can always  
assume

$$\sigma_z = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$$



$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_y \sigma_z = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i \sigma_x$$

$$\sigma_y \sigma_z - \sigma_z \sigma_y = 2i \sigma_x$$

$$\sigma \times \sigma = 2i \sigma$$

For angular momentum vectors

$$M \times M = -\frac{\hbar}{i} M$$

Suggests to take angular momentum associated to  $\sigma$

$$a \sigma \times a \sigma = -\frac{\hbar}{i} a \sigma$$

$$2ia^2 \sigma = -\frac{\hbar}{i} a \sigma$$

$$2a^2 = -\frac{\hbar}{i} \Rightarrow a = \frac{\hbar}{2}$$

Spin angular momentum =  $\frac{\hbar}{2} \sigma$

Spin magn. moment =  ~~$\mu_B$~~   $\frac{e\hbar}{2mc} \sigma$  to fit expt data

or from Dirac theory

$$H = H_0 + H_1 = \frac{p^2}{2m} - eV(r) + \frac{\mu_0 \hbar}{2mc} \frac{F(r)}{r} (l \cdot \sigma)$$

Unpert. e.f

$$\left| \begin{matrix} R_{nl}(r) Y_{lm}(\theta, \varphi) \\ 0 \end{matrix} \right| \text{ and } \left| \begin{matrix} 0 \\ R_{nl} Y_{lm} \end{matrix} \right|$$

$$(l_x + iy_l) Y_{lm} = -\sqrt{(l-m)(l+m+1)} Y_{l, m+1}$$

$$(l_x - iy_l) Y_{lm} = -\sqrt{(l+m)(l-m+1)} Y_{l, m-1}$$

$$l_z Y_{lm} = m Y_{lm}$$

$$(l, \sigma) = l_z \sigma_z + \frac{1}{2}(l_x + i l_y)(\sigma_x - i \sigma_y) + \frac{1}{2}(l_x - i l_y)(\sigma_x + i \sigma_y)$$

$$\frac{\sigma_x + i \sigma_y}{2} = \begin{vmatrix} 0 & 1 \\ 0 & 0 \end{vmatrix}$$

$$(l, \sigma) \begin{vmatrix} Y_{l,m} \\ 0 \end{vmatrix} = \begin{vmatrix} m Y_{l,m} \\ -\sqrt{(l-m)(l+m+1)} Y_{l,m+1} \end{vmatrix}$$

$$\frac{\sigma_x - i \sigma_y}{2} = \begin{vmatrix} 0 & 0 \\ 1 & 0 \end{vmatrix}$$

$$(l, \sigma) \begin{vmatrix} 0 \\ Y_{l,m+1} \end{vmatrix} = \begin{vmatrix} -\sqrt{(l+m+1)(l-m)} Y_{l,m} \\ -(m+1) Y_{l,m+1} \end{vmatrix}$$

Pert. matrix

$$\frac{\mu_0 \hbar}{2mc} \left( \int \frac{F(r)}{r} R_{nl}^2(r) r^2 dr \right) \begin{vmatrix} m & -\sqrt{(l-m)(l+m+1)} \\ -\sqrt{(l+m+1)(l-m)} & -(m+1) \end{vmatrix}$$

$$(m-x)(m+1+x) \neq (l-m)(l+1+m) = 0 \quad x = \begin{cases} l & j = l + \frac{1}{2} \\ -(l+1) & j = l - \frac{1}{2} \end{cases}$$

$$\vec{l} + \frac{1}{2} \vec{\sigma} = \vec{j} \quad j(j+1) = l(l+1) + \frac{3}{4} + (l, \sigma)$$

Eigenfunktionen

$$\text{Splitting} = (2l+1) \frac{\mu_0 \hbar}{2mc} \int \frac{F(r)}{r} R_{nl}^2 r dr$$

e.f.'s

$$j = l + \frac{1}{2} \quad m' = m + \frac{1}{2} \quad l, \sigma = l$$

$$R_{nl}(r) \begin{vmatrix} \sqrt{\frac{l+m+1}{2l+1}} Y_{l,m} \\ -\sqrt{\frac{l-m}{2l+1}} Y_{l,m+1} \end{vmatrix} \quad \begin{vmatrix} R_{nl}(r) \sqrt{(l-m)(l+m+1)} Y_{l,m} \\ \sqrt{(l-m)(2l+1)} \quad - (l-m) Y_{l,m+1} \end{vmatrix}$$

$$R_{nl}(r) \begin{vmatrix} \sqrt{\frac{l-m}{2l+1}} Y_{l,m} \\ \sqrt{\frac{l+m+1}{2l+1}} Y_{l,m+1} \end{vmatrix}$$

50

Systems with several particles &  
~~wave~~ eigenfunctions are products  
~~eigenvalues~~ are sums

$$H = H_1 + H_2 + H_3 + \dots + H_n$$

systems with two identical particles

$H$  is symmetrical

means

$$H \psi(x_1, x_2) = \psi(x_1, x_2)$$

$$H \psi(x_2, x_1) = \psi(x_2, x_1)$$

Follows: if

$$\psi(x_1, x_2) = \pm \psi(x_2, x_1)$$

also

$$\psi(x_1, x_2) = \pm \psi(x_2, x_1)$$

hence complete separation of sym & antisym states

same holds for many identical particles

Pauli principle

If wavefunctions are antisym no two particles can be in one well def quantum state

Bose Einstein statistics

Whereas functions are symmetrical a quantum state is defined by the occupation numbers

Two particle system.

Assume

$$H = H^{(1)} + H^{(2)}$$

$$= \frac{p_1^2}{2m_1} + U_1(x_1) + \frac{p_2^2}{2m_2} + U_2(x_2)$$

$$u_i^{(1)}(x_1) u_k^{(2)}(x_2)$$

Show completeness of system

Effect of interaction

$$H^{(12)}$$

Matrix elements

$$H_{ik,lm}^{(12)} = \int u_i^{(1)*}(x_1) u_k^{(2)*}(x_2) H^{(12)} u_l^{(1)}(x_1) u_m^{(2)}(x_2) dx_1 dx_2$$

So that in general

$$u(x_1, x_2)$$

Identical particles

$u(x_1, x_2)$  is same state as  $u(x_2, x_1)$

Hence

$$u(x_1, x_2) = \pm u(x_2, x_1)$$

Symmetric Hamiltonian does not change symmetry character - Hence character as initial -

Bose Einstein & Pauli particles

Spin and antisymmetry

$$u(x) u_\alpha(x_1, \xi_1) u_\beta(x_2, \xi_2) - u_\alpha(x_2, \xi_2) u_\beta(x_1, \xi_1)$$

He spectrum

1s <sup>2</sup>	1S <sub>0</sub>	198298
1s2s	3S <sub>1</sub>	38455
	1S <sub>0</sub>	32033
1s2p	3P	

mercury

6s <sup>2</sup>	84178
6s6p	46536
	44969
	40138

$$H = H_1 + H_2 + \frac{e^2}{r_{12}}$$

$$H_1 = \frac{p_1^2}{2m} + U(x_1) \quad H_2 = \frac{p_2^2}{2m} + U(x_2)$$

$$u_1(x) \dots u_n(x) \dots u_m(x) \dots$$

$$E_1 \quad E_n \quad E_m$$

$$\alpha(\xi) \text{ define } \alpha(1) = 1 \quad \alpha(-1) = 0$$

$$\beta(\xi) \quad \beta(1) = 0 \quad \beta(-1) = 1$$

one electron states  $n$   
 $u_n(x) \alpha(\xi)$  or  $u_n(x) \beta(\xi)$

two electron states  $n, m$

$$\Psi_1 = \frac{1}{\sqrt{2}} [u_n(x_1) \alpha(\xi_1) u_m(x_2) \alpha(\xi_2) - u_m(x_1) \alpha(\xi_1) u_n(x_2) \alpha(\xi_2)]$$

$$\Psi_2 = \frac{1}{\sqrt{2}} [u_n(x_1) \alpha(\xi_1) u_m(x_2) \beta(\xi_2) - u_m(x_1) \beta(\xi_1) u_n(x_2) \alpha(\xi_2)]$$

$$\Psi_3 = \frac{1}{\sqrt{2}} [u_n(x_1) \beta(\xi_1) u_m(x_2) \alpha(\xi_2) - u_m(x_1) \alpha(\xi_1) u_n(x_2) \beta(\xi_2)]$$

$$\Psi_4 = \frac{1}{\sqrt{2}} [u_n(x_1) \beta(\xi_1) u_m(x_2) \beta(\xi_2) - u_m(x_1) \beta(\xi_1) u_n(x_2) \beta(\xi_2)]$$

normalization  $1/\sqrt{2}$

$$|u_n(x_1)|^2 |u_m(x_2)|^2 \alpha^2(\xi_1) \beta^2(\xi_2) +$$

$$|u_m(x_1)|^2 |u_n(x_2)|^2 \beta^2(\xi_1) \alpha^2(\xi_2) -$$

$$- \underbrace{u_n(x_1) u_m^*(x_1)} \cdot \underbrace{u_m(x_2) u_n^*(x_2)} \alpha(\xi_1) \beta(\xi_1) \alpha(\xi_2) \beta(\xi_2) \cdot$$

- comp cov

$$\int_{\xi_1, \xi_2} \int d^3x_1 d^3x_2 = \left( \int |u_n(x)|^2 dx \right) \left( \int |u_m(x)|^2 dx \right) \left( \sum_{\xi_1=\pm 1} \alpha^2(\xi_1) \right) \left( \sum_{\xi_2=\pm 1} \beta^2(\xi_2) \right)$$



Perturb. matrix  $\times$  4x4 elements

Prove that  
on one or  
two examples

	1	2	3	4
1	0	0	0	
2		0	0	
3	0	0	0	0
4	0	0	0	

so six matrix elements

$$\begin{aligned}
 \mathcal{H}_{11} = \frac{e^2}{2} \iint \sum_{\xi_1 \neq 1} \sum_{\xi_2 \neq 1} \frac{dx_1 dx_2}{r_{12}} & \left( \underbrace{u_n^*(x_1)}_{-} \underbrace{u_m^*(x_2)}_{-} \alpha(\xi_1) \alpha(\xi_2) \underbrace{u_n(x_1)}_{-} \underbrace{u_m(x_2)}_{-} \alpha(\xi_1) \alpha(\xi_2)}_{-} \right. \\
 & - u_n^*(x_1) u_m^*(x_2) \alpha(\xi_1) \alpha(\xi_2) u_n(x_1) u_m(x_2) \alpha(\xi_1) \alpha(\xi_2) \\
 & - u_m^*(x_1) u_n^*(x_2) \alpha(\xi_1) \alpha(\xi_2) u_m(x_1) u_n(x_2) \alpha(\xi_1) \alpha(\xi_2) \\
 & \left. + u_m^*(x_1) u_n^*(x_2) \alpha(\xi_1) \alpha(\xi_2) u_m(x_1) u_n(x_2) \alpha(\xi_1) \alpha(\xi_2) \right)
 \end{aligned}$$

Sum part comes out and is = 1

1st & 4th line equal their sum is

$$A = e^2 \iint \frac{|u_n(x_1)|^2 |u_m(x_2)|^2}{r_{12}} dx_1 dx_2$$

2nd & 3rd lines equal their sum

$$-B = e^2 \iint \frac{u_n^*(x_1) u_m^*(x_2) u_m(x_1) u_n(x_2)}{r_{12}} dx_1 dx_2 \text{ is real}$$

Total

$$\mathcal{H}_{11} = A - B$$

Similar

$$\mathcal{H}_{44} = A - B$$

$$\mathcal{H}_{22} = \mathcal{H}_{33} = A$$

$$\mathcal{H}_{23} = \mathcal{H}_{32} = -B$$

$\mathcal{H}_{23}$

$$\begin{vmatrix}
 A-B & 0 & 0 & 0 \\
 0 & A & -B & 0 \\
 0 & -B & A & 0 \\
 0 & 0 & 0 & A-B
 \end{vmatrix}$$

Find e.v. solving separately

(2) 50

$|A-B|$  has e.v  $\epsilon = A-B$

$$\begin{vmatrix} A-\epsilon-B & \\ -B & A-\epsilon \end{vmatrix} = 0 \quad \epsilon^2 - 2A\epsilon + A^2 - B^2 = 0$$

$$A \pm \sqrt{A^2 - A^2 + B^2} = A \pm \sqrt{B^2} = A \pm B$$

$$\epsilon = \begin{cases} A-B \\ A+B \end{cases}$$

$|A-B| \quad \epsilon = A-B$

three times  $A-B$   
once  $A+B$

Find e.f's to  $\epsilon = A-B$

$$\psi_1 = \frac{1}{\sqrt{2}} \left\{ u_m(x_1) u_m(x_2) - u_m(x_1) u_n(x_2) \right\} \alpha(\epsilon_1) \alpha(\epsilon_2)$$

$$\psi_4 = \frac{1}{\sqrt{2}} \left\{ \beta(\epsilon_1) \beta(\epsilon_2) \right\}$$

also substitute  $\epsilon = A-B$  in sec. determinant

$$\begin{vmatrix} B & -B \\ -B & B \end{vmatrix} = 0$$

minors are coefficients  
they are equal  
hence sum  $\frac{\psi_2 + \psi_3}{\sqrt{2}}$

$$\frac{\psi_2 + \psi_3}{\sqrt{2}} = \frac{1}{\sqrt{2}} \left\{ u_m(x_1) u_m(x_2) - u_m(x_1) u_n(x_2) \right\} \frac{\alpha(\epsilon_1) \beta(\epsilon_2) + \alpha(\epsilon_2) \beta(\epsilon_1)}{\sqrt{2}}$$

Converp to  $\epsilon = A+B$

$$\begin{array}{c} \begin{array}{|cc|} \hline -B & -B \\ \hline -B & -B \\ \hline \end{array} \quad \begin{array}{l} \text{minors } -B, +B \\ \text{or} \\ 1, -1 \end{array} \\ \frac{1}{\sqrt{2}}(\psi_2 - \psi_3) \end{array}$$

$$\frac{\psi_2 - \psi_3}{\sqrt{2}} = \frac{1}{\sqrt{2}} \left\{ u_m(x_1) u_m(x_2) + u_m(x_2) u_m(x_1) \right\} \frac{\alpha(\psi_1) \beta(\psi_2) - \beta(\psi_1) \alpha(\psi_2)}{\sqrt{2}}$$

Notice to  $\epsilon = A - B$   
 e.f. orbital part antisym  
 spin part sym

to  $\epsilon = A + B$   
 orbital anti  
 spin symmetric

Consider spin functions only  
 symmetric

$$\begin{array}{l} \alpha(\psi_1) \alpha(\psi_2) \\ \frac{\alpha(\psi_1) \beta(\psi_2) + \alpha(\psi_2) \beta(\psi_1)}{\sqrt{2}} \\ \beta(\psi_1) \beta(\psi_2) \end{array}$$

antisymmetric

$$\frac{\alpha(\psi_1) \beta(\psi_2) - \beta(\psi_1) \alpha(\psi_2)}{\sqrt{2}}$$

Statement: For sym states  
 For antis state

in units  $\hbar$

$$\begin{array}{l} S = s_1 + s_2 = 1 \text{ or } S^2 = 1 \times 2 = 2 \\ S = 0 \text{ or } S^2 = 0 \end{array}$$

$$\vec{S}_1 = \frac{1}{2} \vec{\sigma}_1 \quad \vec{S}_2 = \frac{1}{2} \vec{\sigma}_2$$

$$S^2 = \frac{1}{4} \left[ (\sigma_{1x} + \sigma_{2x})^2 + (\sigma_{1y} + \sigma_{2y})^2 + (\sigma_{1z} + \sigma_{2z})^2 \right] = \frac{1}{4} (6 + 2(\sigma_{1x}\sigma_{2x} + \dots))$$

$$S^2 = \frac{3}{2} + \frac{1}{2} (\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z})$$

$$\sigma_x \alpha(\beta) = \beta(\beta)$$

$$\sigma_x \beta = \alpha$$

$$\sigma_y \alpha = i\beta$$

$$\sigma_y \beta = -i\alpha$$

$$\sigma_z \alpha = \alpha$$

$$\sigma_z \beta = -\beta$$

(3)<sup>50</sup>

$$(\sigma_1 \cdot \sigma_2) \alpha \alpha = \beta \beta + i^2 \beta \beta + \alpha \alpha = \alpha \alpha$$

$$(\sigma_1 \cdot \sigma_2) \frac{\alpha \beta + \beta \alpha}{\sqrt{2}} = \frac{(\beta \alpha - i^2 \beta \alpha - \alpha \beta) + (\alpha \beta - i^2 \alpha \beta) - \beta \alpha}{\sqrt{2}} = \frac{\beta \alpha + \alpha \beta}{\sqrt{2}}$$

$$(\sigma_1 \cdot \sigma_2) \beta \beta = \beta \beta$$

for sym for  $(\sigma_1 \cdot \sigma_2) = 1$   $S^2 = \frac{3}{2} + \frac{1}{2} = 2$

antis

$$(\sigma_1 \cdot \sigma_2) \frac{\alpha \beta - \beta \alpha}{\sqrt{2}} = \frac{(\quad) - (\quad)}{\sqrt{2}} = -3 \frac{\beta \alpha - \alpha \beta}{\sqrt{2}}$$

$$(\sigma_1 \cdot \sigma_2) = -3 \quad S^2 = \frac{3}{2} - \frac{3}{2} = 0$$

$$S_z = \frac{1}{2} (\sigma_{1z} + \sigma_{2z}) \left\{ \begin{array}{l} \alpha \alpha \\ \frac{\alpha \beta + \beta \alpha}{\sqrt{2}} \\ \beta \beta \end{array} \right\} = 0 \times \frac{\alpha \beta + \beta \alpha}{\sqrt{2}} - 1 \times \beta \beta$$

$$S_z \frac{\alpha \beta - \beta \alpha}{\sqrt{2}} = 0$$

Hence - Spin sym states are said to have  
total spin 1 (Spins ||)

