PHYSICS
251B

QUANTUM
MECHANICS

P 251B

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HARVARD UNIVERSITY

Physics 251b

ANSWER FIVE QUESTIONS

1. Describe the Schrödinger and Heisenberg 'pictures' and the mathematical relation between them, using the notation $\Psi$, A, B, ... for Schrödinger state function and operators and $\Phi$, $\mathcal{A}$, $\mathcal{B}$, ... for Heisenberg state function and operators.

Formulate the transformation from the Schrödinger picture to the interaction picture, and explain the meaning of the interaction picture.

2. For a case in which there is elastic scattering only, the statement of the 'optical theorem' is

$$\sigma = \int |f|^2 \, d\Omega = \frac{4\pi}{k} \operatorname{Im} \left[ f(0) \right]$$

State the theorem for the general case in which inelastic scattering and absorption occur in addition to the elastic scattering.

For the case of elastic scattering only, suppose that all you remember about the partial wave formula is that it has the form

$$f(\theta) = \sum_{\ell} F(\ell) \, (e^{2i\delta_\ell} - 1) \, P_\ell(\cos\theta).$$

By applying the optical theorem, determine the coefficients $F(\ell)$.

3. For a single electron in a central field, we can take as 'orbital' wave functions $f(r)Y_\ell^u(\theta,\varphi)$; these are eigenfunctions of $L^2$, $L_z$ with the eigenvalues $\ell(\ell+1)\hbar^2$, $u\hbar$. The $Y_\ell^u$ are normalized:

$$\int |Y_\ell^u|^2 \, d\Omega = 1$$

As the spin wave functions we can take

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

which are normalized eigenfunctions of $S^2$, $S_z$ with eigenvalues $\frac{1}{2}(\frac{1}{2} + 1)\hbar^2$, $\frac{1}{2}\hbar$ and $\frac{1}{2}(\frac{1}{2} + 1)\hbar^2$, $-\frac{1}{2}\hbar$, respectively.

Any wave function can be expressed as a combination of products of orbital and spin functions. A function of the form

$$f(r) \begin{pmatrix} a \, Y_\ell^{u} \\ b \, Y_\ell^{u+1} \end{pmatrix}$$

is an eigenfunction of $L^2$, $J_z = (L + S)_z$ with eigenvalues $\ell(\ell + 1)\hbar^2$, $m\hbar = (u + \frac{1}{2})\hbar$. Find a and b so that this function is a normalized ($|a|^2 + |b|^2 = 1$) eigenfunction of

$J^2 = |\vec{L} + \vec{S}|^2$ with eigenvalue $j(j + 1)\hbar^2$, $j = \ell + \frac{1}{2}$. Also find the a and b that give the function for $j = \ell - \frac{1}{2}$.

4. A system with angular momentum quantum number $j = 3/2$ is in the eigenstate of $J_z$ with eigenvalue $m\hbar = 3/2\hbar$. Find the probabilities that a measurement of $J_{z'}$ for an axis Oz' at angle $\theta$ with Oz will give the various values $m'\hbar$, $m' = 3/2$, $\frac{1}{2}$, $-\frac{1}{2}$, $-3/2$. Check consistency of your answer for the values $\theta = 0$ and $\theta = \pi$.

5. In Dirac's discussion of the connection between bosons and oscillators he considers a symmetric operator

$$U_T = \sum_r U_r$$

which is a sum of one-particle operators $U_r \left(\equiv U(q_r)\right)$, and expresses it in terms of matrix elements of U $\left(\equiv U(q)\right)$ between one-particle states and the operators $\eta$ (more commonly written $a^+$) and $\bar{\eta}$ (commonly a). State this expression for $U_T$. How is it written in terms of the 'operator wave functions'

$$\psi = \sum_i a_i \, u_i(q)$$

and

$$\psi^+ = \sum_i a_i^+ \, u_i^*(q) \quad ?$$

From the relation of $a^+$ to the appearance (emission, creation) of a boson and of a to its disappearance (absorption, destruction), show how the probabilities for emission and absorption of photons depend on the number of photons present in a given state.

6. State all of the selection rules for electric dipole radiation from an atom with Russell-Saunders coupling. Which of these rules are rigorously valid, and which are only approximate? Under what conditions are there appreciable deviations from the approximate rules? How do the rules for a one-electron system differ from the rules for a many-electron system?

The terms that can arise from the configuration $(1s)^2(2p)^2$ are:

$(2p)^2\ ^1S$, $(2p)^2\ ^3P$, $(2p)^2\ ^1D$

What terms arise from $(1s)^2\ 2s\ 2p$? From $(1s)^2\ 2s\ 3s$? What transitions among all of these terms (of the three configurations) are allowed by the selection rules? For the cases with terms that are triplets, what transitions are allowed between the individual energy levels?

Final, May 1961

# PHYSICS 251 B
## QUANTUM MECHANICS

LECTURE I 2-6-61

Time Dependent Perturbation Theory.

Given: $i\hbar \frac{\partial \psi}{\partial t} = H\psi = (H_0 + H_1)\psi$

knowing $H_0 u_n = E_n u_n$ , with $u_n e^{-iE_nt/\hbar}$

and with $\psi = \sum_n a_n(t) u_n e^{-iE_nt/\hbar}$

We find on substitution:

$$i\hbar \dot{a}_k = \sum_m H^{(1)}_{km} e^{i(E_k - E_m)t/\hbar} a_n$$

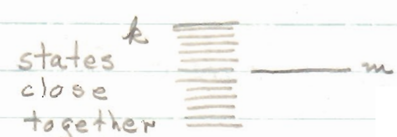
with $a_n^{(0)} = \delta_{nm}$ , $a = a^{(0)} + a^{(1)} + a^{(2)} + \ldots$

$$i\hbar \dot{a}_k^{(1)} = H^{(1)}_{km} e^{i(E_k - E_m)t/\hbar}$$

or $$a_k^{(1)} = \frac{1}{i\hbar}\int_0^t \underset{V_{km}}{\underset{\shortparallel}{H^{(1)}_{km}}} e^{i(E_k - E_m)t'/\hbar} dt'$$

assuming that $H^{(1)}$ is turned on at time zero.

Application:

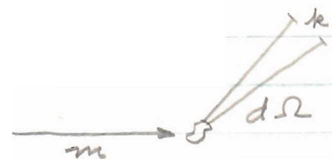



The probability per unit time of transition to the state k from state m is:

$$\frac{2\pi}{\hbar} |H_{km}|^2 \rho(k)$$

This is all in Schiff.

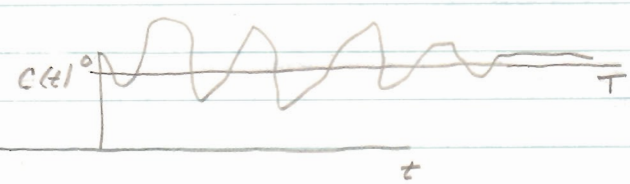
Application to scattering:




All values of $k$ are possible

We assume $H$ turned on at time of collision.

Another application: Atom subjected to Black Body Radiation.


$H^{(1)} = C(t)\cdot O^{(1)}$

assume that perturbation goes to zero at time $T$

Probability of transition $m \to k$ depends on magnitude of proper frequency components in $H^{(1)}$. We examine these components through Fourier transforms:

$$F(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{F}(\omega)\, e^{-i\omega t}\, d\omega$$

$$\mathcal{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(t)\, e^{i\omega t}\, dt$$

with $\int_{-\infty}^{\infty} |F(t)|^2\, dt = \int_{-\infty}^{\infty} |\mathcal{F}(\omega)|^2\, d\omega$ (Parseval's Equation)

If $F(t)$ is real, $\mathcal{F}^*(\omega) = \mathcal{F}(-\omega)$,

then: $\int_{-\infty}^{\infty} |F(t)|^2\, dt = 2\int_{0}^{\infty} |\mathcal{F}(\omega)|^2\, d\omega$

If $F(t)$ is electric field strength, $|F(t)|^2$ is intensity, (per unit time), then $2|F(\omega)|^2$ is intensity per unit frequency.

What we then get for the a's:

$$a_k^{(1)} = \frac{1}{i\hbar}\int_0^T V_{km}\, e^{i(E_k - E_m)t'/\hbar}\, dt' , \quad \omega_{km} = \frac{E_k - E_m}{\hbar}$$

or, using the transforms:

$$a_k^{(1)} = \frac{1}{i\hbar}\sqrt{2\pi}\,\mathcal{V}_{km}(\omega_{km})$$

Thus the transition probability/unit time of $k \leftarrow m$

$$= \frac{|a_k^{(1)}|^2}{T} = \frac{2\pi}{\hbar^2 T}\,|\mathcal{V}_{km}(\omega_{km})|^2$$

We now consider an incident radiation field as a function of position and time, but use the position as the center of the atom as the wavelength is much longer than the dimensions of the atom. That is:


Now V is the product of $\vec{E}$ and the polarization $\vec{p}$ or:

$$V = \vec{E}\cdot\vec{p} = \vec{E}\cdot\sum_a e_a \vec{r}_a$$

The intensity is $\frac{c}{4\pi}E^2$ per unit time

or $I(\omega) = \frac{c}{4\pi}\cdot 2\,|E(\omega)|^2$

We know assume the radiation to be collimated and polarized. Then:

$$\frac{|a_k^{(1)}|^2}{T} = \frac{\pi}{\hbar^2}\cdot\frac{4\pi}{c}\,\left|(P_{\parallel}E)_{km}\right|^2 \underbrace{\left\{\frac{c}{4\pi}\, 2\,\frac{|\mathcal{E}(\omega_{km})|^2}{T}\right\}}_{I(\omega_{km})}$$

Now the energy per unit frequency per unit volume is:

$$\frac{I(\omega)}{c} = U(\omega)$$

Then:
$$\frac{|a_k^{(1)}|^2}{T} = \frac{4\pi^2}{\hbar^2} \left| (p_{\parallel} E)_{km} \right|^2 U(\omega_{km})$$

For the isotropic case where the radiation is in random directions. Thus we have for $p_{\parallel E}$ is $p^2 \overline{\cos^2\theta}$ with $\overline{\cos^2\theta} = 1/3$ in any given direction. Thus:

$$\frac{P_{k\leftarrow m}}{T} = \frac{|a_k^{(1)}|^2}{T} = \frac{4\pi^2}{3\hbar^2} |\vec{p}_{km}|^2 \rho(\omega_{km})$$

making the change in notation $U \to \rho$ for the isotropic case. The Einstein transistion coefficient is:

$$B_{km} = \frac{4\pi^2}{3\hbar^2} |p_{km}|^2$$

Important: note that absorption and emission are equally probable.

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LECTURE II 2-8-61

Recapitulation: For isotropic radiation:

$$\frac{P_{k\leftarrow m}}{T} = \underbrace{\frac{2\pi}{3\hbar^2} |\vec{p}_{km}|^2}_{B_{km}} \rho(\nu_{km})$$

($\rho$: energy / unit volume & unit range of $\nu$)

The Einstein B coefficients is for absorption or stimulated emission.

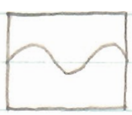
Spontaneous Emission:


If system originally in m, there is probability of transition to k.

None of external field presents. Decay is spontaneous. This is called:

$$\left(\frac{d P_{k \leftarrow m}}{dt}\right)_{spont.} \sim A_{km}, \text{ the Einstein A coefficient.}$$

Method of relating A and B: make up fictitious field assuming $h\nu$ per degree of freedom. Consider a box of unit volume, 1 cm on each side.



This gives for the density of states:

$$\rho' = 2 h\nu \frac{4\pi\nu^2}{c^3}$$

(↑ 2: polarization)

The volume of the box in k space is: $\Delta k_x \Delta k_y \Delta k_z = 8\pi^3$.

The number in k space is: $\frac{d\bar{k}}{\Delta \bar{k}} = \frac{d\bar{k}}{8\pi^3} = \frac{4\pi k^2 dk}{8\pi^3}$

$$= \frac{4\pi\nu^2 d\nu}{c^3}$$

Now $\rho'$ is the "dummy" radiation density. We then get for the spontaneous emission rate:

$$\left(\frac{d P_{k \leftarrow m}}{dt}\right)_{spont.} = \frac{2\pi}{3\hbar^2} \cdot \frac{8\pi h\nu^3}{c^3} \left|\bar{p}_{km}\right|^2$$

We now calculate the spontaneous radiation.

$$\left(\frac{dE}{dt}\right)_{spont.} = h\nu \left(\frac{dP}{dt}\right)_{spont} = \frac{4(2\pi)^4 \nu^4 e^2 \left|\bar{r}_{km}\right|^2}{3c^3}$$

assuming a one-electron atom with
$\bar{p}_{km} = e\,\bar{r}_{km}$

If atom acted as a classical harmonic oscillator:

$$(2\pi\nu)^2\,\bar{r}_{km} = \bar{a}_{km}$$

Then: $$\left(\frac{dE}{dt}\right)_{spont.} = \frac{2e^2}{3c^3}\cdot 2\,|\bar{a}_{km}|^2$$

Now classically:

$$\overline{\left(\frac{dE}{dt}\right)_{rad}} = \frac{2e^2}{3c^3}\,\overline{|\bar{a}|^2} \quad , \quad a \Rightarrow A \text{ in this case}$$
$$\overline{A^2\cos^2\omega t} = \tfrac{1}{2}A^2$$

Classically, we would have Fourier series for acceleration:

$$\bar{a} = \sum_{\tau=1}^{\infty} A_\tau \cos(\tau\omega t + \epsilon_\tau)$$
$$= \sum_{\tau=-\infty}^{\infty} |a_\tau|\, e^{i(\tau\omega t + \epsilon_\tau)}$$

Thus $|A_\tau| = 2\,|a_\tau|$

Thus the $m\,e\ a_{km}$ corresponds exactly to the classical Fourier coefficient $A_\tau$ with $\tau = m-k$, viz: $\bar{a}_{km} \longleftrightarrow \bar{a}_{\tau=m-k}$.
We desire that a relation be obtained between $X_{km} \longleftrightarrow X_{m-k}$. The proper choice led to the development of matrix mechanics.

## Transformation Theory

The model is the one-dimensional Sturm - Liouville system, postulating orthonormality and other usual properties.

Choose a complete orthonormal set; $u_n(q)$, that is:

(1) $\int u_m^* u_n \, dq = \delta_{mn}$ (orthonormal)

(2) $\psi_a(q) = \sum_n a_n u_n(q)$, $a_n = \int u_n^* \psi_a \, dq$ (complete)

We could just as well write:

$$\psi_a(q) = \sum_n u_n(q)\, a_n$$

Another way of stating completeness:

(3) $\sum_n u_n(q)\, u_n^*(q') = \delta(q-q')$

The Parseval equation:

(4) $\int |\psi_a|^2 dq = \sum_n |a_n|^2$

which is also a statement of completeness. We also expand another function the same as (2):

(2') $\psi_b(q) = \sum_n u_n(q)\, b_n$, $b_n = \int u_n^*(q)\, \psi_b \, dq$

which then gives for the inner product or overlap integral:

(5) $\int \psi_b^* \psi_a \, dq = \sum_n b_n^* a_n$

Thus we have two languages or representations: one depending on $q$ and the other on $n$. We then call the $u_n$'s transformation functions.

## LECTURE III  2-10-61

Recapitulation:

(1) $\int u_n^* u_m \, dq = \delta_{mn}$

(2) $\psi_a = \sum_n u_n a_n$ , $a_n = \int u_n^* \psi_a \, dq$

(3) $\sum_n u_n(q) u_n^*(q') = \delta(q-q')$

(4) $\int \psi_b^* \psi_a \, dq = \sum_n b_n^* a_n$

The transformation function are chosen to satisfy:

(6) $\underline{\xi} u_n = \xi u_n$ , $\underline{\xi}$ is a list of a complete set of operators

Suppose that the operator is $\underline{H}$. There is possibility of degeneracy:

For one $\underline{H}$, we could have $E_n = E_{n+1} = \cdots E_{n+f-1}$ for $f$-fold degeneracy. Can choose a different operator to redefine basis functions. Can do this continuously until complete set is formed (operators). Usually $H$ is chosen first.

If for $\underline{A}$ and $\underline{B}$ we have $u_n$ which are eigenfunction of both and form a complete set of functions, then $[\underline{A}, \underline{B}] = 0$

For example, consider: $\psi = \sum_n a_n u_n$

then: $\underline{B}\psi = \sum_n a_n \underline{B} u_n = \sum_n a_n B_n u_n$

and: $\underline{A}\underline{B}\psi = \sum_n a_n B_n \underline{A} u_n = \sum_n a_n B_n A_n u_n$

or: $\underline{B}\underline{A}\psi = \sum_n a_n A_n B_n u_n$ , thus $\underline{B}\underline{A} = \underline{A}\underline{B}$

Now, for hydrogenic cases, consider the operators $\underline{H}$ and $\underline{L}^2$ with eigenvalues $\frac{1}{n^2}$ and $l(l+1)$. Also, consider the operator defined by $\underline{L_z} \rightarrow \frac{1}{i}\frac{\partial}{\partial\varphi}$.

Example: $n = 3$ $\begin{cases} l = 2 \; \{ m = 0, \pm 1, \pm 2 \\ l = 1 \;, \; m = 0, \pm 1 \\ l = 0 \;, \; m = 0 \end{cases}$

Dirac Notation:

(6) $\rightarrow$ $\xi\, u_{\xi'} = \xi' u_{\xi'}$

(7) $u_{\xi'}(q') \longrightarrow (q'|\xi')$ or $\langle q'|\xi'\rangle$

(8) and $u^*_{\xi'}(q') \longrightarrow (\xi'|q')$ or $\langle \xi'|q'\rangle$

These are just numerical quantities because we have a particular eigenvalue $\xi'$ at a specific coordinate $q'$. $\xi'$ is the label and $q'$ is the argument.

In this notation, ① and ③ become:

(9) $\begin{cases} (1) \rightarrow \int (\xi'|q')\,dq'\,(q'|\xi'') = \delta(\xi', \xi'') \\ (3) \rightarrow \sum_{\xi'} (q'|\xi')(\xi'|q'') = \delta(q'-q'') \end{cases}$

and:

(10) $\psi_a(q') \longrightarrow (q'|a)$, if we always consider one state $\psi(q') \rightarrow (q'|)$

(11) $a_{\xi'} \rightarrow (\xi'|a)$ or $C_{\xi'} = (\xi'|)$

The translation rule becomes:

(12) $(q'|a) = \sum_{\xi'} (q'|\xi')(\xi'|a)$

(12) and $\int (\xi'|q')\, dq'\, (q'|a) = (\xi'|a)$

Thus we see that the fluency property enables the elimination of the argument from the notation.

Now our expansion becomes in the Dirac notation becomes (from (4)):

(13) $\int |\psi_a|^2\, dq' = \sum_{\xi'} |a_{\xi'}|^2$

or $\int (a|q')\, dq'\, (q'|a) = \sum_{\xi'} (a|\xi')(\xi'|a) = (a|a)$

$= 1$ for normalization. (Parseval's equation)

(14) $\int (b|q')\, dq'\, (q'|a) = \sum_{\xi'} (b|\xi')(\xi'|a) = (b|a)$

for the overlap integral.

Proof of (4) and (5) from orthonormality and completeness:

$$\int (b|q')\, dq'\, (q'|a) = \iint (b|q')\, dq'\, \underbrace{\delta(q'-q'')}_{\sum_{\xi'} (q'|\xi')(\xi'|q'')}\, dq''\, (q''|a)$$

$$= \sum_{\xi'} (b|\xi')(\xi'|a) = (b|a)$$

This is a common trick that it used often.

# LECTURE IV 2-13-61

Recapitulation:

Wave function : $(q'|\xi')$ ; complex conjugate : $(\xi'|q')$

argument ↗ ↖ label

Case when $q''$ has been measured and we want to get the probability of $q'$:

$$\psi_{q''}(q') = (q'|q'') = \delta(q'-q'')$$

which is not quadratically integrable and represents a continuous spectrum. Now, $\psi$ is normalized in the scale of $q$ and we can write:

$$\int \psi^*_{q'''}(q')\,\psi_{q''}(q')\,dq' = \delta(q'''-q'')$$

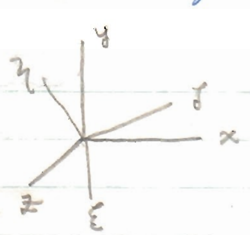
$$\int (q'''|q')\,dq'\,(q'|q'') = (q'''|q'')$$

$$\int \delta(q'''-q')\,\delta(q'-q'')\,dq'$$

We can use different representations:

$(q'|)$ (position)
$(p'|)$ (momentum)
$(\xi'|)$ (eigenvalue)

It is often convenient to represent these quantities independent of their representation. Such a representation would be vectors:




Could represent vector as in terms of basis $A_x, A_y, A_z$ or basis $A_\xi, A_\eta, A_\zeta$, but can represent abstractly as: $\vec{A}$

We can transform between coordinate systems using:

$$(\xi'|) = \sum_{\eta'} (\xi'|\eta')(\eta'|)$$

or $A_x = (\hat{e}_x \cdot \hat{e}_\xi) A_\xi + (\hat{e}_x \cdot \hat{e}_\eta) A_\eta + \cdots$

If space has infinite number of dimensions it is called a Hilbert space.

The most common symbol used to represent states are capital Greek symbols $\Phi$, $\Psi$. We define an inner product as:

$$(\Phi, \Psi) = \text{a number}$$

and $(\Psi, \Phi) = (\Phi, \Psi)^*$

The states can be superposed and the inner products are linear, viz:

(15) $(\Phi, c_1 \Psi_1 + c_2 \Psi_2) = c_1 (\Phi, \Psi_1) + c_2 (\Phi, \Psi_2)$

or $(c_1 \Psi_1 + c_2 \Psi_2, \Phi) = c_1^* (\Psi_1, \Phi) + c_2^* (\Psi_2, \Phi)$

In Dirac's 1st and 2nd editions (D1&2): the representation of the inner product is $\varphi\psi$, or $\varphi_a \psi_a$

In D3&4; the inner product is:

$\langle b|$ $|a\rangle$ or $\langle b|a\rangle$ = a number
bra ket bra (c) ket

Recall: If we apply an operator to a state we get another state: $\xi \Psi$ = another state. If the other state is a number times the first state, it is an eigenvalue equation.

(16) that is, $\xi \Psi_{\xi'} = \xi' \Psi_{\xi'} \longrightarrow \xi | \xi' \rangle = \xi' | \xi' \rangle$

If we have such a function that is a solution to the eigenfunction equation, we can expand in terms of this function:

(17) $\Psi = \sum_{\xi'} \Psi_{\xi'} (\xi' |)$ where $(\xi' |) = (\Psi_{\xi'}, \Psi)$

In the Dirac notation:

(17') $| \rangle = \sum_{\xi'} | \xi' \rangle \underbrace{\langle \xi' | \rangle}_{\text{self-defining}}$

Operators:

(2) Recall: $\psi(q) = \sum_n u_n(q)\, a_n$ , $a_n = \int u_n^* \psi \, dq$

(18) $\underline{F} \psi = \sum_n \underline{F}\, u_n a_n$

or $\underline{F} \psi = \sum_n u_n c_n$

(19) where $c_m = \int u_m^* \underline{F} \psi \, dq = \sum_n \int u_m^* \underline{F}\, u_n a_n \, dq$

and we define the matrix element as:

$\int u_m^* \underline{F}\, u_n \, dq = F_{mn}$ , $\therefore c_m = \sum_n F_{mn} a_n$

In Dirac notation:

(20) $\underset{\substack{\uparrow \\ \text{memorandum}}}{(\xi' | (F\psi))} = \sum_{\xi''} (\xi' | \underline{F} | \xi'')(\xi'' | (\psi))$

(21) $(\xi' | \underline{F} | \xi'') = \int (\xi' | q') \underline{F} (q' | \xi'') \, dq'$ (hybrid notation, not acceptable)

We have $(q' | (F\psi)) = \underline{F} (q' | (\psi))$
but really want:

(22) $(q' | (F\psi)) = \sum_{q''} (q' | F | q'')(q'' | (\psi))$

How do we represent $xe^{-x'^2/2} = x'e^{-x'^2/2}$ as a sum of matrix elements? This is the reason for the birth of the Dirac delta function. Dirac defined a matrix element such that:

(23) $$(x'|x_g|x'') = x_g' \, \delta(x_1'-x_1'') \cdots \delta(x_f'-x_f'')$$

For the QM momentum operator:

(23) $$(x'|p_g|x'') = \frac{\hbar}{i}\delta(x_1'-x_1'') \cdots \delta'(x_g'-x_g'') \cdots \delta(x_f'-x_f'')$$
$$= -\frac{\partial}{\partial x_g'}\delta(x_g'-x_g'')$$

This has all been formally justified in the theory of distributions.

Now, going back to (22):

$$(x'|(\underline{x}_g\psi)) = \int (x'|\underline{x}_g|x'')\,dx''\,(x''|(\psi)) = x_g'\,(x'|(x))$$

$$(x'|(\underline{p}_g\psi)) = \int (x'|p_g|x'')\,dx''\,(x''|(\psi)) = \frac{\hbar}{i}\frac{\partial}{\partial x_g'}(x'|(\psi))$$

The beauty of this is that it puts operators into matrix form so that matrix algebra can be used. Now:

$$(\xi'|F|\xi'') = \iint (\xi'/q')\,dq'\,(q'/F/q'')\,dq''\,(q''/\xi'')$$

which obeys fluency. <u>NOTE</u>: round brackets mean numbers.

We can now make the following identifications.

$(\xi'/)$ : one column matrix "wave function"

$(/\xi')$ : one row matrix "cc of wave function"

$(\xi'/F/\xi'')$ : square Hermitian matrix

$(\xi'/\eta')$ : rectangular unitary matrix

$$\sum_{\eta'} (\xi'/\eta')(\eta'/\xi'') = (\xi'/\xi'') = \delta(\xi',\xi'')$$

LECTURE V    2-15-61

Recapitulation:

(26) $\psi(r) \longrightarrow (r'|) \quad \langle r'| \rangle$

$\varphi(p) \longrightarrow (p'|) \quad \langle p'| \rangle$

the wave function in bra-ket notation.

Recall that wave functions are expressed in terms of Fourier integrals of each other:

(27) $\psi(r) = \frac{1}{h^{3/2}} \int e^{ip\cdot r/\hbar} \varphi(p)\, dp$

$\varphi(p) = \frac{1}{h^{3/2}} \int e^{-ip\cdot r/\hbar} \psi(r)\, dr$

or, in the new notation:

(28) $(r'|) = \int (r'|p')\, dp'\, (p'|)$

$(p'|) = \int (p'|r')\, dr'\, (r'|)$

(29) $(r'|p') = \frac{1}{h^{3/2}} e^{ip'\cdot r'/\hbar}$

$(p'|r') = \overline{(r'|p')} = \frac{1}{h^{3/2}} e^{-ip'\cdot r'/\hbar}$

We require orthonormality,

(30) $\int (p'|r')\, dr'\, (r'|p'') = (p'|p'') = \delta(p'-p'')$

$= \frac{1}{h^3} \int e^{i(p''-p')\cdot r'/\hbar}\, dr' = \frac{1}{(2\pi)^3} \int e^{is'\cdot(p''-p')}\, ds'$

$= \delta(p'-p'')$, when $r' = \hbar s'$

Operators (Observables):

Consider $\langle \xi' | (G F \psi) \rangle = \sum_{\xi''} \langle \xi' | G | \xi'' \rangle \langle \xi'' | (F\psi) \rangle$

$$= \sum_{\xi'' \xi'''} \langle \xi' | G | \xi'' \rangle \langle \xi'' | F | \xi''' \rangle \langle \xi''' | (\psi) \rangle$$

$$= \sum_{\xi'''} \langle \xi' | G F | \xi''' \rangle \langle \xi''' | (\psi) \rangle$$

thus we have the general rule for matrix multiplication:

$$\langle \xi' | GF | \xi'' \rangle = \sum_{\xi'''} \langle \xi' | G | \xi''' \rangle \langle \xi''' | F | \xi'' \rangle$$

Suppose we are working in the $\eta$ representation.

$$\langle \eta' | GF | \eta'' \rangle = \sum_{\eta'''} \langle \eta' | G | \eta''' \rangle \langle \eta''' | F | \eta'' \rangle$$

$$= \sum_{\eta'''} \sum_{\xi' \xi'' \xi''' \xi^{iv}} \langle \eta' | \xi' \rangle \langle \xi' | G | \xi'' \rangle \underbrace{\langle \xi'' | \eta''' \rangle \langle \eta''' | \xi''' \rangle}_{\delta(\xi'', \xi''')} \langle \xi''' | F | \xi^{iv} \rangle \cdot \langle \xi^{iv} | \eta'' \rangle$$

$$= \sum_{\eta'''} \sum_{\xi' \xi'' \xi^{iv}} \langle \eta' | \xi' \rangle \langle \xi' | G | \xi'' \rangle \langle \xi'' | F | \xi^{iv} \rangle \langle \xi^{iv} | \eta'' \rangle$$

$$= \sum_{\eta'''} \langle \eta' | \xi' \rangle \langle \xi' | GF | \xi^{iv} \rangle \langle \xi^{iv} | \eta'' \rangle$$

thus it makes no difference whether we first multiply in $\xi$ representation and transform to $\eta$, or first multiply in $\eta$ last after transforming from $\xi$.

All observables can be represented as square matrices. Introduce the notation:

$F, G$ matrices in $\xi$-rep
$F', G'$ matrices in $\eta$-rep

$S$ = matrix of $\langle \xi' | \eta' \rangle$

$S^{-1}$ = matrix of $\langle \eta' | \xi' \rangle$

now $1 = S^{-1} S \leftrightarrow \sum_{\xi'} \langle \eta' | \xi' \rangle \langle \xi' | \eta'' \rangle = \langle \eta' | \eta'' \rangle$

$= \delta(\eta', \eta'')$

thus: $F' = S^{-1} F S$

or $\langle \eta' | F | \eta'' \rangle = \sum_{\xi' \xi''} \langle \eta' | \xi' \rangle \langle \xi' | F | \xi'' \rangle \langle \xi'' | \eta'' \rangle$

now define $GF = A$ and form:

$S^{-1} \{ GF = A \} S$

or $S^{-1} G S S^{-1} F S = S^{-1} A S$

or we have $G' F' = A'$

It is also possible to show that all algebraic forms in one representation transform to the same algebraic form in another representation by extension of above. Dirac's method gives a method of calculating matrix elements.