Spin antis states have total spin 0  
(Spins antiparallel)

Case  $n = m$  and general discussion  
of the He spectrum

Three states, two particles

~~Boltzmann~~

state	Born	BE	Pauli								
(200)	<table border="1"><tr><td>ab</td><td></td></tr></table>	ab		<table border="1"><tr><td>aa</td><td></td></tr></table>	aa		—				
ab											
aa											
(020)	<del>—</del>		—								
(002)			—								
(011)	<table border="1"><tr><td>a</td><td>b</td></tr></table> <table border="1"><tr><td>b</td><td>a</td></tr></table>	a	b	b	a	<table border="1"><tr><td>a</td><td>a</td></tr></table>	a	a	<table border="1"><tr><td>a</td><td>a</td></tr></table>	a	a
a	b										
b	a										
a	a										
a	a										

Pauli principle with spin

$$\psi(x_1, \xi_1, x_2, \xi_2) = -\psi(x_2, \xi_2, x_1, \xi_1)$$

$$\psi_{++}(x_1, x_2) = -\psi_{++}(x_2, x_1)$$

$$\psi_{--}(x_1, x_2) = -\psi_{--}(x_1, x_2)$$

$$\psi_{+-}(x_1, x_2) = -\psi_{-+}(x_2, x_1)$$

Suppose  $H$  contains only operators acting on the coordinates; then e.v. problem gives

$$H \psi_{++}(x_1, x_2) = E \psi_{++}(x_1, x_2)$$

$$H \psi_{+-}(x_1, x_2) = E \psi_{+-}(x_1, x_2)$$

$$H \psi_{-+}(x_1, x_2) = E \psi_{-+}(x_1, x_2)$$

$$H \psi_{--}(x_1, x_2) = E \psi_{--}(x_1, x_2)$$

Let  $E_a \neq E_s$  be two <sup>non deg</sup> (eigenvalues of  $H$  ~~two~~ with e.f.  $u_a(x_1, x_2) = -u_a(x_2, x_1)$  and  $u_s(x_1, x_2) = u_s(x_2, x_1)$ )

Without symmetry limitations one would expect:

for  $H = E_a$

quadruple degeneracy

$$H = E_a \begin{cases} u_a(x_1, x_2) = \psi_{++} ; \psi_{+-} = \psi_{-+} = \psi_{--} = 0 \\ u_a = \psi_{+-} ; \psi_{++} = \psi_{-+} = \psi_{--} = 0 \\ u_a = \psi_{-+} \text{ others zero} \\ u_a = \psi_{--} \text{ others zero} \end{cases}$$

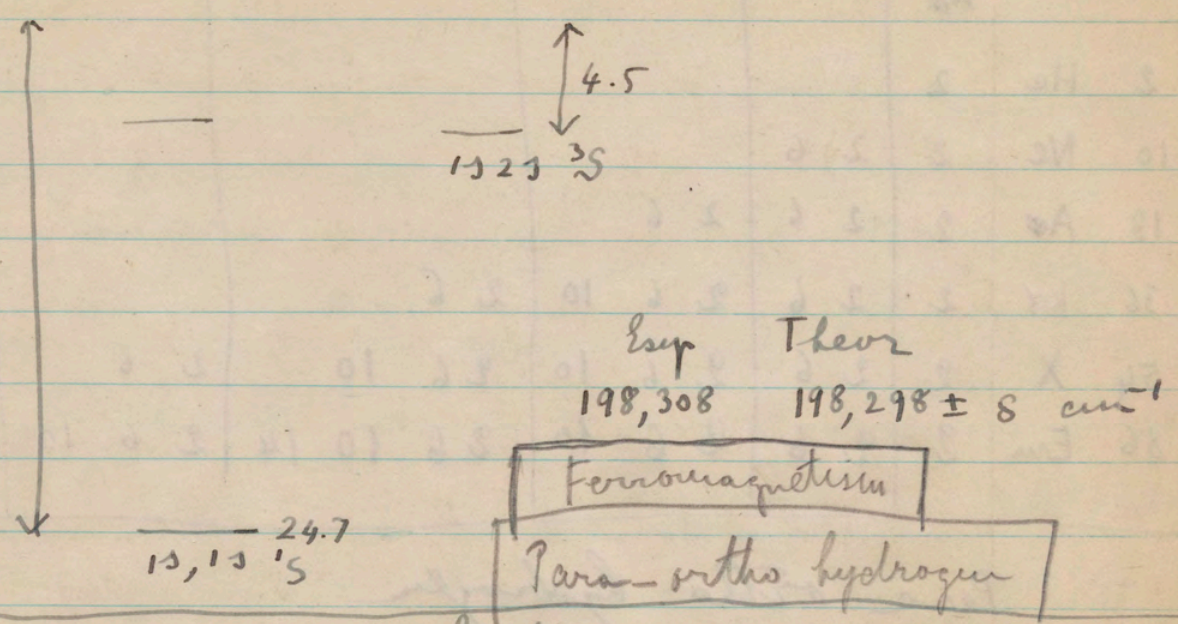
good combinations for electrons

$$H = E_s \begin{cases} u_s = \psi_{++} & \text{others zero} \\ u_s = \psi_{+-} & \text{u} & \text{u} \\ u_s = \psi_{-+} & \text{u} & \text{u} \\ u_s = \psi_{--} & \text{u} & \text{u} \end{cases}$$

$$\begin{aligned} u_s &= \psi_{++} \\ \frac{1}{\sqrt{2}} u_s &= \frac{\psi_{+-}}{\sqrt{2}} ; \frac{\psi_{-+}}{\sqrt{2}} \\ u_s &= \psi_{--} \end{aligned}$$

Helium spectrum

Para Ortho



~~Ortho & Para Hydrogen~~ Periodic System

H								
He								
Li	Be	B	C	N	O	F	Ne	
Na	Mg	Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co Ni
Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	(43)	Ru	Rh Pd
Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	[La	Ce	Pr	Nd	Sm	Eu	Gd Tb Dy Ho Er Tm Yb Lu]
		Hf	Ta	W	Re		Os	Ir Pt
1 Au	Hg	Tl	Pb	Bi	Po	(85)	Em	
(87) Ra	Ac	Th	Pa	U				



54

	1s	2s 2p	3s 3p 3d	4s 4p 4d 4f	5s 5p 5d	6s 6p
2 He	2					
10 Ne	2	2 6				
18 Ar	2	2 6	2 6			
36 Kr	2	2 6	2 6 10	2 6		
54 Xe	2	2 6	2 6 10	2 6 10	2 6	
86 Em	2	2 6	2 6 10	2 6 10 14	2 6 10	2 6

Para or the hydrogen

Atom in the magnetic field.

# Perturbations with quasi degeneracy

$$\begin{array}{cccc} \omega_1 & \approx & \omega_2 & \omega_3 \\ u_1^{(0)} & & u_2^{(0)} & u_3^{(0)} & u_4^{(0)} \end{array}$$

$$u = c_1 u_1^{(0)} + c_2 u_2^{(0)} + c_3 u_3^{(0)} + c_4 u_4^{(0)}$$

$c_1, c_2$  order of magnitude 1

$$c_3 \ll 1 \quad c_4 \ll 1 \dots$$

$$(H_0 + \mathcal{H}) (c_1 u_1^{(0)} + c_2 u_2^{(0)} + c_3 u_3^{(0)} + \dots) = \omega c_1 u_1^{(0)} + \omega c_2 u_2^{(0)} + \omega c_3 u_3^{(0)} + \dots$$

$$c_1 \omega_1^{(0)} u_1^{(0)} + c_2 \omega_2^{(0)} u_2^{(0)} + c_3 \omega_3^{(0)} u_3^{(0)} + \dots$$

$$+ c_1 \mathcal{H} u_1^{(0)} + c_2 \mathcal{H} u_2^{(0)} + c_3 \mathcal{H} u_3^{(0)} + \dots = \omega c_1 u_1^{(0)} + \omega c_2 u_2^{(0)} + \omega c_3 u_3^{(0)} + \dots$$

$$c_1 (\omega_1^{(0)} - \omega) u_1^{(0)} + c_2 (\omega_2^{(0)} - \omega) u_2^{(0)} + c_3 (\omega_3^{(0)} - \omega) u_3^{(0)} +$$

$$+ c_1 \mathcal{H} u_1^{(0)} + c_2 \mathcal{H} u_2^{(0)} + \text{higher terms} = 0$$

56

Exam Winter 1937

An electron is bound to move on a spherical surface of radius  $10^{-8}$  cm. Find its energy levels and the <sup>wavelength of the radiation</sup> emitted in the transition between the two lowest energy levels.

Discuss the  $\psi$  Schrödinger equation of a mass point that moves on a plane in a central field of force. ~~Discuss~~  
~~analogous to that for a~~

A linear harmonic oscillator is per-<sub>2</sub>turbed by a force with potential energy  $kx^4$ . Find the first order perturbation of the first and second energy levels.

An electron movable on a spherical surface is perturbed by a constant electric field. Find the perturbation of the second  $\psi$  energy level.

The four operators  
 $x$ ,  $\frac{d}{dx}$ ,  $\frac{d^2}{dx^2}$ ,  $\log x$   
act on functions of  $x$ .

~~State what~~ For <sup>all pairs</sup> any two of them state whether or not they commute. If they don't commute find the difference between the products taken in different order

## Pauli's theory of spin

$\sigma_x$   $\sigma_y$   $\sigma_z$  are operators on the subspace functions of two valued spin variable with eigenvalues  $\pm 1$

$$\sigma_z u_+ = u_+$$

$$\sigma_z u_- = -u_-$$

$$\text{angular momentum} = \frac{\hbar}{4\pi} \sigma$$

$$\sigma \times \sigma = 2i\sigma$$

$$\sigma_z = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$$

$$\sigma_x = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}$$

$$\sigma_y = \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}$$

Example with  $\alpha, \beta, \gamma$  cosines of direction  
~~Measurement of~~ Eigenvalues of

$$\sigma_n = \alpha \sigma_x + \beta \sigma_y + \gamma \sigma_z = \begin{vmatrix} \gamma & \alpha + i\beta \\ \alpha + i\beta & -\gamma \end{vmatrix}$$

are  $\pm 1$

If measurement gives  $\sigma_n = +1$   
Then

$$\gamma \psi_+ + (\alpha - i\beta) \psi_- = \psi_+$$

$$(\alpha + i\beta) \psi_+ - \gamma \psi_- = \psi_-$$

$$\begin{vmatrix} \psi_+ \\ \psi_- \end{vmatrix} \text{ proportional to } \begin{vmatrix} 1 + \gamma \\ \alpha + i\beta \end{vmatrix} \xrightarrow{\text{normalised}} \frac{1}{\sqrt{2(1+\gamma)}} \begin{vmatrix} 1 + \gamma \\ \alpha + i\beta \end{vmatrix}$$

$$1 + \gamma^2 + 2\gamma \quad 2(1 + \gamma)$$

$$\frac{(1 + \gamma)^2}{2(1 + \gamma)} = \frac{1 + \cos\theta}{2} = \cos^2 \frac{\theta}{2}$$

$$\frac{\alpha^2 + \beta^2}{2(1 + \gamma)} = \frac{1 - \cos\theta}{2} = \sin^2 \frac{\theta}{2}$$

Hamiltonian of electron in <sup>em</sup> field  
(non relativistic)

$$\frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + eV = W$$

$$\dot{x} = \frac{\partial W}{\partial p_x} = \frac{1}{m} \left( p_x - \frac{e}{c} A_x \right) \quad m\dot{x} + \frac{e}{c} A_x = p_x$$

$$\dot{p}_x = m\ddot{x} + \frac{e}{c} \left( \frac{\partial A_x}{\partial t} + \frac{\partial A_x}{\partial x} \dot{x} + \frac{\partial A_x}{\partial y} \dot{y} + \frac{\partial A_x}{\partial z} \dot{z} \right) =$$

$$= - \frac{\partial W}{\partial x} = -e \frac{\partial V}{\partial x} + \frac{e}{c} \left( \dot{z} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_y}{\partial x} + \dot{x} \frac{\partial A_z}{\partial x} \right)$$

$$m\ddot{x} = eE + \frac{e}{c} (\dot{y} H_z - \dot{z} H_y)$$

Uniform magnetic field  $H \parallel z$

$$A_x = -\frac{H}{2} y$$

$$A_y = +\frac{H}{2} x$$

$$W = \frac{p^2}{2m} + eV + \frac{eH}{2mc} (y p_x - x p_y)$$

$$\frac{p^2}{2m} + eV + \frac{eH}{2mc} (y p_x - x p_y)$$

Normal Zeeman effect

Bohr Magneton  
Apparent field due to spin orbit interaction

$$\begin{aligned} \frac{Ze}{r^2} \frac{v}{c} \sin \theta &= \frac{Ze}{mc} \frac{m \vec{v} \times \vec{r}}{r^3} \\ &= \frac{Ze}{mc} \frac{\vec{M}}{r^3} \end{aligned}$$

Thomas factor  $\frac{1}{2}$

In general for electron in <sup>central</sup> field  
Apparent field

$$\left(\frac{1}{2}\right) \frac{v}{c} E(r) \sin \theta = \frac{1}{mc} \frac{E(r)}{r} M_x \left(\frac{1}{2}\right) \quad \left(\frac{1}{2}\right)$$

Complete Hamilton function for electron in central field  $V$  & uniform magnetic field  $H_z$

$$\begin{aligned} \frac{p^2}{2m} + eV(r) - \frac{eH}{2mc} M_z - \frac{e\hbar H}{4\pi mc} \sigma_z + \\ + \frac{1}{2mc} \frac{1}{r} \frac{\partial V}{\partial r} \frac{\hbar}{4\pi mc} (M \sigma) \end{aligned}$$

# Bohr magneton from current density

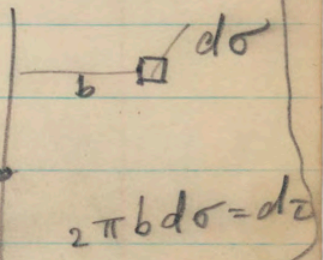
(14) (15)

$$J = \frac{eh}{4\pi m ic} (\psi^* \text{grad} \psi - \psi \text{grad} \psi^*)$$

$$\psi = e^{im\varphi} v(r, \vartheta)$$

$$J = \frac{eh}{4\pi m ic} v^2(r, \vartheta) \frac{2im}{b} \hat{\phi}$$

$$\mu = \int_{\text{half meridian plane}} J d\sigma \times 2\pi b^2 = \frac{eh}{4m\pi c} m \int v^2 d\tau = \frac{eh}{4\pi m c} \underline{m}$$



## Spin in magnetic field

$$\frac{eh}{4\pi m c} (H_x \sigma_x + H_y \sigma_y + H_z \sigma_z)$$

## Description of the spin motion in a magnetic field

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \begin{pmatrix} \gamma & \alpha - i\beta \\ \alpha + i\beta & -\gamma \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$$

$$\begin{aligned} \gamma \psi_+ + (\alpha - i\beta) \psi_- &= \psi_+ \\ (\alpha + i\beta) \psi_+ - \gamma \psi_- &= \psi_- \end{aligned}$$



62

Discussion of  $f(r)$ 

$$\frac{p^2}{2m} + eV(r) + \left( \frac{\mu_0}{2mc} \frac{1}{r} \frac{\partial V}{\partial r} \right) (M \cdot \sigma) = \mathcal{H}$$

$$\frac{\hbar}{i} \dot{M} = \sum_{\mathbf{r}} \left( \mathcal{H} M - M \mathcal{H} \right) = \frac{\mu_0}{2mc} \frac{1}{r} \left( f(r) (M \cdot \sigma) M - M f(r) (M \cdot \sigma) \right)$$

$$M_x \sigma_x f(r) M_x - M_x f(r) M_x$$

$$= f(r) (y p_x - z p_y) - (y p_x - z p_y) f(r) = 0$$

$$\left( f(r) p_x - p_x f(r) \right) = -\frac{\hbar}{i} f'(r) \frac{z}{r}$$

$$(M \cdot \sigma) M - M (M \cdot \sigma)$$

$$(M_x \sigma_x + M_y \sigma_y + M_z \sigma_z) M_x - M_x (M_x \sigma_x + M_y \sigma_y + M_z \sigma_z)$$

$$\sigma_x \sigma_x = 2i \sigma \quad M \times M = -\frac{\hbar}{i} M$$

$$+ \frac{\hbar}{i} (M_z \sigma_y - M_y \sigma_z)$$

$$(M \cdot \sigma) M - M (M \cdot \sigma) =$$

$$= -\frac{\hbar}{i} \{ M \times \sigma \}$$

(r

Conservation of angular momentum

$$(M \cdot \sigma) \sigma - \sigma (M \cdot \sigma) = 2i \sigma$$

Motion of orientation of spin in magnetic field

$$\psi_+ \sim 1 + \gamma = 1 + \cos \vartheta$$

$$\psi_- \sim \alpha + i\beta = \sin \vartheta e^{i\varphi} \quad \frac{\psi_+}{\psi_-} = \frac{\sin \vartheta e^{-i\varphi}}{1 - \cos \vartheta}$$

~~$$\frac{\psi_-}{\psi_+} = \frac{\sin \vartheta e^{i\varphi}}{1 + \cos \vartheta}$$~~

$$\frac{\psi_-}{\psi_+} = \frac{\sin \vartheta}{1 + \cos \vartheta} e^{i\varphi}$$

~~$$\psi_+ = \frac{1}{\sqrt{2(1 + \cos \vartheta)}}$$~~

~~$$\frac{(\alpha + i\beta)(\alpha - i\beta)}{1 - \gamma}$$~~

~~$$H | \gamma \rangle = \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = -\frac{\hbar}{i\mu} \begin{pmatrix} \dot{\psi}_+ \\ \dot{\psi}_- \end{pmatrix}$$~~

~~$$\hat{H}_+ = H_z \quad \dot{\psi}_+ = -\frac{i\mu}{\hbar} (H_z \psi_+ + (H_x - iH_y) \psi_-)$$~~

~~$$\dot{\psi}_- = -\frac{i\mu}{\hbar} ((H_x + iH_y) \psi_+ - H_z \psi_-)$$~~

~~$$\frac{d}{dt} \frac{\psi_-}{\psi_+} = \frac{\dot{\psi}_-}{\psi_+} - \frac{\psi_- \dot{\psi}_+}{\psi_+^2} = -\frac{i\mu}{\hbar} \left[ (H_x + iH_y) - 2H_z \frac{\psi_-}{\psi_+} - \right.$$~~

~~$$\left. - \frac{\psi_-}{\psi_+} (H_x - iH_y) \frac{\psi_-}{\psi_+} \right]$$~~

64

$$l_x = \frac{1}{\hbar} M_x \quad l_y = \frac{1}{\hbar} M_y \quad l_z = \frac{1}{\hbar} M_z$$

$$\vec{l} \times \vec{l} = i \vec{l} \quad l_x = \frac{i}{\hbar} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$l_z Y_{lm}(\vartheta, \varphi) = m Y_{lm}(\vartheta, \varphi)$$

$$(l_x + i l_y) Y_{lm}(\vartheta, \varphi) = -\sqrt{(l-m)(l+m+1)} Y_{l, m+1}(\vartheta, \varphi)$$

$$(l_x - i l_y) Y_{lm}(\vartheta, \varphi) = -\sqrt{(l+m)(l-m+1)} Y_{l, m-1}(\vartheta, \varphi)$$

$$\vec{l} + \frac{1}{2} \vec{\sigma} = \vec{j}$$

$$l_z + \frac{1}{2} \sigma_z = m$$

$$l^2, j^2, m, (\text{etc.})$$

commute among each other and with the energy operator

$$\mathcal{H} = \frac{p^2}{2m} + eV + f(r)(\vec{l} \cdot \vec{\sigma})$$

take therefore  $f(r) = -\frac{\hbar \mu_0}{2mc} \frac{1}{r} \frac{\partial V}{\partial r}$

~~$$l^2 = l(l+1)$$~~

~~$$m = m$$~~

~~$$\sigma^2 = \frac{3}{4}$$~~

~~$$j^2 = l(l+1) + \frac{3}{4} + (\vec{l} \cdot \vec{\sigma})$$~~

eigenvalues of  $\mathcal{J}_m$  are ~~half integral~~ integral +  $\frac{1}{2}$  numbers (half odd numbers)  
Hence to  $l, m$  corresponds e.f.

$$\begin{vmatrix} R Y_{l, m-\frac{1}{2}} \\ Q Y_{l, m+\frac{1}{2}} \end{vmatrix}$$

$(l, \sigma)$  has eigenvalues  $l$   
 $-(l+1)$

Corresponding e.f. are (normalised)

$$(l, l+\frac{1}{2}, m) = \frac{1}{\sqrt{2l+1}} \begin{vmatrix} \sqrt{l+\frac{1}{2}+m} Y_{l, m-\frac{1}{2}} \\ -\sqrt{l+\frac{1}{2}-m} Y_{l, m+\frac{1}{2}} \end{vmatrix} \quad \text{for } (l\sigma)=l$$

~~$l$~~   $j = l + \frac{1}{2}$

and

$$(l, l-\frac{1}{2}, m) = \frac{1}{\sqrt{2l+1}} \begin{vmatrix} \sqrt{l+\frac{1}{2}-m} Y_{l, m-\frac{1}{2}} \\ \sqrt{l+\frac{1}{2}+m} Y_{l, m+\frac{1}{2}} \end{vmatrix} \quad \text{for } (l\sigma)=-l$$

~~$l$~~   $j = l - \frac{1}{2}$

generalised spin functions (note special case of  $l=0$ )  
effective potential

$$-eV + lf(r) \quad \text{for } j = l + \frac{1}{2}$$

$$-eV - (l_{eff})f(r) \quad \text{for } j = l - \frac{1}{2}$$

Systematic spectroscopic notations

$A$  is an operator  
 classify the functions (vectors of Hilbert space)  
 calling a class of functions (or vectors)  
 those that fulfill

$$A\psi = a\psi \quad (\text{Class } A=a)$$

If  $a$  is a non-degenerate e.v. of  $A$   
 there ~~is~~ the class is made by the vectors  
 parallel to one - When there is degeneracy  
 the class has a subspace of the Hilbert  
 space of ~~at~~ more than one dimension

Theorem:

If  $AB = BA$   
 and  $\psi$  belongs to the  $A=a$  class  
 also

By  $B\psi$   
 belongs to the  $A=a$  class

Proof

$$A\psi = a\psi$$

$$BA\psi = aB\psi$$

$$A(B\psi) = a(B\psi)$$

Q.E.D.

Since ~~the~~ ~~class~~ ~~belongs~~ belongs to the  $A=a$  class we may consider the operator  $B$  in this Hilbert sub-space

There  $B$  will have eigen values and e.f in number equal to the dimensions of the sub-space - They are obtained as solutions of the system

$$\begin{cases} A\psi = a\psi \\ B\psi = b\psi \end{cases}$$

Such a system defines a sub-class of the class  $A=a$  that may have any number of dimensions  $\geq 1$  and  $\leq$  the no of dimensions of class  $A=a$ ; we call this sub class class  $A=a, B=b$

Let  $C$  be a third operator that commutes with both  $A$  and  $B$

$$AC=CA, \quad BC=CB$$

All we said of  $B$  with respect to class  $A=a$  holds of  $C$  with respect to the class  $A=a, B=b$

And so forth

Example  $\mathcal{H}_0 = \frac{r^2}{2m} - eV(r) + f(r)(l, \sigma)$

~~group~~ The operators  $\mathcal{H}_0, \vec{L}^2, \vec{j}^2$   $j_z = m$  intercommute (hence classification of terms)

From spin spherical functions follows

$$\bar{\sigma}_z = \pm \frac{2m}{2l+1} \quad \text{for } j = l \pm \frac{1}{2}$$

Zeeman effect  
perturbation

$$W_{\text{mag}} = H\mu_0 (l_z + \sigma_z) = H\mu_0 \left( m + \frac{1}{2}\bar{\sigma}_z \right)$$

Since  $m$  commutes with the perturbation we can neglect the degeneracy; hence in first approximation

$$\bar{W}_{\text{mag}} = H\mu_0 m \left( 1 \pm \frac{1}{2l+1} \right) \quad \text{for } j = l \pm \frac{1}{2}$$

Discussion: semiclassical derivation of  $g$  factors of Landé

$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

$$\sigma_z(l, l+\frac{1}{2}, m) = \frac{2m}{2l+1} (l, l+\frac{1}{2}, m) + \frac{2\sqrt{(l+\frac{1}{2})^2 - m^2}}{2l+1} (l, l-\frac{1}{2}, m)$$

$$\sigma_z(l, l-\frac{1}{2}, m) = \frac{2\sqrt{(l+\frac{1}{2})^2 - m^2}}{2l+1} (l, l+\frac{1}{2}, m) - \frac{2m}{2l+1} (l, l-\frac{1}{2}, m)$$

Perturbation matrix of Paschen-Back effect is

$$H\mu_0(m + \frac{1}{2}\sigma) + \mathcal{H}_0$$

$$H\mu_0 m + \begin{vmatrix} w + a & \\ 0 & 0 \end{vmatrix} + \frac{H\mu_0}{2l+1} \begin{vmatrix} m \sqrt{(l+\frac{1}{2})^2 - m^2} & \\ \sqrt{\quad} & -m \end{vmatrix}$$

$w$  = energy difference between terms with  $j = l + \frac{1}{2}$  and  $j = l - \frac{1}{2}$

Put

$$a = \frac{2l+1}{H\mu_0} w$$

$$\begin{vmatrix} m+a & \sqrt{\quad} \\ \sqrt{\quad} & -m \end{vmatrix} \text{ has e. values } \frac{a \pm \sqrt{a^2 + 4am + 4(l+\frac{1}{2})^2}}{2}$$



# Identical particles

Operator  $H$  is symmetrical

$H\psi_{\text{sim}}$  is symmetrical

$H\psi_{\text{antis}}$  is antisymmetrical

Particles with sym and antis wave functions.

Individual quantum states

$$H = H_1 + H_2$$

a) System of independent particles

$$SH = HS$$

Symmetrical operators

$S$  = symmetrical operator

a) Independent particles

Energy sum

Wave functions products

Individual quantum states

Symmetry properties of operators

Symmetry operation  $S$

b)  $SA = AS$  is equivalent to say that  $A$  has the symmetry  $S$

Examples (rotation of space — Reflection exchange of identical particles)

See pages 50-54

$$H = H_1 + H_2 + \mathcal{H}_2$$

$H_1(q_1)$      $H_2 = H_1(q_1)$      $\mathcal{H}_2$  symmetrical

Degeneracy with individual states

$$\psi_m(x_1) \psi_m(x_2) \quad \psi_m(x_1) \psi_m(x_2) \quad E = W_m + W_m$$

Several particles

Definition of symm and antis

$$H \psi = W \psi$$

Case of individual quantum states

~~W~~  $\sum_{(P)} \psi_{m_{p1}}(x_1) \psi_{m_{p2}}(x_2) \dots \psi_{m_{pA}}(x_A)$  [(-1)^P]

Pauli principle (go back pages 50-54)  
Statistics (50-51)

Pauli principle with Spin (p. 51)

Para & orthohelium (p. 52, 53)

Periodic system p 53-54

Diracs Wave function

$$\gamma_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \gamma_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

$$\gamma_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \quad \delta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$W = eV - c\left(\boldsymbol{\gamma} \cdot \mathbf{p} - \frac{e\mathbf{A}}{c}\right) - mc^2\delta$$

$$(W - eV)^2 = c^2\left(\mathbf{p} - \frac{e\mathbf{A}}{c}\right)^2 + m^2c^4$$

$$W\psi_1 - \frac{\hbar}{i} \frac{\partial \psi_1}{\partial t} = \cancel{eV\psi_1} - \frac{c\hbar}{i} \left[ \frac{\partial \psi_4}{\partial x} - i \frac{\partial \psi_4}{\partial y} + \frac{\partial \psi_3}{\partial z} \right] + e \left[ (A_x - iA_y)\psi_4 + A_z\psi_3 \right]$$

$$W\psi_2 - \frac{\hbar}{i} \frac{\partial \psi_2}{\partial t} = \cancel{eV\psi_2} - \frac{c\hbar}{i} \left[ \frac{\partial \psi_3}{\partial x} + i \frac{\partial \psi_3}{\partial y} - \frac{\partial \psi_4}{\partial z} \right] + e \left[ (A_x + iA_y)\psi_3 - A_z\psi_4 \right]$$

$$W\psi_3 - \frac{\hbar}{i} \frac{\partial \psi_3}{\partial t} = \cancel{eV\psi_3} - \frac{c\hbar}{i} \left[ \frac{\partial \psi_2}{\partial x} - i \frac{\partial \psi_2}{\partial y} + \frac{\partial \psi_1}{\partial z} \right] + e \left[ (A_x - iA_y)\psi_2 + A_z\psi_1 \right]$$

$$W\psi_4 - \frac{\hbar}{i} \frac{\partial \psi_4}{\partial t} = \cancel{eV\psi_4} - \frac{c\hbar}{i} \left[ \frac{\partial \psi_1}{\partial x} + i \frac{\partial \psi_1}{\partial y} - \frac{\partial \psi_2}{\partial z} \right] + e \left[ (A_x + iA_y)\psi_1 - A_z\psi_2 \right]$$

Plane waves

$$W \text{ near } mc^2$$

$$W = mc^2 + E$$

$$E \ll mc^2$$

$$2m\psi_1 = -\frac{e\hbar}{2mic} \left[ \frac{\partial \psi_4}{\partial x} - i \frac{\partial \psi_4}{\partial y} + \frac{\partial \psi_3}{\partial z} \right]$$

$$\psi_2 = -\frac{\hbar}{2imc} \left[ \frac{\partial \psi_3}{\partial x} + i \frac{\partial \psi_3}{\partial y} - \frac{\partial \psi_4}{\partial z} \right]$$

Plane waves

$$E\psi_3 = eV\psi_3 + \frac{c\hbar}{i} \frac{\hbar}{2mic} \Delta \psi_3$$

$$2mc^2 \left( 1 + \frac{E-eV}{2mc^2} \right)$$

$$(2mc^2 + E - eV)\psi_1 = -\frac{c\hbar}{i} \left[ \frac{\partial \psi_4}{\partial x} - \dots \right] + e \left[ (A_x - iA_y)\psi_4 + \dots \right]$$

$$\psi_1 = -\frac{\hbar}{2imc} \left[ \frac{\partial \psi_4}{\partial x} - \dots \right] + \frac{e}{2mc^2} \left[ (A_x - iA_y)\psi_4 + A_z\psi_3 \right]$$

~~Back~~

$$(E - eV)\psi_3 = -\frac{\hbar^2}{2m} \Delta \psi_3 + \frac{e\hbar}{2mci} \left[ (A_x - iA_y) \frac{\partial \psi_3}{\partial x} + \dots \right]$$