$\langle \eta' | F | \eta'' \rangle = \int \psi_{\eta'}^{*} F \psi_{\eta''} \, dr$

but the dirac notation is independent of the coordinate representation.

Statistical Interpretation:

$|(\xi'|a)|^2$ is a probability density that a measurement of $\xi$ gives $\xi'$

↑ state label

If the eigenvalues are continuous and denoted by $\xi_l'$ and the discrete by $\xi_k'$, then:

$$|(\xi'/a)|^2 \, d\xi_{l_1}' \, d\xi_{l_2}' \cdots = \text{probability that } \xi_k$$

will be found to have values $\xi_k'$ and $\xi_l$ in $d\xi_l'$ {for system in state a}

In general:

$$|(\xi'|\eta')|^2 \, d\xi_{l_1}' \cdots \begin{cases} = \text{probability, if } \eta \text{ all discrete} \\ \propto \text{probability, if any } \eta \text{ continuous} \end{cases}$$

which is for system in eigenstate with eigenvalue $\eta'$.

Actually eigenstates of continuous spectrum are not physically realizable.

All of above depends on the postulate (0th law) is that a measurement gives one of the eigenvalues.

The diagonals of matrices are the expectation values of the observable:

$$(a|\xi_k|a) = \text{Expectation of } \xi_k = \overline{\xi_k'} = \langle \xi_k \rangle$$

LECTURE VI    2-17-61

Statistical Interpretation:

$(\xi'|a)$ is a probability amplitude

and $(a|\xi_k|a)$ = Expectation$_a$ $(\xi_k)$

From ordinary statistical theory on expectation values:

$$\mathrm{Exp}_a(\xi_k) = \sum_{\xi'} \xi_k' \,|(\xi'|a)|^2 = \sum_{\xi'} (a|\xi')\xi_k'(\xi'|a)$$

Recall: $(\xi''|\xi_k|\xi') = \xi_k'(\xi''|\xi') = \xi_k' \,\delta_{\xi''\xi'}$

Then: $\mathrm{Exp}_a(\xi_k) = \sum_{\xi'} (a|\xi')\xi_k'(\xi'|a)$

$$= \sum_{\xi'\xi''} (a|\xi')\xi_k' \,\delta(\xi',\xi'')(\xi''|a) = \sum_{\xi'\xi''} (a|\xi')(\xi'|\xi_k|\xi'')(\xi''|a)$$

$$= (a|\xi_k|a)$$

This is the usual statistical interpretation of the theory, but is not most general.

Take $(q'|\xi')$ which means that we have completely determined $\xi'$ and now want to find $q'$. Completely determined states are called pure states. A pure state is also denoted by $\Phi$ or $|\xi'\rangle$ also. If we want to use wave functions, however, we must use the argument, viz $(q'|\xi')$.

For a mixed state, we cannot write the wave function. We only give a list of probabilities $w_{\xi'}$ for states $|\xi'\rangle$, $\sum_{\xi'} w_{\xi'} = 1$. This situation corresponds better with physical reality. We suppose that some of the possible values of measurements are $\eta_k$ (discrete), $\eta_e$ (continuous).

Consider an electron which has two spin directions. The a priori probability of each spin is 1/2, up or down, where the spin up and spin down are pure states.

Then, for the pure state, the Prob of $\eta'_{\xi}$ in $(d\eta'_{\xi})$ is:

$$|(\eta'|\xi')|^2 \, d\eta'_{\xi} \ldots$$

or

$$\sum_{\xi'} w_{\xi'} |(\eta'|\xi')|^2 \, d\eta'_{\xi} \ldots$$

or

$$\left\{ w_a |(\eta'|a)|^2 + w_b |(\eta'|b)|^2 + \cdots \right\} d\eta'_{\xi} \ldots$$

for the mixed state. This does not mean we are representing a mixed state by a expanded wave function as a mixed state cannot be represented by wave functions. The word mixing is sometimes used colloqually as the mixing of states which does not apply here. This mixing (here) results from the fact that all the observables are not measured.

If we tried to represent a mixed state by a wave function by:

$$(q'|) = \sum_{\xi'} \sqrt{w_{\xi'}} \, (q'|\xi')$$

We have merely supperposed pure states resulting in another pure state.

which represents a pure state and not a mixed state. Forming the probability:

$$|(q|)|^2 = \sum_{\xi'} w_{\xi'} |(q'|\xi')|^2 + \sum_{\xi'' \neq \xi} \sqrt{w_{\xi'} w_{\xi''}} \, (q'|\xi')(\xi''|q')$$

Now the mixed state, as above, does not have the cross-product terms which arise from using wave function. One way to fix this is to include a phase factor in the expansion $e^{i\varphi_{\xi'}}$. Then, averaging over the phase factors will remove the cross-product. The phase factor must be unspecified over the states. This lack of information about phase characterizes the mixed state (see Von Neumann).

Density matrix (Example: polarized beam on unpolarized target)

Definition for mixed states:

$$(q'|P|q'') = \sum_{\xi'} w_{\xi'} (q'|\xi')(\xi'|q'') = \sum_{\xi'} w_{\xi'} \psi_{\xi'}(q')\psi^*_{\xi'}(q'')$$

which gives a matrix whose diagonal gives the probability. This can be written, per Dirac:

$P = \sum_a w_a |a\rangle\langle a|$ , $|a\rangle\langle a|$ is an operator

Analogous to scalar product and dyadic:

$\vec{A}\cdot\vec{B} = \sum_i A_i B_i$

$\vec{A}\,\vec{B} = A_j B_j$ usually used in conjunction with other vectors.

now: Prob. of in $dq' = (q'|P|q'')\,dq'$

Prob of $\eta' = (\eta'|P|\eta')$

Therefore, we can write $Exp(F) = Tr(PF)$
↑ some operator

$$Exp(\eta_k) = \sum_{\xi'} w_{\xi'} \left[ Exp(\eta_k) \right]_{\xi'}$$

— expectancy of $\eta_k$ if it belonged to a pure state $\xi'$. From definition.

$$= \sum_{\xi'} w_{\xi'} (\xi'/\eta_k/\xi') = \sum_{\xi'} w_{\xi'} \iint (\xi'/q')\,dq'\,(q'/\eta_k/q'')\,dq''\,(q''/\xi')$$

$$= \iint (q''/P/q')\,dq'\,(q'/\eta_k/q'')\,dq'' = Trace\,(\eta_k P)$$

$= Trace\,(P\eta_k)$ , thus proving the above statement.

LECTURE VII    2-20-61

$$\text{Exp}\{F\} = \text{Tr}\, PF \quad , \quad \text{Tr}\, P = 1$$

$$P = \sum_{\xi'} \omega_{\xi'} |\xi'\rangle\langle\xi'|$$

$$\langle\eta'|P|\eta''\rangle = \sum_{\xi'} \langle\eta'|\xi'\rangle \omega_{\xi'} \langle\xi'|\eta''\rangle$$

Note that the ω's are eigenvalues of P:

$$P|\xi''\rangle = \omega_{\xi''}|\xi''\rangle$$

Pure State:

$$(\eta'|P|\eta'') = (\eta'|\xi')(\xi'|\eta'')$$

$$(\eta'|P^2|\eta'') = \sum_{\eta'''} (\eta'|P|\eta''')(\eta'''|P|\eta'')$$

$$= \sum_{\eta'''} (\eta'|\xi')\underbrace{(\xi'|\eta''')(\eta'''|\xi')}_{1}(\xi'|\eta'')$$

$$= (\eta'|\xi')(\xi'|\eta'') = (\eta'|P|\eta'')$$

Therefore: $P^2 = P$ is implied.
This property is called idempotent and the operator is called a projection operator.

Examples: Dyadic: $\hat{i}\hat{i}\cdot A = \hat{i}A_x = A_x$

In old-fashioned notation:

$$P_{mn} = C_m C_n^* \quad \text{or} \quad W_a a_m a_n^* + W_b b_m b_n^* + \dots$$

and $(x'|P|x'') = \psi(x')\,\psi^*(x'')$

Some Von Neumann Arguments:

1. No Hidden Parameter Argument (Von Neumann)

Quantum mechanics is inconsistent with hidden parameters which would remove uncertainty. V.N. did not prove hidden parameters do not exist in universe, but that if quantum mechanics is strictly true, the concept of hidden parameters cannot exist.

Pure State: Classical Physics: - know every dynamical variable of system when prepared - mechanical determinism, everything that happens henceforth is completely determined.

V.N.'s proof does not indicate how much error would have to occur in QM to indicate hidden parameters.

Mixed State: Classical Physics: - Gibb's ensemble of states and systems. However, still assume that dynamical variables could in principle be measured. A pure state would be an ensembles of systems all in the same state. Thus we see two definitions for pure states.

If hidden parameters existed, it would be possible to form a pure state from mixed states. Von Neumann's theorem proves this untrue.

These definitions are not identical in QM. It is possible to have Gibb's ensemble of systems in same state, however, that of knowing dynamical variables of system does not exist. A mixed state in CM can only be formed from Gibb's ensemble of systems of different states. Thus QM contains probabilities of two types, that of statistical mechanics and that of Born interpretation. V.N.'s argument is that:

If $P^2 = P$ and $P = wQ + (1-w)R$

Then $Q = R = P$ and a pure state cannot be formed as composed of mixed states.

2. The act of measurement causes the state of the object to be mixed. We have object with suitably prepared instrument coupled by suitable Hamiltonian; after a certain time we decouple and observe instrument, whereupon, we find a particular $\varphi_i(p)$ corresponding to a particular $\psi_i(q)$

$$\varphi(p)\,\psi(q) \xrightarrow[\text{Hamiltonian}]{} \sum_n w_n\, \varphi_n(p)\, \psi_n(q)$$, when brought together, we have no knowledge of phase factor.

$\varphi(p) \to$ original state of instrument, $\psi(q) \to$ original state of object

Degenerate Mixture: $n$ states:

$$(\eta'|P|\eta'') = \sum_{k=1}^{n} \frac{1}{n} (\eta'|\xi^{(k)})(\xi^{(k)}|\eta'')$$

Probabilities of different states assumed equal (reason for $\frac{1}{n}$ term).

Suppose we have sets $|\xi^{(k)}\rangle$, $|\zeta^{(j)}\rangle$ that span the same manifold. Now there are certain states that can be written:

$$|\;\rangle = \sum_{k=1}^{n} |\xi^{(k)}\rangle\langle\xi^{(k)}|\;\rangle \quad \text{(but not all)}$$

Any set that spans the same manifold would yield a similar expansion:

$$|\;\rangle = \sum_{j=1}^{n} |\zeta^{(j)}\rangle\langle\zeta^{(j)}|\;\rangle$$

manifold = some $n$ dimensions of the Hilbert space.

Then:

$$(\eta'|P|\eta'') = \sum_{j=1}^{n} \frac{1}{n} (\eta'|\zeta^{(j)})(\zeta^{(j)}|\eta'')$$

The relation between the two sets is:

$$|\zeta^{(j)}\rangle = \sum_{k=1}^{n} |\xi^{(k)}\rangle\langle\xi^{(k)}|\zeta^{(j)}\rangle$$

with:

$$\sum_{k=1}^{n} \langle\zeta^{(j)}|\xi^{(k)}\rangle\langle\xi^{(k)}|\zeta^{(l)}\rangle = \delta_{jl}$$

Therefore:

$$(\eta'|P|\eta'') = \sum_{\substack{k=1\\ l=1}}^{n} \frac{1}{n} (\eta'|\xi^{(k)}) \, \delta_{kl} \, (\xi^{(l)}|\eta'')$$

$$= \sum_{k,l} \sum_{j} \frac{1}{n} (\eta'|\xi^{(k)})(\xi^{(k)}|\gamma^{(j)})(\gamma^{(j)}|\xi^{(l)})(\xi^{(l)}|\eta'')$$

which yields of the same as before. What this says is that, for example, states composed of spin, it makes no difference if half the spins are up and some down, or if half to left and half to right. A similar analogy holds in unpolarized light being considered as composed of polarized light independent of the scheme of polarization, that is, at right angles, or in opposite circular directions.

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LECTURE VIII    2-24-61

Time Dependence:

In non-relativistic QM, time is not an observable but merely a parameter. Analytic measurements determine quantities but destroy the system, called retrospective. Those putting system in another eigenstate are called predictive.

If we measure the observable at time $t_0$ we get $\xi'$, this means that we get $\xi'$ at time $t_0$ again (no time lapse). If we measure $\xi$ at $t > t_0$ may not get $\xi'$ again. We indicate the preparedness of the system at $t_0$ by

$$|\xi', t_0\rangle \quad \text{means} \quad |(\xi(t_0))'\rangle$$

The usual base of time is 0, hence $|\xi', 0\rangle$ indicates initial preparedness.

We denote a "frozen" state by $|\xi', t\rangle$ which means that this state gives $\xi'$ at any time $t$. That is,

$$\xi\,|\xi', t\rangle = \xi'\,|\xi', t\rangle \qquad \text{at time } t$$

Also we require for "frozen" state:

$$\langle \eta', t\,|\,\xi', t\rangle = \text{constant}$$

If we change all states by phase factor $e^{i\gamma(t)}$, they cancel in the inner products so we have still "frozen" states. Thus we say that at time $t$ we have:

$$|\xi', t\rangle_t = \text{constant ket} = |\xi', t\rangle$$

$$|\xi', 0\rangle = \text{physical ket or physical state}$$

Constant kets have little physical significance and are available primarily for expansion purposes.

Now for the physical states $|\xi', 0\rangle$, we hold that all superposition properties are independent of time. Consider:

$$|(a), 0\rangle = c_1|\xi', 0\rangle + c_2|\xi'', 0\rangle + \ldots$$

which is independent of time (the $c$'s are time independent, so superposition is held as a physical postulate) (Dirac, pp 109–110).

Now we postulate:

$$|\xi', a\rangle_t = T(t)|\xi', 0\rangle_0 \quad , \; T \text{ is linear}$$

and describes the course of events as time progresses. $T$ cannot be shown to be an observable.

Consider the bra ${}_t\langle\xi',0|$, then:

$${}_t\langle\xi',0| = {}_0\langle\xi',0|T^\dagger$$

is the definition of $T^\dagger$.

We require as another postulate:

$${}_t\langle\xi',0|\xi',0\rangle_t = 1 \quad \text{independent of } t>0$$

Using this, we have immediately $T^\dagger T = 1$ which shows that it might be unitary (we need $TT^\dagger = 1$ for sure proof). We will postulate that $T$ is unitary.

Now write:

$$|\xi',0\rangle_{t+\Delta t} = (T+\Delta T)\,|\xi',0\rangle_0$$

$$= (T+\Delta T)\,T^\dagger\,|\xi',0\rangle_t$$

from $T^\dagger|\xi',0\rangle_t = |\xi',0\rangle_0$. Now assume $TT^\dagger = 1$:
(not necessary)

Now we can write:

$$|\xi',0\rangle_{t+\Delta t} - |\xi',0\rangle_t = \Delta T\,T^\dagger\,|\xi',0\rangle_t$$

Now: $(1+\Delta T\,T^\dagger)$ is unitary since origin of time is arbitrary.

Then: $(1+\Delta T\,T^\dagger)(1+\Delta T\,T^\dagger)^\dagger = 1$

$$\text{or} \quad \Delta T\,T^\dagger + T(\Delta T)^\dagger + \Delta T\,\underbrace{T^\dagger T}_{1}\,(\Delta T)^\dagger = 0$$

Now divide by $\Delta t$ and let $\Delta t \to 0$ and get:

$$\frac{d}{dt}|\xi',0\rangle_t = \frac{dT}{dt}\,T^\dagger\,|\xi',0\rangle_t \quad \text{and:}$$

$$\frac{dT}{dt}T^\dagger + \left(\frac{dT}{dt}T^\dagger\right)^\dagger = 0$$

which shows that $\frac{dT}{dt}T^\dagger$ is anti-Hermitean.

We then write $\frac{dT}{dt} T^{+} = i\left(-\frac{H}{\hbar}\right)$

as a definition where $H$ is a Hermitean operator. Then we have:

(1) $H\,|\xi',0\rangle = i\hbar \frac{d}{dt}\,|\xi',0\rangle$

and for physical cases, we postulate that $H$ is the Hamiltonian. Then this describes the behaviour of the state as time moves along.

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## LECTURE IX    2-27-61

Can show that $_0\langle\xi'',0|T^{+}T|\xi',0\rangle_0$ is sufficient to show that $T^{+}T$ is unitary, so separate assumption is not necessary.

We had shown that:

(1) $i\hbar \frac{d}{dt}\,|\xi',0\rangle_t = H\,|\xi',0\rangle_t$

where $H$ is some Hermitean operator and in $|\xi,0\rangle_t$ $t$ is a label, not an argument; the time is the present but the system is prepared at 0. If we write $|\eta',t\rangle$ this means that state is freshly prepared every instant. Then:

(2) $i\hbar \frac{d}{dt}\,\langle\eta',t|\xi',0\rangle_t = \langle\eta',t|H|\xi',0\rangle_t$

$|\eta',t\rangle$ is a constant.

If $\eta' = x$: coordinate rep.
$\eta' = p$: momentum rep.

Now:

(3) $i\hbar \frac{d}{dt}\,\langle\eta',t|\xi',0\rangle_t = \sum_{\eta''} \langle\eta',t|H|\eta'',t\rangle\langle\eta'',t|\xi',0\rangle_t$

which is the Schroedinger equation.
$|\xi',0\rangle_t$ is called a physical ket and is time dependent.

We can expand any ket as:

(4) $| \rangle = \sum_{\xi'} |\xi',0\rangle_{t\,t}\langle\xi',0| \rangle$

independent of time per assumption for inner products, ∴ numbers

Then we write (3) as:

(5) $i\hbar \frac{d}{dt} \langle\eta',t| \rangle = \sum_{\eta''} \langle\eta',t|H|\eta'',t\rangle\langle\eta'',t| \rangle$

This is Schroedinger equation in the $\eta'$ representation. Consider $H$ independent of time and the expression:

(6) $\langle\eta',t| e^{-iHt/\hbar} |\xi',t\rangle$ (6), $|\xi',t\rangle$ = constant ket, $\langle\eta',t|$ = constant bra

Take time derivative:

$$i\hbar \frac{d}{dt} \langle\eta',t| e^{-iHt/\hbar} |\xi',t\rangle = \langle\eta',t| H e^{-iHt/\hbar} |\xi',t\rangle$$

$$= \sum_{\eta''} \langle\eta',t|H|\eta'',t\rangle\langle\eta'',t| e^{-iHt/\hbar} |\xi',t\rangle$$

Now; to satisfy the boundary conditions:

$$\left[{}_t\langle\eta',t| e^{-iHt/\hbar} |\xi',t\rangle_t\right]_{t=0} = \left[\langle\eta',t|\xi',0\rangle\right]_{t=0}$$

Therefore:

(7) $\langle\eta',t|\xi',0\rangle = \langle\eta',t| e^{-iHt/\hbar} |\xi',t\rangle$

(7)* $\langle\xi',0|\eta',t\rangle = \langle\xi',t| e^{iHt/\hbar} |\eta',t\rangle$

This is formal solution to Schroedinger equation. The time dependence is removed from $|\xi',0\rangle$ and put in an operator.

Consider a Hermitean operator which is an observable:

$$\langle\eta',0|\alpha|\xi',0\rangle = \sum_{\eta''\xi''} \langle\eta',0|\eta'',t\rangle\langle\eta'',t|\alpha|\xi'',t\rangle\langle\xi'',t|\xi',0\rangle$$

Then:

$$\langle \eta';0|\alpha|\xi';0\rangle = \sum_{\eta''\xi''} \langle \eta';t|e^{iHt/\hbar}|\eta'';t\rangle\langle \eta'';t|\alpha|\xi'';t\rangle \langle \xi'';t|e^{-iHt/\hbar}|\xi';t\rangle$$

or:

(8) $$\langle \eta';0|\alpha|\xi';0\rangle = \langle \eta';t|e^{iHt/\hbar}\,\alpha\, e^{-iHt/\hbar}|\xi';t\rangle$$

This (LHS) is the matrix elements between physical states in the Schroedinger picture. The operator is independent of time (except explicitly). The state vectors are time dependent. The RHS of (8) is the Heisenberg picture: state vectors independent of time, operators have dynamical dependence on time. The LHS is the Schroedinger picture. In other notation:

(9) $$\underbrace{\alpha(t)}_{\text{Heisenberg}} = e^{iH\hbar/t}\,\underbrace{\alpha(0)}_{\text{Schroedinger}}\, e^{-iH\hbar/t}$$

For no explicit time dependence:

(10) $$\frac{d}{dt}\alpha(t) = \frac{i}{\hbar}\left[H, \alpha(t)\right]$$

From last term:

(11) $$\left(\frac{d}{dt}\alpha(0)\right) = \frac{i}{\hbar}\left[H, \alpha(0)\right]$$

In a representation with $H$ diagonal: $H_{nm} = E_n \delta_{nm}$
Then; from (8):

(12) $$\alpha_{nm}(t) = e^{i(E_n - E_m)t/\hbar}\,\alpha_{nm}(0)$$

which is the original assertion of Heisenberg for time dependence of matrix elements. In Schroedinger, we separate $\psi$-function, rather than operators.

manipulating (9) some more:

$$\alpha(t) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \left(\frac{it}{\hbar}\right)^{k+l} \frac{(-1)^l}{k!\,l!} H^k \alpha(0) H^l$$

Consider the $n$-fold commutator:

$$[H, \{H, \cdots \{H, \alpha(0)\} \cdots]_{n \text{ times}} = \sum_{k+l=n} \frac{(-1)^l n!}{k!\,l!} H^k \alpha(0) H^l$$

as can be found thru deduction: Then:

$$\alpha(t) = \sum_{n=0}^{\infty} \left(\frac{it}{\hbar}\right)^n \frac{1}{n!} [H, \{H, \cdots \{H, \alpha(0)\}_{(n)} \cdots]$$

and finally:

$$(13) \quad \alpha(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \left(\frac{d^n}{dt^n} \alpha(0)\right) \qquad \text{(Mac Laurin Series)}$$

Note on Notation:

$\Psi$ : Schroedinger state vector (Time dependent)
$\Phi$ : Heisenberg state vector (constant)

Then:

$$(14) \quad (\Psi_a, \alpha(0) \Psi_b) = (\Phi_a, \alpha(t) \Phi_b)$$

where $\alpha(t) = e^{iHt/\hbar} \alpha(0) e^{-iHt/\hbar}$

and:

$$(15) \quad \Psi = e^{-iHt/\hbar} \Phi$$

$$(16) \quad i\hbar \frac{\partial}{\partial t} \Psi = H \Psi$$

LECTURE X    3-1-61

In the Schroedinger representation:

(12) $i\hbar \frac{\partial}{\partial t} \Psi = H \Psi$ , $(\Psi_a, \alpha(0) \Psi_b)$

The state vector contains the time.

In The Heisenberg representation:

$$\frac{\partial}{\partial t} \Phi = 0 , \quad (\Phi_a, \alpha(t) \Phi_b)$$

$\alpha(t)$ is the Heisenberg operator, $\Phi$ is constant in Time.

The connecting relation is:

$$\alpha(t) = e^{iHt/\hbar} \alpha(0) e^{-iHt/\hbar}$$

$$\Psi = e^{-iHt/\hbar} \Phi$$ where $H$ is time independent.

Now consider:

(14) $H = H_0 + V$

where $H_0$ is time independent but $V$ is time dependent

A possible form for $V(0)$ could be:

$$V(0) = \dots + f(p,q) e^{i\omega t}$$ (not dynamically time dep.)

and still be a Schroedinger operator. This could possibly be an external EM field. In the most general type of physical theory, time dependence does not occur. $V(0)$ above has the time dependence introduced by an external system. Now:

(12)' $i\hbar \frac{\partial \Psi}{\partial t} = (H_0 + V(0)) \Psi$

(19) $\Psi = e^{-iH_0t/\hbar}\,\Psi'$

Take (12)' times $e^{iH_0t/\hbar}$ :

} we are making a transformation to a mixed representation. Called interaction representation

(20) $$i\hbar\frac{\partial}{\partial t}\Psi' = \underbrace{e^{iH_0t/\hbar}\,V(0)\,e^{-iH_0t/\hbar}}_{V}\,\Psi'$$

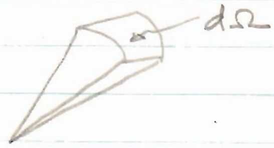
$\Psi'$ carries time dependence of unperturbed Hamiltonian. This is called the interaction picture.

(21) $$(\Psi_a, \alpha(0)\,\Psi_b) = (\Psi_a', e^{iH_0t/\hbar}\,\alpha(0)\,e^{-iH_0t/\hbar}\,\Psi_b')$$

Dirac claims to switch from Sch. rep. to Hes. rep., but really goes to interaction rep.

<u>Collision Theory</u>:

Scattering cross-section:




$\sigma(\theta,\varphi)\,d\Omega =$

Methods:

1. Exact solution
2. Partial Waves

} elastic

3. Born Approximation
4. Time Dependent Perturbation Theory

} inelastic

Rutherford scattering:

Use parabolic coordinates, hydrogen atom can be solved in this system. It seems that if accidental degenerate states occur in one system, the problem is solvable in another system: Accidental degeneracy because $E$ independent of $l$.

Spherical: $r, \theta, \varphi$ $\qquad \psi = R(r)\,\Theta(\theta)\,e^{im\varphi}$

Parabolic: $\xi = r + z$, $\eta = r - z$, $\varphi$ $\qquad \psi = F(\xi)\,G(\eta)\,e^{im\varphi}$

$$\xi = r(1+\cos\theta), \quad \eta = r(1-\cos\theta)$$

We find for the case $E > 0$:

$$F(\xi) \rightarrow e^{ik\xi/2} \, {}_1F_1(\sim\sim ; -ik\xi)$$

$$G(\eta) \rightarrow e^{-ik\eta/2} \, {}_1F_1(\sim\sim ; ik\eta)$$

For scattering we want a wave function of the form of the incoming plane wave plus the spherical wave from the scattering center.

$$\boxed{\psi \sim e^{ikz} + \frac{f(\theta)}{r} e^{ikr}}$$

This would be good if coulomb field did not fall off so rapidly. $f(\theta)$ is the scattering coefficient. We find that:

$$f(\theta) \sim \frac{1}{\eta} \, , \quad \eta = r - z = r(1 - \cos\theta) = 2r \sin^2\frac{\theta}{2}$$

Then: $f(\theta) \propto \dfrac{1}{2r \sin^2\frac{\theta}{2}}$

However, there is really a creeping phase factor in the asymptotic expansion. Then,

$$f(\theta) \propto \frac{e^{-i\nu \log(-ik\eta)}}{\eta}$$

$$\sigma \, d\Omega = |f(\theta)|^2 \, d\Omega$$

which will eventually give the Rutherford results.

LECTURE XI    3-3-61

Scattering Problem: want to find a wave function of asymptotic form:

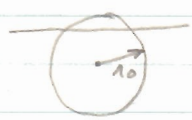
$$\psi \sim e^{ikz} + \frac{f(\theta)}{r} e^{ik \cdot r} \qquad \text{(elastic scattering)}$$

$f(\theta)$ = scattering amplitude. We take $V$ as:

$$V \leq \frac{\text{constant}}{r^{\alpha}}, \quad \alpha > 1$$

When can we use static $V$?
Adiabatic

Assume $V$ limited to range $r_0$, $V = 0$, $r > r_0$



For adiabatic, $\frac{v}{r_0} \ll$ all natural frequencies of system.

That is, the speed of the particle that collides with the system is much less than the speed of the particles which make up the system.

Can use static $V$ for anti-adiabatic scattering where opposite of above is true. $v \gg v$ part in system. However, there will be quite a bit of inelastic scattering. Thus static $V$ is good only for elastic scattering.

The Method of Partial Waves:

We can take solutions of form $Y_l^m(\theta,\varphi)\, g_l(r)$ or $P_l(\cos\theta)\, g_l(r)$ for spherical symmetry and build up solution for scattering.

We consider potential $V(r)$, with $V = 0$, $r > r_0$. Then the solution is written:

$$\psi = \sum_l B_l P_l(\cos\theta) \frac{v_l(r)}{r}$$

where $v_l(r)$ satisfies:

$$v_l'' + \left[ k^2 - \frac{2mV}{\hbar^2} - \frac{l(l+1)}{r^2} \right] v_l = 0$$

with $v_l(0) = 0$

This is the most general form for an axially symmetric scattering potential.

Now, for the free particle:

$$\psi_{free} = \sum_l C_l P_l \frac{u_l}{r}$$

where $u_l$ satisfies: $u_l'' + \left[ k^2 - \frac{l(l+1)}{r^2} \right] u_l = 0$
with $u_l(0) = 0$

For $r > r_0$, $kr \gg l$, we have:

$$v'' + k^2 v = 0 \quad , \quad u'' + k^2 u = 0$$

which gives immediately: $u_l \sim \sin(kr + \epsilon_l)$
where $\epsilon_l$ is an important quantity which must make $u_l(0) = 0$. Now, for $v_l$ we get:

$$v_l \sim \sin(kr + \epsilon_l + \delta_l)$$

← phase shift

$\delta_l$ controls the condition $v_l(0) = 0$. These phase shifts are very hard to find and usually cannot be found generally. The problem here is to determine the scattering in terms of the phases.

Choose: $C_l$ such that: $\sum_l C_l P_l \frac{u_l}{r} \sim e^{ikz}$

We now equate $\psi$ for large $r$ to initial equation:

$$\sum_l b_l P_l \frac{\sin(kr + \epsilon_l + \delta_l)}{r} = \sum_l C_l P_l \frac{\sin(kr + \epsilon_l)}{r} + \sum_l a_l P_l \frac{e^{ikr}}{r}$$

since: $f(\theta) = \sum_l a_l P_l(\cos\theta)$

Expand sines as exponentials; equating coefficients of similiar exponentials:

$\frac{P_l e^{-ikr}}{r}$ : $+\frac{B_l e^{-i(\epsilon_l+\delta_l)}}{2i} = +\frac{C_l e^{-i\epsilon_l}}{2i}$

or $B_l = C_l e^{i\delta_l}$

$\frac{P_l e^{+ikr}}{r}$ : $C_l e^{i\delta_l} \frac{e^{i(\epsilon_l+\delta_l)}}{2i} = \frac{C_l e^{i\epsilon_l}}{2i} + a_l$

or $a_l = \frac{(e^{2i\delta_l}-1)}{2i} C_l e^{i\epsilon_l} = C_l e^{i(\epsilon_l+\delta_l)} \sin\delta_l$

Then: $f = \sum_l C_l e^{i(\epsilon_l+\delta_l)} \sin\delta_l \, P_l(\cos\theta)$

Now: $\sigma = \int \sigma(\theta)\, d\Omega = \int |f|^2 d\Omega = \int |f|^2 d(\cos\theta)\, d\varphi$

$$= 4\pi \sum_l \frac{|C_l|^2}{2l+1} \sin^2\delta_l$$

We must now determine $C_l$: For large $r$, we want:

$$\sum_l C_l P_l(\mu) \frac{u_l}{r} = e^{ikr\mu} \quad , \mu = \cos\theta$$

Multiply by some $P_{l'}(\mu)$ and integrate:

$$C_l \frac{u_l}{r} \frac{2}{2l+1} = \int_{-1}^{1} e^{ikr\mu} P_l(\mu)\, d\mu$$

Integrate by parts:

$$C_l \frac{u_l}{r} = \frac{2l+1}{2} \frac{1}{ikr} \left[ e^{ikr\mu} P_l(\mu) \right]_{-1}^{1}$$

$$- \frac{2l+1}{2} \frac{1}{ikr} \int_{-1}^{1} e^{ikr\mu} P_l'(\mu)\, d\mu$$

This process can be repeated indefinitely until we run out of $l$'s. Since $r \gg r_0$, we write $u_l = \sin(kr + \epsilon_l)$. Then:

$$C_l \sin(kr + \epsilon_l) = \frac{2l+1}{2ik}\left[e^{ikr} - (-1)^l e^{-ikr}\right]$$

$$= \begin{cases} \frac{2l+1}{k} \sin kr & l \text{ even} \\ \frac{2l+1}{ik} \cos kr & l \text{ odd} \end{cases}$$

We could have:

$$C_l = \frac{2l+1}{k}, \quad \epsilon_l = 0, \quad l \text{ even}$$

$$C_l = \frac{2l+1}{ik}, \quad \epsilon = \pi/2, \quad l \text{ odd}$$

Conventionally; we use:

$$C_l = \frac{2l+1}{k} i^l, \quad \epsilon_l = -\frac{l\pi}{2}$$

Then, finally: $f = \frac{1}{k} \sum_l (2l+1) e^{i\delta_l} \sin \delta_l \cdot P_l$

and $\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l$

---

LECTURE XII 3-6-61

Recall: $f = \frac{1}{k} \sum_l (2l+1) e^{i\delta_l} \sin \delta_l \, P_l(\cos\theta)$

$$\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l$$

Usually see this result in terms in Bessel functions:

$(\nabla^2 + k^2) u = 0$ in spherical coordinates has solution:

$$e^{ikr\cos\theta}, \quad Y_l^m \frac{J_{l+\frac{1}{2}}(kr)}{\sqrt{kr}}$$

now: $$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} A_l \underbrace{\frac{J_{l+1/2}(kr)}{\sqrt{kr}}}_{j_l(kr)} P_l(\cos\theta)$$

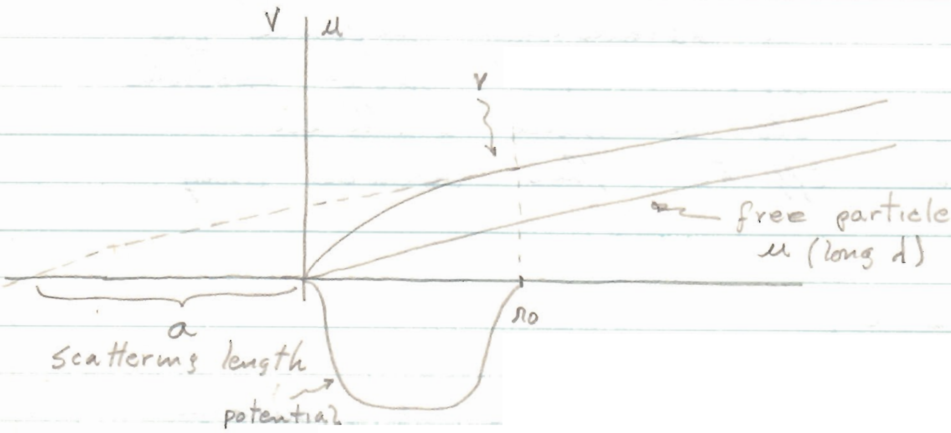
and: $$A_l \frac{J_{l+1/2}(kr)}{\sqrt{kr}} = \frac{2l+1}{2} \int e^{ikr\cos\theta} P_l(\cos\theta)\, d(\cos\theta)$$

$$= \frac{2l+1}{2} \int_{-1}^{1} e^{ikru} P_l(u)\, du$$

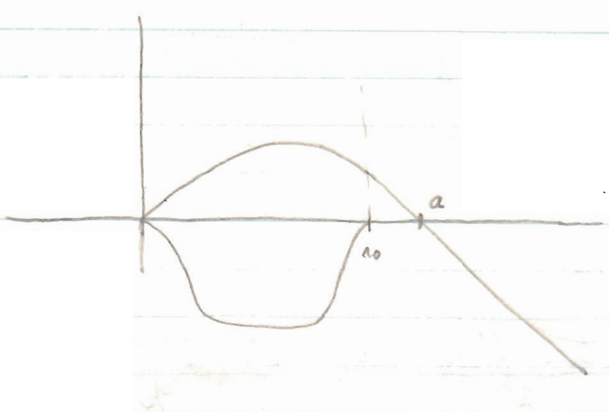
Could find the $A_l$ by expanding for small $kr$. Result is:

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1)\, i^l \sqrt{\frac{\pi}{2kr}}\, J_{l+\frac{1}{2}}(kr)\, P_l(\cos\theta)$$

Recall $V=0$, $r \geq r_0$ and consider the case $kr_0 << 1$.




Only case where particle sees V is when $l=0$ otherwise centripetal barrier potential is far outside range of V and keeps particle from approaching.
$\therefore\ \delta_l \approx 0,\ l \neq 0$



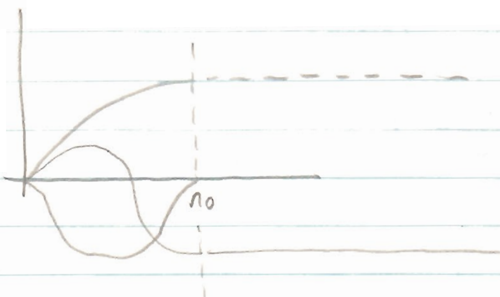

$\delta_0 = ka$,
If $\delta_0 << 1$, we have:

$$\sigma = \frac{4\pi}{k^2} \cdot 1 \cdot (ka)^2$$

$$\sigma = 4\pi a^2$$

(spherical cross-section of radius a).

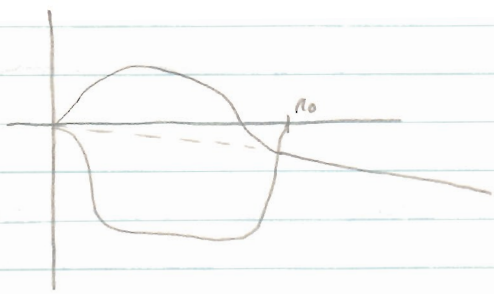
If phase is $\pi/2$: Resonance, $\delta_0 = \pi/2$




scattering length is infinite.

$$\sigma = \frac{4\pi}{k^2} = \frac{\lambda^2}{\pi}$$

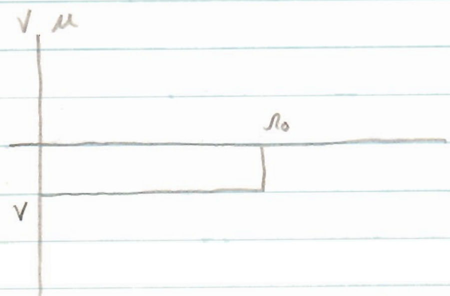
We see that in this case, nature of potential is unimportant, that is, wavelength $\lambda$ is much longer than extent of V. Or, the energy is much less than V, $E << V$. Thus we have $\sigma \sim \frac{1}{E}$




Case of $\delta_0 = \pi$, with scattering length = 0. Means no scattering, which is paradoxial because one would expect slow particles to be more scattered.

Called the Ramshauer Effect. This occurs only in certain atoms.

Consider Potential Well:




Consider $kr_0 << 1$, means only $\delta_0$ counts, $\delta_0 << 1$

Now: $k' = \sqrt{\frac{2m(E-V)}{\hbar^2}}$

$C \sin k'r, \quad r < r_0$

$\sin(kr + \delta_0), \quad r > r_0$

Equate $\frac{u}{u'}$ at $r_0$: $\quad \frac{\tan k'r_0}{k'} = \frac{\tan(kr_0 + \delta_0)}{k}$

Since the potential is small, we can take a series expansion of each side:

$$r_0 + \frac{1}{3} k'^2 r_0^3 + \cdots = r_0 + \frac{\delta_0}{k} + \frac{1}{3} k^2 r_0^3 + \cdots$$

Then: $\delta_0 \doteq \frac{1}{3} k \left( k'^2 - k^2 \right) r_0^3$

Now: $k'^2 - k^2 \sim V$, and $\delta_0 \propto k\, V$ (volume)
then:

$$\sigma \propto V^2 \,(\text{volume})^2$$

Note that $V$ does not have to be small, just that $k' r_0 \ll 1$.

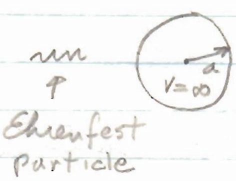
For light and EM waves: $k = \frac{2\pi}{\lambda}$, $k' = \frac{2\pi}{\lambda} n$
with $\delta_0 \ll 1$. Then:

$$\sigma = \frac{4\pi}{k^2} \cdot \frac{1}{9} k^2 \left( k^2 n^2 - k^2 \right)^2 r_0^6$$

or $\sigma \propto \frac{(\text{volume})^2}{\lambda^4}$ (Rayleigh scattering)

Another Case: large rigid sphere, where particles cannot get in:

$ka \ll 1$




Would expect $\sigma = 4\pi a^2$, but actually get $\sigma = 2\pi a^2$. Illustrates the difference between particles and waves

# LECTURE XIII    3-8-61

Born Approximation:

We can treat a wider class of cases with this than with plane wave method. Can do inelastic cases. Method is really Schroedinger stationary perturbation theory where we are concerned now with wave functions rather than energy. Problem is to find correct combination of incident waves and scattered waves: We proceed in a general method:

Scatterer: coordinates $q$; with $H(q)$, $u_m(q)$
and $H(q)\, u_m(q) = W_m\, u_m(q)$

Particle: initially $\vec{k_0}$, K.E.: $T = \frac{(\hbar k_0)^2}{2m}$ | Hamiltonian is $-\frac{\hbar^2}{2m}\nabla^2$

Interaction: $V(r, q)$

Case of Center of Force: $V(r)$

Assume: only one state of scatterer, such that $|u_m(q)|^2 = \delta(q)$ which makes the scatterer is a point. We do this after general development.

We take for the unperturbed wave function:

$$u^{(0)} = e^{i k_0 \cdot r}\, u_n(q) \quad \text{where } n \text{ is the initial state}$$

Then the unperturbed Schroedinger equation is:

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + H(q) - (W_n + T) \right\} u^{(0)} = 0$$

Now: $u = u^{(0)} + u^{(1)} + u^{(2)} + \dots$

Then, to the first order:

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + H(q) - (W_n + T) \right\} u^{(1)} = -V(r, q)\, u^{(0)}$$

In general, to $\alpha^{th}$ order:

$$\{\quad\} u^{(\alpha)} = -V(r,q)\, u^{(\alpha-1)}$$

NB: Total energy does not change; only $W_n$ and $T$ change if $W_n + T$ is constant.

We take $u^{(\alpha)}$ to be expanded in terms of scatterer functions:

$$u^{(\alpha)} = \sum_m v_m^{(\alpha)}(r)\, u_m(q)$$

Call: $\frac{2m}{\hbar^2}\left(W_n - W_m + T\right) = k_{nm}^2$

Then: $\sum_m \left\{\nabla^2 + k_{nm}^2\right\} v_m^{(\alpha)} u_m(q) = \frac{2m}{\hbar^2} V(r,q) \underbrace{\sum_m v_m^{(\alpha-1)} u_m(q)}_{u^{(\alpha-1)}}$

Multiply by $u_m^*(q)$:

$$\left(\nabla^2 + k_{nm}^2\right) v_m^{(\alpha)} = \frac{2m}{\hbar^2}\int u_m^*(q)\, V(r,q)\, u^{(\alpha-1)}\, dq$$

This corresponds to the electrodynamic equation for the retarded potential:

$$\left(\nabla^2 + k^2\right) v = \rho \quad , \quad w = e^{-ikct}\, v(r)$$

which gives: $\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) w = \rho$

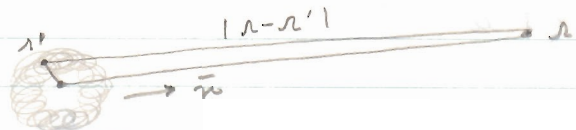
$$w = -\int \frac{\rho\left\{r' ; t - \frac{|r-r'|}{c}\right\}}{4\pi\, |r-r'|}\, dr'$$

Then the result for scattering:

$$v = -\frac{1}{4\pi}\int dr'\, \rho(r')\, \frac{e^{ik|r-r'|}}{|r-r'|}$$

which contains the Green function of the problem.

The physical picture is somewhat like this:




We can then write $|r - r'| = r - r' \cdot \bar{n}$

Then, in the first order;

$$v_m^{(1)}(r) \sim -\frac{e^{ik_{nm}r}}{r} \frac{m}{2\pi\hbar^2} \int dr' \, e^{i(\bar{k}_0 - \bar{n} k_{nm}) \cdot r'}$$

$$\cdot \int dq \, u_m^*(q) \, V(r', q) \, u_n(q)$$

$$u^{(0)} + u^{(1)} \sim e^{ik_0 \cdot r} u_n(q) + \frac{e^{ik_0 \cdot r}}{r} f_n \, u_n(q)$$

$$+ \sum_{m \neq n} \frac{e^{ik_{nm}r}}{r} f_m \, u_m(q)$$

This is coherent elastic scattering for the first two terms. The last term includes incoherent, inelastic scattering.

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LECTURE XIV 3-10-61

Recall: $v_m^{(1)}(r) \sim -\frac{e^{ik_{nm}r}}{r} \frac{m}{2\pi\hbar^2} \int dr' \, e^{i(\vec{k}_0 - \vec{k}_{nm}) r'}$

$$\cdot \int dq \, u_m^*(q) \, V(r', q) \, u_n(q)$$

with $\vec{k}_{nn} = k_{nm} \hat{n}$, $\hat{n} = \frac{\mathbf{r}}{r}$, $\vec{k}_0 = k_0 \hat{e}_3$

Fixed Center: 1 state: Elastic scattering; Symmetric V

$$v^{(1)}(r) \sim -\frac{e^{ikr}}{r} \underbrace{\frac{m}{2\pi\hbar^2} \int dr' \, e^{i(k_0 - k) \cdot r} \, V(r')}_{f(\theta)}$$

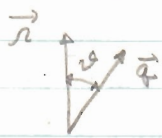
Coulomb scattering: $V(r') = \dfrac{Ze^2}{r'}$

now: $$\left(\frac{1}{r}\right)_{k,k_0} = \frac{1}{(2\pi)^3}\int \frac{e^{i(k_0-k)\cdot r}}{r}\,dr$$

$$f(\theta) = -\frac{me^2(2\pi)^2}{\hbar^2}\left(\frac{1}{r}\right)_{k,k_0}$$

$$\sigma(\theta)\,d\Omega = |f|^2\,d\Omega = \left(\frac{4\pi^2 mZe^2}{\hbar^2}\right)^2 \left|\left(\frac{1}{r}\right)_{k,k_0}\right|^2 d\Omega$$

Define: $\vec{k_0} - \vec{k} = \vec{q}$




$\cos\vartheta = \mu$

Then: $$\left(\frac{1}{r}\right)_{k,k_0} = \frac{1}{(2\pi)^2}\int_0^\infty r\,dr \int_{-1}^{1} d\mu\, e^{iqr\mu}$$

$$= \frac{1}{2\pi^2 q}\int_0^\infty dr\,\sin qr$$

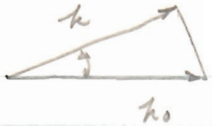
This integral does not exist nor converge but it is summable. The trouble is large values of $r$, however, waves are never scattered at this distance. We then use an Abelian integral:

$$\left(\frac{1}{r}\right)_{k,k_0} = \frac{1}{2\pi^2 q}\lim_{\alpha\to 0}\underbrace{\int_0^\infty e^{-\alpha r}\sin qr\,dr}_{\operatorname{Im}\int_0^\infty e^{-(\alpha - iq)r}\,dr}$$

$$\operatorname{Im}\frac{1}{\alpha - iq} = \operatorname{Im}\frac{\alpha + iq}{\alpha^2+q^2} = \frac{q}{\alpha^2+q^2}$$

and then:

$$\sigma(\theta)\,d\Omega = \left(\frac{4\pi^2 mZe^2}{\hbar^2}\right)^2\left(\frac{1}{2\pi^2|k-k_0|^2}\right)^2 d\Omega$$




$$|k_0 - k| = 2k \sin\frac{\theta}{2} = \frac{2mv}{\hbar} \sin\frac{\theta}{2}$$

which is the classical result for Rutherford scattering.

Optical Theorem:

Two Types of cross-section:

$$\sigma_{tot} \begin{cases} \sigma_{el} = \int |f_{el}|^2 \, d\Omega \quad (m=n) \\ \sigma_{nm} = \frac{v_{nm}}{v} \int |f_{nm}|^2 \, d\Omega \\ \sigma_{abs} \end{cases}$$

The theorem is that $\sigma_{tot}$ can be written:

$$\sigma_{tot} = \frac{4\pi}{k} \, \mathrm{Im} \left\{ f_{el}(0) \right\}$$

Proof: The asymptotic wave function is:

$$\psi \sim e^{ikz} u_n(q) + \frac{f_{el} \, e^{ikr}}{r} u_n(q) + \underbrace{\sum_{m \neq n} \frac{f_{nm} \, e^{ik_{nm} r}}{r} u_m(q)}_{\text{incoherent part}}$$

Recall: $j = \frac{\hbar}{2mi} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right)$

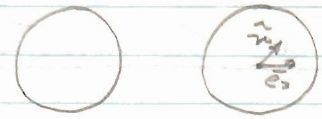
which is the probability current for one particle with the coordinates known. However, $\psi$ contains the scatterer, so must use joint probability techniques and integrate over scatterer coordinates:

$$j = \int \frac{\hbar}{2mi} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) dq = \mathrm{Im} \int \frac{\hbar}{m} \psi^* \nabla \psi \, dq$$

Using a Gauss' law argument:

$$\int \vec{J} \cdot \hat{n} \, r^2 \, d\Omega = - v \, \sigma_{abs}$$

($v$ ↑ velocity)



Thus:

$$\int \vec{J} \cdot \hat{n} \, r^2 \, d\Omega = \underbrace{\int \sum_{m \neq n} v_{nm} \, |f_{nm}|^2 \, d\Omega}_{\sum_{m \neq n} v \, \sigma_{nm}}$$

$$+ \ \mathrm{Re} \ v \int \left\{ \cos\theta + f(\theta) \frac{e^{ikr(1-\cos\theta)}}{r} \right.$$

$$\left. + \cos\theta \, f^*(\theta) \frac{e^{-ikr(1-\cos\theta)}}{r} + \frac{|f|^2}{r^2} \right\} r^2 \, d\Omega$$

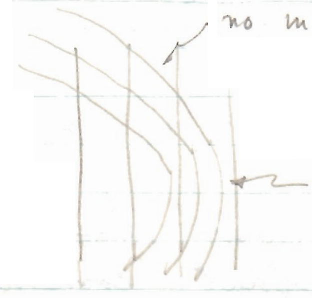
In differentiating $\frac{e^{ikr}}{r}$, we do not differentiate the $\frac{1}{r}$ part.

$$\sigma_{tot} = - \mathrm{Re} \int_{-1}^{1} 2\pi f(\theta) \, (1 + \cos\theta) \, e^{ikr(1-\cos\theta)} \, r \, d(\cos\theta)$$

Define: $kr(1 - \cos\theta) = \xi$

$$\sigma_{tot} = - \mathrm{Re} \int_0^{2kr} \frac{2\pi}{k} f \cdot \left( 2 - \frac{\xi}{kr} \right) e^{i\xi} \, d\xi$$

$$= \frac{4\pi}{k} \, \mathrm{Im} \, f(0)$$



LECTURE XV    3-13-61

## Angular Momentum

Orbital angular momentum of a particle:

$$\vec{m} = r \times p \quad ; \quad m_x = y p_z - z p_y$$

Does this commute with the Hamiltonian components $p^2$, $V(r)$?

$$[m_x, V(r)] = y[p_z, V] - z[p_y, V]$$

$$= y \frac{\hbar}{i} V'(r) \frac{z}{r} - y \frac{\hbar}{i} V'(r) \frac{z}{r} = 0$$

since $\frac{\partial r}{\partial z} = \frac{\partial}{\partial z}\{x^2+y^2+z^2\}^{1/2} = \frac{z}{r}$

In the central field case: $[\vec{m}, H] = 0$

How about: $[m_x, m_y] = [y p_z - z p_y, z p_x - x p_z]$

$$= [y p_z, z p_x] - \dots \quad = \frac{\hbar}{i} y p_x - \frac{\hbar}{i} x p_y$$

$= i\hbar m_z$ , $\therefore$ $[m_x, m_y] = i\hbar m_z$

In general: $[m_j, m_k] = i\hbar \epsilon_{jkl} m_l$

where: $\epsilon_{jkl} = \begin{cases} 0 & \text{unless } jkl \text{ all different} \\ 1 & \text{for } 123, 231, 312 \\ -1 & \text{for } 132, 321, 213 \end{cases}$

Consider: $m^2 = m_x^2 + m_y^2 + m_z^2$

$$[m_x, m^2] = [m_x, m_y] m_y + m_y [m_x, m_y] + \dots$$

$$= i\hbar m_z m_y + i\hbar m_y m_z - \dots \quad = 0$$

$\therefore$ $[m_x, m^2] = 0$ , so we now have two operators that commute with $H$; viz, $m_x$, $m^2$

Examine these in spherical coordinates:

$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi \\ y &= r\sin\theta\sin\varphi \\ z &= r\cos\theta \end{aligned}\right\} \qquad \begin{aligned} r &= \{x^2+y^2+z^2\}^{1/2} \\ \theta &= \cos^{-1} z/r \\ \varphi &= \tan^{-1} y/x \end{aligned}$$

Now $M_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}$$

Thus:

$$\frac{\partial}{\partial x} = \frac{x}{r}\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial y} = \frac{y}{r}\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial z} = \frac{z}{r}\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

Then:

$$M_x = \frac{\hbar}{i}\left\{-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right\}$$

$$M_y = \frac{\hbar}{i}\left\{\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right\}$$

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

Now we form $M^2$:

$$M^2 = -\hbar^2\left\{\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \csc^2\theta\frac{\partial^2}{\partial\varphi^2}\right\}$$

$$= -\hbar^2 r^2\left\{\nabla^2 - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right\}$$

Recall for the central field problem:

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

where we can now write:

$$H = \frac{-\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r) + \frac{M^2}{2mr^2}$$

Now we already know the result for the central field problem: $Hu = Eu$:

$$u = Y_\ell^m(\theta,\varphi)\, R(r)$$

which gives for the R equation upon separation of variables:

$$\frac{-\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left(V - E + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right)R = 0$$

We see that $\hbar^2 \ell(\ell+1)$ must be the eigenvalues of $\mathcal{M}^2$ and we can write the eigenvalue equation

$$\mathcal{M}^2 Y_\ell^m = \hbar^2 \ell(\ell+1) Y_\ell^m$$
$$\mathcal{M}_z Y_\ell^m = \hbar m\, Y_\ell^m$$

or
$$\mathcal{M}^{2\prime} = \hbar^2 \ell(\ell+1)$$
$$\mathcal{M}_z' = \hbar m \quad , \quad m = -\ell, -\ell+1, \dots +\ell$$

We have generated a set of commuting observables that operate on simultaneous eigenfunctions.

Consider in the abstract, the operators defined by:
$$[\mathcal{M}_j, \mathcal{M}_k] = i\hbar\, \epsilon_{jk\ell}\, \mathcal{M}_\ell$$

Take as eigenvalues:

$\mathcal{M}^{2\prime}, \mathcal{M}_z', \gamma'$ where $\gamma$ is a set of other commuting observables.

We will invoke ladder method: Define;

$$\mathcal{M}_+ = \mathcal{M}_x + i\,\mathcal{M}_y$$

$$\mathcal{M}_+^{+} = \mathcal{M}_- = \mathcal{M}_x - i\,\mathcal{M}_y$$

Let's see these commute:

$$M_+ M_- = M_x^2 + M_y^2 + \hbar M_z = M^2 - M_z^2 + \hbar M_z$$

$$M_- M_+ = M^2 - M_z^2 - \hbar M_z$$

$$[M_+, M_z] = -i\hbar M_y - \hbar M_x = -\hbar M_+$$

$$[M_-, M_z] = \hbar M_-$$

$$\left.\right\} \quad [M_\pm, M^2] = 0 \qquad [M_\pm, \gamma] = 0$$

which give: $M_z M_+ = M_+ (M_z + \hbar)$
$M_z M_- = M_- (M_z - \hbar)$

Now take the normalized ket of commuting observables $|M^{2\prime}, M_z^\prime, \gamma^\prime\rangle$ and operate with $M^2 M_+$:

$$M^2 \underbrace{M_+ |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle} = M_+ M^2 |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle$$

$$= M^{2\prime} \underbrace{M_+ |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle}_{\text{new unnormalized eigenket of } M^{2\prime}.}$$

Now try $M_z M_+$:

$$M_z M_+ |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle = M_+ (M_z + \hbar) |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle$$

$$= (M_z^\prime + \hbar) \underbrace{M_+ |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle}_{\text{also eigenket of } M_z}$$

We now normalize by forming its inner product:

$$\langle M^{2\prime}, M_z^\prime, \gamma^\prime | M_- M_+ | M^{2\prime}, M_z^\prime, \gamma^\prime\rangle$$

$$= \langle | M^2 - M_z^2 - \hbar M_z | \rangle = M^{2\prime} - M_z^{\prime 2} - \hbar M_z^\prime$$

Thus: $M_+ |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle = \{M^{2\prime} - M_z^{\prime 2} - \hbar M_z^\prime\}^{1/2} |M^{2\prime}, M_z^\prime + \hbar, \gamma^\prime\rangle$

$M_- |M^{2\prime}, M_z^\prime, \gamma^\prime\rangle = \{M^{2\prime} - M_z^{\prime 2} + \hbar M_z^\prime\}^{1/2} |M^{2\prime}, M_z^\prime - \hbar, \gamma^\prime\rangle$

now: $\mathcal{M}_-(+) = \left\{ \mathcal{M}^{2'} - \mathcal{M}_z'^2 - \hbar \mathcal{M}_z' \right\}^{1/2} | \mathcal{M}^{2'}, \mathcal{M}_z', \gamma' \rangle$

$= \{ \quad \}^{1/2} \left\{ \mathcal{M}^{2'} - (\mathcal{M}_z' + \hbar)^2 + \hbar (\mathcal{M}_z' + \hbar) \right\}^{1/2} | \mathcal{M}^{2'}, \mathcal{M}_z', \gamma' \rangle$

Thus showing that choice of + sign for square roots is consistent.

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LECTURE ~~XVI~~ 3-15-61

Recap: $\mathcal{M}_+ = \mathcal{M}_x + i\mathcal{M}_y$

(+) $\mathcal{M}_+ | \mathcal{M}^{2'}, \mathcal{M}_z', \gamma' \rangle = \left\{ \mathcal{M}^{2'} - \mathcal{M}_z'^2 - \hbar \mathcal{M}_z' \right\}^{1/2} | \mathcal{M}^{2'}, \mathcal{M}_z' + \hbar, \gamma' \rangle$

(−) $\mathcal{M}_- | \mathcal{M}^{2'}, \mathcal{M}_z', \gamma' \rangle = \left\{ \mathcal{M}^{2'} - \mathcal{M}_z'^2 + \hbar \mathcal{M}_z' \right\}^{1/2} | \mathcal{M}^{2'}, \mathcal{M}_z' - \hbar, \gamma' \rangle$

This problem is much like the ladder method of treating the harmonic oscillator where we had to restrict the eigenvalues to a certain range to keep out negative values.