74

$$\frac{\partial \psi_3}{\partial x} + i \frac{\partial \psi_3}{\partial y} - \frac{\partial \psi_4}{\partial z}$$

$$(A_x + iA_y)\psi_3 - A_z \psi_4$$

$$2mc^2 \left(1 + \frac{E - eV}{2mc^2}\right) \psi_1 = -\frac{c\hbar}{i} \left(\frac{\partial \psi_4}{\partial x} - i \frac{\partial \psi_4}{\partial y} + \frac{\partial \psi_3}{\partial z}\right) + e \left[ (A_x - iA_y)\psi_4 + A_z \psi_3 \right]$$

$$\psi_1 = -\frac{\hbar}{2imc} \left(\frac{\partial \psi_4}{\partial x} \dots\right) + \frac{e}{2mc^2} (A_x \psi_4 \dots) + \frac{E - eV}{2mc^2} \frac{\hbar}{2imc} \left(\frac{\partial \psi_4}{\partial x} \dots\right)$$

$$\psi_2 = -\frac{\hbar}{2imc} \left(\frac{\partial \psi_3}{\partial x} \dots\right) + \frac{e}{2mc^2} (A_x \psi_3 \dots) + \frac{E - eV}{2mc^2} \frac{\hbar}{2imc} \left(\frac{\partial \psi_3}{\partial x} \dots\right)$$

$$(E - eV)\psi_3 = -\frac{c\hbar}{i} \left(\frac{\partial \psi_2}{\partial x} - i \frac{\partial \psi_2}{\partial y} + \frac{\partial \psi_1}{\partial z}\right) + e \left[ (A_x - iA_y)\psi_2 + A_z \psi_1 \right]$$

$$(E - eV)\psi_3 = -\frac{\hbar^2}{2m} \Delta \psi_3 - \frac{e\hbar}{2mci} \left[ A_x \frac{\partial \psi_3}{\partial x} + \frac{\partial A_x}{\partial x} \psi_3 + \right.$$

$$\left. + i A_y \frac{\partial \psi_3}{\partial x} + i \frac{\partial A_y}{\partial x} \psi_3 - A_z \frac{\partial \psi_4}{\partial x} - \frac{\partial A_z}{\partial x} \psi_4 - i A_x \frac{\partial \psi_3}{\partial y} - i \frac{\partial A_x}{\partial y} \psi_3 \right.$$

$$\left. + A_y \frac{\partial \psi_3}{\partial y} + \frac{\partial A_y}{\partial y} \psi_3 + i \frac{\partial A_z}{\partial y} \psi_4 - i A_z \frac{\partial \psi_4}{\partial y} + A_x \frac{\partial \psi_4}{\partial z} + \frac{\partial A_x}{\partial z} \psi_4 \right.$$

$$\left. - i A_y \frac{\partial \psi_4}{\partial z} - i \frac{\partial A_y}{\partial z} \psi_4 \right.$$

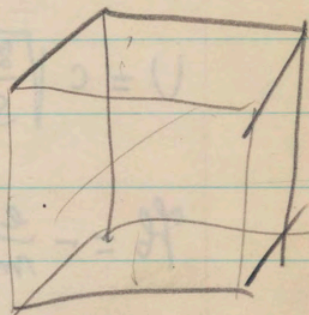
$$dN = \frac{8\pi}{c^3} \Omega v^2 dv$$

$$U = A u(t) \sin\left(\frac{2\pi v}{c} (\alpha \cdot r) + \beta\right)$$

$$U = \sum_s A_s u_s(t) \sin \Gamma_s = \sum U_s$$

$$\Gamma_s = \frac{2\pi v_s}{c} \alpha_s \cdot r + \beta_s$$

$$E = -\frac{1}{c} \frac{\partial U}{\partial t} \quad H = \text{rot } U$$



$$E = -\frac{1}{c} \sum_s A_s \dot{u}_s \sin \Gamma_s$$

$$H = \sum_s \frac{2\pi v_s}{c} [\alpha_s \times A_s] u_s \cos \Gamma_s$$

$$\overline{E^2} = \frac{1}{2c^2} \sum_s \dot{u}_s^2 \quad \overline{H^2} = \sum \frac{2\pi^2 v_s^2}{c^2} u_s^2$$

$$W_e = \frac{\Omega}{8\pi c^2} \sum_s$$

$$v = \frac{c}{a} (n_x^2 + n_y^2 + n_z^2)$$

$$\sin\left(\frac{2\pi}{a} (n_x x + \dots)\right) = \frac{2\pi v}{c}$$

$$\frac{\pi}{6} \frac{a^3 v^3}{c^3} \quad \frac{\pi}{2} \frac{a^3}{c^3} v^2 dv \quad \frac{2\pi}{c} \left(\frac{a}{c} v\right)^2 \frac{a}{c} dv$$

$$8\pi \frac{a^3}{c^3} v^2 dv$$

76

$$H = \frac{p^2}{2m} + eV + \sum_s \left( \frac{p_s^2}{2} + 2\pi^2 \gamma_s^2 q_s^2 \right) + \mathcal{H}_b$$

$$\mathcal{H}_b = -\frac{e}{mc} (\mathbf{U} \cdot \mathbf{p})$$

$$\mathbf{U} = c \sqrt{\frac{8\pi}{\Omega}} \sum_s \mathbf{A}_s q_s \sin \Gamma_s$$

$$\mathcal{H}_b = -\frac{e}{m} \sqrt{\frac{8\pi}{\Omega}} \sum_s (\mathbf{A}_s \cdot \mathbf{p}) q_s \sin \Gamma_s$$

for

$$\int q_s u_{n_s} u_{m_s} dq_s = \begin{cases} 0 & m_s \neq n_s \pm 1 \\ \sqrt{\frac{\hbar}{8\pi^2 \gamma_s}} \sqrt{n_s + 1} & m_s = n_s + 1 \\ \sqrt{\frac{\hbar}{8\pi^2 \gamma_s}} \sqrt{n_s} & m_s = n_s - 1 \end{cases}$$

$$\mathcal{H}_b_{n n_s; m n_s \pm 1} = -\frac{e}{m} \sqrt{\frac{8\pi}{\Omega}} \sqrt{\frac{\hbar}{8\pi^2 \gamma_s}} \begin{cases} \sqrt{n_s + 1} \\ \text{or} \\ \sqrt{n_s} \end{cases} (\mathbf{A}_s \cdot \mathbf{P}_{snm})$$

$$P_{snm} = \int u_n^* \left( \frac{\partial}{\partial z} \sin \Gamma_s \right) u_m dz =$$

$$= \frac{\hbar}{2\pi i} \int \sin \Gamma_s u_n^* \frac{\partial u_m}{\partial z} dz$$

$$\int u_m^* \frac{\partial u_n}{\partial x} d\tau =$$

$$\Delta u_n + \frac{8\pi^2 m}{h^2} (E_n - eV) u_n = 0$$

$$\Delta u_m^* + \frac{8\pi^2 m}{h^2} (E_m - eV) u_m^* \neq 0$$

$$u_m^* \Delta u_n - u_n \Delta u_m^* = \frac{8\pi^2 m}{h^2} (E_n - E_m) u_n u_m^*$$

$$\text{div} (u_m^* \text{grad} u_n - u_n \text{grad} u_m^*) = \frac{8\pi^2 m}{h^2} (E_n - E_m) u_n u_m^*$$

$$\mathcal{R} \text{div} ( \quad ) = \frac{8\pi^2 m}{h^2} (E_n - E_m) \mathcal{R} u_n u_m^*$$

$$- \int \left( u_m^* \frac{\partial u_n}{\partial x} - u_n \frac{\partial u_m^*}{\partial x} \right) d\tau = \frac{8\pi^2 m}{h^2} (E_n - E_m) \chi_{mn}$$

$$- \int u_m^* \frac{\partial u_n}{\partial x} d\tau = \frac{4\pi^2 m}{h^2} (E_n - E_m) \chi_{mn}$$

$$- \frac{2\pi i}{h} p_{mn} = \frac{4\pi^2 m}{h^2} (E_n - E_m) \chi_{mn}$$

$$p_{mn} = 2\pi i m \chi_{mn}$$



78

$$\dot{a}_{n n_s} = \frac{4\pi^{3/2} e}{\sqrt{h\Omega}} \sum_{ms} \frac{\nu_{mn}}{\sqrt{\nu_s}} (A_s \cdot r_{nm}) \sin \Gamma_s \times$$

$$\times \left[ a_{m n_{s+1}} \sqrt{n_{s+1}} e^{-2\pi i (\nu_{mn} + \nu_s) t} + a_{m n_{s-1}} \sqrt{n_{s-1}} e^{-2\pi i (\nu_{mn} - \nu_s) t} \right]$$

Emission of radiation

$$a_{m 0}(0) = 1$$

$$\dot{a}_{n 1_s} = \frac{4\pi^{3/2} e}{\sqrt{h\Omega}} \frac{\nu_{mn}}{\sqrt{\nu_s}} (A_s \cdot r_{nm}) \sin \Gamma_s e^{-2\pi i (\nu_{mn} - \nu_s) t}$$

$$a_{n 1_s} = \frac{4\pi^{3/2} e}{\sqrt{h\Omega}} \frac{\nu_{mn}}{\sqrt{\nu_s}} (A_s \cdot r_{nm}) \sin \Gamma_s \frac{e^{-2\pi i (\nu_{mn} - \nu_s) t} - 1}{-2\pi i (\nu_{mn} - \nu_s)}$$

$$|a_{n 1_s}|^2 = \frac{16\pi e^2}{h\Omega} \frac{\nu_{mn}^2}{\nu_s} |A_s \cdot r_{nm}|^2 \sin^2 \Gamma_s \frac{\sin^2 \pi t (\nu_{mn} - \nu_s)}{(\nu_{mn} - \nu_s)^2}$$

H. W. W. W. W.

Physics 238 Def ~~Sept~~ 1940

- 1) Discuss the meaning of the following Pauli operators:

$$\sigma_z, \sigma_x + i\sigma_y, \sigma_x \sigma_y \sigma_z.$$

- 2) Discuss the electronic configurations of the fundamental states of the following elements:  
Al ( $Z=13$ ); Kr ( $Z=36$ ).

- 3) Discuss the lowest energy levels of the element Ca ( $Z=20$ ).

- 4) Find the Zeeman effect pattern of a  ${}^2F_{5/2}$  and  ${}^2F_{7/2}$  terms of the spectrum of an alkali atom.

Born theory

Born + classical theory for Coulomb field

Exact collision theory

Born theory of anelastic collision

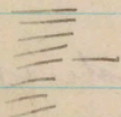
Born theory of collisions in which a particle is absorbed and a different particle is emitted ( $n, \gamma$ ) - processes

Compound nucleus

Physics 247 (Winter 1940-41) 81  
Collision theory

$$a_{\mathbf{k}} = -\frac{i}{\hbar} \sum_m \int \mathcal{H}_{\mathbf{k}j} a_{mj} e^{\frac{i}{\hbar} (w_{\mathbf{k}} - w_{mj}) t}$$

prob of transition =  $\frac{2\pi}{\hbar} |\mathcal{H}_{\mathbf{k}j}|^2$  <sup>n</sup> ~~number of states~~  
per unit energy



Born approximation

$$\psi_{jn} = \frac{1}{\sqrt{\Omega}} e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}}$$

$$\psi_{\mathbf{k}} = \frac{1}{\sqrt{\Omega}} e^{\frac{i}{\hbar} \mathbf{q} \cdot \mathbf{r}}$$

$$\mathcal{H}_{\mathbf{k}j} = \frac{1}{\Omega} \int V(\mathbf{r}) e^{\frac{i}{\hbar} (\vec{\mathbf{p}} - \vec{\mathbf{q}} \cdot \vec{\mathbf{r}})}$$

no of states  $\frac{\Omega}{h^3} p^2 dp d\omega$

energy interval  $v dp$

$$n = \frac{\Omega}{8\pi^3 \hbar^3} \frac{p^2 d\omega}{v}$$

prob of transition =  $\frac{1}{\Omega} v \sigma_{d\omega} = \frac{2\pi}{\hbar} \frac{1}{\Omega^2} \left| \int V e^{\frac{i}{\hbar} (\vec{\mathbf{p}} - \vec{\mathbf{q}} \cdot \vec{\mathbf{r}})} d\tau \right|^2$

$$\sigma_{d\omega} = \frac{1}{4\pi^2 \hbar^4} \frac{p^2}{v^2} \left| \int V e^{\frac{i}{\hbar} (\vec{\mathbf{j}} - \vec{\mathbf{k}} \cdot \vec{\mathbf{r}})} d\tau \right|^2 d\omega$$

$\times \frac{2}{8\pi^3 \hbar^3} \frac{p^2}{v} d\omega$

Conditions:

no substantial perturbation of the e.f. hence either

a) very large energy

$$W \gg |V|$$

b) for small energy: small radius of action  $\rho$  and precisely

$$\frac{\hbar}{\sqrt{mV}} \gg \rho \quad \text{or} \quad \frac{mV\rho^2}{\hbar^2} \ll 1$$

Condition b) is equivalent to

$$\frac{V\rho^2}{\hbar^2} \ll 1$$

scattering cross-section  $\ll$  geometrical cross-section

Special cases ~~a) b)~~

Coulomb field

$$V = \frac{Ze^2}{r}$$

$$Ze^2 \int \frac{1}{r} e^{\frac{i}{\hbar} P \cdot r} = \frac{4\pi\hbar^2}{p^2} Ze^2$$

$$P = \rho p \sin \frac{\theta}{2}$$

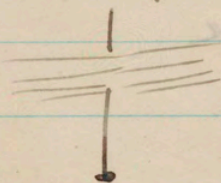
$$-\sqrt{\frac{p^2}{\hbar^2}} \dots = + \frac{4\pi Ze^2 \hbar^2}{p^2}$$

$$\sigma_{d\omega} = \frac{m^2 d\omega}{4\pi^2 \hbar^4} \frac{16\pi^2 \hbar^4 Z^2 e^4}{16\rho^4 \sin^4 \frac{\theta}{2}} =$$

Limit to validity

$$\frac{Ze^2}{mv^2} \ll \frac{\hbar}{mv} \quad \text{or} \quad \frac{Ze^2}{\hbar v} \ll 1$$

Limit of classical theory



$$\frac{Ze^2}{r^2} \frac{\hbar}{v} \gg \frac{\hbar}{mv} \quad \text{or} \quad \frac{Ze^2}{\hbar v} \gg 1$$

hence two limitations are complementary since result is the same for Born & classical theory it may be expected to be exact

Small energy: isotropic scattering

$$\sigma = \frac{m^2}{\pi \hbar^4} \left| \int V d\tau \right|^2$$

valid provided  $\sigma \ll \rho^2$

Large energies: scattering within angle

$$\frac{\hbar}{m} \rho \theta < 1 \quad \theta < \frac{\hbar}{\rho}$$

84

See QG 6

$$\psi = e^{\frac{i}{\hbar} p z} + \sum_{l=0}^{\infty} P_l^{(0)}(\cos\theta) \frac{a_l}{z} e^{\frac{i}{\hbar} p z}$$

$$\overline{P_l^{(0)2}} = \frac{1}{2l+1}$$

incident  $\frac{p}{l}$  per  $\text{cm}^2 \text{ sec}$

$$\frac{4\pi}{2l+1} |a_l|^2 \frac{p}{m} = \sigma_l \frac{p}{m}$$

$$\sigma_l = \frac{4\pi}{2l+1} |a_l|^2$$

$P_l^0$  (page 10)

$$e^{\frac{i}{\hbar} p z} = \sum_l \varphi_l(z) P_l^{(0)}(\cos\theta)$$

$$\frac{4\pi}{2l+1} \varphi_l(z) = \int_0^\pi e^{\frac{i}{\hbar} p z \cos\theta} P_l^{(0)}(\cos\theta) 2\pi \sin\theta d\theta$$

$$\frac{2}{2l+1} \varphi_l(z) = \int_{-1}^1 e^{\frac{i p z}{\hbar} x} P_l^{(0)}(x) dx$$

$$2\varphi_0(z) = \frac{2\hbar}{p z} \left( \sin \frac{p z}{\hbar} \right)$$

$$\varphi_0(z) = \frac{\hbar}{p z} \sin \frac{p z}{\hbar}$$

$$\varphi_l(z) = \sqrt{\frac{\pi}{2}} \sqrt{\frac{\hbar}{p z}} i^l (2l+1) P_l^{(0)}(\cos\theta) J_{l+\frac{1}{2}}\left(\frac{p z}{\hbar}\right)$$

$$a(1)b(2) \pm b(1)a(2) = \begin{matrix} \psi_+ \\ \psi_- \end{matrix}$$

$$H = \frac{p_1^2 + p_2^2}{2m} + \frac{e^2}{r} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} - \frac{e^2}{r_{b2}}$$

$$\int \psi_+^* H \psi_+ \mathcal{Q}$$

Step a (normalisation)

$$\begin{aligned} & \iint (a(1)b(2) + b(1)a(2))^2 d\tau_1 d\tau_2 = \\ & = \int a^2(1) d\tau_1 \int b^2(2) d\tau_2 + \int b^2(1) d\tau_1 \int a^2(2) d\tau_2 + \\ & \quad + 2 \int a(1)b(1) d\tau_1 \int a(2)b(2) d\tau_2 \\ & = 2 [1 + \beta^2] \quad \beta = \int a(1)b(1) d\tau_1 \end{aligned}$$

$$\psi_+ = \frac{a(1)b(2) + b(1)a(2)}{\sqrt{2(1 + \beta^2)}}$$

$$\psi_- = \frac{a(1)b(2) - b(1)a(2)}{\sqrt{2(1 - \beta^2)}}$$

spins  
antipar

spins  
parallel

Note  $\beta = 0$  if  
e.f. do not overlap.  
Would be 1 for  
coincident nuclei



The density of neutrons of any given energy in a lattice containing a large number of cells is a function of the position in the lattice. One can arrive at a simple mathematical description of the behavior of such a system by neglecting in first approximation the local variation of such functions due to the periodic structure of the lattice and substituting for the actually inhomogeneous system an equivalent homogeneous system. In this section we shall accordingly simplify the problem by substituting for all densities of neutron values obtained by averaging the actual values over the volume of the cell. The densities will then be represented by smooth functions such as one would expect in a homogeneous uranium-graphite mixture.