Note:

$|\mathcal{M}_z'| \leq \sqrt{\mathcal{M}^{2'}}$

because $\mathcal{M}^2 - \mathcal{M}_z^2 = \mathcal{M}_x^2 + \mathcal{M}_y^2$

now: $\langle | \mathcal{M}_x \mathcal{M}_x | \rangle$ must be positive, which proves the above inequality. We thus stipulate:

$\mathcal{M}_+ | \mathcal{M}^{2'}, (\mathcal{M}_z')_{max}, \gamma' \rangle = 0$

Apply $\mathcal{M}_-$ and get: $\mathcal{M}^{2'} - (\mathcal{M}_z')^2_{max} - \hbar (\mathcal{M}_z')_{max} = 0$

Similarly: $\mathcal{M}^{2'} - (\mathcal{M}_z')^2_{min} + \hbar (\mathcal{M}_z')_{min} = 0$

Thus: $(\mathcal{M}_z')_{max} = \dfrac{-\hbar \pm \sqrt{4\mathcal{M}^{2'} + \hbar^2}}{2}$

$(\mathcal{M}_z')_{min} = \dfrac{\hbar \pm \sqrt{\quad}}{2}$

must choose + for max, and − for min.
Thus:

$$(M_z')_{max} = -(M_z')_{min}$$

Now the number of steps taken from max to min is twice from 0 to max or min:

$$2(M_z')_{max} = -2(M_z')_{min} = 2j\hbar$$

Possible values of $j$ are $0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ and allows the calculation:

$$M^{2\prime} = (j\hbar)^2 + \hbar(j\hbar) = j(j+1)\hbar^2$$

Thus: $\hbar^{-1} M_z' = -j, -j+1, \ldots, j-1, j$

or $M_z' = m\hbar$

We can then change the notation, dropping $\gamma$, of the eigenket to: $|jm\rangle$. Then:

(1) $(M_x + i M_y)|jm\rangle = \hbar\{(j-m)(j+m+1)\}^{1/2}|j, m+1\rangle$

from $j(j+1) - m^2 - m$

(2) $(M_x - i M_y)|jm\rangle = \hbar\{(j+m)(j-m+1)\}^{1/2}|j, m-1\rangle$

Other notations: $M^2 \psi_{j,m} = j(j+1)\hbar^2 \psi_{j,m}$
$M_z \psi_{j,m} = m\hbar\, \psi_{j,m}$

$$\psi_{j,m} = \langle \theta, \varphi | jm\rangle$$

(1′) $\therefore$ $(M_x + i M_y)\psi_{jm} = \hbar\{(j-m)(j+m+1)\}^{1/2}\psi_{j,m+1}$

(2′) $(M_x - i M_y)\psi_{jm} = \hbar\{(j+m)(j-m+1)\}^{1/2}\psi_{j,m-1}$

We can represent these operators in matrix form as follows:

(3) $\langle j'm' | m_x + i m_y | j m \rangle = \hbar \{(j-m)(j+m+1)\}^{1/2} \delta_{jj'} \delta_{m',m+1}$

(4) $\langle j'm' | m_x - i m_y | j m \rangle = \hbar \{(j+m)(j-m+1)\}^{1/2} \delta_{jj'} \delta_{m',m-1}$

(3) and (4) are adjoints of each other.

Note that $\psi_{j,m}$ are normalized eigenfunctions of *any* variables. Thus, we form:

$$|(\psi)\rangle = \sum_{jm}{}' |jm\rangle\langle jm|(\psi)\rangle$$

We can write, following Dirac:

$$(m_x + i m_y)|(\psi)\rangle = |(m_x + i m_y)\psi\rangle$$

$$= \sum_{j''m'} \hbar \{(j''-m')(j''+m'+1)\}^{1/2} |j'', m'+1\rangle\langle j''m'|(\psi)\rangle$$

Then:

$$\langle jm|((m_x + i m_y)\psi)\rangle = \hbar \{(j-m+1)(j+m)\}^{1/2} \langle j, m-1|(\psi)\rangle$$

(5) $\left((m_x + i m_y)\psi\right)_{(jm)} = \hbar \{(j-m+1)(j+m)\}^{1/2} \psi(j, m-1)$

(6) $\left((m_x - i m_y)\psi\right)_{(jm)} = \hbar \{(j+m+1)(j-m)\}^{1/2} \psi(j, m+1)$

Much confusion exists between equations (5) and (6) and (1') and (2'). The difference is that in (1'), (2') $j\,m$ are *labels*, in (5), (6), $j\,m$ are *arguments*

LECTURE XVII    3-17-61

Consider two dynamically independent systems: $\vec{M}_1$, $\vec{M}_2$ with the commutation rules:

$$[M_{1j}, M_{1k}] = i\hbar\, \epsilon_{jkl} M_{1l}$$

$$[M_{2j}, M_{2k}] = i\hbar\, \epsilon_{jkl} M_{2l}$$

$$[M_{1k}, M_{2l}] = 0$$

Now suppose $\vec{M} = \vec{M}_1 + \vec{M}_2$ , $M_z = M_{1z} + M_{2z}$ with $[M_j, M_k] = i\hbar\, \epsilon_{jkl} M_l$

and that $M_1$, $M_2$ have eigenvalues and eigenstates such that:

$$M_1^{2\prime} = j_1(j_1+1)\hbar^2 \quad ; \quad M_{1z}' = m_1\hbar$$

$$M_2^{2\prime} = j_2(j_2+1)\hbar^2 \quad ; \quad M_{2z}' = m_2\hbar$$

This is one possible set of commuting operators. Another set:

$$M_1^{2\prime} = j_1(j_1+1)\hbar^2 \quad ; \quad M_2^{2\prime} = j_2(j_2+1)\hbar^2$$

$$M^{2\prime} = j(j+1)\hbar^2 \quad ; \quad M_z' = m\hbar$$

but now cannot include $M_{1z}'$ or $M_{2z}'$.

Thus one set can be described by the quantum numbers $j_1, j_2, m_1, m_2$ and the other by $j_1, j_2, j, m$.
Suppose we label states of the first kind, then eigenket is:

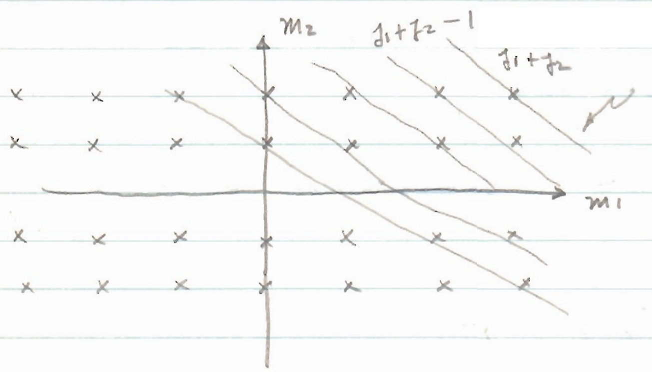
$$|j_1 m_1)\,|j_2 m_2) = |j_1 j_2 m_1 m_2>$$

The kets for the other system can be found by expansion in terms of the first.

$|j_1 j_2 m_1 m_2\rangle$ will be used as the basis:

$$|j_1, j_2, j, m\rangle = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \underbrace{\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle}$$

How does one find these coefficients?
Called Clebsch-Gordon coefficients.
The sum is really over $m_1 + m_2 = m$
since $M_z = M_{1z} + M_{2z}$
Can we show that list of $j$ is:
$j = j_1 + j_2,\ j_1 + j_2 - 1,\ \dots\ |j_1 + j_2|$




Take $j_1 = 3$
$j_2 = 3/2$

We can go to wave functions:

$$\psi_{jm} = \sum_{m_1 + m_2 = m} \varphi_{m_1} \chi_{m_2} \langle \sim | \sim \rangle$$

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $m$ | $j_1 + j_2$ | $j_1 + j_2 - 1$ | ... | $j_1 - j_2$ | ... | $-j_1 + j_2$ | ... | $-j_1 - j_2$ |
| available products | 1 | 2 | ... | $2j_2 + 1$ | ... | $2j_2 + 1$ | ... | 1 |

$$|j_1, j_2, \underbrace{j_1 + j_2}_{\text{particular } j}, \underbrace{j_1 + j_2}_{\text{particular } m}\rangle\rangle = |j_1, j_2, j_1, j_2\rangle$$

Apply $M_- = M_x - i M_y$ to step down above ket.

Plot of available products:


Example: Take $j_1 = 2$, $j_2 = 1$

$\psi^{(1)}_{j_1, m_1} = u_{m_1}$
$\psi^{(2)}_{j_2, m_2} = v_{m_2}$
$\psi^{(total)}_{j, m} =$ for total system.

Available wave functions:

| | |
|---|---|
| $u_2$ | |
| $u_1$ | $v_1$ |
| $u_0$ | $v_0$ |
| $u_{-1}$ | $v_{-1}$ |
| $u_{-2}$ | |

| $m =$ | 3 | 2 | 1 | 0 | −1 | −2 | −3 |
|---|---|---|---|---|---|---|---|
| | $u_2 v_1$ | $u_2 v_0$ | $u_2 v_{-1}$ | $u_1 v_{-1}$ | $u_0 v_{-1}$ | $u_{-1} v_{-1}$ | $u_{-2} v_{-1}$ |
| | | $u_0 v_1$ | $u_1 v_0$ | $u_0 v_0$ | $u_{-1} v_0$ | $u_{-2} v_0$ | |
| | | | $u_0 v_1$ | $u_{-1} v_1$ | $u_{-2} v_1$ | | |

Now: $\varphi_{33} = u_2 v_1$

Operate with $\frac{M_-}{\hbar}$ on $\varphi_{33}$:

$$\sqrt{6\cdot 1}\ \varphi_{3,2} = \sqrt{4\cdot 1}\ u_1 v_1 + \sqrt{2\cdot 1}\ u_2 v_0$$

or $$\varphi_{32} = \sqrt{\frac{2}{3}}\ u_1 v_1 + \sqrt{\frac{1}{3}}\ u_2 v_0$$

We similarly generate $\varphi_{31}$:

$$\sqrt{5\cdot 2}\ \varphi_{31} = \sqrt{\frac{2}{3}}\left(\sqrt{3\cdot 2}\ u_0 v_1 + \sqrt{2\cdot 1}\ u_1 v_0\right)$$
$$+ \sqrt{\frac{1}{3}}\left(\sqrt{4\cdot 1}\ u_1 v_0 + \sqrt{1\cdot 2}\ u_2 v_{-1}\right)$$

$$\varphi_{31} = \sqrt{\frac{2}{30}}\ u_2 v_{-1} + \sqrt{\frac{16}{30}}\ u_1 v_0 + \sqrt{\frac{12}{30}}\ u_0 v_1$$

or $$\varphi_{31} = \sqrt{\frac{1}{15}}\ u_2 v_{-1} + \sqrt{\frac{8}{15}}\ u_1 v_0 + \sqrt{\frac{6}{15}}\ u_0 v_1$$

which we can see is normalized. The others $\varphi_{3,0}$ etc, can be found in a similar manner.

Now: $$\varphi_{22} = \sqrt{\frac{1}{3}}\ u_1 v_1 - \sqrt{\frac{2}{3}}\ u_2 v_0$$

Can find using $\frac{M_-}{\hbar}\varphi_{j,m} = \{(j+m)(j-m+1)\}^{1/2}\varphi_{j,m-1}$

$\varphi_{21}$, $\varphi_{20}$, etc.

LECTURE XVIII 3-20-61

Since we have $\varphi_{3,2} = \sqrt{\frac{1}{3}}\, u_2 v_0 + \sqrt{\frac{2}{3}}\, u_1 v_1$
we can write using orthogonality:

$$\varphi_{22} = \sqrt{\frac{2}{3}}\, u_2 v_0 - \sqrt{\frac{1}{3}}\, u_1 v_1$$

and using the ladder operator:

$$\varphi_{21} = \sqrt{\frac{2}{6}}\, u_2 v_{-1} + \sqrt{\frac{1}{6}}\, u_1 v_0 - \sqrt{\frac{3}{6}}\, u_0 v_1 \quad , \text{etc.}$$

We now move on to $\varphi_{1,1}$.

$$\varphi_{1,1} = a\, u_2 v_{-1} + b\, u_1 v_0 + c\, u_0 v_1$$

where $a, b, c$ must be such that $\varphi_{1,1}$ are orthogonal to $\varphi_{2,1}$ and $\varphi_{3,1}$, or the coefficients match as:

| | | |
|---|---|---|
| $\sqrt{\frac{1}{15}}$ | $\sqrt{\frac{8}{15}}$ | $\sqrt{\frac{6}{15}}$ |
| $\sqrt{\frac{2}{6}}$ | $\sqrt{\frac{1}{6}}$ | $-\sqrt{\frac{3}{6}}$ |
| $a$ | $b$ | $c$ |

Since all $\varphi$'s are orthogonal and normalized the rows are orthogonal and so are the columns.

$$a^2 = 1 - \frac{1}{15} - \frac{2}{6} = \frac{15-1-5}{15}$$

$$b^2 = 1 - \frac{8}{15} - \frac{1}{6} = \frac{30-16-5}{30}$$

$$c^2 = \frac{30-12-15}{30}$$

We can choose signs by inspection and find $a = \sqrt{\frac{18}{30}}$, $b = -\sqrt{\frac{9}{30}}$, $c = \sqrt{\frac{3}{30}}$

then: $\varphi_{1,1} = \sqrt{\frac{6}{10}}\, u_2 v_{-1} - \sqrt{\frac{3}{10}}\, u_1 v_0 + \sqrt{\frac{1}{10}}\, u_0 v_1$

and the rest can be found with the ladder operator.

Suppose, though, we have available $j_1 = 7$, $j_2 = 4$ and we want the state for $j = 4$, $m = 0$ or $\varphi_{40}$. There is a simpler way.

Use fact that $\frac{M_+}{\hbar}$ must annihilate $\varphi_{1,1}$:

$$\frac{M_+}{\hbar} = \sqrt{(j-m)(j+m+1)}$$

$$\frac{M_+}{\hbar}\left\{ \begin{array}{l} \varphi_{1,1} = a\, u_2 v_{-1} + b\, u_1 v_0 + c\, u_0 v_1 \\ 0 = a\, u_2 \cdot \sqrt{2\cdot 1}\, v_0 + b\left( u_1 \sqrt{1\cdot 2}\, v_1 + \sqrt{1\cdot 4}\, u_2 v_0 \right) \end{array}\right.$$

$$+ c \sqrt{2\cdot 3}\, u_1 v_1$$

The coefficients must equal to zero:

$$\sqrt{2}\, a + \sqrt{4}\, b = 0 \quad ; \quad \sqrt{2}\, b + \sqrt{6}\, c = 0$$

$$a = -\sqrt{2}\, b \quad , \quad c = -\sqrt{\tfrac{1}{3}}\, b$$

So by using $M_+$ we can find the initial $\varphi$ of each group. Suppose we wanted $\varphi_{7,0}$. Even with initial $\varphi$, it is tedious to find.

Take $j_1$ anything such that $j_1 \geq j_2 = 1$. Try to find formula for $\varphi_{j_1,m}$. Use fact that $\varphi$'s are eigenfunctions of some operators. The values of $\varphi_{j_1,m}$ are:

$$\varphi_{j_1,m} = A\, u_{m+1} v_{-1} + B\, u_m v_0 + C\, u_{m-1} v_1$$

Now: $M^2 = |M_1 + M_2|^2 = M_1^2 + M_2^2 + 2 M_{1z} M_{2z}$

$$+ 2 M_{1x} M_{2x} + 2 M_{1y} M_{2y}$$

or $$\boxed{M^2 = M_1^2 + M_2^2 + 2 M_{1z} M_{2z} + M_{1+} M_{2-} + M_{1-} M_{2+}}$$

Now apply $\frac{M^2}{\hbar^2}$ onto $\varphi_{j_1,m}$: $\frac{M_+}{\hbar} = \sqrt{(j-m)(j+m+1)}$

$$\frac{M_-}{\hbar} = \sqrt{(j+m)(j-m+1)}$$

Since $\varphi_{j_1,m}$ is an eigenfunction of $M^2$, its application results in:

$$j_1(j_1+1)\,\varphi_{j_1,m} = A\Big\{\big[j_1(j_1+1)+2-2(m+1)\big]u_{m+1}v_{-1}$$

$$+\sqrt{(j_1+m+1)(j_1-m)}\,\sqrt{2}\,u_m v_0\Big\} + B\Big\{\sqrt{(j_1-m)(j_1+m+1)}\,\sqrt{2}\,u_{m+1}v_{-1}$$

$$+\big[j_1(j_1+1)+2\big]u_m v_0 + (j_1+m)(j_1-m+1)\sqrt{2}\,u_{m-1}v_1\Big\}$$

$$+\,C\Big\{\sqrt{(j_1-m+1)(j_1+m)}\,\sqrt{2}\,u_m v_0 + \big[j_1(j_1+1)+2+2(m-1)\big]u_{m-1}v_1\Big\}$$

Equating coefficients:

$$u_{m+1}v_{-1}: \quad -2mA + \sqrt{2(j_1-m)(j_1+m+1)}\;B = 0$$

$$u_m v_0: \quad \sim A + \sim B + \sim C = 0$$

$$u_{m-1}v_1: \quad \sqrt{2(j_1+m)(j_1-m+1)}\;B + 2mC = 0$$

The middle equation is seen to be not needed.
Take $B = 2m$:

$$A = \sqrt{2(j_1-m)(j_1+m+1)}$$

$$C = -\sqrt{2(j_1+m)(j_1-m+1)}$$

Since there are proportionalities, we can make equalities by taking the sum of squares of A and C:

$$4j_1(j_1+1) - 4m^2 + 4m^2 = 4j_1(j_1+1)$$

Tables: $\boxed{j_2=1}$ $\langle j_1, 1; m_1, m_2 \mid j_1, 1; j, m\rangle$

| $j \setminus m_2$ | $-1$ | $0$ | $1$ |
|---|---|---|---|
| $j_1-1$ | | | |
| $j_1$ | $\dfrac{(j_1-m)(j_1+m+1)}{2j_1(j_1+1)}$ | $\dfrac{m}{j_1(j_1+1)}$ | $-\;\underline{(j_1+m)(j_1-m+1)}$ |
| $j_1+1$ | | | |

LECTURE XIX    3-20-61

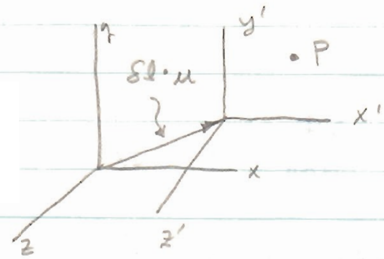
Infinitesimal Transformations:

Transformation: shift of coordinates
or: shift of state with respect to coordinates.

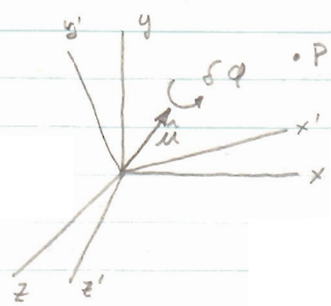
Here we take transformation as shifting coordinate system with respect to state. We will examine connection with angular momentum. Standard reference in Pauli's Quantumechanik. Also see Rose, Edmonds, and Dirac on angular momentum. Also new book by Powell and Crasimann.

Two different types of infinitesimal transformation in rectangular coordinate system:

Translation:




Rotation:



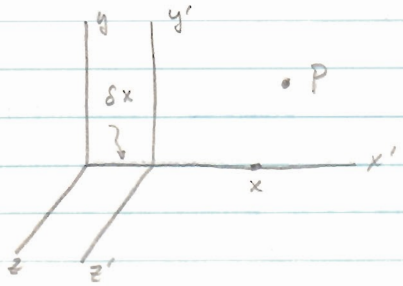

Consider a scalar wave function at P: $\psi(P) = \psi(x,y,z) = \psi'(x',y',z')$ which is a different function but has the same value at P as $\psi(x,y,z)$. The rule to get $\psi'(x',y',z')$ is:

$$\psi'(x',y',z') = \psi\{x(x',y',z'),\ y(x',y',z'),\ z(x',y',z')\}$$

Definition: $\psi'(x,y,z) - \psi(x,y,z) = \delta\psi(x,y,z)$

What is $\delta$? Consider small enough to work out to first order in $\delta l$ or $\delta\varphi$.

Consider translation along x:




$$x' = x - \delta x \quad \text{or} \quad x = x' + \delta x$$
$$y' = y$$
$$z' = z$$

Then: $\psi'(x', y', z') = \psi(x' + \delta x, y', z')$

and $\delta\psi = \delta x \dfrac{\partial\psi}{\partial x}$

Suppose we had more particles in system:

$x_1 = x_1' + \delta x$ etc. for the rest of particles;
$y_1 = y_1'$
$z_1 = z_1'$

Then; $\delta\psi = \delta x \sum_a \dfrac{\partial\psi}{\partial x_a} = \delta x \cdot T_x \psi$

Call $P_x = \frac{\hbar}{i} T_x$ : Then $P_x = \sum_a p_{ax} = \sum_a \frac{\hbar}{i} \frac{\partial}{\partial x_a}$

or the linear momentum.
Therefore,

$$\delta\psi = \delta x \cdot \frac{i}{\hbar} P_x \psi$$

For $\hat{u}\cdot\delta l$ translation, $\delta\psi = \delta l \cdot \frac{i}{\hbar}(\hat{u}\cdot\bar{P})\psi$

where $\vec{P} = \sum_a \vec{p_a} = \sum_a \frac{\hbar}{i} \nabla_a$

Suppose we have a Hamiltonian whose potential function depends only on the relative position of the particles:

$$H = \sum_a \frac{p_a^2}{2m_a} + V(r_1 - r_2, r_1 - r_3, \dots)$$

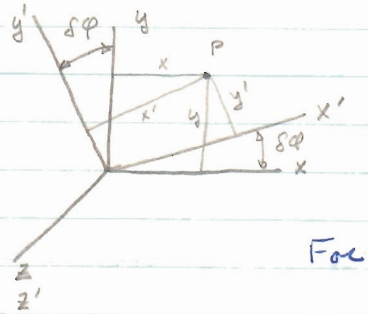
We now note the important fact that:

$$[H, \vec{P}] = 0$$

If we had a term such as $V(r_1)$, $H$ would not commute with the translation operator. Since $\vec{P}$ commutes with $H$, $\vec{P}$ is a constant of the motion, since the Hamiltonian is invariant under the infinitesimal translation.

Infinitesimal Rotation:

Consider rotation around z axis:




$$x = x' - y\,\delta\varphi$$
$$y = y' + x\,\delta\varphi$$
$$z = z'$$

For $x', y', z'$: $\delta\psi = \psi(x' - y\,\delta\varphi,\ y' + x\,\delta\varphi,\ z') - \psi(x', y', z')$

Since we are working in the first order in $\delta\varphi$, we can drop primes:

$$\delta\psi = \delta\varphi \cdot x\frac{\partial\psi}{\partial y} - \delta\varphi \cdot y\frac{\partial\psi}{\partial x} = \delta\varphi\underbrace{\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)}_{R_z}\psi$$

Then we see: $\delta\psi = \delta\varphi \cdot R_z\psi = \delta\varphi \cdot \frac{i}{\hbar} m_z \psi$

In general: $\delta\psi = \delta\varphi\,\frac{1}{\hbar}(\hat{u}\cdot\vec{m})\psi$

For several particles: $\vec{m} = \sum_a \vec{m}_a = \sum_a r_a \times p_a$

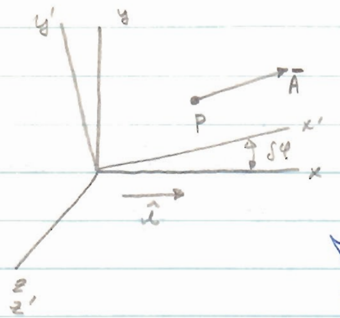
Now suppose a Hamiltonian of the form:

$$H = \sum_a \frac{p_a^2}{2m} + \sum_a V_a(r_a) + V(|r_1 - r_2|, |r_1 - r_3|, \ldots)$$

Then it can be shown: $[H, \vec{m}] = 0$

hence, $\vec{m}$ is a constant of the motion, and is thus conserved.

For preparation for spin, consider <u>vector</u> wave functions. We call this wave function $\vec{A}$.




For $\hat{\imath}\cdot\bar{A}$ we have scalar. Then:

$$\delta\, \hat{\imath}\cdot\bar{A} = \delta\varphi\cdot\underbrace{\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)}_{\frac{i}{\hbar}\mathcal{L}_z}\hat{\imath}\cdot\bar{A}$$

This is not $\delta A_x$, since rotation changes meaning of x.

orbital angular momentum

Now: $\delta A_x = A_{x'}\{x(x',y',z'),\, y(x',y',z'),\, z(x',y',z')\} - A_x(x,y,z)$

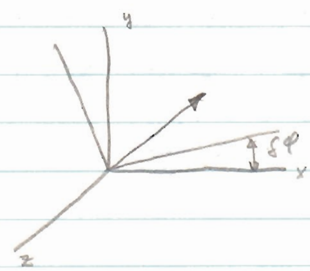
Then we could write:

$$\delta A_x = \delta\varphi\cdot\frac{i}{\hbar}\mathcal{L}_z A_x + \delta\varphi\cdot\frac{i}{\hbar}(S_z A)_x$$

It will turn that $S_z$ is the spin angular momentum. It can be shown geometrically that:

$$A_{x'}(P) = A_x(P) + \delta\varphi\, A_y(P)$$

$$A_{y'}(P) = A_y(P) - \delta\varphi\, A_x(P)$$




Then: $\delta A_x = \delta\varphi\,\frac{i}{\hbar}\mathcal{L}_z A_x + \delta\varphi\, A_y$

and:
$$\frac{i}{\hbar}(S_z A)_x = A_y$$
$$\frac{i}{\hbar}(S_z A)_y = -A_x$$
$$\frac{i}{\hbar}(S_z A)_z = 0$$

Then in vector-matrix notation:

$$S_z = \frac{\hbar}{i}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

We finally can write for the general rotation:

$$\delta \vec{A} = \delta\varphi \cdot \frac{1}{\hbar} (\hat{u} \cdot \vec{m}) \vec{A}$$

where now: $\vec{m} = \vec{L} + \vec{S}$

Also:

$$S_x = \frac{\hbar}{i} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} ; \quad S_y = \frac{\hbar}{i} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Now:

$$S_x^2 = -\hbar^2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} ; \quad S_y^2 = -\hbar^2 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$S_z^2 = -\hbar^2 \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Then:

$$S^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Thus the eigenvalues of $S^2$ are $2\hbar^2$

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<u>LECTURE XX</u> 3-24-61

Recapitulation:

$$\delta \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \frac{i}{\hbar} \delta\varphi (\hat{u} \cdot \vec{m}) \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

where $\vec{m} = \vec{L} + \vec{S}$, and $\vec{L}$ is the angular momentum operator and $\vec{S}$ is the spin operator

Consider rotation around the $z$-axis and $\vec{A}$ constant in space or for <u>fixed</u> point P.

$$\begin{pmatrix} A_x' \\ A_y' \\ A_z' \end{pmatrix} = [1 + \delta\varphi \cdot R_z] \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} \qquad \text{Rotation about } OZ$$

where $R_z = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Now: $R_x R_y = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, can find $[R_x, R_y] = -R_z$

or $[S_x, S_y] = i\hbar S_z$

so the spin operators commute as angular momentum operators as would be expected since they are generated by infinitesimal rotations.

However, one usually says that infinitesimal rotations commute in the first order:

$$[1 + \delta\varphi R_z][1 + \delta\varphi R_y] = 1 + \delta\varphi R_z + \delta\varphi R_z + \underbrace{(\delta\varphi)^2}\, R_y R_z$$

Now take rotation by finite $\varphi$ around $Oz$ or, we repeat the rotation "$\delta\varphi$" $\frac{\varphi}{\delta\varphi}$ times, viz:

$$\begin{pmatrix} A_x' \\ A_y' \\ A_z' \end{pmatrix} = \lim_{\delta\varphi \to 0} [I + \delta\varphi R_z]^{\frac{\varphi}{\delta\varphi}} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

Use the binomial theorem:

$$I + \frac{\varphi}{\delta\varphi} \cdot \delta\varphi R_z + \frac{\frac{\varphi}{\delta\varphi}\left(\frac{\varphi}{\delta\varphi} - 1\right)}{2!} (\delta\varphi)^2 R_z^2 + \ldots$$

Note that $\lim_{\delta\varphi \to 0} [I + \delta\varphi R_z]^{\frac{\varphi}{\delta\varphi}}$

is the definition of $e^{\varphi R_z}$ as the series shows also. Thus:

$$\begin{pmatrix} A_x' \\ A_y' \\ A_z' \end{pmatrix} = e^{\varphi R_z} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

Recall $S_x^2 + S_y^2 + S_z^2 = S^2 = 1 \cdot (1+1)\hbar^2$

gives the eigenvalue $j = 1$

and for $S_z$, $m = -1, 0, +1$.

$$R_z^2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad R_z^3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = -R_z$$

Thus we would find: $R_z^4 = -R_z^2$, etc,
or we have found all the powers of $R_z$:
From:

$$e^{\varphi R_z} = 1 + \varphi R_z + \frac{\varphi^2 R_z^2}{2!} + \frac{\varphi^3 R_z^3}{3!} + \cdots$$

Then:

$$e^{\varphi R_z} = 1 + R_z\left(\varphi - \frac{\varphi^3}{3!} + \frac{\varphi^5}{5!} + \cdots\right)$$

$$+ R_z^2\left(\frac{\varphi^2}{2!} - \frac{\varphi^4}{4!} + \frac{\varphi^6}{6!}\right)$$

$$= 1 + R_z \sin\varphi + R_z^2(1 - \cos\varphi)$$

and finally:

$$\begin{pmatrix} A_x' \\ A_y' \\ A_z' \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

or the usual result.

What diagonalizes $R_z$? Its eigenvalues are $i, 0, -i$ for $R_z$. Then:

$$R_z \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} = \begin{pmatrix} i \\ -1 \\ 0 \end{pmatrix} = i \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$$ — seen to be one of eigenvectors by trial.

For $S_z$: Eigenvectors Eigenvalues

| Eigenvectors | Eigenvalues |
|---|---|
| $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \\ 0 \end{pmatrix}$ | $\hbar$ |
| $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ | $0$ |
| $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \\ 0 \end{pmatrix}$ | $-\hbar$ |

In Dirac notation: $\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} \rightarrow \begin{pmatrix} \langle \hat{i} | \rangle \\ \langle \hat{j} | \rangle \\ \langle \hat{k} | \rangle \end{pmatrix}$

and any ket can be written:

$$| \rangle = \sum_{i j k} | \hat{i} \rangle \langle \hat{i} | \rangle$$

We can write the vector components:

$$\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = a \overset{\hbar}{\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \\ 0 \end{pmatrix}} + b \overset{0}{\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}} + c \overset{-\hbar}{\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \\ 0 \end{pmatrix}}$$

$a \rightarrow \frac{A_x - i A_y}{\sqrt{2}} = A_-$, $\quad b \rightarrow A_z$, $\quad c \rightarrow \frac{A_x + i A_y}{\sqrt{2}} = A_+$

Then:

$$\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}}_{U} \begin{pmatrix} A_- \\ A_z \\ A_+ \end{pmatrix}$$

We can now write a new operator $\mathcal{S}_z$ such that:

$$\mathcal{S}_z \begin{pmatrix} A_- \\ A_z \\ A_+ \end{pmatrix} = U^{-1} S_z U \begin{pmatrix} A_- \\ A_z \\ A_+ \end{pmatrix}$$

or $\mathcal{S}_z = U^{-1} S_z U$

Then we can find: $\mathcal{S}_x = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \hbar$

$\mathcal{S}_y = \hbar \begin{pmatrix} 0 & \frac{i}{\sqrt{2}} & 0 \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}$, $\quad \mathcal{S}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

Then we can form the ladder operators:

$$S_+ = S_x + i\,S_y = \begin{pmatrix} 0 & -\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \hbar$$

$$S_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

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LECTURE XXI    3-27-61

Electron Spin

We need to define a new two component quantity called a spinor. The representation of these quantities in described by square matrices.

Suppose there are two ways to spin might point. If we can locate a particle in $d\tau$ volume, we may be able to which direction the spin goes.

□ $d\tau$    Probability in $d\tau$: "spin up $(m_s = \frac{1}{2})$" $= |\psi(r, 1/2)|^2 d\tau$
" " " : "spin down $(m_s = -\frac{1}{2})$" $= |\psi(r, -1/2)|^2 d\tau$

Note that we include the discrete variable of $\pm\frac{1}{2}$ with the continuous variable $r$. However, we could define a new wave function in $r$ for each spin, such that, "up" $= |f(r)|^2 d\tau$
"down" $= |g(r)|^2 d\tau$

and these form a two-component wave function $\begin{pmatrix} f(r) \\ g(r) \end{pmatrix}$

We must have: $\int (|f|^2 + |g|^2)\, d\tau = 1$

If we have usual functions $u(r)$, $v(r)$ and orthonormal, we can write:

$f = \alpha u$ , $g = \beta v$ so that $|\alpha|^2 + |\beta|^2 = 1$

We can construct using spin eigenvalues :

$$\begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = f(r)\begin{pmatrix} 1 \\ 0 \end{pmatrix} + g(r)\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and for arbitrary function :

$$\begin{pmatrix} a \\ b \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

so that $\psi_{+1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ , $\psi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\left.\begin{aligned} S_z \psi_{+1/2} &= \tfrac{1}{2}\hbar \psi_{+1/2} \\ S_z \psi_{-1/2} &= -\tfrac{1}{2}\hbar \psi_{-1/2} \end{aligned}\right\}$$

and the operator is written $S_z = \hbar \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$

Recall: $M_\pm \psi_{jm} = \hbar \sqrt{(j \mp m)(j \pm m + 1)}\, \psi_{j, m\pm 1}$

then: $S_+ = (S_x + i S_y) = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

$S_- = (S_x - i S_y) = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

and $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ; $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y$

$= \frac{\hbar}{2}\sigma_x$

$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$

where the matrices $\sigma_k$ are the Pauli spin matrices.
Note $\sigma_k^2 = 1$ , $k = x, y, z$.
Also, all these matrices anti-commute:

$$\boxed{\sigma_k \sigma_l + \sigma_l \sigma_k = 2\,\delta_{kl}\, 1}$$

and:

$$\boxed{\sigma_k \sigma_l = i\,\epsilon_{klm}\,\sigma_m + \delta_{kl}\, 1}$$

} contains all information about $\sigma$ matrices

Also: $[\sigma_k, \sigma_l] = 2i\,\epsilon_{klm}\,\sigma_m$

$[S_k, S_l] = i\hbar\,\epsilon_{klm}\, S_m$

Now in a magnetic field, we can define a magnetic moment:

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \quad , \quad \vec{\mu} = \frac{e}{mc}\vec{S} = \frac{e\hbar}{2mc}\vec{\sigma}$$

$\therefore$ in a magnetic field: $-(\vec{\mu}\cdot\vec{H}) = -\frac{e\hbar}{2mc}(\vec{\sigma}\cdot\vec{H})$ will appear in the Hamiltonian.

Suppose we rotate $\delta\varphi$ around $\hat{u}$:

$$\psi' = \left[1 + \frac{i}{\hbar}(\hat{u}\cdot\vec{S})\,\delta\varphi\right]\psi$$

$$= \left[1 + \frac{i}{2}(\hat{u}\cdot\vec{\sigma})\,\delta\varphi\right]\psi$$

For a finite rotation $\varphi$:

$$\psi' = \lim_{\delta\varphi\to 0}\left[1 + \frac{i}{2}(\hat{u}\cdot\vec{\sigma})\,\delta\varphi\right]^{\frac{\varphi}{\delta\varphi}}\psi$$

$$= e^{i\frac{\varphi}{2}(\hat{u}\cdot\vec{\sigma})}\,\psi$$

Now: $\hat{u}\cdot\vec{\sigma} = \begin{pmatrix} u_z & u_x - i u_y \\ u_x + i u_y & -u_z \end{pmatrix}$

and $(\hat{u}\cdot\vec{\sigma})^2 = (u_x\sigma_x + u_y\sigma_y + u_z\sigma_z)(u_x\sigma_x + u_y\sigma_y + u_z\sigma_z)$

$= 1$

$$e^{\frac{\varphi}{2}i(\hat{u}\cdot\vec{\sigma})} = \cos\frac{\varphi}{2} + i(\hat{u}\cdot\vec{\sigma})\sin\frac{\varphi}{2}$$

$$= \begin{pmatrix} \cos\frac{\varphi}{2} + i u_z \sin\frac{\varphi}{2} & (i u_x + u_y)\sin\frac{\varphi}{2} \\ (i u_x - u_y)\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} - i u_z \sin\frac{\varphi}{2} \end{pmatrix}$$

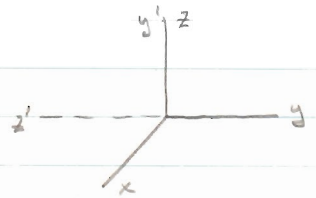
Example:


Rotate around $x$ by $180° = \varphi$

$\begin{pmatrix}1\\0\end{pmatrix} \parallel z$

$\psi' = i\sigma_x\psi \equiv \begin{pmatrix}0\\i\end{pmatrix}$

Now take $\varphi = \pi/2$ around x axis




$$\psi' = \begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{i\sqrt{2}}{2} \\ \frac{i\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{i\sqrt{2}}{2} \end{pmatrix}$$

which gives probability ½ for left or right as it should.

For $\varphi = 2\pi$ around x-axis:
Get:

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

so that we get negative of identity. Thus our rotation matrix is double-valued.

However, probabalities are still the same. There are then two matrices per rotation.

Quaternions: 1, i, j, k with properties
$$i^2 = j^2 = k^2 = -1$$

Hamiltons method of rotation was to sandwich the vector between two quaternions.

$$\left(\cos\frac{\varphi}{2} - i\,u_x - j\,u_y - k\,u_z\right)\left(A_x i + A_y j + A_z k\right)\left(\cos\frac{\varphi}{2} + i\,u_x + j\,u_y + k\,u_z\right)$$

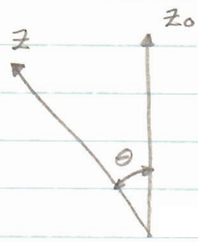
Now this representation is isomorphic to the Pauli matrices:

$$i\sigma_x \rightarrow i$$
$$i\sigma_y \rightarrow j$$
$$i\sigma_z \rightarrow k$$

Must watch difference in meaning which is similar to difference between Schroedinger and Heisenberg representations.

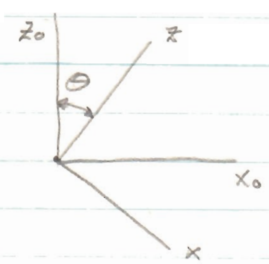
## LECTURE XXII     3-29-61

Suppose we know $j$ (total angular momentum) which is in a state such that we know a component along an axis.




$j$ is fixed along $z_0$. Probability for $m$ along $z$, given $m_0$ along $z_0$ in the initial preparation of the state, is:

$$|(\Phi_m, \Phi_{m_0})|^2$$




Now:

$$|\langle m|m_0\rangle|^2 : \quad |m_0\rangle = \sum_m |m\rangle\langle m|m_0\rangle$$

Can do same with rotation operator:

$$\lim_{\delta\theta\to 0}\left[ I + \delta\theta \frac{1}{\hbar} M_y \right]^{\frac{\theta}{\delta\theta}} \varphi_{m_0} = \varphi_m$$

Take $j=1$: $\quad r f(r) Y_1^{m_0}$

for $m_0 = 0$: $\quad r f(r) \cos\theta_0 = f(r)\, z_0$

$$= f(r)\,(\cos\theta \cdot z - \sin\theta \cdot x)$$

$\langle 0|0\rangle = \cos\theta$

$$f(r) = \begin{cases} z & 0 \\ \frac{x+iy}{\sqrt{2}} & 1 \\ \frac{x-iy}{\sqrt{2}} & -1 \end{cases}$$

$\langle 1|0\rangle = \langle -1|0\rangle = -\frac{\sin\theta}{\sqrt{2}}$

Then $m_0$

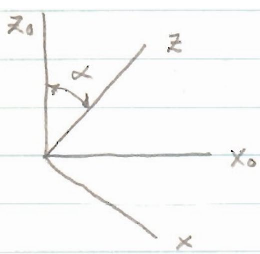
$$0 \longrightarrow \begin{cases} m & \\ 1 & \frac{\sin^2\theta}{2} \\ 0 & \cos^2\theta \\ -1 & \frac{\sin^2\theta}{2} \end{cases}$$

$m_0 = 1$ : $\quad f(r) \cdot \dfrac{x_0 + i y_0}{\sqrt{2}} = f(r) \dfrac{x \cos\theta + i y + z \sin\theta}{\sqrt{2}}$

$$x \cos\theta + i y = a(x + iy) + b(x - iy)$$
$$a + b = \cos\theta \,, \quad a - b = 1$$

$$m_0 \qquad m$$
$$1 \to \begin{cases} 1 & \left(\dfrac{1+\cos\theta}{2}\right)^2 = \cos^4 \dfrac{\theta}{2} \\ 0 & \dfrac{\sin^2\theta}{2} = 2 \sin^2 \dfrac{\theta}{2} \cos^2 \dfrac{\theta}{2} \\ -1 & \left(\dfrac{1-\cos\theta}{2}\right)^2 = \sin^4 \dfrac{\theta}{2} \end{cases}$$

## More General Method




$$|m_0\rangle = \sum_m |m\rangle \langle m | m_0 \rangle$$

$$M_{z_0} |m_0\rangle = m_0 \hbar |m_0\rangle$$

$$M_{z_0} = M_z \cos\alpha - M_x \sin\alpha$$

$$= M_z \cos\alpha - M_+ \frac{\sin\alpha}{2} - M_- \frac{\sin\alpha}{2}$$

Now apply $M_{z_0}$ to $|m_0\rangle$ :

$$\sum_m \Big\{ -\frac{\sin\alpha}{2} \sqrt{(j-m)(j+m+1)}\, |m+1\rangle + (m \cos\alpha - m_0) |m\rangle$$
$$- \frac{\sin\alpha}{2} \sqrt{(j+m)(j-m+1)}\, |m-1\rangle \Big\} \langle m | m_0 \rangle = 0$$

or :

$$\sum_m |m\rangle \Big\{ -\frac{\sin\alpha}{2} \sqrt{(j-m+1)(j+m)}\, \langle m-1 | m_0 \rangle$$

$$+ (m \cos\alpha - m_0) \langle m | m_0 \rangle - \frac{\sin\alpha}{2} \sqrt{(j+m+1)(j-m)}\, \langle m+1 | m_0 \rangle \Big\}$$

$$= 0$$

Take $j = 1$:

$m = 1$: $\quad -\frac{\sin\alpha}{2}\sqrt{2}\,\langle 0|m_0\rangle + (\cos\alpha - m_0)\langle 1|m_0\rangle = 0$

$m = -1$: $\quad (-\cos\alpha - m_0)\langle -1|m_0\rangle - \frac{\sin\alpha}{2}\sqrt{2}\,\langle 0|m_0\rangle = 0$

$$\langle 1|m_0\rangle = \frac{\sin\alpha}{\sqrt{2}\,(\cos\alpha - m_0)}\langle 0|m_0\rangle$$

$$\langle -1|m_0\rangle = \frac{\sin\alpha}{\sqrt{2}\,(-\cos\alpha - m_0)}\langle 0|m_0\rangle$$

$$|\langle 0|m_0\rangle|^2 \left\{1 + \frac{\sin^2\alpha}{2(m_0-\cos\alpha)^2} + \frac{\sin^2\alpha}{2(m_0+\cos\alpha)^2}\right\} = 1$$

$$\{\} = \frac{2(m_0^2-\cos^2\alpha)^2 + \sin^2\alpha\,[(m_0+\cos\alpha)^2 + (m_0-\cos\alpha)^2]}{2(m_0^2-\cos^2\alpha)^2}$$

$$= \frac{m_0^4 - 2m_0^2\cos^2\alpha + \cos^4\alpha + \sin^2\alpha\, m_0^2 + \sin^2\alpha\cos^2\alpha}{(m_0^2-\cos^2\alpha)^2}$$

$$|\langle 0|m_0\rangle|^2 = \frac{(m_0^2-\cos^2\alpha)^2}{m_0^4 + (1-3\cos^2\alpha)m_0^2 + \cos^2\alpha}$$

$$|\langle 1|m_0\rangle|^2 = \frac{\frac{\sin^2\alpha}{2}(m_0+\cos\alpha)^2}{\text{denominator}}$$

$$|\langle -1|m_0\rangle|^2 = \frac{\frac{\sin^2\alpha}{2}(m_0-\cos\alpha)^2}{\text{denominator}}$$

LECTURE XXIII 3-31-61

## Systems Containing Elementary Particles

We take the state described by $\psi(r_1, r_2, \cdots r_N)$ in which:

$|\psi(r_1, r_2, \cdots r_N)|^2 dr_1 \cdots dr_N$ = probability of finding 1 in $dr_1$, 2 in $dr_2$, etc.

Prob. of 1 in $dr_1 = dr_1 \int |\psi(r_1, \cdots r_N)|^2 dr_2 \cdots dr_N$

With spins, we have to include reference to orientation in wave function argument, viz; $r_1, m_{1s} \rightarrow r_1, s_1$. Then; state is:

$\psi(r_1, s_1; r_2, s_2; \cdots)$

For two particle system:

$\psi(r_1 \tfrac{1}{2}; r_2 \tfrac{1}{2})$
$\psi(r_1 \tfrac{1}{2}; r_2 -\tfrac{1}{2})$
$\psi(r_1 -\tfrac{1}{2}; r_2 \tfrac{1}{2})$
$\psi(r_1 -\tfrac{1}{2}; r_2 -\tfrac{1}{2})$

One can think of these as elements of a column matrix:

$\begin{pmatrix} f \\ g \\ h \\ k \end{pmatrix}$ : $|f(r_1, r_2)|^2 dr_1 dr_2$ = Prob. 1 in $dr_1$ and has $m_{1s} = 1/2$ and 2 in $dr_2$ and has $m_{2s} = 1/2$

Can have Prob. 1 in $dr_1$, 2 in $dr_2$

$$= \sum_{s_1 = \frac{1}{2}, -\frac{1}{2}} \sum_{s_2 = \frac{1}{2}, -\frac{1}{2}} |\psi(r_1, s_1; r_2, s_2)|^2 dr_1 dr_2$$

Prob. 1 in $dr_1$ and with $\tfrac{1}{2}$ = $dr_1 \sum_{s_2} \int dr_2 |\psi(r_1, \tfrac{1}{2}; r_2, s_2)|^2$

Recall: $\vec{j}_1 = \sum_{s_1} \sum_{s_2} \frac{\hbar}{2mi} \int dr_2 (\psi^* \nabla_1 \psi - \psi \nabla_1 \psi^*)$

We now consider particles which are identical:

Now, in classical physics, there are several ways to tell particles apart.

① Measure or detect difference in intrinsic properties

② Trace paths.

Now, in QM, ① is still possible. However, if ① is not available, ② can never be because of uncertainty principle when particles are closely interacting, like in Helium or any atom.

Now, if all particles are identical, we have for the Hamiltonian (which must involve each particle the same way):

$$H(r_1, p_1, \vec{S}_1; r_2, p_2, \vec{S}_2; \dots)$$

$$= H(r_2, p_2, \vec{S}_2; r_1, p_1, \vec{S}_1; \dots), \quad \text{etc.}$$

Define the operator $P_{12}$ that exchanges the particles, such that:

$$P_{12} H = H P_{12} \quad \text{or} \quad [P_{12}, H] = 0$$

or, define the general permutation operator:

$$PH = HP \quad \text{or} \quad [P, H] = 0$$

Consider 3 particles: P's operate such that:

| | | | | |
|---|---|---|---|---|
| 1, 2, 3 $\longrightarrow$ | 1, 2, 3 | (identity operator) | even | By using P's can form antisymmetric or symmetric wave function. |
| | 2, 1, 3 | ($P_{12}$) | odd | $\sum_{\text{all } P} (P_{even} - P_{odd})\psi$ for antisymmetric |
| | 1, 3, 2 | | odd | |
| | 3, 2, 1 | | odd | |
| | 3, 1, 2 | | even | |
| | 2, 3, 1 | | even | |

For $n$ particles, there are always $n!$ operators, with 1/2 odd and 1/2 even.

We can even include perturbations because they treat each particle the same.
The operators do not commute with each other.

The operators not only could commute with $H$ but also with other quantities.

Now, we have:

$$H\psi = E\psi$$
$$PH\psi = EP\psi = HP\psi$$

so That $P\psi$ is also an eigenfunction. If $\psi$ is non-degenerate $P\psi$ is just a multiple of $\psi$, that is: $P_{jk}\psi = c\psi$, applying $P_{jk}$ again we get $\psi = c^2\psi$, $c = \pm 1$
If $c$ is $+1$, $\psi$ is symmetric; $c = 1$, $\psi$ antisymmetric
Can show by $P_{34} = P_{24}\,P_{13}\,P_{12}\,P_{13}\,P_{24}$, that $P_{34}$ is same as $P_{12}$.
Particles which are antisymmetric are called Fermions, symmetric particles are called Bosons.

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LECTURE XXIV    4-10-61

Recall: $[P, H] = 0$
$H\psi = E\psi$
$HP\psi = EP\psi$

Non Degenerate: $P\psi = \text{constant} \cdot \psi$
Symmetric: $P\psi = \psi$
Anti-symmetric $P_{ab}\psi = -\psi$
$\therefore\ P\psi = \pm\psi$

If degenerate, get linear combination:

$$P\psi_i = \sum_{j=1}^{f} p_{ij}\,\psi_j$$

If we add perturbation to H, the result still commutes with P. The effect of time on the permutation is nill since P commutes with all H, even H time dependent:

$$P \frac{\partial \psi_i}{\partial t} = \sum_{j=1}^{f} p_{ij} \frac{\partial \psi_j}{\partial t}$$

Example: Spin Functions; spin 1/2

Define: eigenfunction $\left\{ \begin{array}{l} a : \ 1/2 \\ b : \ -1/2 \end{array} \right\}$ eigenvalues

For two electrons, define $ab \equiv a(1)\, b(2)$

| | | $m_s$ |
|---|---|---|
| Then: | $aa$ | 1 |
| | $\frac{1}{\sqrt{2}}(ab+ba)$ | 0 |
| | $bb$ | -1 |

These are all symmetric with $s=1$ and is called the triple state. For anti-symmetric:

$\frac{1}{\sqrt{2}}(ab-ba) \Leftrightarrow 0$ ($m_s$) called singlet

For 3 particles (not electrons)

| | $m_s$ |
|---|---|
| $aaa$ | 3/2 |
| $\frac{1}{\sqrt{3}}(aab+aba+baa)$ | 1/2 |
| $\frac{1}{\sqrt{3}}(abb+bab+bba)$ | -1/2 |
| $bbb$ | -3/2 |

These are symmetric; impossible to make antisymmetric. Corresponds to $s = 3/2$. If we look for combination orthogonal to above combinations, we get:

| $m_s$ | | |
|---|---|---|
| 1/2 | $\frac{1}{\sqrt{2}}(aab - baa) = u$ | $s = 1/2$ |
| -1/2 | $\frac{1}{\sqrt{2}}(abb - bba)$ | |

which are neither symmetric or antisymmetric.

If we look further:

$$v = \frac{1}{\sqrt{6}}(aab - 2\,aba + baa) \qquad \begin{matrix} m_s \\ 1/2 \end{matrix}$$
$$-\frac{1}{\sqrt{6}}(abb - 2\,bab + bba) \qquad -1/2$$
} $S = 1/2$

If we apply the permutation $P_{12}$ to $u$:

$$P_{12}\,u = \frac{1}{\sqrt{2}}(aab - aba) = \frac{1}{2}u + \frac{\sqrt{3}}{2}v$$

and $$P_{12}\,v = \frac{\sqrt{3}}{2}u - \frac{1}{2}v$$

Can show: $P_{13}\,u = -u$
$P_{13}\,v = v$

$u$ and $v$ are said to be the basis of the group. That is, if:

$$P_{12}(Au + Bv) = (\mathcal{A}u + \mathcal{B}v)$$

then $$\begin{pmatrix} \mathcal{A} \\ \mathcal{B} \end{pmatrix} = \begin{pmatrix} \sim & \sim \\ \sim & \sim \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$$ exists

For symmetric basis, representation is unity.
For antisymmetric wave function, half of representation is +1, other half is −1.

For 4 particles:

| $m_s$ | |
|---|---|
| 2 | $aaaa$ |
| 1 | $\frac{1}{2}(aaab + aaba + abaa + baaa)$ |
| −1 | $\frac{1}{2}(abbb + babb + bbab + bbba)$ |
| −2 | $bbbb$ |
| 0 | $\frac{1}{\sqrt{6}}(aabb + abab + abba + bbaa + baab + baba)$ |

symmetric: $S = 2$
For $m_s = 1$: $u_1 = \frac{1}{2}(aaab + aaba + abaa + baaa)$
Look for $v_1 = \frac{1}{2}(\quad - \quad + \quad - \quad)$
orthogonal combinations $w_1 = \frac{1}{2}(\quad - \quad - \quad + \quad)$

$P_{12}\, u_1 = u_1$ $\qquad P_{23}\, u_1 = v_1$

$P_{12}\, v_1 = w_1$ $\qquad P_{23}\, v_1 = u_1$

$P_{12}\, w_1 = v_1$ $\qquad P_{23}\, w_1 = w_1$

Can find for $m_s = 0$:

$$u_0 = \frac{1}{\sqrt{2}}(aabb - bbaa)$$
$$v_0 = \frac{1}{\sqrt{2}}(abab - baba)$$
$$w_0 = \frac{1}{\sqrt{2}}(baab - abba)$$

We need two more to get 16, these are singlets

$$x_0 = \frac{1}{2}\left[(aabb + bbaa) - (baab + abba)\right]$$

$$y_0 = \frac{1}{\sqrt{12}}\left[(aabb + bbaa) - 2(abab + baba) + (baab + abba)\right]$$

However, in nature, only states with symmetric or antisymmetric wave functions exist.

If we take a particle with spin 1:

| a | b | c |
|---|---|---|
| +1 | 0 | −1 |

Then for three particles, there are 27 functions:

| | | | |
|---|---|---|---|
| 3 | aaa | symmetric | $S = 3, 1$ |
| ⋮ | | 2 rowed | $S = 2, 1$ |
| −3 | ccc | antisymmetric | $S = 0$ |

Then, the antisymmetric must have the form:

$$\begin{vmatrix} a(1) & b(1) & c(1) \\ a(2) & b(2) & c(2) \\ a(3) & b(3) & c(3) \end{vmatrix}$$

If wave function can be written as products of individual states, then determinant forms antisymmetric wave functions.

LECTURE XXV 4-12-61

Consider two electrons and write an unsymmetric wave function between them

$$\psi_{un} = \psi_1(r_1)\,\psi_2(r_2)$$

$$\psi_{anti} = c\left\{ \psi_1(r_1)\,\psi_2(r_2) - \psi_1(r_2)\,\psi_2(r_1) \right\}$$

Consider the point operator F which acts only on the coordinates: $\frac{e^2}{r_{12}}$ is an example.
Consider $\bar{F}$: F is symmetric:

$$(\bar{F})_{un} = \int \psi_1^*(r_1)\,\psi_2^*(r_2)\,F\,\psi_1(r_1)\,\psi_2(r_2)\,dr_1\,dr_2$$

$$(\bar{F})_{anti} = |c|^2 \int \psi_1^*(r_1)\,\psi_2^*(r_2)\,F\,\psi_1(r_1)\,\psi_2(r_2)\,dr_1\,dr_2$$
$$- |c|^2 \int \psi_1^*(r_1)\,\psi_2^*(r_2)\,F\,\psi_1(r_2)\,\psi_2(r_1)\,dr_1\,dr_2 \quad + 2 \text{ terms.}$$

Only need antisymmetry when possibly wave functions of two electrons overlap. Since F is symmetric:

$$(\bar{F})_{anti} = 2|c|^2 \int \psi_1^*(r_1)\,\psi_2^*(r_2)\,F\,\psi_1(r_1)\,\psi_2(r_2)\,dr_1\,dr_2$$

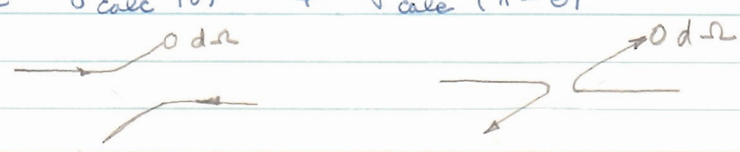
$$- 2|c|^2 \underbrace{\int \psi_1^*(r_1)\,\psi_2^*(r_2)\,F\,\psi_1(r_2)\,\psi_2(r_1)\,dr_1\,dr_2}_{\text{exchange integral}}$$

If no overlap, exchange integral is zero, thus $c = \frac{1}{\sqrt{2}}$. Then, if wave function do not overlap, can use either symmetry or antisymmetry combinations.

Example: Consider the Collision of Identical Particles.

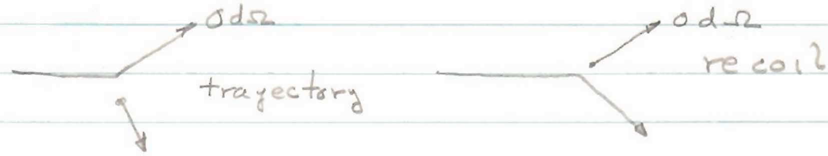
Classical Treatment in center of mass system:

$$\sigma_{obs}(\theta) = \sigma_{calc}(\theta) + \sigma_{calc}(\pi - \theta)$$



In the laboratory coordinate system:

$$\sigma_{obs}(\vartheta) = \sigma_{calc}(\vartheta) + \sigma_{calc}(\tfrac{\pi}{2} - \vartheta)$$




Consider QM treatment of spinless α-particles which are symmetric: 4 particles in nucleus.
Using c. of m. coordinates:

$$\psi(r_1, r_2) \;:\; R = \frac{r_1 + r_2}{2} \;;\; r = r_1 - r_2$$

Then the wave function of the particle and scatterer is:

$$\psi \sim e^{ikz} + e^{-ikz} + \{ f(\theta) + f(\pi - \theta) \} \frac{e^{ikr}}{r}$$

Then: $\sigma(\theta) = | f(\theta) + f(\pi-\theta) |^2 = | f(\theta) |^2 + | f(\pi - \theta) |^2 + \underbrace{2 \,\mathrm{Re} \{ f^*(\theta) f(\pi - \theta) \}}_{\text{interference terms}}$

Note that interference term is typically QM. Also depends on phase. However, at high energy collisions, wave packets form, and fluctuation from Rutherford scattering are so rapid that they smear out to classical result. Low energys, plane waves, produce deviations from Rutherford result.

Example: Electrons, polarized, so that spins are in same direction.
The spin function is symmetric $\alpha(1)\alpha(2)$, thus must be antisymmetric in coordinates.
Then:

$$\sigma(\theta) = |\,|^2 + |\,|^2 - 2\,\mathrm{Re}\,(\sim)$$

Example: Electrons, unpolarized, 4 possibilities:

$$\alpha\alpha$$
$$\frac{1}{\sqrt{2}}(\alpha\beta + \beta\alpha) \qquad \frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$$
$$\beta\beta$$

Symmetric                Antisymmetric

In coordinates: $\frac{3}{4}$ antisymmetric    $\frac{1}{4}$ symmetric

$$\sigma(\theta) = |\,|^2 + |\,|^2 - \mathrm{Re}(\ )$$

Example: Electrons, opposite in spin, 2 possibilities

$$\sigma(\theta) = |\,|^2 + |\,|^2$$

Traditional case is unpolarized electrons.