Let  $\rho(x, y, z)$  be the number of fast neutrons produced per unit time and unit volume at each position in the lattice. These neutrons diffuse through the mass and are slowed down. During this process some of the neutrons are absorbed at resonance. Let  $q(x, y, z)$  be the number of neutrons per unit time and unit volume which become thermal at the position  $x, y, z$ . We shall assume that if an original fast neutron is generated at a point  $O$  the probability that it becomes thermal at a given place has a Gaussian distribution around  $O$ . This assumption may be justified by considering that the diffusion process of slowing down consists of very many free paths. Experimentally one finds that the distribution curve of the nascent thermal neutrons around a point source of fast neutrons is represented only approximately by a Gaussian distribution and formulas have been used in which the actual distribution is described as a super-position of two or three Gaussian curves with different ranges. For the purpose of the present discussion, however, we shall take only one. For each fast neutron produced

Lattice Containing a Large Number of Cells

$$E_+ = \iint \psi_+^\dagger H \psi_+ d\tau_1 d\tau_2$$

R = Rydberg energy

Use

$$\left( \frac{p_1^2}{2m} - \frac{e^2}{r_{a1}} \right) a(1) = -R a(1)$$

~~$$H \psi_+ = \frac{1}{\sqrt{2(1+\beta^2)}} \left( \frac{p_1^2}{2m} a(1) b(2) + \frac{p_2^2}{2m} a(2) b(1) + \frac{e^2}{r} a(1) b(2) + \frac{e^2}{r} a(2) b(1) - \frac{e^2}{r_{a1}} a(1) b(2) - \frac{e^2}{r_{a2}} a(2) b(1) - \frac{e^2}{r_{b1}} a(1) b(2) - \frac{e^2}{r_{b2}} a(2) b(1) \right)$$~~

$$\frac{p_1^2}{2m} a(1) = \left( \frac{e^2}{r_{a1}} - R \right) a(1)$$

$$H a(1) b(2) = \frac{e^2}{r_{a1}} - R + \frac{e^2}{r_{b2}} - R + \frac{e^2}{r} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}}$$

$$= -2R + \frac{e^2}{r} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}}$$

$$E_+ = -2R + \frac{e^2}{r} + \frac{1}{2(1+\beta^2)} \iint (a(1)b(2) + b(1)a(2)) \times$$

$$\times \left[ \left( \frac{e^2}{r_{12}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} \right) a(1)b(2) + \left( \frac{e^2}{r_{12}} - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{b2}} \right) b(1)a(2) \right] d\tau_1 d\tau_2$$

$$E_{\pm} = -2R + \frac{e^2}{r} + \frac{1}{1 \pm \beta^2} \iint \left( \frac{e^2}{r_{12}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} \right) a^2(1) b^2(2) d\tau_1 d\tau_2 +$$

$$\pm \frac{1}{1 \pm \beta^2} \iint \left( \frac{e^2}{r_{12}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} \right) a(1) b(1) a(2) b(2) d\tau_1 d\tau_2$$

where  $\lambda$  is the reflection coefficient of the jump for thermal neutrons.

$$(9) \quad \lambda = \frac{\sqrt{3} \lambda' (1 - \lambda')}{\lambda' + \lambda}$$

of length. It is further

expressed taking the diffusion length in graphite  $L = \sqrt{\lambda' V/3}$  as unit where  $\alpha$  and  $\beta$  represent the radius of the lump and the radius of the cell

$$(8) \quad f = \frac{3\alpha^2}{3\alpha^2 - \beta^2} \frac{(\alpha + \lambda - \alpha\lambda)(1 + \beta)^2 - (\alpha + \lambda + \alpha\lambda)^2}{(1 - \alpha)(1 + \beta)^2 - (\beta + \alpha)^2 - (1 + \alpha)(1 - \beta)^2 - \beta - \alpha}$$

be absorbed by uranium:

Finds the following formula for the probability  $f$  that thermal neutrons the dimensions of the cell are not too large. With these assumptions one graphite part of the cell. This approximation is fairly correct provided energies per unit time and unit volume is constant throughout in the also assumed that the number of neutrons that are slowed down to thermal of the density of neutrons vanishes at the surface of the sphere. It is of the actual cell with the boundary condition that the radial derivative substitute the lattice cell by a spherical cell having volume equal to that  $n_G$  and  $n_U$  using the diffusion theory. The approximation is made to sub- For practical purposes it is usually sufficiently accurate to calculate

$$(7) \quad f = \frac{N_U \sigma_U n_U}{N_U \sigma_U n_U + N_G \sigma_G n_G}$$

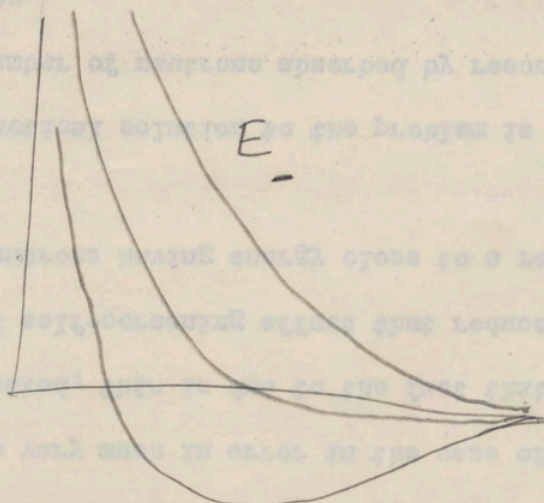
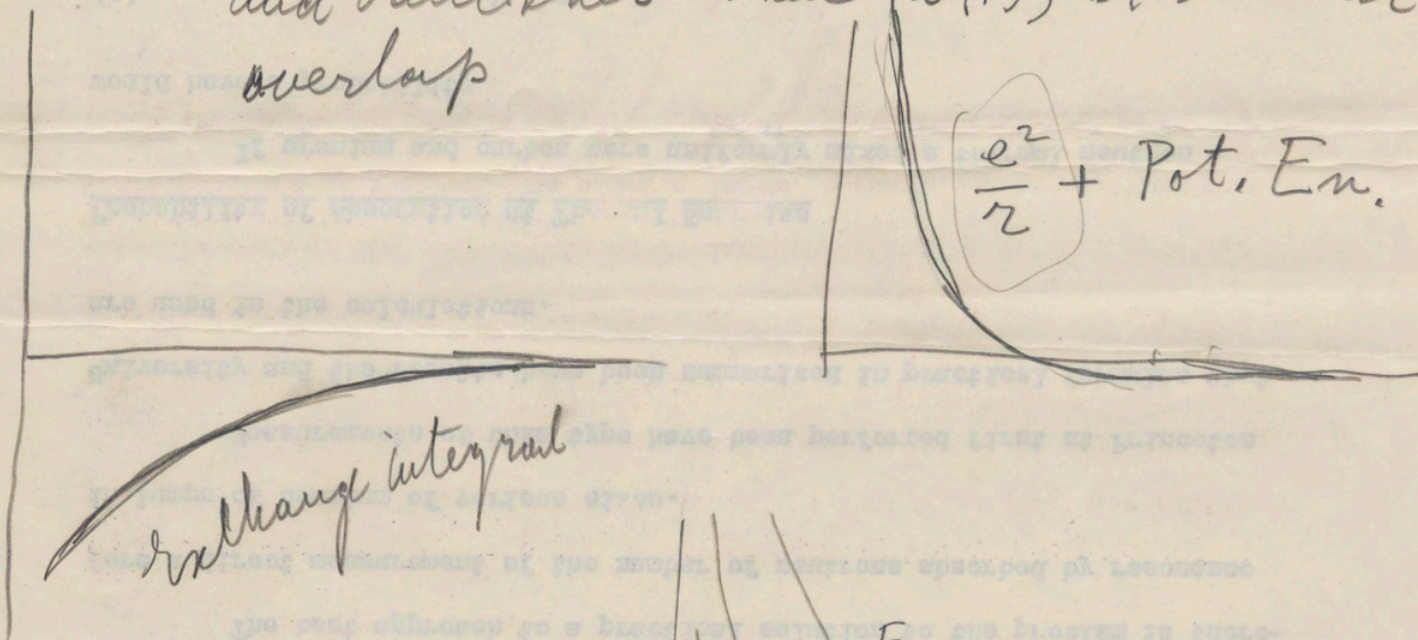
and we will have therefore, instead of Eq. (6) the corrected formula uranium and by carbon will be proportional to  $N_U \sigma_U n_U$  and  $N_G \sigma_G n_G$

Discussion

take this as  $-2R$  is the energy of the two separate atoms  
 zero energy  $\frac{e^2}{r}$  " " pot energy of the nuclei

3rd factor apart of  $\beta$  which is small  
 $\int \psi(1) \psi(2)$  is electrostatic interaction

4th factor is called exchange  
 and vanishes when  $a(1), b(1)$  don't overlap



$E_+$  solution stable  
 $E_-$  solution repulsive ) In normal  $H_2$  molecule, spins N electrons

The above formula would be very much in error in the case of a lattice of lumps. As already indicated, this is due to the fact that inside a lump there is an important self-screening effect that reduces very considerably the density of neutrons having energy close to a resonance maximum. The best approach to a practical solution to the problem is therefore a direct measurement of the number of neutrons absorbed by resonance in lumps of uranium of various sizes. Measurements of this type have been performed first at Princeton University and the results have been summarized in practical formulas that are used in the calculations.

Probability of Absorption at Thermal Energies

If uranium and carbon were uniformly mixed a thermal neutron would have a probability

$$(6) \quad \frac{N_C \sigma_C + N_U \sigma_U}{N_U \sigma_U}$$

to be absorbed by uranium. In this formula  $N_C$  and  $N_U$  represent the numbers of atoms of carbon and of uranium per unit volume; and  $\sigma_C$  and  $\sigma_U$  represent the cross-sections of carbon and uranium for thermal neutrons. More complicated is the case of a lattice distribution of lumps of uranium in graphite, since the density of thermal neutrons throughout the system is not uniform but is large at the places far from the uranium lumps and smaller near and inside the uranium lumps, due to the fact that the absorption of thermal neutrons is much greater in uranium than in graphite. Let  $n_U$  and  $n_G$  be the average densities of thermal neutrons in the graphite and in the uranium lumps. The number of thermal neutrons absorbed by

# Different approx

Consider as zero approx

1 electron in field of 2 nuclei



or  $a(1) + b(1)$   
 and  $a(1) - b(1)$

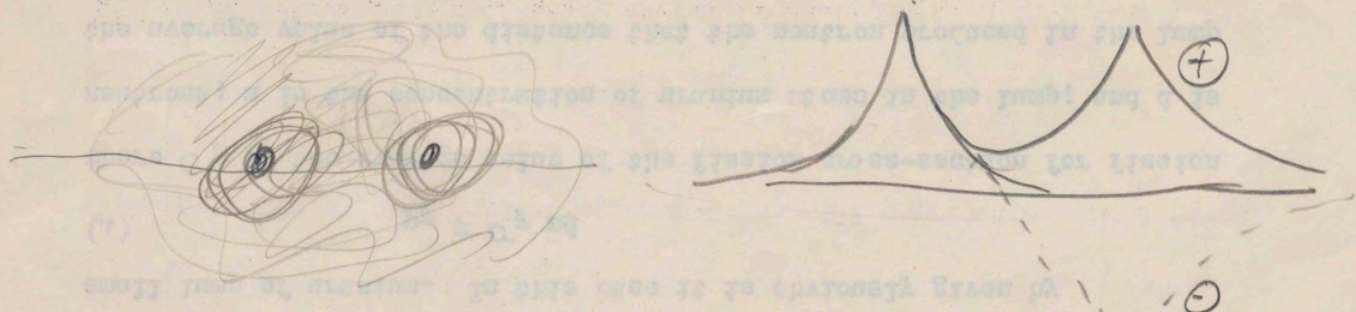
These are degenerate

Solving perturbation problem one finds

$a(1) + b(1)$  is the lowest state

(has no nodes while  $a(1) - b(1)$  solution has median plane as a node)

One electron state would be



Two electrons can go in lowest orbit if ↑↓

— UP TO HERE —  
 Start with Ritz next time

contribution to the integral will be due to the Breit-Wigner peaks of  $\sigma(E)$ . average energy of the fission neutrons. One will expect that the largest a low limit just above thermal energy and an upper limit equal to the absorption cross-section at energy  $E$ . The integral must be taken between and unit volume;  $\lambda$  is the mean free path and  $\sigma(E)$  is the resonance where  $q$  is the number of fast neutrons entering the system per unit time

$$(5) \quad \int \frac{q}{\lambda} \sigma(E) dE$$

than thermal energy would be given by the following expression: unit time of a resonance absorption process of neutrons with energy larger neutrons are produced and slowed down to thermal energy, the probability per If we had a single atom of uranium in a graphite medium where fast

Resonance Absorption

by the resonance process. and brings them down to an energy level in which they are readily absorbed effectively slows down the neutrons before the fission threshold of  $^{238}\text{U}$  erable role. In particular the last process for a lump of large size become important and both elastic and inelastic scattering play a consid- of larger size is more complicated since then multiple collision processes must travel before reaching the surface of the lump. The case of a lump the average value of the distance that the neutron produced in the lump neutrons;  $n$  is the concentration of uranium atoms in the lump; and  $d$  is where  $\sigma_f$  is the average value of the fission cross-section for fission

$$(1) \quad p_f = \sigma_f n d$$

small lump of uranium. In this case it is obviously given by The value of this quantity is very easily calculable for a very

Probability of Fission Before Slowing Down

UP TO 458 - 8 -  
 Start with part 3 next time

# Wang solution

Uses Ritz method

Theorem I: if  $u$  is arbitrary function normalized

to 1 
$$\int |u|^2 dz = 1$$

then

$$\int u^* H u dz \geq \text{min } e. v$$

Proof: develop  $u$  in e.f. of  $H$

$$H \psi_n = E_n \psi_n$$

$$u = \sum c_n \psi_n$$

$$H u = \sum c_n E_n \psi_n$$

$$u^* = \sum c_m^* \psi_m^*$$

$$\int u^* H u = \sum_{m,n} c_m^* c_n E_n \underbrace{\int \psi_m^* \psi_n}_{\delta_{mn}} = \sum_n |c_n|^2 E_n$$

Theorem II: if  $u$  differs from  $\psi_1$  by inf. of 1st

order  $\int u^* H u$  differs from  $E_1$  by 2nd order terms

In this case  $c_2, c_3, \dots$  are 1st order

Since  $|c_1|^2 + |c_2|^2 + \dots = 1$   $|c_1|^2 = 1 - |c_2|^2 - \dots = 1 - 2nd\ order$



figures for a good lattice will be given as an example. When a neutron is first produced by a fission taking place in a lump of uranium it may have a probability of the order of say 3 percent of being absorbed giving rise to fission before losing any appreciable amount of energy. In 97 percent of the cases when this does not happen the neutron will initiate its slowing down process and it may either be absorbed by the resonance process during the slowing down or reach thermal energy. The probability of resonance absorption during the slowing down may be of the order of 10 percent so that 87 percent of the original neutrons will be slowed down to thermal energies. Of these perhaps 10 percent may be absorbed by carbon and the remaining 77 percent by uranium. If we assume for the purpose of example that  $\nu = 2$ , we shall have in one generation the processes summarized by the table.