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## LECTURE XXVI    4-14-61

Theory of many-electron atoms:

Take for unperturbed problem a common central field $V(r)$ which is screened from the usual coulomb field. Recall the shell structure of atom:

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f

If one takes this model, a high degree of degeneracy occurs. For ~~nitrogen~~ Carbon: $(1s)^2(2s)^2(2p)^2$

For perturbations:

Main one (electrostatic): $$H_1 = \sum_{\text{electrons}} \left(-\frac{Ze^2}{r} + V(r)\right) + \sum_{\text{pairs}}' \frac{e^2}{R_{ij}}$$

Smaller ones: $H_2$ = spin-orbit coupling and interactions

$H_3$ = spin-spin interaction

Can also have H term for external magnetic field. Waves functions are antisymmetric since no two can occupy the same point.

Example: Two Electrons:

Possibilities for spins:

$$\left.\begin{array}{c} \alpha(1)\,\alpha(2) \\ \dfrac{\alpha(1)\,\beta(2) + \beta(1)\,\alpha(2)}{\sqrt{2}} \\ \beta(1)\,\beta(2) \end{array}\right\} \quad S = 1,\ \text{singlet symmetric}$$

$$\left.\dfrac{\alpha(1)\,\beta(2) - \beta(1)\,\alpha(2)}{\sqrt{2}}\right\} \quad S = 0,\ \text{triplet antisymmetric}$$

All right to be symmetric in spin as have not considered orbital functions.

Possibilities for orbitals:

$$\left.\dfrac{u(1)\,v(2) - u(2)\,v(1)}{\sqrt{2}}\right\} \quad \text{antisymmetric}$$

$$\left.\dfrac{u(1)\,v(2) + u(2)\,v(1)}{\sqrt{2}}\right\} \quad \text{symmetric}$$

Thus, we must combine with spins to form completely antisymmetric wave functions. We find the average value of $H_1$: First term vanishes;

$$S=1: \quad \overline{\left(\frac{e^2}{r_{12}}\right)} = e^2 \int |u(1)|^2 \, |v(2)|^2 \, \frac{1}{r_{12}} \, dr_1 \, dr_2$$

$$- \; e \underbrace{\int u^*(1)\, v^*(2) \, \frac{1}{r_{12}} \, u(2)\, v(1)\, dr_1\, dr_2}_{\text{Exchange integral}}$$

$+$ for $S=0$

Exchange integral: also almost always + for simple atomic case. Thus can see triplet state lies lowest.

Note difference between states and terms:

Consider Carbon: $(1s)^2 (2s)^2 (2p)^2$

The term values of Carbon are: $^1S$, $^3P$, $^1D$.
The states are $(1s)^2(2s)^2(2p)^2$. The terms split into levels; upon introduction of magnetic fields.

$$^3P \rightarrow {}^3P_2, {}^3P_1, {}^3P_0$$
one level → 3 levels

This should show large effect due to spin interaction and coupling being more large than their magnetic field interaction.

Dirac and Van Vleck assume strong interaction exist: Form:

$$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)\sigma_{1x} = \sigma_{2x} - i\sigma_{2y}\sigma_{1z} + i\sigma_{2z}\sigma_{1y}$$

Also form: $\sigma_{2x}(\vec{\sigma}_1 \cdot \vec{\sigma}_2) = \sigma_{1x} + i\sigma_{1y}\sigma_{2z} - i\sigma_{1z}\sigma_{2y}$

using $\vec{s} = \frac{\hbar}{2}\vec{\sigma}$ and $\sigma_j\sigma_k = \delta_{jk} + i\epsilon_{jkl}\sigma_l$

We can see that:

$$\underbrace{[1 + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)]}_{P_{12}^{\sigma}}\sigma_{1x} = \sigma_{2x}[1 + (\sigma_1 \cdot \sigma_2)]$$

Thus we can write: $P_{12}^{\sigma^{-1}}\sigma_{2x}P_{12}^{\sigma} = \sigma_{1x}$

or $P_{12}^{\sigma^{-1}}\sigma_{2x}P_{12}^{\sigma}\psi = \sigma_{1x}\psi$

Actually Dirac calls $[1 + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)] = O_{12}^{\sigma}$. We don't have $P_{12}^{\sigma}$ yet. Form:

$$(O_{12}^{\sigma})^2 = \{1 + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\}^2 = (1 + \sigma_{1j}\sigma_{2j})^2$$

$$= 1 + 2(\sigma_1 \cdot \sigma_2) + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$$

now: $\sigma_{1j} \cdot \sigma_{2j} \cdot \sigma_{1k} \cdot \sigma_{2k} = (\delta_{jk} + i\epsilon_{jkl}\sigma_{1l})(\delta_{jk} + i\epsilon_{jkm}\sigma_{m})$

$$= \delta_{kk} - 2(\vec{\sigma}_1 \cdot \sigma_2)$$

$\therefore \quad (O_{12}^{\sigma})^2 = 4$

Then define: $\quad P_{12}^{\sigma} = \frac{1}{2}\left\{1 + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\right\}$

Recall: $\quad P_{12}\,\psi = -\psi$

$$P_{12}^{x}\,P_{12}^{\sigma}\,\psi = -\psi$$

Then $\quad P_{12}^{x}\,\psi = -P_{12}^{\sigma}\,\psi$

and: $\quad P_{12}^{x}\,\psi = -\frac{1}{2}\left\{1 + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\right\}\psi$

which shows the apparent spin interaction.

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LECTURE XXVII $\qquad$ 4-17-61

One can justify neglecting closed shells and treat just outer electrons because they have no angular momentum and no current. Consider the operator $O$ applied to a product antisymmetric wave function which can be written as a determinant:

$$\mathcal{O} = O_1 + O_2 + \cdots$$

$$\begin{vmatrix} \psi_1(1) & \psi_1(2) & \psi_1(3) & \cdots \\ \psi_2(1) & \psi_2(2) & \psi_2(3) & \cdots \\ \psi_3(1) & \psi_3(2) & \psi_3(3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix}$$

$O_1$ applies to first column, $O_2$ to second, etc: We want to write result as sum:

$$\mathcal{O}\begin{vmatrix} \psi_1(1) & \cdots \\ \vdots & \cdots \\ \vdots & \cdots \end{vmatrix} = \sum_{k,\alpha} O_k\,\psi_\alpha(k)\left\{\text{cofactor of } \psi_\alpha(k)\right\}$$

O means single-particle operator:

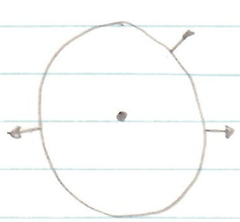
$$\therefore \sum_{\alpha} \text{---} = \begin{vmatrix} (O\psi_1)(1) & (O\psi_1)(2) & \cdots \\ \psi_2(1) & \psi_2(2) & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} + \begin{vmatrix} \psi_1(1) & \psi_1(2) & \cdots \\ (O\psi_2)(1) & (O\psi_2)(2) & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} + \cdots$$

Can talk of 1s 2s electrons because we can apply operator to states of 1s 2s.
If closed shells: 1st m rows are fixed. If we apply operator $M_z$, will get all $m_s + m_l$ for closed shells which will add up to zero and will get only contribution from unclosed shells. Same for $M_x$ and $M_y$.
Suppose we have:

$$\begin{vmatrix} \psi_{1s+}(1) & \psi_{1s+}(2) & \psi_{1s+}(3) & \psi_{1s+}(4) \\ \psi_{1s-}(1) & \psi_{1s-}(2) & \psi_{1s-}(3) & \psi_{1s-}(4) \\ \psi_{2s}(1) & \psi_{2s}(2) & \psi_{2s}(3) & \psi_{2s}(4) \\ \psi_{2p}(1) & \psi_{2p}(2) & \psi_{2p}(3) & \psi_{2p}(4) \end{vmatrix}$$

Use Laplace expansion to find 6 determinantal products.

Closed shell has no current: closed shell is isotropic, so current must be isotropic



Assume current (isotropic): current would be outward thus depleting inside of charge, violating conservation of charge.

Consider excited Carbon (neglect filled shells) $2p\,3p$

| $m_l$ | $m_s$ |
|---|---|
| $-1$ | $+$ |
| $0$ | $-$ |
| $1$ | |

$$\begin{vmatrix} u_{21 m_{l_1} m_{s_1}}(1) & u_{21 m_{l_1} m_{s_1}}(2) \\ u_{31 m_{l_2} m_{s_2}}(1) & u_{31 m_{l_2} m_{s_2}}(2) \end{vmatrix}$$

For $l_1 = 1 \quad s_1 = 1/2$

$l_2 = 1 \quad s_2 = 1/2$

$L = 2, 1, 0 \;\} \; S = 1, 0$

| | |
|---|---|
| $^3D$ | $^1D$ |
| $^3P$ | $^1P$ |
| $^3S$ | $^1S$ |

Can write $\left\{ u_1(1) v_0(2) + u_0(1) v_1(2) \right\} \alpha(1) \alpha(2)$

Can form such terms, after finding by Clebsch-Gordan coefficients, and anti-symmetrize by forming determinants.

Equivalent Electrons : $l = m_l$

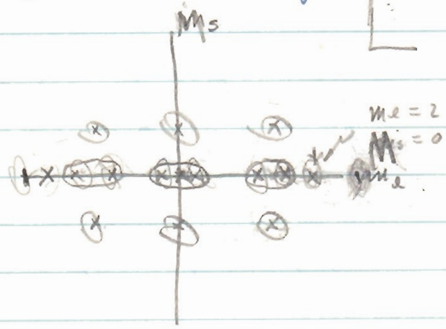
consider:

$n \; l$

$(2 \; p)^2$

| $m_{l1}$ | $m_{s1}$ | $m_{l2}$ | $m_{s2}$ | number |
|---|---|---|---|---|
| 1 | + | 1 | — | 1 |
| 1 | ± | 0 | ± | 4 |
| 1 | ± | −1 | ± | 4 |
| 0 | + | 0 | — | 1 |
| 0 | ± | −1 | ± | 4 |
| −1 | + | −1 | — | 1 |
| | | | | 15 |

What are possibilities of combination of $m_l$ and $m_s$ to get antisymmetric wave functions?




Can form 3 terms:

$^1D$ , $^3P$ , $^1S$

Operate on these terms with $H = \sum_{ij} \frac{e^2}{r_{ij}} - \sum_i V_0(r_i)$ to get splitting into usual levels.

LECTURE XXVIII 4-19-61

Spin - Orbit Interaction:

$$\frac{\text{magnetic moment}}{\text{angular momentum}} = \text{gyromagnetic ratio} = \frac{\mu}{\mathcal{M}}$$

For Orbit: $\frac{\mu}{\mathcal{M}} = \frac{e}{2mc}$

(for circular orbit)


$\mu = \frac{iA}{c} = \frac{\pi a^2 e \nu}{c}$

$\mathcal{M} = m\, 2\pi a \nu \cdot a$ , $\therefore$ $\frac{\mu}{\mathcal{M}} = \frac{e}{2mc}$

For spin, $\frac{\mu}{\mathcal{M}}$ is twice as large: $\frac{e}{mc}$

Infers precession twice as fast as orbit. Total precession is struggle between spin and orbit.

For electron; charge $-e$, and spin:

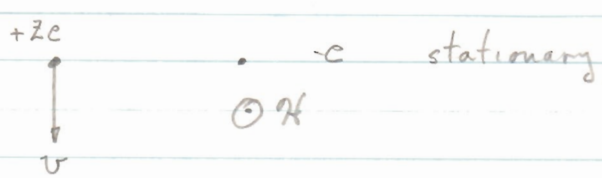
$$\vec{\mu} = -\frac{e\hbar}{2mc}\vec{\sigma}$$

The Hamiltonian in magnetic field is:

$$H_{spin-\mathcal{H}} = -(\vec{\mu}\cdot\vec{\mathcal{H}}) = \frac{e\hbar}{2mc}(\vec{\sigma}\cdot\vec{\mathcal{H}})$$

We want to talk about SO splitting of levels like $^3P_{2,1,0}$

Consider fixed electron and moving nucleus:




Electron sees magnetic field $\mathcal{H}'$:

$$\mathcal{H}' = \mathcal{E}\frac{v}{c} = \frac{Zev}{cr^2}$$

In actual case:


or $\vec{\mathcal{H}}' = \vec{\mathcal{E}} \times \frac{\vec{v}}{c}$

This suggests that we take for $H_{s\text{-}o}$:

$$H_{so} = \frac{e\hbar}{2mc}\,\vec{\sigma}\cdot\left(\vec{\mathcal{E}} \times \frac{\vec{v}}{c}\right)$$

Now the force on the electron is
$-e\vec{\mathcal{E}} = -\nabla V$

Then:

$$H_{so} = \frac{e\hbar}{e2mc}\,\vec{\sigma}\cdot\left(\nabla V \times \frac{\vec{v}}{c}\right) = \frac{\hbar}{2m^2c^2}\,\vec{\sigma}\cdot\left(\nabla V \times \vec{p}\right)$$

Now: $\nabla V = \frac{\vec{r}}{r}\frac{dV}{dr}$ for central field.

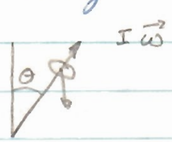
$$\therefore \quad H_{so} = \frac{\hbar}{2m^2c^2}\,\frac{1}{r}\frac{dV}{dr}\,\vec{\sigma}\cdot\underbrace{\left(\vec{r}\times\vec{p}\right)}_{\hbar\vec{L}}$$

Therefore, there is coupling between spin and angular orbital momentum. However, this Hamiltonian gives twice the splitting observed. The factor $\frac{1}{2}$ needed because of Thomas effect. Called Thomas factor, but comes from different effect than this coupling. In general, we write for gyromagnetic ratio:

$g\frac{e}{2mc}$ : Thomas factor is $\frac{1}{g}$, not always $\frac{1}{2}$

Precessional angular velocity:

Top:




Classically: $I\omega\sin\theta\,\Omega = L$

Now the magnitude of the precession angular velocity is:

$$\frac{\mathcal{H}'e}{mc}$$

For difference in energy: $\hbar \frac{\mathcal{H}'e}{mc}$

We write the precession frequency as a vector:

$$\vec{\omega}'_{\text{relative to local system or electron}} = \frac{e}{mc}\vec{\mathcal{E}} \times \frac{\vec{v}}{c} = \frac{1}{c^2}(\vec{v} \times \vec{a})$$

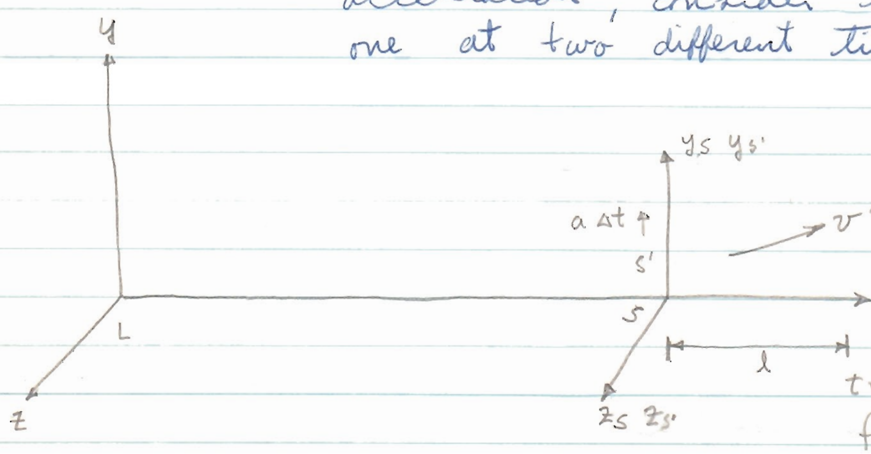
However, local system is precessing:

$$\vec{\omega}_T = \vec{\omega}''_{\text{of local system}} = \frac{1}{2c^2}(\vec{a} \times \vec{v})$$

Sum of both gives $\frac{1}{2c^2}(\vec{v} \times \vec{a})$


We now make a simple proof of Thomas precession. Actually Thomas precession is a lower order effect than addition of velocities. We consider case where $\vec{v} \perp \vec{a}$

L = laboratory system. Because of acceleration, consider two systems; actually one at two different times:



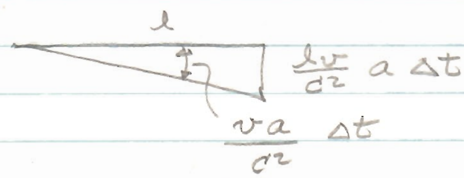

$t_m = \frac{t_1+t_2}{2} = t_1 + \frac{l}{c}$

from view of S.

Consider system S' moving with velocity $\vec{a}\,\Delta t$, coinciding with $y_s$ axis; light signal is sent from S and reflected, giving $t_m = t_1 + \frac{l}{c}$ from point of view of S. From point of view of L, second mirror appears to move a distance $\frac{l}{c} v$. Thus L sees:

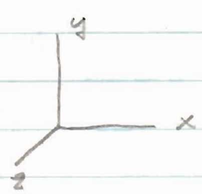
$$t = t_1 + \frac{l}{c} + \frac{lv}{c^2}$$

Thus L says that altho S and S' coincide at some time, the times differ at some other point




When separating Lorentz contraction from rotation, we get Thomas precession. Lorentz contraction squashes angles.

If we use infinitesimal rotation operators




$$\left[ \frac{M_x}{\hbar}, \frac{M_y}{\hbar} \right] = i \frac{M_z}{\hbar}$$

If one of axes is time, Thomas precession is result of commutator of Lorentz rotations.

## LECTURE XXIX 4-21-61

Spin-orbit coupling:

Undisturbed:

configuration

$(n_1, n_2, n_3, \dots)(l_1, l_2, l_3, \dots)(m_{l_1}, m_{l_2}, \dots m_{s_1}, m_{s_2}, \dots)$

Electrostatic coupling splits and gives terms:
$L, S, (M_L, M_S)$

Spin-orbit coupling splits further; and gives levels: $L, S, J (M)$

Finally, upon introduction of magnetic field: get states: $L, S, J, M$.

Electrostatic coupling >> spin orbit coupling. Called Russell-Saunders coupling. What are sizes of es and so coupling?

Electrostatic : $\sim \frac{e^2}{a}$, $a$ = Bohr orbit

Consider for a moment some elementary atomic units:

| | | | |
|---|---|---|---|
| Bohr radius : | $a_0 = \frac{\hbar^2}{me^2}$ | larger | each |
| Compton $\lambda$ ; | $\bar{\lambda} = \frac{\hbar}{mc}$ | to | differ by about |
| Classical electron radius ; | $e^2/mc^2 = r_0$ | smaller | $\frac{1}{137} = \alpha$ |

Typical optical wavelengths are larger than any above.

Electrostatic: $\sim \frac{e^2}{a} \sim \alpha^2 mc^2$

Spin-orbit : $\sim \frac{e\hbar}{mc} \cdot \frac{v}{c} \frac{(Z)e}{(a_0/(Z))^2}$ ; $\left(\frac{v}{c}\right) \sim \alpha (Z)$ for atom with outer electrons

$Z$ is effective atomic number:

$$\sim \frac{e^2}{a_0} \underbrace{\left(\frac{\hbar/mc}{a_0}\right)}_{\alpha} \alpha (Z)^4 \sim (Z)^4 \alpha^4 mc^2$$

Therefore, the ratio of so to es coupling:

$$\text{Ratio } \frac{so}{es} \sim (Z)^4 \alpha^2$$

so so small if Z is small, light atom.
For heavy atom, it will be bigger and so could be larger than es. If so >> es, we get so-called j-j coupling; must reverse process outlined above:

$l_1, l_2, \ldots$
↘ so
$j_1, j_2$
↓ es
$(j_1, j_2, \ldots), J, (M)$

This case is very rare, since Z rarely reaches its full value for heavy atoms because of screening.

For visible light, it can be shown $\lambda \sim \frac{10}{\alpha} a$ since the Rydberg constant is 10 times too large for visible spectra.

Selection Rules:

Electric dipole transitions, Electric quadrapole, etc. and Magnetic dipole, etc.
Nuclear transitions are much more fine and complex. Labelled $E_1$, $E_2$, $M_1$, etc.
We limit to electric dipole transitions in atoms:

$$\frac{\text{Intensity } (E_2)}{\text{Intensity } (E_1)} \sim \left(\frac{a}{\lambda}\right)^2$$

or $E_2$ is less intense than $E_1$ by many orders of magnitude. The dipole matrix elements can be written:

$$\int \psi_f^* \sum_a e^{i\vec{k}\cdot\vec{r}_a} e_a \vec{r}_a \, \psi_i \prod_a d\vec{r}_a$$

(Spontaneous emission)

The magnetic dipole moment is written: The Intensity are:

$$\frac{(M_1)}{(E_1)} = \left(\frac{\frac{e\hbar}{2mc}}{ea}\right)^2 \sim \left(\frac{v}{c}\right)^2 \sim \left(\frac{a}{\lambda}\right)^2$$

so $M_1$ is less intense than $E_1$.

We write for the dipole moment (electric):

$\vec{P} = e \sum_a r_a$ : $\langle f | \vec{P} | i \rangle$

---

LECTURE XXX  4-24-61

The intense transitions are the electric dipole transitions, and are of the order of $10^6$ greater than the electric quadrupole.

Selections are obtained thru angular momentum symmetry properties. Consider definition of orbital angular momentum:

One particle:

$$L_j = \epsilon_{jkl} \, x_k p_l$$

$$[L_j, x_m] = \epsilon_{jkl} \, x_k \underbrace{[p_l, x_m]}_{-i\hbar\delta_{lm}} = i\hbar \epsilon_{jmk} \, x_k$$

Now for Total: $\vec{L} = \sum_a \vec{L}_a$

$$[M_j, x_{am}] = i\hbar \epsilon_{jmk} \, x_{ak}$$

$$[L_j, x_{am}] = i\hbar \epsilon_{jmk} \, x_{ak}$$

since $\{M_j, M_m\} = i\hbar \epsilon_{jmk} M_k$

Now the angular momentum operator is the generator of infinitesimal rotations, and their results can be expressed by the commutators of these operators with vectors.

Therefore, if $\vec{P} = e \sum_a r_a$, then:

$$[M_j, P_k] = i\hbar \epsilon_{jkl} P_l$$

Recall ladder operators: define similar quantities can be defined for $P$, viz:

$$P_+ = P_x + iP_y \quad ; \quad P_- = P_x - iP_y$$

$$[P_+, M_z] = -\hbar P_+$$

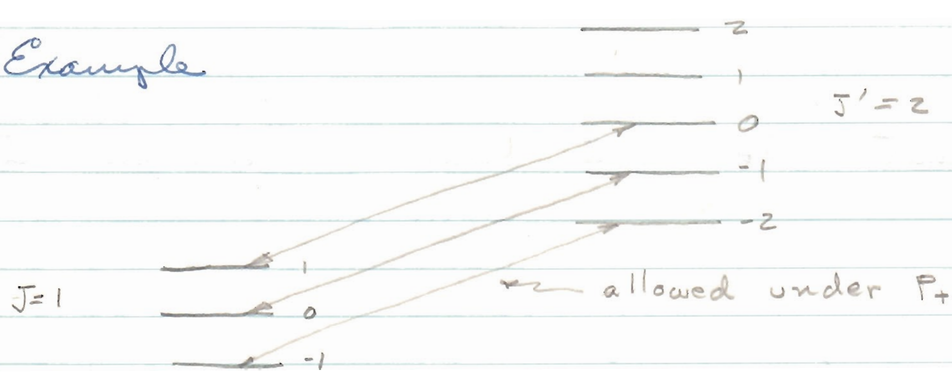
since $P_+ (M_z + \hbar) = M_z P_+$

and: $P_- (M_z - \hbar) = M_z P_-$

suppose a state $\langle M^2, M_z, \gamma' )$, then:

$\langle J, M, \gamma' | P_+ | J', M', \gamma'' \rangle = 0$ unless $M = M' + 1$ } allowed $\Delta M = +1$

Example




For $P_-$ : $\langle J, M, \gamma' | P_- | J', M', \gamma'' \rangle = 0$ unless $M = M' - 1$ } Allowed $\Delta M = -1$

For $P_z$ : $\langle J, M, \gamma' | P_z | J', M', \gamma'' \rangle = 0$ unless $M = M'$ } allowed $\Delta M = 0$

Observe in z direction: $\langle f | P_x + iP_y | i \rangle = \text{constant}\, e^{i\omega t}$

$P_x \propto \cos\omega t$
$P_y \propto -\sin\omega t$

for $P_-$

| Observation | Zeeman Effect | | |
|---|---|---|---|
| $\parallel z$ | ||| | ||| | |
| $\parallel x$ | ||| | ||| | ||| |
| | $\sigma$ | $\pi$ | $\sigma$ |

What about selection rules for J?
Can be extracted from commutation laws but very tedious. Consider:

$$\int \psi^*_{JM\gamma'} P_x \psi_{J'M'\gamma''} \, dr_1 dr_2 \ldots$$

and same for $P_y$ and $P_z$. Write coordinates in terms of spherical harmonics:

$$x = C r \left( Y_1^1 + Y_1^{-1} \right)$$

$$y = C r \left( Y_1^1 - Y_1^{-1} \right)$$

$$z = C' r Y_1^0$$

Thus we see that $P_*$ acts like a wave function with $J=1$, ∴

$$\int \psi^*_{JM\gamma'} P_* \psi_{J'M'\gamma''} \, dr_1 dr_2$$

$$J \qquad 1 \qquad J'$$

From previous discussion on Clebsch-Jordan orthogonization methods, can only step by one, when forming products of wave functions: therefore:

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

$$\text{not } 0 \to 0$$

are the proper selection rules. These are all the rigorous selection rules in angular momentum.

Consider some examples in the lighter atoms where we have R-S coupling:

$^3P_{0,1,2}$

$S=1,\ L=1$


Since electric dipole contains no spin coordinates all ed transitions must be between same spins. Thus all triplets go to triplets, singlets to singlets. However, in heavier atoms, Hg get green line between singlet and triplet. In He, people thought two different substances existed because two separate spectra. Thus the selection rules are:

$$\Delta S = 0\ , \quad \Delta L = \pm 1, 0$$

These break down when no RS coupling, ie, SO coupling too strong.

For one electron case, me is:

$$\int f(r)\, Y_{l'}^{m'*} \times Y_l^m\, g(r)\, r^2\, dr\, d\Omega$$

Recall recurrence formulae:

$$(l+1) P_{l+1} - (2l+1) \cos\theta\, P_l + l P_{l-1} = 0$$

from which we can see: $\Delta l = \pm 1$ as the famous selection rule.

LECTURE XXXI    4-26-61

Recall: $L, S, l$    s-o coupling small.

$\Delta J = \pm 1, 0$ (dipole)

$J = 0 \rightarrow 0$ forbidden (all 1-quantum radiation transmissions)

Recall: initial state $J$: $\psi_i$

dipole operator $D$: $J = 1$

Thus: $\psi_f$ $D$ $\psi_i$ } not allowed for any

$J=0$ $J=1$ $J=0$ } one quantum emission

Usually have intermediate states for multiphoton emission. However do not have this in Schroedinger scheme.

Another kind of selection rule arises from inversion of axes if Hamiltonian is invariant under this operation, that is:

$[H, P] = 0$ which leads to, if $H\psi = E\psi$,

$HP\psi = EP\psi$

since $PP\psi = \psi$, for nondegenerate state, then:

$P\psi = c\psi$ ; $c^2 = 1$, $P\psi = \pm\psi$

or: $P\psi(x,y,z) = \psi(-x,-y,-z) = +\psi(x,y,z)$ even

$-\psi(x,y,z)$ odd

For degenerate states, will get splitting of degeneracy.

$[H,P] = 0$ still holds under magnetic fields because $H$ vectors are vectors of rotation and direction of rotation is not changed by inversion. Not true for $E$ fields. When Zeeman splitting occurs into nondegenerate states, will get states of same parity since they combine and coalesce when magnetic field is removed. The rule is that the same parity goes with all of the terms of the configuration.

That is: parity of configuration = parity of $\sum_a l_a$

The selection rule is that the parity changes in a transition.

$$\int \psi_f^* \, D \, \psi_i \, dr_1 \, dr_2$$
$- \quad - \quad +$

inversion $+ \quad - \quad -$

either the parity changes or the integral is zero. ($a$ —— does not change)

Selection rule is called Laporte's rule.

## Interaction of Electron with Electromagnetic Field

$$\vec{\mathcal{H}} = \nabla \times \vec{A} \quad ; \quad \vec{\mathcal{E}} = -\nabla\varphi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$\vec{F} = e\vec{\mathcal{E}} + e\left[\frac{\vec{v}}{c} \times \vec{\mathcal{H}}\right]$$

$$\mathcal{H}_j = \epsilon_{jkl}\frac{\partial A_l}{\partial x_k}$$

$$F_j = e\mathcal{E}_j + \frac{e}{c}\epsilon_{jkl}\epsilon_{lmn} v_k \frac{\partial A_n}{\partial x_m}$$

$$\epsilon_{jkl}\epsilon_{lmn} = \delta_{mj}\delta_{nk} - \delta_{mk}\delta_{nj}$$

$$\therefore \quad F_j = e\mathcal{E}_j + \frac{e}{c}v_k\frac{\partial A_k}{\partial x_j} - \frac{e}{c}v_k\frac{\partial A_j}{\partial x_k}$$

$$\text{or} \quad F_j = -e\frac{\partial\varphi}{\partial x_j} + \frac{e}{c}v_k\frac{\partial A_k}{\partial x_j} - \frac{e}{c}v_k\frac{\partial A_j}{\partial x_k} - \frac{e}{c}\frac{\partial A_j}{\partial t}$$

$$\text{or} \quad F_j = -e\frac{\partial\varphi}{\partial x_j} + \frac{e}{c}v_k\frac{\partial A_k}{\partial x_j} - \frac{e}{c}\frac{dA_j}{dt} = m\dot{v}_j$$

$$\text{or} \quad \frac{d}{dt}\left(mv_j + \frac{e}{c}A_j\right) = -e\frac{\partial\varphi}{\partial x_j} + \frac{e}{c}v_k\frac{\partial A_k}{\partial x_j}$$

Now $E = \frac{1}{2}mv^2 + e\varphi$

so we call $mv_j + \frac{e}{c}A_j = p_j$ (dynamical momentum)

and write $\vec{v} = \frac{1}{m}(\vec{p} - \frac{e}{c}\vec{A})$

Thus, one is tempted to take for the Hamiltonian:

$$H = \frac{1}{2m} \left| \vec{p} - \frac{e}{c} \vec{A} \right|^2 + e\varphi$$

from the definition of the total energy. Thus, from Hamiltonians equations:

$$\dot{x}_j = \frac{\partial H}{\partial p_j} = \frac{1}{m}\left(p_j - \frac{e}{c} A_j\right)$$

$$\dot{p}_j = -\frac{\partial H}{\partial x_j} = -e\frac{\partial \varphi}{\partial x_j} - \underbrace{\frac{1}{m}\left(p_k - \frac{e}{c} A_k\right)}_{\dot{x}_k}\left(-\frac{e}{c}\frac{\partial A_k}{\partial x_j}\right)$$

which gives previous equation for $\dot{p}_j$.