Probability	Type of Process	Neutrons Produced per Neutron absorbed	Neutrons per Generation by One Neutron
3%	Fast Fission	2	0.06
10%	Resonance Absorption	0	0
10%	Absorption by Carbon	0	0
77%	Absorption by Uranium at thermal energies	$\eta$	$0.77\eta$

For the example given the reproduction factor will be, therefore,

$$k = 0.06 + 0.77\eta \quad (3)$$

Consequently, a lattice of the type as described would have a reproduction factor larger than 1 provided  $\eta$  is larger than 1.22.

In order to evaluate the reproduction factor one must be able to

calculate the probabilities for the various processes mentioned. We shall

briefly indicate some points of view which may be used in the practical

calculation.

$$\int u^* H u = \underbrace{|c_1|^2 E_1}_{1 + 2nd\ order} + \underbrace{|c_2|^2 E_2 + \dots}_{2nd\ order}$$

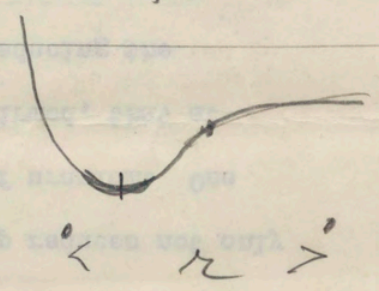
Hence method: Guess a wave function

Wang's guess was

$$u = \text{Norm. factor} \times \left\{ e^{-\frac{z}{a}(r_{1a} + r_{2b})} + e^{-\frac{z}{a}(r_{2a} + r_{1b})} \right\}$$

a = Bohr radius

z = adjustable parameter



Calculate

$$\int u^* H u = f(z)$$

Minimise this with resp. to z

	Wang	Experiment
Energy	-2.278 Ryd	-2.326
Mom. of inertia	.459 x 10 <sup>-40</sup>	.467
Oscill. freq	4900 cm <sup>-1</sup>	4360

not restrict ourselves, however, to homogeneous mixtures only, one can try to obtain a more favorable situation by proper arrangement of the geometrical distribution of the two components. This actually is possible to a considerable extent due to the following circumstances. The resonance absorption which is responsible for the loss of neutrons during the slowing down has very sharp cross-section maxima of the Breit-Wigner type. If the uranium, therefore, instead of being spread through the graphite mass is concentrated in rather sizeable lumps, we will expect that the uranium in the interior of a lump will be shielded by a thin surface layer from the action of neutrons with energy close to a resonance maximum. Therefore, the resonance absorption of a uranium atom inside the lump will be much less than it would be for an isolated atom. Of course, self-absorption in a lump reduces not only the resonance absorption but also the thermal absorption of uranium. One can expect theoretically, however, and experiment has confirmed, that at least up to a certain size of lumps the gain obtained by reducing the resonance loss of neutrons over-balances by a considerable amount the loss due to a lesser absorption of thermal neutrons.

The typical structure of a pile is a lattice of uranium lumps embedded in a matrix of graphite. The lattice may be for instance a cubic lattice of lumps or a lattice of rods of uranium. This latter arrangement is slightly less efficient from the point of view of the neutron absorption balance but often presents some practical advantages since it makes the removal of the heat produced by the pile more easy. In the present discussion we shall consider only lattices of lumps.

It is useful to give some typical figures for the probabilities of the various absorption processes. These probabilities of course, are not constant but depend on the details of the structure of the lattice. Average

London Eisenhitz

$$\psi_m \psi_m \quad E_{nm} = A_n + B_m$$

$$H = \frac{2Z\xi - X\xi - Y\eta}{r^3}$$

$$H_{00,00} = \frac{2Z_{00}\xi_{00}}{r^3} = 0$$

$$\Delta W = - \sum_{n,m} \frac{|H_{00, nm}|^2}{E_{nm} - E_{00}} \approx - \frac{K}{r^6}$$

$$(Z\xi)_{00, nm} = Z_{0m} \xi_{0n}$$

$$K = \sum_{nm} \frac{|2Z_{0m} \xi_{0n} - \dots|^2}{A_m - A_0 + B_n - B_0}$$

$$Z \sim \frac{1}{e^2} \left( \frac{\hbar^2}{me^2} \right)^{\frac{1}{2}}$$

$$10^{-32} \frac{10^{-32} e^4}{1/2}$$

$$e^2 \times 5 \quad e^2 \left( \frac{\hbar^2}{me^2} \right)^5 \quad 10^{-40}$$

$$E = E_e + \hbar c \omega \left( \nu + \frac{1}{2} \right) + \hbar c B \left[ J(J+1) - \Omega^2 \right]$$

## ELEMENTARY THEORY OF THE PILE

by E. Fermi  
Institute for Nuclear Studies, University of Chicago

I shall attempt in what follows to give an outline of the theory of a chain reacting pile working with natural uranium and graphite.

The results and the methods that I am going to discuss have been obtained partly independently and partly in collaboration by many people who participated in the early development work on the chain reaction. Very important contributions to the theoretical ideas were given by Szilard and Wigner. Many physicists contributed experimental results that helped to lead the way. Among them H. L. Anderson and W. H. Zinn first at Columbia University and later at the Metallurgical Laboratory of the University of Chicago; R. R. Wilson and E. Greutz at Princeton; Allison, Whitaker and V. G. Wilson at the University of Chicago. The production of the chain reaction was finally achieved in the Metallurgical Laboratory directed by A. H. Compton.

### Absorption and Production of Neutrons in a Pile

We consider a mass, "the pile", containing uranium spread in some suitable arrangement throughout a block of graphite. Whenever a fission takes place in this system an average number  $\nu$  of neutrons is emitted with a continuous distribution of energy of the order of magnitude of a million of electron volts. After a neutron is emitted, its energy decreases by elastic collisions with the atoms of carbon and to some extent also by inelastic collisions with the uranium atoms. In the majority of cases the neutrons will be slowed down to thermal energies. This process

*Handwritten signatures:*  
Bartlett  
P. A. M. S. C.  
E. Fermi

$$\dot{a}_m = -\frac{i}{\hbar} \sum_n \mathcal{H}_{mn} a_n e^{\frac{i}{\hbar} (W_m - W_n) t}$$

$$a_m = 1 \quad a_n = -\frac{\mathcal{H}_{mn}}{W_m - W_n} \left( e^{\frac{i}{\hbar} (W_m - W_n) t} - 1 \right)$$

$$|a_n|^2 = \frac{|\mathcal{H}_{mn}|^2}{(W_m - W_n)^2} 4 \sin^2 \frac{(W_m - W_n) t}{2\hbar}$$

$$\begin{aligned} \sum |a_n|^2 &= 4 |\mathcal{H}_{mn}|^2 \frac{dn}{dW_m} \int \frac{\sin^2\left(\frac{t}{2\hbar} \epsilon\right)}{\epsilon^2} \\ &= \frac{2\pi}{\hbar} |\mathcal{H}_{mn}|^2 \frac{dn}{dW_m} t \quad \frac{\pi t}{2\hbar} \end{aligned}$$

$$\text{Prob of transition per unit time} = \frac{2\pi}{\hbar} |\mathcal{H}_{mn}|^2 \frac{dn}{dW_m}$$

$$\mathcal{H}_{mn} = \frac{1}{\Omega} \int U e^{\frac{i}{\hbar} (p' - p) \cdot r} d\tau$$

$$\frac{dn}{dW_m} = \frac{p^2 dp d\omega \Omega}{8\pi^3 \hbar^3 v dp}$$

$$\frac{\sigma_{d\omega}}{\Omega} = \frac{2\pi}{\hbar} \frac{1}{\Omega} \left| \int U e^{\frac{i}{\hbar} (p' - p) \cdot r} d\tau \right|^2 \frac{p^2 d\omega \Omega}{8\pi^3 \hbar^3 v}$$

$$\sigma_{d\omega} = \frac{p^2/v^2}{4\pi^2 \hbar^4} \left| \int U e^{\frac{i}{\hbar} p' - p \cdot r} d\tau \right|^2 d\omega$$

requires about 100 collisions with carbon atoms. After the energy of the neutron is reduced to thermal value, the neutron keeps on diffusing until it is finally absorbed. In several cases, however, it will happen that the neutron is absorbed before the slowing down process is completed.

The neutron may be absorbed by either the carbon or the uranium. The absorption cross-section of carbon for neutrons of thermal energy is quite small; its value being approximately  $.005 \times 10^{-24} \text{ cm}^2$ . For graphite of density 1.6 this corresponds to a mean free path for absorption of about 25 m. It is believed that the absorption cross-section follows the  $1/v$  law and consequently the absorption cross-section which is already quite small at thermal energies becomes practically negligible for neutrons of higher energy. It is, therefore, a sufficiently good approximation to assume that absorption by carbon during the slowing down process can be neglected.

The absorption of a neutron by uranium may lead either to fission or to absorption by an  $(n, \gamma)$  process. We shall refer to this last possibility as the process of resonance absorption. The relative importance of fission and resonance absorption in the different energy intervals is not the same. In this respect we can consider roughly three intervals.

a. Neutrons with energy above the fission threshold of  $U^{238}$ . We can call these conventionally "fast neutrons". For fast neutrons the most important absorption process is fission which normally takes place in the abundant isotope  $U^{238}$ . Resonance absorption is smaller but not negligible.

b. Neutrons of energy below the fission threshold of  $U^{238}$  and above thermal energy. We shall refer to these neutrons as "epi-thermal neutrons". For epi-thermal neutrons the most important absorption process

$$\psi \rightarrow e^{\frac{i}{\hbar} p r} + \sum_l P_l^{(0)}(\theta) \frac{a_l}{r} e^{\frac{i}{\hbar} p r}$$

$$\frac{4\pi}{2l+1} \frac{p_m}{m} |a_l|^2 \quad \overline{P_l^2} = \frac{1}{2l+1}$$

$$\sigma_l = \frac{4\pi}{2l+1} |a_l|^2$$

$$e^{\frac{i}{\hbar} p r} = \sqrt{\frac{\pi}{2}} \sqrt{\frac{\hbar}{p r}} \sum_l i^l (2l+1) P_l J_{l+\frac{1}{2}}\left(\frac{p r}{\hbar}\right)$$

$$J_{l+\frac{1}{2}}(z) = \frac{2\left(\frac{1}{2}z\right)^{l+\frac{1}{2}}}{\sqrt{\pi} l!} \left(1 + \frac{d^2}{dz^2}\right)^l \frac{\sin z}{z}$$

$$\rightarrow \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi}{4} - \frac{l\pi}{2}\right)$$

$$\psi \rightarrow \sum_{l=0}^{\infty} \frac{1}{r} P_l^{(0)}(\theta) \left\{ e^{\frac{i}{\hbar} p r} \left[ a_l - \frac{i}{2} \frac{\hbar(2l+1)}{p} \right] + e^{-\frac{i}{\hbar} p r} (-1)^l \frac{i}{2} \frac{\hbar(2l+1)}{p} \right\}$$

$$\psi = \sum \frac{1}{r} P_l^{(0)}(\theta) c_l v_l(r)$$

$$v_l'' + \left[ \frac{2mE}{\hbar^2} - \frac{2mU}{\hbar^2} - \frac{l(l+1)}{r^2} \right] v$$

$$r^{l+1} \leftrightarrow v_l \leftrightarrow A_l \cos\left(\frac{p r}{\hbar} - \frac{l+1}{2} \pi + \beta_l\right)$$

$$a_l = \frac{\hbar(2l+1)}{p} e^{i\beta_l} \sin \beta_l \quad c_l = (-1)^l e^{i\left(\beta_l - \frac{\pi l}{2}\right)} \frac{\hbar(2l+1)}{p A_l}$$



$$\sigma = \sum \frac{4\pi\hbar^2}{p^2} (2l+1) \sin^2 \beta_l$$

# Inelastic collisions (Born)

$$\frac{1}{\sqrt{\Omega}} e^{i \frac{p \cdot r}{\hbar}} \Psi_i(q)$$

$$\frac{1}{\sqrt{\Omega}} e^{i \frac{p' \cdot r}{\hbar}} \Psi_f(q)$$

$$g_b = \frac{1}{\Omega} \int V(q, r) \Psi_i^* \Psi_f e^{i \frac{p' - p \cdot r}{\hbar}}$$

$$\frac{\Omega}{p^3}$$

$$\Delta \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$V = V_0 + \sum V_n$$

$$\Delta \psi - \frac{2m}{\hbar^2} V_n \psi = 0$$

$$\psi = \frac{v}{r}$$

$$v'' = \frac{2m}{\hbar^2} V_n v = 0$$

$$\int V_n \psi d\tau = 4\pi \int_0^\rho r V_n v dr$$

$$= \frac{2\pi \hbar^2}{m} \int_0^\rho r v'' dr = \frac{2\pi \hbar^2}{m} [ \rho v'(\rho) - v(\rho) ]$$

$$v(r) = \bar{\psi} \left( r + \frac{a}{2} \right)$$

$$v'(r) = \bar{\psi}$$

$$\int V_m \psi d\tau = - \frac{2\pi\hbar^2}{m} a \bar{\psi}$$

$$\overline{\Delta V \psi} = - \frac{2\pi\hbar^2 a}{m} n \bar{\psi}$$

$$\frac{2m}{\hbar^2} E$$

inelastic collisions

Born

$$\sigma_{dw} = \frac{m^2}{4\pi^2\hbar^4} \frac{1}{v'} \int |V(q,r)|^2 e^{\frac{i}{\hbar}(q,p)r} dq$$

Capture process (Born)

$$\frac{1}{\sqrt{\Omega}} e^{\frac{i}{\hbar}(p,r)} \psi_i(q) \quad \frac{1}{\sqrt{\Omega}} e^{\frac{i}{\hbar}(q,p)} \psi_f(r,q)$$

$$\mathcal{H}_0 = \frac{1}{\sqrt{\Omega}} \iint e^{\frac{i}{\hbar}(p,r)} \psi_i(q) \psi_f^*(q,r) dq$$

$$\mathcal{H}_0 = \frac{1}{\Omega} \iint V(r,p,q) e^{\frac{i}{\hbar}[(p,r)-(q,p)]} \psi_f^* \psi_i$$

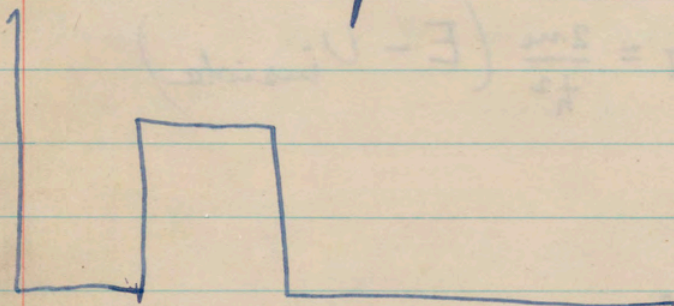
$$\frac{\Omega}{8\pi^3\hbar^3} m^2 v' d\omega$$

~~Capture process~~

sp heat

$$\bar{L} = \frac{3}{40} \left(\frac{6}{\pi}\right)^{3/2} \frac{h^2 n^{2/3}}{m g^{2/3}} + \frac{2^{1/3} \pi^{8/3} g^{2/3}}{3^{2/3}} \frac{m k^2 T^2}{h^2 n^{2/3}}$$

Compound nucleus



~~$A + B \Delta E^2$~~

~~$B \sim \frac{1}{kv}$~~

88

$$A^2 = \frac{G}{\sqrt{r}g(\rho)} e^{-2 \int_{\rho}^b \sqrt{g} dr}$$

$$B^2 = \frac{\cancel{h^2} m^2 \rho^2 \sqrt{g(\rho)}}{h^4 G \sqrt{r}} e^{2 \int_{\rho}^b \sqrt{g} dr}$$