Now, for QM Hamiltonian, use for dynamical momentum $\frac{\hbar}{i}\frac{\partial}{\partial x_k} = p_k$

$\therefore$

(1) $$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_k} - \frac{e}{c}A_k\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x_k} - \frac{e}{c}A_k\right)\psi + e\varphi\psi$$

$$= -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{ie\hbar}{2mc}\underbrace{\left(\frac{\partial}{\partial x_k}A_k + A_k\frac{\partial}{\partial x_k}\right)}_{\text{symeterized and Hermitean}}\psi + \frac{e^2}{2mc^2}|\vec{A}|^2\psi + e\varphi\psi$$

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## LECTURE XXXII    4-28-61

One symmetry type not covered is Kramer's degeneracy or time-reversal symmetry.
Magnetic Field Continued: Recall above equation;

Gauge Invariance: gauge term comes from attempts to set up unified field theory in terms of length transformations.

We have $\vec{E}$ and $\vec{\mathcal{H}}$ in terms of $\varphi$ and $\vec{A}$ but phenomena (beam experiments) can be explained using only $\vec{E}$ and $\vec{\mathcal{H}}$.

$$\vec{\mathcal{E}} = -\nabla\varphi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$\vec{\mathcal{H}} = \nabla \times \vec{A}$$

Consider some function $\lambda(x,y,z,t)$

$$\varphi' = \varphi - \frac{1}{c}\frac{\partial \lambda}{\partial t} \quad , \quad \vec{A}' = \vec{A} + \nabla\lambda$$

Then $\vec{\mathcal{H}} = \nabla \times \vec{A} = \nabla \times \vec{A}'$

$$\vec{\mathcal{E}} = -\nabla\varphi' - \frac{1}{c}\frac{\partial \vec{A}'}{\partial t}$$

Therefore different potentials give the same fields. The transformation is called a gauge transformation. The gauge transformation for the wave function must be:

$$\psi' = \psi e^{\frac{ie}{\hbar c}\lambda}$$

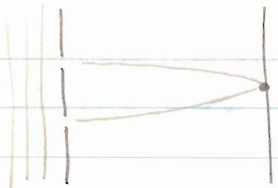
which is $\psi$ modified by a phase factor. These three equations make up the gauge transformation. We then get for the time derivative and the gradient in the Schroedinger equation:

$$\underbrace{-\frac{\hbar}{i}\frac{\partial}{\partial t} - e\varphi}_{KE} \quad ; \quad \underbrace{\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}}_{\vec{\pi}}$$

$\vec{\pi}$ (kinetic momentum)
actual $m\vec{v}$ of particle

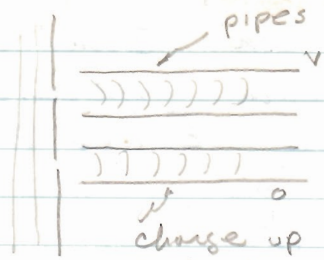
Thus if we add an arbitrary potential energy, we change total energy, but not kinetic energy. Similar to elementary physics experiments illustrating only difference in energy. However, angular momentum would not be conserved in a magnetic field (one of those lesser known facts of physics).

Bohm & Aharonov have shown that interference effects depends on potential.



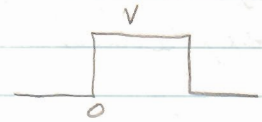
change in $A$
same along
both paths
from time integral

Ordinary

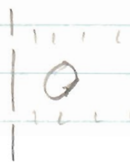



charge up
to high potential
and turn off
while still in pipe

B & A




We have not changed group velocity, however total energy has so that $e^{-Et/\hbar}$ is different for each pipe and waves emerge at different phases. Same thing can happen around a magnetic field.



Line integral of $A$ gives change in phase.

This has almost been observed experimentally and can be shown that it must exist to make quantum theory consistent. Take equation (1) of last lecture:

$\psi^*(1) - \psi(1)^*$ and get: the divergence of a current density, which is gauge invariant:

$$i\hbar \frac{\partial}{\partial t}\psi^*\psi = \nabla\cdot\left\{-\frac{\hbar^2}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) + \frac{ie\hbar}{mc}\vec{A}\,\psi^*\psi\right\}$$

Probability Density: $\rho = \psi^*\psi$

Probability Current: $\vec{J} = -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) - \frac{e}{mc}\vec{A}\,\psi^*\psi$

Don't use any old gauge; use gauge to fit paoblem. Can choose to minimize last term of $\vec{J}$. Take a circular gauge: $\left(\frac{c}{v}\right)\left(\frac{eA}{mc^2}\right)$ : this term is responsible for scattering of soft light.

however, small this term must be considered

Next time describe gauge.

LECTURE XXXIII 5-1-61

Uniform Magnetic Field:

Recall:

$$m\vec{v}\times\vec{r} \longrightarrow \vec{\pi}\times\vec{r}$$
$$(\vec{p}-\tfrac{e}{c}\vec{A})\times\vec{r}$$

Angular momentum is not conserved except in the case when the electron is injected into a circular orbit centered about the nucleus. However, there is a candidate for angular momentum that is conserved which is given by infinitesimal rotations. That is, look for conservation of $\vec{r}\times\vec{p}$. However, $\vec{p}$ is not gauge invariant. We want the Hamiltonian to remain invariant under an infinitesimal rotation thus conserving $\vec{r}\times\vec{p}$. A way to do this is to choose $\vec{\mathcal{H}}$ in the z direction with a circular potential A about the z axis whose strength goes as r. Then $(\vec{r}\times\vec{p})_z$ is conserved and the Hamiltonian remains invariant.

$$|\vec{A}| = Cr \; ; \quad \int \vec{A}\cdot d\vec{s} = Cr\cdot 2\pi r = 2C\,(\text{area}) = \mathcal{H}\,(\text{area})$$

Take: $\vec{A} = -\frac{1}{2}\left[\vec{r}\times\vec{\mathcal{H}}\right]$ or $A_j = \frac{1}{2}\,\epsilon_{j3k}\,x_k\,\mathcal{H}$

$$\vec{\mathcal{H}} = \vec{k}\,\mathcal{H} = \nabla\times\vec{A}$$

$$\mathcal{H}\,\delta_{m3} = \epsilon_{mns}\frac{\partial A_s}{\partial x_n} = \frac{1}{2}\,\epsilon_{mns}\underbrace{\frac{\partial}{\partial x_n}\,\epsilon_{s3k}\,x_k}_{\delta_{kn}}\,\mathcal{H}$$

The interaction terms are:

$$-\frac{e}{2mc}\left(\vec{A}\cdot\vec{p}+\vec{p}\cdot\vec{A}\right) + \frac{e^2}{2mc^2}\,|\vec{A}|^2$$

Neglect last term as it is completely negligible in any field that has ever been produced.

check relative magnitudes:

$$-\frac{e}{4mc}\left\{\underbrace{[\vec{\mathcal{H}}\times\vec{r}]\cdot\vec{p}}_{\vec{\mathcal{H}}\cdot\vec{L}} + \underbrace{\vec{p}\,[\vec{\mathcal{H}}\times\vec{r}]}_{-\vec{p}\cdot\underbrace{[\vec{r}\times\vec{\mathcal{H}}]}_{\vec{L}\cdot\vec{\mathcal{H}}}}\right\}$$

all right to commute x-product since different components are involved

now: $\vec{r}\times\vec{p} = \vec{L}$ ;
and we get:

$$-\frac{e}{2mc}\,\vec{\mathcal{H}}\cdot\vec{L}$$

Take $L \sim \hbar$ so we get: $\frac{e\hbar\mathcal{H}}{mc}$

now $\frac{e^2}{2mc^2}|\vec{A}|^2 \sim \frac{e^2}{mc^2}\mathcal{H}^2\frac{\hbar^4}{m^2e^4}$

and the ratio of the two terms is:

$$\frac{\hbar^3 e\mathcal{H}}{m^2ce^4}$$

now if this ratio is about 1:

$$e\mathcal{H} = \frac{m^2ce^4}{\hbar^3} = \frac{mc^2}{\frac{\hbar}{mc}}\cdot\left(\frac{e^2}{\hbar c}\right)^2$$

or $$\mathcal{H} = \frac{e}{\left(\frac{\hbar}{mc}\right)^2}\frac{e^2}{\hbar c} = \frac{e}{a_0^2}\cdot\frac{1}{\alpha}\ ;\quad \alpha = \frac{1}{137}$$

Thus the field must be of the order of 137 times the field at the Bohr radius of the H atom.
Or:

$$\mathcal{H} \sim \frac{137}{300}\,\frac{25\text{ volts}}{5\cdot 10^{-9}} > 10^9\text{ gauss}\quad\text{since } a_0\mathcal{E} = 25\text{ volts.}$$

so last term can be neglected as far as energy level calculation is concerned, but not susceptibility

Instead of one electron, we write the total interaction energy, including spin, we have:

$$-\frac{e}{2mc}(\vec{\mathcal{H}}\cdot\vec{\mathcal{L}}) - \frac{e}{mc}(\vec{\mathcal{H}}\cdot\vec{\mathcal{S}})$$

($\vec{\mathcal{L}}$ ↑ total)

Since $\vec{\mathcal{L}} = \vec{L}\hbar$ and $\vec{\mathcal{S}} = \vec{S}\hbar$ :

$$\boxed{-\frac{e\hbar}{2mc}\vec{\mathcal{H}}\cdot(\vec{L}+2\vec{S}) = -\frac{e\hbar}{2mc}\vec{\mathcal{H}}\cdot(\vec{J}+\vec{S})}$$

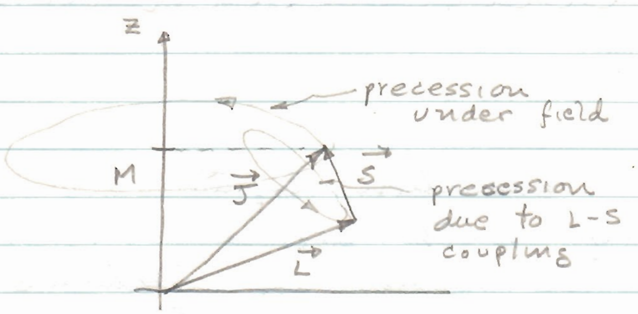
Anomalous Zeeman Effect;

Zeeman splitting << spin-orbit coupling (splitting)

$\vec{\mathcal{H}} = \hat{k}\mathcal{H}$ and we write; using first order perturbation theory:

$$\Delta E = \frac{-e\hbar\mathcal{H}}{2mc}\left(M + \langle S_z\rangle\right)$$

Qualitative Argument:




In semiclassical picture the time average $\langle S_z\rangle$ would be:

$$\langle S_z\rangle = \frac{\vec{S}\cdot\vec{J}}{|\vec{J}|^2}M$$

Thus we anticipate:

$$\Delta E = \frac{-e\hbar\mathcal{H}}{2mc}\underbrace{\left(1+\frac{\vec{S}\cdot\vec{J}}{|\vec{J}|^2}\right)}_{\text{Landé "g" factor}}M$$

How do we do this in QM? Consider:

$$S_z|\vec{J}|^2 = S_z(J_x^2 + J_y^2 + J_z^2)$$

Do algebra to get $\vec{S}\cdot\vec{J}$ part:

$$S_z |\vec{J}|^2 = J_z (S_x J_x + S_y J_y + S_z J_z)$$

$$+ \underbrace{(S_z J_x - J_z S_x)}_{-\gamma_y} J_x + \underbrace{(S_z J_y - J_z S_y)}_{\gamma_x} J_y$$

and recall $\vec{S}$ and $\vec{J}$ commute.

Define a new vector $\vec{\gamma}$ which has the properties:

$$[J_k, \gamma_l] = i\,\epsilon_{klm}\,\gamma_m \quad ; \quad (\vec{J}\cdot\vec{\gamma}) = 0$$

which corresponds to in the one electron atom:

$$[l_m, x_n] = i\,\epsilon_{mns}\,x_s \quad , \quad (\vec{l}\cdot\vec{r}) = 0$$

selection rule: $\Delta l = \pm 1$

However: $\Delta L = \pm 1, 0 \quad ; \quad (\vec{L}\cdot\sum_i \vec{r}_i) \neq 0$

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## LECTURE XXXIV 5-3-61

Reading Period Assignment: Radiation Chapter in Dirac: Concern yourself with second quantitization which will be needed for relativistic treatment of QM. Deals with wave functions as operators which can create and annihilate particles, hence quantization (second).

Magnetic Field:
Recall:

$$\Delta E = -\frac{e\hbar\mathcal{H}}{2\mu c}\langle J_z + S_z\rangle_{\text{diagonal}}$$

We consider L and S to be well enough coupled to form a J.

For classical vectors:

$$\left[ \vec{J} \times [\vec{S} \times \vec{J}] \right]_z = S_z (\vec{J} \cdot \vec{J}) - (\vec{J} \cdot \vec{S}) J_z$$

In QM, must watch commutation: call $\vec{\gamma} = [\vec{S} \times \vec{J}]$
Recall the commutation rule:

$$[J_n, \gamma_r] = i \epsilon_{nrs} \gamma_s$$

$\Delta J = \pm 1$ ; $(\vec{J} \cdot \vec{\gamma}) = 0$ ; $\therefore \Delta J = 0$ not allowed ; $\gamma$ has no diagonal

In one particle system : $[l_n, x_r] = i \epsilon_{nrs} x_s$

$\Delta l = \pm 1$ ; $\Delta l \neq 0$ since $(\vec{l} \cdot \vec{r}) = 0$

$$\Delta E = -\frac{e \hbar H}{2 \mu c} \underbrace{\left\{ 1 + \frac{(\vec{J} \cdot \vec{S})}{|\vec{J}|^2} \right\}}_{\text{Landé } g} M$$

which gives split levels which are $\frac{e \hbar H g}{2 \mu c}$ apart

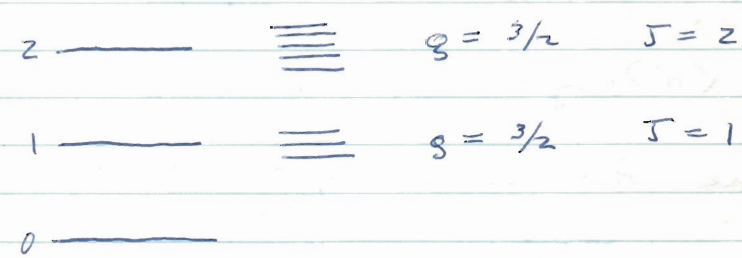
Find: $|\vec{J}|^2$ : $\vec{J} - \vec{S} = \vec{L}$ which leads to:

$$J(J+1) + S(S+1) - 2(J \cdot S) = L(L+1)$$

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

For singlet level: $J = L$, $S = 0$ ; $\therefore g = 1$

For Triplet P: $^3P$



Consider Electrostatic interaction with the spin-orbit coupling:

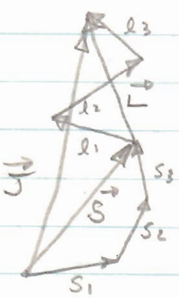
$$H' = \sum_a -\frac{\hbar}{4\mu^2c^2}\,\vec{\sigma}_a \cdot \left[\vec{p} \times \nabla V\right]$$

where $V = V(r)$ ; $\nabla V = \frac{\vec{r}}{r}\frac{dV}{dr}$ , then:

$$H' = \sum_a \frac{\hbar}{4\mu^2c^2}\,\vec{\sigma}_a \cdot (\vec{r} \times \vec{p})\,\frac{1}{r}\frac{dV}{dr}$$

$$= \sum_a \frac{\hbar}{2\mu^2c^2}\,\frac{1}{r}\frac{dV}{dr}\,(\vec{s}_a \cdot \vec{l}_a)$$

where all the s's are tightly coupled together by apparent electrostatic interaction to form S:




We change index from a to i
Then we write:

$$H' = \sum_i a_i\,(s_i \cdot l_i)$$

$$= \sum_i a_i\,(s_{ix} l_{ix} + s_{iy} l_{iy} + s_{iz} l_{iz})$$

Now take diagonal; as in Zeeman effect:

$$(s_{iz})_{diag} = \frac{\vec{s}_i \cdot \vec{S}}{S(S+1)}\,S_z \quad ; \quad (l_{iz})_{diag} = \frac{\vec{l}_i \cdot \vec{L}}{L(L+1)}\,L_z$$

Thus, for the constancy of L and S:

$$\langle H' \rangle_{diag} = A\,(L \cdot S)$$

where $A = \sum_i a_i \frac{\vec{s}_i \cdot \vec{S}}{S(S+1)}\,\frac{\vec{l}_i \cdot \vec{L}}{L(L+1)}$

since $\vec{L} + \vec{S} = \vec{J}$ : $L(L+1) + 2(\vec{L} \cdot \vec{S}) + S(S+1) = J(J+1)$

$$\langle H' \rangle_{diag} = A\,\frac{J(J+1) - L(L+1) - S(S+1)}{2}$$

Compare splitting :

$$(H')_{J,J} - (H')_{J-1,J-1} = A\left[\frac{J(J+1)-(J-1)J}{2}\right] = AJ$$

Called Landé interval rule.

READING NOTES FROM DIRAC'S P. of QM

I. The Principle of Superposition
   A. The need for a quantum theory.
      1. Classical electrodynamics cannot explain remarkable stability of atoms and molecules
      2. Frequencies of atomic spectra not in harmonic relationship but follow Ritz combination law.
      3. Anomalies in the theory of specific heats.
      4. Wave - particle duality of light, and of matter, which illustrates the inadequacy of the concepts of classical mechanics to supply us with a description of atomic events.
      5. On the matter of the act of measurement disturbing the quantities about which information is desired: It is usually assumed that, by being careful, we may cut down the disturbance accompanying our observation to any desired extent. The concepts of big and small are then purely relative and refer to the gentleness of our means of observation as well as to the object being described. In order to give an absolute meaning to size, such as is required for any of the ultimate structure of matter, we have to assume that there is a limit to the fineness of our powers of observation and the smallness of the accompanying disturbance; a limit which is inherent in the nature of things and can never be surpassed by improved technique or increased skill on the part of the observer.
      6. Causality applies only to a system which is left undisturbed, such as classical systems where measurement does not disturb the system. Causal relations are used in Q.M. between the probabilities.

B. The polarization of light.

1. A new set of laws of nature are needed, the most fundamental of which is the Principle of Superposition.
2. When photons are polarized obliquely to the optic axis of a tourmaline crystal, it is found that a fraction $\sin^2\alpha$ go thru.
3. The result of an experiment using one photon at a time will be that sometimes the photon will pass thru the tourmaline retaining its complete quanta or otherwise be absorbed completely. One never finds part of a photon. The emerging photon is polarized ⊥ to the optic axis of the crystal.
4. Questions of how it changes its polarization and whether or not the photon passes thru or not are outside the realm of science.
5. We assume that the state of oblique polarization can be thought of as a superposition of ⊥ and ∥ states, each weighted in a manner to produce the correct angle of polarization. Then, this weight of the ⊥ state could be thought as related to the probability of passing the photon.
6. The effect of making the observation is to force the photon to jump completely into one or the other states, the particular state being governed by probability laws.

C. Interference of photons.

1. When a beam of light is incident on some kind of interferometer, it gets split up into two components which are made to interfere.
2. When the incident beam is one photon, it must go partly into each of the

components into which the original beam was split. Thus we can say that the translational state of the photon is a superposition of the two states in which it should split.

3. We know that fractions of photons never occur, so the act of observation of energy forces the photon completely into either of the two component states, in analogy with the polarization case. In this manner, the photon cannot be made to interfere with itself.

4. The above phenomena is also associated with matter.

D. Superposition and Indeterminacy

1. We must extend the idea of "physical picture" to include any way of looking at the fundamental laws of nature which makes their self-consistency obvious.

2. The complication of indeterminacy in nature is offset by the simplification of the general principle of superposition of states.

3. Definition of state: the state of an atomic system must be specified by fewer data than classically needed because of indeterminacy. The state of a single photon is given by its translational state together with its polarization state. A state of a system may be defined as an undisturbed motion that is restricted by as many conditions or data as are theoretically possible without mutual interference or contradiction. These conditions could be those imposed by some suitable preparation of the system.

4. The General Principle of Superposition of Quantum Mechanics requires us to assume that between the states of any one dynamical system there exist peculiar relationships such that whenever the system is definitely in one state we can

consider it as being partly in each of two or more other states.

5. One cannot in the classical sense picture a system being partly in each of two states and see the equivalence of this to the system being completely in some other state.

6. When a state is formed by the superposition of two other states, it will have properties somewhat vaguely intermediate between the two states.

7. If we say that an observation on a certain state A leads to the certain result a, and on a state B to b, then the result of an observation on a state formed by the superposition of A and B will give sometimes a and sometimes b according to some probability law, and the result will never be different from a or b. The intermediate character of the state formed by superposition thus expresses itself through the probability of a particular result for an observation being intermediate between the corresponding probabilities for the original states, not through the results itself being intermediate between the corresponding results for the original states. This is a drastic departure from the classical ideas of superposition.

8. The assumption of superposition relationships between the states leads to a mathematical theory in which the equations for the unknowns are linear, but is different from the classical case in that the superposition principle of quantum mechanics demands indeterminacy in the results.

E. Mathematical Formulation of the principle.

1. The principle of superposition suggests an additive process among the states of a dynamical system. We now associate mathematical quantities with these states that obey rules of the additive process. We shall take these quantities to be vectors in an infinitely-dimensioned space (vectors added to vectors give vectors).

2. We denote the vector associated with a state by $| \rangle$ and call it a ket. The ket associated with the state A is denoted $|A\rangle$.

3. From superposition:

$$c_1 |A\rangle + c_2 |B\rangle = |R\rangle$$

where $c_1, c_2$ are complex numbers. In general,

$$\int |x\rangle \, dx = |Q\rangle$$

A set of ket vectors are called independent if no one of them can be expressed as a sum of the others

4. The assumption is implicit that each state of a dynamical system at a particular time corresponds to a ket vector, the correspondence being such that if a state results from the superposition of certain other states, its corresponding ket vector is expressible linearly in terms of the corresponding ket vectors of the other states, and conversely.

5. A set of states will be called independent if no one of them is expressible linearly in terms of the others.

6. Since the superposition of the same state should yield the same state;

$$c_1 |A\rangle + c_2 |A\rangle = (c_1 + c_2) |A\rangle$$

thus a state is specified by the direction of a ket and not its magnitude.

7. If the ket vector corresponding to a state is multiplied by any complex number, not zero, the resulting ket will correspond to the same state. There is no distinction between $|A\rangle$ and $-|A\rangle$. This clearly is not classical as the superposition of the same state of a vibrating string leads to a state with higher oscillations.

8. Note that if $c_1$ and $c_2$ are complex numbers only two real numbers characterize the new state as only the ratio of $c_1$ to $c_2$ is important. From two different states, a two-fold infinity of new states is obtained. This is in accordance with the polarization and interference examples.

F. Bra and Ket Vectors.

1. When we have a set of vectors in a mathematical theory, we can construct the dual vectors (for example, $\vec{r}$ and $\vec{k}$ vectors in solid state theory).
2. These new vectors are called <u>bras</u> and denoted by $\langle|$, or, for a particular state B, by $\langle B|$
3. The scalar product of a bra and a ket is denoted by $\langle B|A\rangle$ and is a number.
4. Any complete bracket expression denotes a number and any incomplete bracket expression denotes a vector.
5. A bra vector is defined when its scalar product with every ket vector is given.
6. Also:

$$\{\langle B| + \langle B'|\}|A\rangle = \langle B|A\rangle + \langle B'|A\rangle$$

$$\{c\langle B|\}|A\rangle = c\langle B|A\rangle$$

thus the scalar product of bras and kets satisfy the distributive law of multiplication

7. We make the important assumption that: there is a one-to-one correspondence between the bras and kets, such that the bra corresponding to the ket $|A\rangle + |A'\rangle$ is the sum of the bras corresponding to $|A\rangle$ and $|A'\rangle$, and the bra corresponding to $c|A\rangle$ is $\bar{c}$ times the bra corresponding to $|A\rangle$, $\bar{c}$ being the complex conjugate of $c$.

8. The bra corresponding to $|A\rangle$ is written $\langle A|$.

9. The bra and ket vectors are imaginary quantities as each can be multiplied by complex numbers without having their natures changed. However, they cannot be separated into real and imaginary parts. The usual method of doing this cannot be done since bras and kets cannot be added. However, the relationship between a bra and a ket is such that it is reasonable to say that one is the <u>imaginary conjugate</u> of the other. This is a definition.

10. Any physical state can be specified by the direction of a bra as well as a ket.

11. Given any two kets $|A\rangle$ and $|B\rangle$ we can form a number $\langle B|A\rangle$. We can also form the number $\langle A|B\rangle$. We assume that the following is true: $\langle B|A\rangle = \overline{\langle A|B\rangle}$. If $|A\rangle = |B\rangle$, it is obvious that $\langle A|A\rangle$ is real and we assume that it is greater than zero.

12. If the scalar product of a bra and ket is zero, we say that they are <u>orthogonal</u>

13. We define the length of the bra $|A\rangle$ or the ket $|A\rangle$ as the square root of the positive number $\langle A|A\rangle$. If this number is unity, the vectors are <u>normalized</u>.

14. The vectors are still not completely determined as one can multiply it by the phase factor $e^{i\gamma}$ without changing its length or direction.

# I. Principle of Superposition

Failure of classical mechanics to explain experimental evidence of atomic physics

Limit to experimental accuracy due to absolute size of atomic systems and disturbance of system when performing measurements

Obliquely polarised photon will be completely passed or completely absorbed. Can be thought of as superposition of ⊥ and ∥ states, and observation forces photon to one state or the other

Beam of photons incident on interferometer splits into two beams. Single photon thought of as superposition of these two states. An attempt at observation forces photon into either one of the two states according to probability laws

Principle of superposition asserts that whenever a system is definitely in one state, it may be considered to be partly in each of two or more other states.

Intermediate character of state formed by superposition is manifested as an intermediate probability for one of the particular results.

Ket vectors: $| \rangle$
Superposition of states corresponds to linear combination of corresponding kets, a ket denoting the state of the system

The superposition of identical states yields the same state:
$c_1|A\rangle + c_2|A\rangle = (c_1+c_2)|A\rangle$

Bra vectors: $\langle |$
Defined as duals of kets. The scalar product of a bra and ket, $\langle B|A\rangle$, is a number. Bras and kets are complex imaginaries of each other. ∴ $\langle B|A\rangle = \overline{\langle A|B\rangle}$

If $\langle B|A\rangle = 0$, $|A\rangle \neq |B\rangle$, then $|A\rangle$ and $|B\rangle$ are orthogonal. Also, if $\langle A|A\rangle = 1$, the vectors are normalized.

## II. Dynamical Variables and Observables

### A. Linear Operators

1. If we have a ket $|F\rangle$ which is a <u>linear</u> function of a ket $|A\rangle$, we may think of $|F\rangle$ being formed by the application of a linear operator on $|A\rangle$, viz; $|F\rangle = \alpha |A\rangle$
2. Similarly $\langle F| = \langle A|\alpha$, thus setting the convention for the order of operator and vector.
3. The algebra of linear operators is defined by their operations on vectors of the Hilbert space (bras and kets) and is identical to regular algebra except that the law of multiplicative commutation is not obeyed.
4. As a special kind of operator, consider $|A\rangle\langle B|$ and multiply it on the left by $|P\rangle$: $|A\rangle\langle B|P\rangle$, which is a number times the ket $|A\rangle$, so the application of the linear operator $|A\rangle\langle B|$ onto a ket is to yield a constant times the ket $|A\rangle$. A similar manipulation holds for bras.
5. We assume that the physical significance of linear operators is that they represent the dynamical variables of a system <u>at a given time</u>, just as vectors in the Hilbert space represent states of the system <u>at a given time</u>. Dynamical variables are the variables in terms of which classical mechanics is built.

### B. Conjugate Relations

1. Take the ket which is the complex imaginary of $\langle P|\alpha$. This ket depends antilinearly on $\langle P|$ and thus linearly on $|P\rangle$. We define $\bar{\alpha}$ as the adjoint of $\alpha$ and then $\bar{\alpha}|P\rangle$ is the complex imaginary of $\langle P|\alpha$.

B. 2. It is obvious that $\langle B|\bar{\alpha}|P\rangle = \overline{\langle P|\alpha|A\rangle}$ by considering $\langle B|A\rangle = \overline{\langle A|B\rangle}$ and putting $|A\rangle = \bar{\alpha}|P\rangle$.