~~$$g = \frac{2m}{h^2} (U - E)$$~~

$$g = \frac{2m}{h^2} (U - E)_{\text{barrier}}$$

~~$$\frac{m^2 \rho^2}{h^4 \sqrt{r} h^2 r^2}$$~~

$$r = \frac{2m}{h^2} (E - U_{\text{inside}})_{\text{outside}}$$

$$G = \frac{2m}{h^2} (E - U_{\text{inside}})$$

$$\tau = \frac{h B}{2 A}$$

$$\left( \frac{\text{Amp outside}}{\text{Amp inside}} \right)^2 = A^2 + B^2 \delta E^2$$

$$A \sim e^{-2 \int_{\rho}^b \sqrt{g} d\rho}$$

$$B \sim \frac{1}{h v_0} e^{2 \int_{\rho}^b \sqrt{g} d\rho}$$

$$\tau \sim \frac{h}{2} \frac{1}{h v} e^{2 \int_{\rho}^b \sqrt{g} d\rho}$$

$$r^{l+1} \leftrightarrow v_l(r) \leftrightarrow \frac{A}{r} \cos\left(\frac{pr}{\hbar} - \frac{l+1}{2}\pi + \beta_l\right)$$

$$\psi \rightarrow e^{\frac{i}{\hbar} pr} + \sum_l P_l^{(0)} \frac{a_l}{r} e^{\frac{i}{\hbar} pr}$$

$$\psi = \sum \frac{1}{r} P_l^{(0)} c_l v_l(r)$$

$$a_l = \frac{\hbar(2l+1)}{p} e^{i\beta_l} \sin \beta_l$$

$$c_l = (-1)^l e^{i(\beta_l - \frac{l\pi}{2})} \frac{\hbar(2l+1)}{p A_l}$$

~~$$\dot{a} = -\frac{i}{\hbar} \hbar a_n e^{\frac{i}{\hbar} (\omega_0 - \omega_n) t} - \frac{a}{\tau}$$~~

~~$$a = \hbar a_n \frac{1}{\omega_0 - \omega_n} \left( e^{\frac{i}{\hbar} (\omega_0 - \omega_n) t} \right)$$~~

~~$$\dot{a} + \frac{a}{\tau} = -\frac{i}{\hbar} \hbar a e^{\frac{i}{\hbar} (\omega_0 - \omega) t}$$~~

~~$$-\frac{i}{\hbar} \hbar \sum a_n e^{\frac{i}{\hbar} (\omega_0 - \omega_n) t}$$~~

90

$$\dot{a}_0 = -\frac{i}{\hbar} a_0 \mathcal{H}_0 e^{\frac{i}{\hbar}(\omega_0 - \omega_i)t}$$

$$-\frac{i}{\hbar} \sum_n a_n \mathcal{H}_{n0} e^{\frac{i}{\hbar}(\omega_0 - \omega_n)t}$$

$$\dot{a}_n = -\frac{i}{\hbar} a_0 \mathcal{H}_{0n} e^{\frac{i}{\hbar}(\omega_n - \omega_0)t}$$

 ~~$a_n = a_i$~~ 

$$\dot{a}_0 + \frac{a_0}{\tau} = -\frac{i}{\hbar} a_i \mathcal{H}_{i0} e^{\frac{i}{\hbar}(\omega_0 - \omega_i)t}$$

$$-\frac{i}{\hbar} a_i \mathcal{H}_{i0} e^{\frac{i}{\hbar}(\omega_0 - \omega_i)t}$$

$$a_0 = \frac{-\frac{i}{\hbar} a_i \mathcal{H}_{i0} e^{\frac{i}{\hbar}(\omega_0 - \omega_i)t}}{\frac{1}{\tau} + \frac{i}{\hbar}(\omega_0 - \omega_i)}$$

$$\dot{a}_n = -\frac{1}{\hbar^2} a_i \mathcal{H}_{i0} \mathcal{H}_{0n} e^{\frac{i}{\hbar}(\omega_n - \omega_i)t} \frac{1}{\frac{1}{\tau} + \frac{i}{\hbar}(\omega_0 - \omega_i)}$$

$$a_n = \frac{i}{\hbar} a_i \mathcal{H}_{i0} \mathcal{H}_{0n} \frac{e^{\frac{i}{\hbar}(\omega_n - \omega_i)t} (-1)}{\left[ \frac{1}{\tau} + \frac{i}{\hbar}(\omega_0 - \omega_i) \right] (\omega_n - \omega_i)}$$

$$= -a_0 \frac{e^{\frac{i}{\hbar}(\omega_n - \omega_0)t} - e^{\frac{i}{\hbar}(\omega_i - \omega_0)t}}{\omega_n - \omega_i} \mathcal{H}_{0n}$$

$$\frac{1}{\tau} = \frac{i}{\hbar} \sum_n \frac{e^{\frac{i}{\hbar}(\omega_n - \omega_0)t} - e^{\frac{i}{\hbar}(\omega_i - \omega_0)t}}{\omega_n - \omega_i} |\mathcal{H}_{0n}|^2$$

$$\int_{-\infty}^{\infty} \frac{\sin qx}{x} dx = \pi$$

$$\int_{-\infty}^{\infty} \frac{\sin^2 kx}{x^2} dx = \pi k$$

$$\int_{-\infty}^{\infty} \frac{1 - \cos kx}{x} dx = 0$$

Gamma

Virtual states

Virtual state (A) amplitude  
 Continuous states

$$\frac{2\pi}{h} |\mathcal{H}|^2 n$$

$$\mathcal{H} = \frac{H}{\sqrt{\Omega}} \quad n = \frac{4\pi p^2 dp \Omega}{8\pi^3 h^3 v dp} = \frac{\Omega}{2\pi^2 h^3} \frac{p^2}{v}$$

$$\frac{1}{\tau} = \frac{|H|^2}{\pi h^4} \frac{p^2}{v}$$

$$\Gamma = \frac{|H|^2}{\pi h^4} \frac{p^2}{v}$$

$$\frac{1}{\tau} = \sum \Gamma$$

$$A = -\frac{i}{h} a_1 \frac{H}{\sqrt{\Omega}}$$



92

$$\dot{A} = -\frac{i}{\hbar} a \sqrt{n} H_a e^{\frac{i}{\hbar} (\omega_A - \omega_a) t}$$

$$= \frac{i}{\hbar} \left[ b_s \frac{H_b}{\sqrt{2}} e^{\frac{i}{\hbar} (\omega_A - \omega_s) t} \right.$$

$$\left. - \frac{i}{\hbar} \sum_{c \neq s} c \frac{H_c}{\sqrt{2}} e^{\frac{i}{\hbar} (\omega_0 - \omega_c) t} \right]$$

$$\dot{A} + \frac{1}{2\tau} A = -\frac{i}{\hbar} a \sqrt{n} H_a e^{\frac{i}{\hbar} (\omega_0 - \omega_a) t}$$

$$A = \frac{-\frac{i}{\hbar} a \sqrt{n} H_a e^{\frac{i}{\hbar} (\omega_A - \omega_a) t}}{\frac{1}{2\tau} + \frac{i}{\hbar} H_a (\omega_0 - \omega_a)}$$

$$\dot{b}_s = -\frac{i}{\hbar} A \frac{H_b^*}{\sqrt{2}} e^{\frac{i}{\hbar} (\omega_s - \omega_A) t}$$

$$b_s = + \frac{i}{\hbar} a A \frac{\sqrt{n} H_a H_b^*}{\sqrt{2}} \frac{e^{\frac{i}{\hbar} (\omega_s - \omega_a) t}}{\frac{1}{2\tau} + \frac{i}{\hbar} H_a (\omega_0 - \omega_a)}$$

$$b_s = \frac{\dot{b}_s}{\frac{i}{\hbar} (\omega_s - \omega_a)}$$

$$e^{\frac{i}{\hbar} (\omega_s - \omega_a) t} - 1$$

$$A = \frac{i}{\hbar}$$

$$\dot{A} + \frac{A}{2\tau} = -\frac{i}{\hbar} \sqrt{n} H_a e^{\frac{i}{\hbar} (\omega_A - \omega_a) t}$$

$$A = - \frac{\frac{i}{\hbar} \sqrt{n} H_a e^{\frac{i}{\hbar} (\omega_A - \omega_a) t}}{\frac{1}{2\tau} + \frac{i}{\hbar} (\omega_A - \omega_a)}$$

$$\frac{|A|^2}{n} = \frac{|H_a / \hbar|^2}{\frac{1}{4\tau^2} + \frac{1}{\hbar^2} (\omega_A - \omega_0)^2} = \frac{\pi \hbar^2}{p^2}$$

Discuss width of resonance

$$\dot{b}_s = -\frac{i}{\hbar} A \frac{H_b}{\sqrt{\Omega}} e^{\frac{i}{\hbar} (\omega_b - \omega_A) t}$$

$$|H_a|^2 = \pi \hbar^4 \frac{v}{p^2} \Gamma_a$$

$$\Gamma_b |A|^2 = \frac{n v \hbar^2}{p^2} \frac{\Gamma_a \Gamma_b}{\frac{\Gamma^2}{4} + \frac{(\omega_a - \omega_0)^2}{\hbar^2}} = n v \sigma(a, b)$$

$$\sigma(a, b) = 4 \lambda^2 \frac{\Gamma_a \Gamma_b}{\Gamma^2 + \frac{4}{\hbar^2} (\omega_a - \omega_0)^2}$$

~~1000~~

$$\frac{1000}{10^6}$$

$$\frac{F_a \Gamma_b}{\Gamma^2}$$

$$\frac{10^2}{10^6}$$

$$\frac{10^2}{10^6}$$

94

$$A = - \frac{\frac{i}{\hbar} \sqrt{n} H_a e^{\frac{i}{\hbar} (\omega_A - \omega_0) t}}{\frac{\Gamma}{2} + \frac{i}{\hbar} (\omega_A - \omega_0)}$$

$$a_s = - \frac{\frac{i}{\hbar} H_a^*}{\sqrt{2}} \left( \frac{-\frac{i}{\hbar} \sqrt{n} H_a}{\frac{\Gamma}{2} + \frac{i}{\hbar} (\omega_A - \omega_0)} \right) \frac{e^{\frac{i}{\hbar} (\omega_s - \omega_0) t} - 1}{\omega_s - \omega_0}$$

$$b_k = - \frac{\frac{i}{\hbar} H_b^*}{\sqrt{2}} \left( \frac{-\frac{i}{\hbar} \sqrt{n} H_a}{\frac{\Gamma}{2} + \frac{i}{\hbar} (\omega_A - \omega_0)} \right) \frac{e^{\frac{i}{\hbar} (\omega_k - \omega_0) t} - 1}{\omega_k - \omega_0}$$

$$|b_k|^2 = \frac{1}{\hbar^2} \frac{|H_a|^2 |H_b|^2 n}{\Omega \left( \frac{\Gamma^2}{4} + \frac{1}{\hbar^2} (\omega_A - \omega_0)^2 \right)} \frac{4 \sin^2 \left( \frac{\omega_k - \omega_0}{2\hbar} t \right)}{(\omega_k - \omega_0)^2}$$

$$\sum |b_k|^2 = \frac{4}{\hbar^2} \frac{|H_a|^2 |H_b|^2 n}{\left( \frac{\Gamma^2}{4} + \frac{1}{\hbar^2} (\omega_A - \omega_0)^2 \right)} \frac{\pi t}{\hbar} \frac{p_b^2}{v_b} \frac{1}{\pi^2 \hbar^3} = v_0 t \sigma_b n$$

$$\sigma_b = \frac{1}{v_0} \frac{1}{\pi \hbar^3}$$

$$\sigma_b = \frac{1}{v_0} \frac{1}{\pi \hbar^3} \frac{p_b^2}{v_b} \frac{|H_a|^2 |H_b|^2}{\frac{\Gamma^2}{4} + \frac{(\omega_A - \omega_0)^2}{\hbar^2}}$$

$$\frac{1}{2} \frac{A^2}{\hbar}$$

$$\frac{1}{2} \frac{A^2}{\hbar}$$

$$\Gamma = \frac{1}{\pi \hbar^4} \left\{ |H_a|^2 \frac{p_0^2}{v_0} + |H_b|^2 \frac{p_b^2}{v_b} \right\}$$

$$\sigma(n, r) = \frac{1}{v} \frac{\hbar^2 \pi \hbar^4}{\hbar^4} \frac{\Gamma r \frac{\hbar^4}{\hbar^4} \frac{v_0}{p_0^2} \Gamma n}{\frac{\Gamma^2}{4} + \frac{\Delta \omega^2}{\hbar^2}}$$

Hombostel

95

$$\sim 1 \text{ eV} \left\{ \begin{array}{l} \sigma_{\text{max}} = 8200 \times 10^{-24} \quad \hbar\Gamma = .13 \text{ eV} \quad \hbar\Gamma_n = 3.7 \times 10^{-4} \\ \sigma_{\text{max}} = 46000 \times 10^{-24} \quad \hbar\Gamma = .07 \quad \hbar\Gamma_n = 1 \times 10^{-3} \end{array} \right.$$

Rh  
In

~~$$\sigma(n, \gamma) = 4\pi \lambda^2 \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} \frac{1}{1 + \frac{4}{\hbar^2 \Gamma^2} (\omega_n - \omega_0)^2}$$~~

$$\left\{ \begin{array}{l} \sigma(n, \gamma) = \frac{v_0}{v} 4\pi \lambda_0^2 \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} \frac{1}{1 + \frac{4}{\hbar^2 \Gamma^2} (\omega_n - \omega_0)^2} \\ \sigma_{\text{max}}(n, \gamma) = 4\pi \lambda_0^2 \frac{\Gamma_\gamma \Gamma_n}{\Gamma^2} \end{array} \right.$$

$$1 \text{ eV} \quad \lambda = \frac{1.052 \times 10^{-27}}{2.3 \times 10^{-13}} = 4.56 \times 10^{-10}$$

$$\frac{p^2}{2m} = 1.6 \times 10^{-12} \quad p^2 = 5.31 \times 10^{-36} \quad p = 2.3 \times 10^{-18}$$

$$4\pi \lambda^2 = 2.6 \times 10^{-18}$$

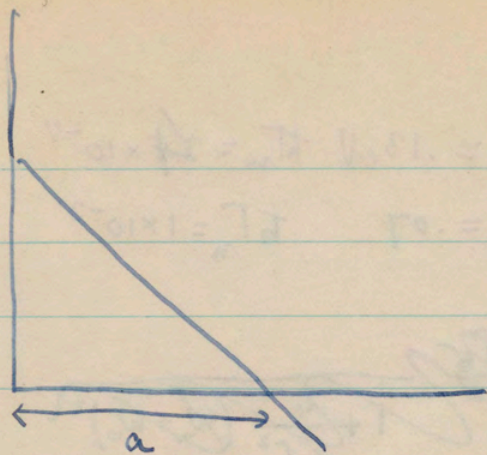
$10^{-18}$

$$\frac{2.6 \times 10^{-18}}{\sqrt{1 \times 0.025}} \quad \frac{.13 \times 4 \times 10^{-4}}{1^2} \quad \frac{0.07 \times 1 \times 10^{-3}}{1^2}$$

850

$$\frac{2.3 \times 10^{-18} \times 10^{-4}}{2.6 \times 10^{-18}} = 2.3 \times 10^{-2}$$

96



$$u'' + \frac{m}{\hbar^2} (E - W) u = 0$$

$$E = -W$$

$$e^{-\sqrt{\frac{m}{\hbar^2} W} x}$$

$$\sqrt{\frac{m W_0}{\hbar^2}} a = 1$$

$$a = \frac{\hbar}{\sqrt{m W_0}}$$

~~$$\frac{1}{2} \frac{m v^2}{2} = E$$~~

$$\frac{m v^2}{4} = E = \frac{W}{2}$$

$$u'' + \frac{m W}{2 \hbar^2} u = 0$$

$$u = \frac{\sin\left(\sqrt{\frac{m W}{2 \hbar^2}} x\right)}{\sin \beta}$$

$$-\frac{1}{a} = \sqrt{\frac{m W}{2 \hbar^2}} \frac{\cos \beta}{\sin \beta}$$

$$\sigma = \frac{4 \pi \hbar^2}{2 a^2} \sin^2 \beta$$

$$-\sqrt{\frac{m\omega_0}{\hbar^2}} = \sqrt{\frac{m\omega}{2\hbar^2}} \cot\beta$$

$$\tan\beta = -\sqrt{\frac{\omega}{2\omega_0}}$$

$$\sin^2\beta = \frac{\frac{\omega}{2\omega_0}}{1 + \frac{\omega}{2\omega_0}}$$

$$\sigma = \frac{4\pi\hbar^2}{m} \frac{1/2\omega_0}{1 + \frac{\omega}{2\omega_0}}$$

$$\sigma = \frac{4\pi\hbar^2}{m} \left\{ \frac{3}{4|\omega_0| + \frac{\omega}{2}} + \frac{1}{4|\omega_1| + \frac{\omega}{2}} \right\}$$

$$\omega_0 = 2.17 \text{ MeV}$$

$$\omega = 0 \quad \sigma = 20 \times 10^{-24}$$

$$\frac{4\pi\hbar^2}{m(1\text{MeV})} = \frac{4\pi \times 1.054^2 \times 10^{-54}}{1.67 \times 10^{-24} \times 1.6 \times 10^{-6}} = 5.2 \times 10^{-24}$$

$$\frac{3}{4 \times 2.17} + \frac{1}{4|\omega_1|} = 3.85$$

$$\frac{334}{758} = 3.51$$

$$\omega_1 = 0.034 \text{ MeV}$$

$$|\omega_1| = 0.071 \text{ MeV}$$

98

$$a \ll R$$

$$\rho \ll R$$

$$10^{-12}$$

$$R \ll \lambda$$

$$10^{-9}$$

X, Y, Z

(H)

x y z

(neut)

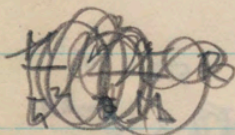
$$-\frac{\hbar}{i} \dot{\psi} = -\frac{\hbar^2}{2M} \left( \frac{\partial^2 \psi}{\partial x^2} + \dots + \frac{\partial^2 \psi}{\partial X^2} + \dots \right) + U(x, Y, Z) \psi + \overline{g(z)} \psi$$

$$\overline{\psi} = \frac{1}{\frac{4}{3} \pi R^3} \iiint \psi(\xi, \eta, \epsilon, X, Y, Z) d\xi d\eta d\epsilon$$

(R) around x y z

$$-\frac{\hbar}{i} \dot{\overline{\psi}} = -\frac{\hbar^2}{2M} \left( \frac{\partial^2 \overline{\psi}}{\partial x^2} + \dots + \frac{\partial^2 \overline{\psi}}{\partial X^2} + \dots \right) + U \overline{\psi} + \overline{g(z)} \overline{\psi}$$

$$\overline{g(z)} \overline{\psi} = -\frac{4\pi \hbar^2 a}{M} \delta_R(z)$$



$$\sigma_{mn, d\omega} = 4a^2 \frac{p}{p_0} d\omega \left| \int u_m^* u_n e^{\frac{i}{\hbar}(\vec{p} - \vec{p}_0, x)} d\tau \right|^2$$

Strong binding

$$\sigma = 16\pi a^2$$

No binding:  $u_n = e^{\frac{i}{\hbar}(p_n x)} \frac{1}{\sqrt{2}}$        $u_m = \frac{1}{\sqrt{2}}$

$$\vec{p}_0 = \vec{p}_m + \vec{p}$$

$$p_0^2 = p_m^2 + p^2$$

$$|p| = |p_0| \cos \vartheta$$

$$\sigma_{d\omega} = 4a^2 \cos \vartheta d\omega$$

$$\sigma = 4a^2 \int_0^{\pi/2} \cos \vartheta \cdot 2\pi \sin \vartheta d\vartheta = 4\pi a^2$$



a) The state of the system is defined by the knowledge of the wave function.

~~b) Wave functions~~

b) Given a physical magnitude we ~~are~~ Hermitian operator corresponding to a physical magnitude  $A$

~~If~~

$$A\psi = a\psi$$

follows

~~if not only the prob. dist. of the~~  
The only allowed values of  $A$  are its proper values.

If  $\psi$  is a proper function of  $A$  namely

$$A\psi = a\psi$$

a measurement of  $A$  gives certainly

$$A = a$$

If not develop  $\psi$  in proper functions of  $A$

$$\psi = \sum c_n \psi_n$$

if everything is normalized

$$|c_n|^2$$

is the probability of  $A = a_n$

If measurements give

$$A = a_n$$

the measurement affects the state bringing it to

$$\psi = \phi_n$$

c)  $\psi$  varies with time according to the Schrödinger equation

$$H\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

Time derivative

~~$$A\psi(t)$$~~

$$A\left(\psi(t) + \tau \frac{\partial \psi}{\partial t}\right)$$

$$\left(1 - \frac{i\tau}{\hbar} H\right) \psi(t) = \psi(t + \tau)$$

$$\left(1 + \frac{i\tau}{\hbar} H\right) \psi(t + \tau) = \psi(t)$$

$$A\psi(t + \tau) = \phi(t + \tau)$$

$$A\left(1 - \frac{i\tau}{\hbar} H\right) \psi(t) = \left(1 - \frac{i\tau}{\hbar} H\right) \phi(t)$$

$$\psi(t + \tau) = \sum c_n^{(t)} \phi_n$$

102

$$A u_n = a_n u_n$$

 ~~$\psi(x)$~~ 

$$\psi(x) = \sum c_n u_n$$

$$A \psi(x) = \sum c_n a_n u_n$$

$$\begin{aligned} A \left(1 - \frac{i\tau H}{\hbar}\right) \psi(0) &= \sum c_n a_n u_n \\ &= A \sum c_n u_n \end{aligned}$$

$$\left(1 + \frac{i\tau H}{\hbar} A\right) A \left(1 - \frac{i\tau H}{\hbar}\right)$$

$$\begin{aligned} \left(1 + \frac{i\tau H}{\hbar} A\right) \left(1 - \frac{i\tau H}{\hbar}\right) \psi_0 &= \left(1 + \frac{i\tau H}{\hbar} A\right) \sum c_n a_n u_n \\ &= \sum c_n a_n \left(1 + \frac{i\tau H}{\hbar} A\right) u_n \end{aligned}$$

$$\left(1 + \frac{i\tau H}{\hbar} A\right) \left(1 - \frac{i\tau H}{\hbar}\right) \left(1 + \frac{i\tau H}{\hbar} A\right) u_n = a_n \left(1 + \frac{i\tau H}{\hbar} A\right) u_n$$

A

$$\begin{array}{cccc} a_1 & a_2 & \dots & a_n \\ u^{(1)} & u^{(2)} & & u^{(n)} \end{array}$$

Transformation matrix

$$T \quad t_{ik}$$

$$T^{-1} \quad \text{inverse } (t_{ki})$$

$$T T^{-1} = T^{-1} T = I$$

$$|T|$$

$TAT^{-1}$  has p.val.  $a_1, a_2, \dots, a_n$   
 prop funct  $Ta_1, Ta_2, \dots, Ta_n$

~~has~~ **proof**

$$A u^{(r)} = a_r u^{(r)}$$

$$TAT^{-1} T u^{(r)} = a_r T u^{(r)}$$

Unitarian matrix:  $\tilde{T}T = I \quad \tilde{T} = T^{-1}$

if  ~~$u^{(r)}$~~   $\sum_k u_k^{(r)*} u_k^{(s)} = \delta_{rs}$

follows  $\sum_k u_k^{(r)*} \tilde{T} T u_k^{(s)} = \delta_{rs} \quad \tilde{T}T = I$

~~Matrix~~  $u_k^{(s)}$  is unitarian

~~$t_{sk} = \delta_{kl}$~~   $\sum_k u_k^{(s)} u_k^{(l)*} = \delta_{sl}$

$T_{sk} = u_k^{(s)}$  is a unitarian matrix

$\tilde{T}_{ks} = u_k^{(s)*}$

$\tilde{T}AT$

~~$\tilde{T}AT\tilde{T}$~~

$\tilde{T}f = u_k^{(s)*}$

104

Matrix

$$T_{ks} = u_k^{(s)}$$

is unitarian.

Proof

$$\tilde{T}_{jk} = u_k^{(j)*}$$

$$(\tilde{T}T)_{js} = \sum_k \tilde{T}_{jk} T_{ks} = \sum_k u_k^{(j)*} u_k^{(s)} = \delta_{js}$$

$$T_{ks} = u_k^{(s)}$$

Transforms A in the diagonal matrix

$$\tilde{T}AT = \begin{vmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & & \\ & & \ddots & \\ 0 & & & a_n \end{vmatrix}$$

Proof

$$\begin{aligned} \tilde{T}AT &= u_k^{(s)*} a_{kl} u_l^{(r)} \\ &= a_{rs} u_k^{(s)*} u_k^{(r)} = a_{rs} \delta_{rs} \end{aligned}$$

The proper functions are at pos  $s$ 

$$\tilde{T}u^{(s)} = \begin{vmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{vmatrix}$$

$$(\tilde{T}f) = u_k^{(s)*} f_k = \text{coeff of expansion}$$

Meaning of  $T \tilde{T} = 1$

$$u_k^{(s)} u_j^{(s)*} = \delta_{kj}$$

or orthogonality for summation on the upper index

case of continuum

$$u_s(x)$$

$$\int u_s^*(x) u_n(x) dx = \delta_{ns}$$

$$\sum_s \int u_s^*(x') u_s(x) dx = \delta(x-x')$$

Proof: Develop  $\delta(x-x')$  in a series of p.f.

Average value of an operator

$$\bar{\psi} A \psi \quad \text{or} \quad \int \psi^* (A \psi) dx$$

(25)

# Perturbations with degeneracy or quasi-degeneracy

(See pages 35-36)

$$u_1^0 \quad u_2^0 \quad u_3^{(0)} \quad \dots \quad u_g^{(0)} \quad | \quad u_{g+1}^{(0)} \quad u_{g+2}^{(0)} \quad \dots$$

$$\sum_1^g c_i u_i^{(0)} + \sum_{g+1}^{\infty} c_\alpha u_\alpha^{(0)} = u$$

$\left\{ \begin{array}{l} c_\alpha \text{ small} \\ c_i \text{ large} \end{array} \right.$

~~$$(H_0 + \mathcal{H})u = \sum_1^g c_i w_i^0 u_i^0 + \sum_1^g c_i \mathcal{H} u_i^{(0)} + \sum_{g+1}^{\infty} c_\alpha \mathcal{H} u_\alpha^{(0)} = w \left( \sum c_i u_i^0 + \sum c_\alpha u_\alpha^{(0)} \right)$$~~

$$H = H_0 + \mathcal{H}$$

$$\sum_1^g c_i H u_i^0 + \sum_{g+1}^{\infty} c_\alpha w_\alpha^0 u_\alpha^0 = w \sum_1^g c_i u_i^0 + w^{(0)} \sum_g^{\infty} c_\alpha u_\alpha^0$$

$$w c_i = \sum_1^g c_k H_{ik}$$

Secular equation for  $w$  with  $g$  solutions

$$c_\alpha (w_\alpha^0 - w^0) + \sum c_i H_{\alpha i} = 0$$

no infinity

$HA - AH = 0$

$H_0 A - A H_0 = 0$

Classes with respect to A do not mix

~~Perturbation~~ theory of ~~for the case that~~  
(4) Discuss the ~~perturbations problem~~ ~~when~~  
the unperturbed state is degenerate or  
quasi-degenerate

~~Calculate the life-time of the sp. state~~  
~~of hydrogen~~ Discuss the uncertainty

~~The energy operator of a~~ ~~segment~~  
an electron ~~is movable~~ on a segment

2 of length  $a$ . Find the probability  
of spontaneous transition from the second  
to the first energy level.

1 Find whether or not  
which of the following operators  
are hermitian:

$\frac{d}{dx}, \frac{d^2}{dx^2}, \frac{d^3}{dx^3}, x^2 p + x p^2$

$x p^2 + p^2 x$



# Outline of Quantum Mechanics Course (Chicago - Fall + Winter 1948)

- Oct 1 x 1 Historical Resume up to 1925
- ⑩ x 2 Mechanics - Optics analogy
- x 3 Time dependent + time independent Schrodinger equation
- x 4 Generalisations to simple cases.
- x 5 Examples. Point on closed line + rotator with fixed axis - Normalization integral
- x 6 Density of probability + Density of current
- x 7 The linear oscillator
- 2 x 8 Orthogonality in one dimension - Point on a spherical surface - Resume on spherical harmonics - Reduction of the <sup>Schrodinger</sup> equation of ~~motion~~ of a point in a central field.
- x 9 Hydrogenlike atoms: negative energy levels.
- x 10 Positive energy levels - Expression of e.f. in terms of Laguerre polynomials.
- x 11 Degeneracy of the hydrogen levels. Notation s, p, d, ...
- x 12 Potential energy  $-\frac{ze^2}{r} (1 + \frac{\beta}{r})$  and qualitative discussion of one electron problem approximation of heavy atoms.

- 13 x WKB method x
- 14 x Orthogonality in three dimensions -1
- 15 x Degenerate eigenfunctions x
- 16 x Operators - Linear operators - Matrices x
- 17 x Factorization of vectors - Scalar product Add Hamiltonian
- Sum Difference + Product of operators
- 18 x Sum, difference + products of matrices.
- 19 x Eigenvalues & e. f. of operators - Secular equation for the e. v. of a matrix - Hermitian matrices have real e. v.
- 20 x Geom. interpretation of e. v. + e. f. - Hermitian operators of continuous fields.
- 21 x Development in e. f. - Geom. discussion
- Functions of operators - State of a system
- x 22 Examples on  $\Delta p \Delta q \sim \hbar$  and  $\Delta W \Delta T \sim \hbar$  x
- x 23 Wave interpretation of uncertainty principle x
- x 24 Operator  $p = \frac{\hbar}{i} \frac{d}{dx}$  x
- x 25 Operator  $x$  -  $\delta$ -function - Operators corresponding to physical quantities. x
- Dec 1 x 26 Schrödinger function as state function x
- x 27 Commutation and its significance x
- 28 Properties of angular momentum operators x
- 29 Time independent perturbation theory x

- 30 Discussion on preceding lecture x-57  
 31 Stark effect on Hydrogen atom x-51  
 32 Zeeman effect without spin  
 33 Discussion of time dependent Schrodinger equation  
 34 Time dependent perturbation theory

### Winter Quarter

Jan 5  
1948

- 1 Discussion of time dependent perturb. theory
- 2 Absorption of light (From perturbation by electric field of wave)
- 3 Emission of light (From  $A'$ 's and  $B'$ 's)
- 4 Selection rules  $l \rightarrow l \pm 1$   $m \rightarrow m \pm 1$ , Quadrupole radiation
- 5 Spin of the electron - generalities
- 6 The Pauli operators
- 7 Electron in central field - unperturbed problem
- 8 Perturbation matrix.
- 9 Perturbation of energy levels
- 10 Interpretation with vectors - Description of the Hydrogen fine-structure.
- 11 Anomalous Zeeman effect
- 12 Landé  $g$ -formula with vector model
- Feb 2 13 Many (two) particle systems.

- Systems with two equal particles - Symmetry & antisymmetry
- 14 Antisymmetric functions & Pauli principle
- 15 Exchange integral splitting of terms of 2-electron system
- 16 Discussion of preceding case
- 17 The helium spectrum
- 18 Selection rules - Even and odd states
- 19 Electron orbits & periodic table
- 20 Spectra of alkali atoms & alkaline earths
- 21 Spectra of earths - Various types of couplings.
- 22 X-Ray spectra
- 23 Molecules - Polar Bond
- 24 Heitler-London theory of H<sub>2</sub> molecule
- 25 Single orbit approximation - ~~Wang~~  
Ritz method - Wang eigenfunctions
- 26 Theory of Van der Waals forces
- 27 Terms of a diatomic molecule  
Rotation-oscillation bands
- 28 Electronic band spectra
- 29 Alternating intensities
- 30 Formula for prob. of transition  $\frac{2\pi}{h} |\langle \psi_{final} | \hat{H}_{pert} | \psi_{initial} \rangle|^2 N$
- 31 Born approximation of collision theory
- 32 Case of spherical symmetry - Case of identical particles

112

33

The exact theory of collision <sup>for</sup> ~~against~~  
~~spherical~~ <sup>central</sup> forces, ~~center~~



VERNON

COMPOSITION BOOKS

NO.	LVS.	SIZE
101-40	40	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
101 $\frac{1}{2}$	48	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
101	60	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
101X	72	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
102	84	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
103	96	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
104	120	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$
104 $\frac{1}{2}$	144	9 $\frac{3}{4}$ x 7 $\frac{3}{8}$

MADE IN U. S. A.