3. Also $\langle B|\bar{\bar{\alpha}}|P\rangle = \overline{\langle P|\bar{\alpha}|B\rangle} = \langle B|\alpha|P\rangle$ from which we infer $\bar{\bar{\alpha}} = \alpha$, so that the adjoint of the adjoint is equal to the original linear operator, or it is reasonable to say that taking the adjoint is equivalent to taking the complex conjugate.

4. If a linear operator equals its adjoint, $\alpha = \bar{\alpha}$, it is called <u>self-adjoint</u> or <u>Hermitean</u> and corresponds to a real dynamical variable.

5. Define: $\langle A| = \langle P|\alpha$ , $\langle B| = \langle Q|\bar{\beta}$
so that: $|A\rangle = \bar{\alpha}|P\rangle$ and $|B\rangle = \beta|Q\rangle$
and recall $\langle B|A\rangle = \overline{\langle A|B\rangle}$, then:
$\langle Q|\bar{\beta}\bar{\alpha}|P\rangle = \overline{\langle P|\alpha\beta|Q\rangle} = \langle Q|\overline{\alpha\beta}|P\rangle$
which implies $\bar{\beta}\bar{\alpha} = \overline{\alpha\beta}$. This can be easily generalized to $\bar{\gamma}\bar{\beta}\bar{\alpha}\ldots = \overline{\alpha\beta\gamma\ldots}$
and $\overline{|A\rangle\langle B|} = |B\rangle\langle A|$

6. General Rule: The conjugate complex or the conjugate imaginary of any product of bra vectors, ket vectors, and linear operators is obtained by taking the conjugate complex (conjugate imaginary) of each factor and reversing their order.

7. Theorem: If $\xi$ is a real linear operator and $\xi^m|P\rangle = 0$ for a particular ket $|P\rangle$, $m$ a positive integer, then $\xi|P\rangle = 0$.
Proof: Consider $m = 2$. Then $\langle P|\xi^2|P\rangle = 0$. Because if $\langle A|A\rangle = 0$, $|A\rangle = 0$, we then have $\xi|P\rangle = 0$ and we have the proof for $m = 2$. For $m > 2$, form $\xi^{m-2}|P\rangle = |Q\rangle$ or $\xi^m|P\rangle = \xi^2|Q\rangle = 0$, and, from the proof for $m = 2$, $\xi|Q\rangle = 0$ or $\xi^{m-1}|P\rangle = 0$ and upon repetition we can prove the general case, and arrive eventually at $\xi|P\rangle = 0$

C. Eigenvalues and Eigenvectors.

1. Consider the following effect of the linear operator $\alpha$:

$$\alpha |P\rangle = a |P\rangle$$

where $\alpha$ is known; $|P\rangle$, $a$ are unknown. That is, the effect of the linear operator is merely to lengthen the vector in the Hilbert space. Also, we could have the equation $\langle Q|\alpha = b\langle Q|$.

2. If this equation is satisfied, $a$ is called an <u>eigenvalue</u> of the dynamical variable and $|P\rangle$ is an <u>eigenket</u> of the dynamical variable.

3. If degeneracy is present, we could have several eigenvectors belonging to the same eigenvalue, all of which are independent. A linear combination of the degenerate eigenvectors is another eigenvector belonging to the same eigenvalue.

4. We shall find that Hermitean operators will correspond to observable quantities and will therefore limit ourselves to these. A Hermitean operator will be called $\xi$

5. Some important results:

(i) The eigenvalues are all real numbers.

Form $\langle P|\xi|P\rangle = a\langle P|P\rangle$ from $\xi|P\rangle = a|P\rangle$

Now $\langle P|\xi|P\rangle = \overline{\langle P|\xi|P\rangle}$ and is thus real. Also $\langle P|P\rangle$ is real, therefore $a$ is real.

(ii) The eigenvalues associated to the eigenbras are just the same as those associated with the eigenkets.

(iii) The conjugate imaginary of any eigenket is an eigenbra belonging to the same eigenvalue, and conversely. This makes it possible to call the state corresponding to any eigenvector an <u>eigenstate</u> of the dynamical variable $\xi$.

C. 6. Notation: We denote the eigenvalues of the dynamical variable $\xi$ by $\xi', \xi''$, etc. and $|\xi'\rangle$ as the eigenket belonging to the eigenvalue $\xi'$. If the eigenkets belonging to $\xi'$ are degenerate, we label them by $|\xi'1\rangle$, $|\xi'2\rangle$, $|\xi'3\rangle$, etc.

7. Theorem: Two eigenvectors of a real dynamical variable belonging to different eigenvalues are orthogonal.

Proof: Consider: $\xi|\xi'\rangle = \xi'|\xi'\rangle$

and: $\xi|\xi''\rangle = \xi''|\xi''\rangle$

Form $\langle\xi'|\xi = \xi'\langle\xi'|$ and multiply by $|\xi''\rangle$.

$\langle\xi'|\xi|\xi''\rangle = \xi'\langle\xi'|\xi''\rangle$

Similarly: $\langle\xi'|\xi|\xi''\rangle = \xi''\langle\xi'|\xi''\rangle$

Therefore: $(\xi''-\xi')\langle\xi'|\xi''\rangle = 0$

or $\langle\xi'|\xi''\rangle = 0$, $\xi' \neq \xi''$, QED.

8. Theorem: If $\xi|\xi'\rangle = \xi'|\xi'\rangle$, then any reasonably behaved function of the dynamical variable, say $\phi(\xi)$, satisfies $\phi(\xi)|\xi'\rangle = \phi(\xi')|\xi'\rangle$.

Proof: If $\phi(\xi)$ is well behaved, it can be expanded in a Taylor series analytic in some region about the point c, viz: $\phi(\xi) = \sum_{n=1}^{\infty} a_n(\xi-c)^n$. It is necessary to consider only the nth term $(\xi-c)^n$ which can be expanded by the binomial theorem in powers of $\xi$ such that if we can prove $\xi^n|\xi'\rangle = \xi'^n|\xi'\rangle$, the above theorem is obviously true.

Consider: $\xi^n|\xi'\rangle = \xi^{n-1}\xi|\xi'\rangle = \xi'\xi^{n-1}|\xi'\rangle = \xi'^2\xi^{n-2}|\xi'\rangle = \cdots = \xi'^n|\xi'\rangle$, so the theorem is proved.

D. Observables

1. We now develop a physical interpretation for the mathematics based on the fact that any observable we measure must result in a real number and thus must be represented by a real dynamical variable.

D.2. All the dynamical variables of use in Quantum Mechanics must be Hermitean operators.

3. Assumptions:

(i) If the dynamical system is in an eigenstate of the Hermitean operator $\xi$, belonging to the eigenvalue $\xi'$, then a measurement of $\xi$ will certainly give as a result the number $\xi'$; and conversely.

(ii). If we have two or more eigenstates (degenerate) belonging to the same eigenvalue $\xi'$, then any state formed by superposition of these eigenstates will also be an eigenstate of $\xi'$.

4. From this we can infer that the set of eigenvalues of a real dynamical variable (Hermitean operator) are the possible results of the measurements of the dynamical variable.

5. If a certain $\xi$ is measured with the system in a particular state, the states into which the measurement causes the system to jump into states upon which the original state is dependent (Principle of Superposition) and these states are all eigenstates of the system. We define a complete set of states to be such that any one state depends upon the set of eigenstates of the system — the eigenstates of $\xi$ form a complete set.

6. If the system is not originally in an eigenstate, a measurement will cause it to jump into an eigenstate which will be the observation of the measurement. Subsequent measurements will yield the same eigenstate.

7. A real dynamical variable whose eigenstates do not form a complete set is a quantity that cannot be measured.

D. 8. The condition that $\xi$ be an <u>observable</u> is that the eigenkets of $\xi$ can be used to express any arbitrary ket; that is:

$$|P\rangle = \int |\xi' c\rangle \, d\xi' + \sum_r |\xi^r d\rangle$$

where the $\int$ is over the range of continuous eigenvalues and the sum is over selected eigenvalues in the continuous range plus any discrete range outside the continuous range, the c and d being labels used to distinguish the eigenvalues when they are equal. Evidently the eigenkets above must contain their own multiplicative constants explicitly.

9. Sometimes a quantity can be considered an observable although it cannot be proved because of the difficulty of finding the eigenvalues and eigenstates of the system.

E. Functions of Observables

1. Dirac defines a function of an operator in terms of the eigenvalue equation;
$f(\xi)|\xi'\rangle = f(\xi')|\xi'\rangle$
immediately without resort to power series.

2. It is obvious from the proof given before that $\overline{f(\xi)}\,|\xi'\rangle = \bar{f}(\xi')|\xi'\rangle$ since $\xi'$ is real if $\xi$ is an observable.

3. Also, the following is evident from the above expansion:

$$\langle \xi''|\overline{f(\xi)}|P\rangle = \bar{f}(\xi'')\langle \xi''|P\rangle = \int \bar{f}(\xi')\langle \xi''|\xi' c\rangle \, d\xi'$$

$$+ \sum_r \bar{f}(\xi'')\langle \xi''|\xi^r d\rangle = \int \bar{f}(\xi'')\langle \xi''|\xi' c\rangle + \bar{f}(\xi'')\langle \xi''|\xi'' d\rangle$$

However, $\langle \xi''|\bar{f}(\xi)|P\rangle = \langle \xi''|\overline{f(\xi)}|P\rangle$ from which we infer $\overline{f(\xi)} = \bar{f}(\xi)$ which should be as $\xi$ is a real linear operator.

E. 4. If $f(\xi')$ is real, it follows that $f(\xi)$ is an observable.

5. We are able to give a meaning to any function $f$ of an observable, provided only that the domain of existence of the function of a real variable $f(x)$ includes all the eigenvalues of the observable. Also, the function must be single-valued so that the inverse exists, that is, so that $\xi$ is a function of $f(\xi)$.

6. All of the above statements apply equally well to functions of an observable operating on bras as well as kets.

F. The General Physical Interpretation

1. Theorem: If the measurement of the observable $\xi$ for the system in the state corresponding to $|x\rangle$ is made a large number of times, the average of all the results obtained will be $\langle x|\xi|x\rangle$, provided $|x\rangle$ is normalized. If $|x\rangle$ is not normalized, then $\langle x|\xi|x\rangle$ is proportional to the mean value of $\xi$.

2. The observable $\xi$ will have a defined value for a state if it is an eigenvalue of the state. Otherwise, we can only talk about its average value.

3. If the observable is $\xi$, we can talk about mean values of $f(\xi)$, viz, $\langle x|f(\xi)|x\rangle$. Consider the function $\delta_{\xi a}$ where $a$ is some real number. Then $\langle x|\delta_{\xi a}|x\rangle = P_a$ which is the probability of $\xi$ having the value $a$. If $a$ is not an eigenvalue of $\xi$, $\delta_{\xi a}$ times any eigenket of $\xi$ is zero, since the result of the measurement of an observable must be one of its eigenvalues.

4. If the possible results of a measurement of $\xi$ form a continuous range, then

we can only talk about $\xi$ having a value in the range $a$ and $a+da$. We denote the required function to give us this probability be $\chi(\xi)$. Then $P(a)\,da = \langle x|\chi(\xi)|x\rangle$. Statements (3) and (4) imply:

$\delta_{\xi a}|\xi'\rangle = 0$ unless $\xi = a$ (discrete)

and $\chi(\xi)|\xi'\rangle = 0$ unless $\xi$ is in $da$ (continuous)

5. Continuous eigenstates are not realizable in practice.

G. Commutability and Compatibility

1. If a state is simultaneously an eigenstate of two observables, that is,

$$\xi|A\rangle = \xi'|A\rangle$$
$$\eta|A\rangle = \eta'|A\rangle$$

then it is easily shown that $\xi\eta - \eta\xi = 0$ or that the observables commute. This idea of simultaneous eigenstates can be extended to more than two observables in general.

2. It can be shown that if a set of observables do commute, there exists so many simultaneous eigenstates that they form a complete set.

3. We also can define $f(\xi, \eta, \zeta)$ where $\xi, \eta, \zeta$ are commuting observables such that: $f(\xi, \eta, \zeta, \ldots)|\xi', \eta', \zeta', \ldots\rangle = f(\xi', \eta', \zeta', \ldots)|\xi', \eta', \zeta', \ldots\rangle$.

4. We can also generalize the definition for a state to have a given value for an observable to:

$$P_{abc\ldots} = \langle x|\delta_{\xi a}\,\delta_{\eta b}\,\delta_{\zeta c}\ldots|x\rangle$$

5. The importance of this section lies in the fact that: one can give a meaning to several commuting observables having values at the same time. The observations are then said to be compatible. Thus any two or more commuting observables can be counted as one observable, the resulting measurement giving two or more numbers. Example: Energy, angular momentum and linear momentum in H-case.

## III. Representations

### A. Basic Vectors:

We have been working with bra and ket vectors in Hilbert space which represent the various states of a dynamical system. To solve practicle problems and to advanse the theory, we must introduce a representation in which to work. This is analogous to the coordinate components of an ordinary vector in 3-dimensional space.

This is usualy done by choosing a system of basis vectors and taking the components of a general vector as the scalar product of the vector with each one of the basis vectors. Thus we take as basic vectors in Hilbert space a set (complete) of bras (basic bras) and the representation (components) of a general ket as the scalar product of this ket with each of the bras in turn.

The representatives may be either numbers as they would be if both the basic bras and the general ket represented eigenstates of the same dynamical variable, or, they could be functions of the labels of the basic bras as they would be if the bras were the eigenbras of the displacement dynamical variable and the ket was an eigenket belonging to the Hamiltonian operator.

Theorem: If $\xi_1, \xi_2, \ldots \xi_u$ are any set of commuting observables, we can set up an orthogonal representation in which the basic bras are simultaneous eigenbras of $\xi_1, \xi_2, \ldots \xi_u$.

An example of a set of commuting observables are $H, L^2, L_z$ of the central field problem. There is only one simultaneous eigenket for each set of eigenvalues for this problem. The theorem, however, can be extended to the degenerate case.

If the eigenvectors forming the basis vectors form a complete orthogonal set, we can normalize them to unit length. This is only possible if the eigenvalues that label them are of a discreet nature. If the eigenvalues are continuous, the basis vectors will be of infinite length. This brings us to the $\delta$ function.

B. The $\delta$ Function:

The $\delta$ function performs essentially the same operation in an integral that the Kronecker delta performs in a sum. It only has meaning when used in a sum.

C. Properties of the Basic Vectors:

If we have given the observable $\xi$ which forms by itself a commuting set, and has discrete eigenvalues $\xi'$, then we have a complete set of orthonormal basis vectors with the following properties:

$$\langle \xi' | \xi'' \rangle = \delta_{\xi'\xi''}$$

Recalling the function that the Kronecker $\delta$ performs in a sum, we can construct:

$$\sum_{\xi''} | \xi'' \rangle \delta_{\xi''\xi'} = | \xi' \rangle = \sum_{\xi''} | \xi'' \rangle \langle \xi'' | \xi' \rangle$$

hence we can think of $\sum_{\xi'} | \xi' \rangle \langle \xi' |$ as the unit operator. If we apply the unit operator on an arbitrary ket $| P \rangle$ we have:

$$| P \rangle = \sum_{\xi'} | \xi' \rangle \langle \xi' | P \rangle$$

thus giving the important result that any arbitrary ket can be expanded in terms of the basic kets.

D. The Representation of Linear Operators:

If we have the observable $\xi$, forming a complete commuting set with itself, and another operator $\alpha$, in general not commuting with $\xi$, we can form the number: $\langle \xi'' | \alpha | \xi' \rangle$. We see that this can be arranged according to its eigenvalues in an infinite square matrix. If we have $\alpha$ real, then $\langle \xi'' | \alpha | \xi' \rangle = \overline{\langle \xi' | \alpha | \xi'' \rangle}$ and the matrix is Hermitian. If $\alpha = \xi$, the matrix is obviously diagonal. If we consider the matrix of the product of two operators, we have:

$$\langle \xi'' | \alpha\beta | \xi' \rangle = \langle \xi'' | \alpha \sum_{\xi'''} | \xi''' \rangle \langle \xi''' | \beta | \xi' \rangle$$

$$= \sum_{\xi'''} \langle \xi'' | \alpha | \xi''' \rangle \langle \xi''' | \beta | \xi' \rangle$$

The notion of matrices is even continued to the case where $\xi''$, $\xi'$ are continuous eiginvalues using integration and the Dirac $\delta$ function. All matrices of linear operators are subject to the same algebraic laws as the linear operators themselves. The extension of this idea to bras (basic) as row matrices and basic kets as columns is obvious. These will be unit columns and rows. The elements of the rows and columns of and bra or ket will be the components of the vectors.

PURE AND MIXED STATES    Kemble, p. 320

We hold that we can prepare an ensemble of identical systems such that their statistical properties can be described by a quantum mechanical wave function or a vector in the Hilbert space. It necessarily follows that it is possible to unite the systems of two or more ensembles into a single superensemble. The constituent ensembles are said to represent pure states since their statistical properties are given by a wave function (or point in Hilbert space). If the constituent ensembles are all in the same state, the resulting superensemble is also a pure state. However, if the ensembles differ, the resulting superensemble represents a mixed state.

All information that can be known about the constituent ensembles is assumed to be known, hence this is why they are said to be pure states. All the systems in the pure state ensembles are in the same state which is another reason why they are pure state ensembles.

Let us take two pure state ensembles A and B with $N_A$ systems in A and $N_B$ systems in B. The quantities:

$$w_A = \frac{N_A}{N_A + N_B} \quad ; \quad w_B = \frac{N_B}{N_A + N_B}$$

are the wieghts of A and B in any superensemble composed of them. Let $W_A$ be the probability of an event in A and $W_B$ be the probability of the same event in B. Since the systems of A and B are independent of each other, the probability of the event in the superensemble is the sum of the probabilities of the events in the sub-ensembles:

$$W_{A+B} = w_A W_A + w_B W_B$$

The expectation value of a dynamical variable $\alpha$ in a pure state ensemble is $\langle \xi' | \alpha | \xi' \rangle$. The expectation value of this same dynamical variable in the superensemble follows the usual statistical laws governing probability distributions and averages. Therefore, it follows that in general:

$$Exp(\alpha) = \bar{\alpha} = \sum_{\xi'} w_{\xi'} \langle \xi' | \alpha | \xi' \rangle$$

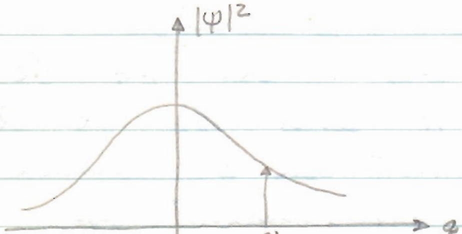
This was shown in lecture. It was also shown that a mixed state cannot be represented by a wave function.

Further Thoughts on Quantum Statistical Mechanics:

We begin with the Born interpretation of the Schroedinger wave function, namely, that:

$|\psi_{\xi'}(q)|^2$ is a probability density function for the configuration of the system. We consider that $\xi'$ labels the state to which the sub-ensemble belongs and that the state of the sub-ensemble is represented by the ket $|\xi'\rangle$ which we assume to be expressible in terms of a complete set of basic kets $|q'\rangle$.

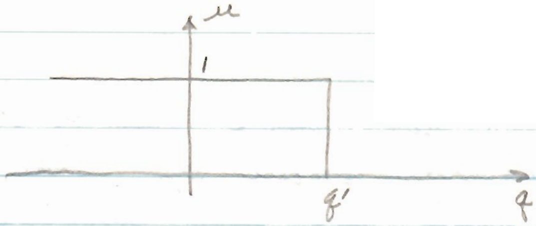
Although $q$ is the configuration space of the sub-ensemble, we denote the probability distribution function in one dimension for simplicity.




In probability theory, we can talk about the probability of obtaining a value less than a given value. In this case, the probability of the sub-system having a given configuration less than $q'$ is:

$$P(q < q') = \int_{-\infty}^{q'} |\psi_{\xi'}(q)|^2 \, dq$$

By defining the unit step function $u(q-q')$ as:




Then: $$P(q<q') = \int_{-\infty}^{\infty} \psi_{\xi'}^{*}(q)\, u(q-q')\, \psi_{\xi'}(q)\, dq$$

$$= \langle \xi' | u(q-q') | \xi' \rangle$$

Now, the probability for the super-ensemble formed by a collection of the above sub-ensembles to have a configuration $q<q'$ is the sum of the weighted probabilities of each sub-ensemble to have a configuration $q<q'$. Another way to say this is to say that the probability of the sub-ensembles to have the same configuration is the sum of their probabilities (wieghted and independent) as follows from statistical independence. That is:

$$P_T(q<q') = \sum_{\xi'} w_{\xi'} \langle \xi' | u(q-q') | \xi' \rangle \quad , \quad \sum_{\xi'} w_{\xi'} = 1$$

Expand $|\xi'\rangle$ in terms of a complete set of suitable basis functions $|\eta'\rangle$:

$$|\xi'\rangle = \sum_{\eta'} |\eta'\rangle\langle\eta'|\xi'\rangle \quad \text{and} \quad \langle\xi'| = \sum_{\eta''} \langle\xi'|\eta''\rangle\langle\eta''|$$

Then:

$$P_T(q<q') = \sum_{\eta'\eta''\xi'} \langle\eta'|\xi'\rangle\, w_{\xi'}\, \langle\xi'|\eta''\rangle\langle\eta''| u(q-q') |\eta'\rangle$$

$$= \sum_{\eta'\eta''} \langle\eta'| \left\{ \sum_{\xi'} w_{\xi'} |\xi'\rangle\langle\xi'| \right\} |\eta''\rangle\langle\eta''| u(q-q') |\eta'\rangle$$

$$= \sum_{\eta'} \langle\eta'| \left\{ \sum_{\xi'} w_{\xi'} |\xi'\rangle\langle\xi'| \right\} u(q-q') |\eta'\rangle = \mathrm{Tr}\left\{ \rho\, u(q-q') \right\}$$

We thus define as the <u>density matrix operator</u>:

$$\rho = \sum_{\xi'} w_{\xi'} |\xi'\rangle\langle\xi'|$$

On closer inspection, what we have really done is to find the expectation value of the unit step function. Thus we can generalize immediately to the expectation value of any dynamical variable:

$$\bar{\alpha} = Exp(\alpha) = Tr(\rho\alpha) = Tr(\alpha\rho)$$

We should expect to find $Tr\,\rho = 1$ and indeed this is the case upon setting $\alpha = 1$:

$$Tr\,\rho = \sum_{\eta'} \langle\eta'| \left\{ \sum_{\xi'} w_{\xi'} |\xi'\rangle\langle\xi'| \right\} |\eta'\rangle$$

$$= \sum_{\eta'\xi'} w_{\xi'} \langle\eta'|\xi'\rangle\langle\xi'|\eta'\rangle = \sum_{\xi'} w_{\xi'} = 1$$

## RESUME' OF CLASSICAL MECHANICS

We shall show that the following holds in expressing Newton's second law for a simple non-relativistic system.

(1) $$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \qquad (i = 1, 2, 3, \cdots f)$$

where $L(q_i, \dot{q}_i) = T - V$ and is called the Lagrangian of the system. The $q_i$ are generalized coordinates and stand for a coordinate in the configuration space of the system.

If the $q_i$ are cartesian components, then:

(2) $$L = \frac{1}{2}\sum_j M_j \dot{q}_j^2 - V$$

and if $q_i = x$ (one dimensional):

(3) $$M\ddot{x} = -\frac{\partial V}{\partial x} = F_x$$

if $V$ is a conservative force field.

It is easy to see that the following relations hold:

(4) $$p_i = \frac{\partial L}{\partial \dot{q}_i} \qquad\qquad \dot{p}_i = \frac{\partial L}{\partial q_i}$$

These are the Lagrangian equations of motion.

We can form $2f$ first order differential equations by defining the so-called Hamiltonian:

(5) $$H(p_i, q_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$$

If we take the total differential of the Hamiltonian function:

(6) $$dH = \sum_i \left\{ \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q_i} dq_i \right\}$$

$$= \sum_i \left\{ \left[ \dot{q}_i - \frac{\partial L}{\partial p_i} \right] dp_i + \left[ \underbrace{\frac{\partial}{\partial q_i}(p_i \dot{q}_i)}_{p_i \frac{\partial \dot{q}_i}{\partial q_i}} - \frac{\partial L}{\partial q_i} \right] dq_i \right\}$$

$$= \sum_i \left\{ \left[ \dot{q}_i \, dp_i + p_i \, d\dot{q}_i \right] - \left[ \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i \right] \right\}$$

using the fact that:

$$\frac{\partial L(q_i, \dot{q}_i)}{\partial p_i} dp_i = \left\{ \frac{\partial L}{\partial q_i} \underset{0}{\underset{\parallel}{\frac{\partial q_i}{\partial p_i}}} + \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial p_i} \right\} dp_i$$

$$= \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i$$

From the Lagrangian equation $p_i = \frac{\partial L}{\partial \dot{q}_i}$:

$$dH = \sum_i \left\{ \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q_i} dq_i \right\}$$

$$= \sum_i \left\{ \dot{q}_i \, dp_i - \dot{p}_i \, dq_i \right\}$$

using $\dot{p}_i = \frac{\partial L}{\partial q_i}$. We see immediately:

(7) $$\boxed{\dot{q}_i = \frac{\partial H}{\partial p_i}} \qquad \boxed{\dot{p}_i = -\frac{\partial H}{\partial q_i}}$$

which are called the Hamiltonian equations of motion.

For simple, conservative, non-relativistic systems, we can write the Hamiltonian as:

(8) $$H = T + V = \sum_i \frac{p_i^2}{2m_i} + V$$

# Physics 251b : Final Exams

1957 – 1958

① a. Prove that the quantum number $j$ for the total angular momentum can have only integral or half-integral values.

b. Show further that if the system is composed of spinless particles the half integral values cannot occur.

② State the asymptotic form of the wave function as used in 3-D problems of scattering by a fixed center of force. In terms of the scattering amplitude, state the formula for the differential cross-section, and from it derive two different expressions for the total cross-section.

③ Use time-dependent perturbation theory to obtain the first-order probability for transition between two discrete states. Explain how this result is used to establish the formula for the Einstein B coefficient in terms of the matrix element.

④ A system has $j=1$. Measurement of the angular momentum component $m'\hbar$ along the $z'$ axis has given the value $m'=1$. The component $m\hbar$ along the $z$ axis is now measured. Calculate the probabilities for the different values of $m$ as functions of the angle $\theta$ between the $z$ and $z'$ axis, and check against results naturally expected for $\theta = 0, \pi/2, \pi$. (Take $Oz'$ in the $xz$ plane. Work in representation with $M_z = m\hbar$ diagonal. Find one-column matrix $\langle m|m'=1\rangle$ as eigenvector of operator $M_{z'}$).

(5) Two partial systems have angular momentum quantum numbers $j_1 = j_2 = 2$ and wave functions $u_{m_1}$, $v_{m_2}$. Find the wave function of the combined systems for $j=1, m=0$. (Use fact that this is an eigenfunction of the operator $|\vec{M}_1 + \vec{M}_2|^2$; express this operator in terms of $j_1$, $j_2$, $m_1$, $m_2$, and ladder operators.).

(6) What is meant by an antisymmetric wave function? Show how to antisymmetrize an arbitrary function, and give the special formula that results when the given function is a product of single-electron functions. Describe the way two widely separated energy levels arise from the configuration 1s2s of the helium atom.

(7) Explain the meaning of "pure state", and "mixed state", giving formulas for probabilities and for expectation values. Define the statistical matrix, and show how it is used to calculate expectation values. State and prove an important theorem about any mixed state in which all the weights are equal.

1954-1955

(1) Write the Schroedinger equation for an electron in an electromagnetic field. Explain what is meant by gauge invariance; write a general gauge transformation of the potentials and the corresponding transformation of the wave function $\psi$. Derive the form of the probability current vector; show that it is a gauge-invariant quantity.

② Phase Integral 4 Last year

③ State the asymptotic form of the wave function as used in 3-D scattering problems; identify the quantity "scattering amplitude": state two different formulas for the total cross-section in terms of the scattering amplitude. Apply both formulas in the case of a scattering amplitude given in terms of phase shifts,

$$f(\theta) = (ik)^{-1} \sum_l (l+\tfrac{1}{2})\,(e^{2i\delta_l} - 1)\,P_l(\cos\theta)$$

and show they give the same result.

④ A system with $j = 3/2$ has been found to have magnetic quantum number $m$ with respect to the $z$ axis. Find the probabilities of the various results $m'$, if a new measurement is made using the $x$-axis instead of the $z$-axis: (a) For $m = \frac{3}{2}$; (b) for $m = 1/2$.

⑤ Two systems treated separately have angular momentum quantum numbers $j_1 = j_2 = \frac{3}{2}$; write $u_{m_1}$ for the wave function of the first system, $v_{m_2}$ for those of the second. What values are possible for the resultant quantum numbers $j, m$ of the two systems taken together? Determine all the wave functions $\psi_{j,m}$ in terms of the products $u_{m_1} v_{m_2}$. (For this case with $j_1 = j_2$, symmetry is of particular assistance in compiling and checking the results.)

(6) Discuss the use of antisymmetric wave functions for electrons:
(a) in connection with Pauli's exclusion principle and the periodic table; and also
(b) with particular attention to the location of the terms of the normal helium atom (He I), and the dependence of the energy of a term on its multiplicity.

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1953 - 1954

(1)
(2)
(3)
(4)
} Questions covered last semester or not covered now.

(5) Compute all the normalized wave functions $\varphi_{j,m}$ in terms of the normalized product functions $\psi_{m_1} \chi_{m_2}$ for $j_1 = 1$, $j_2 = 1$.

(6) Tabulate the possible values of $M_L$ and $M_S$ and determine the spectral terms that exist for the configuration $(nd)^2$.

(7) Explain the meaning of "pure state" and "mixed states", giving formulas for probabilities and for expectation values. Same as (7) in 1957 - 1958.

Due 15th

# Physics 251b Problems, 1961

1. Apply the transformation function $(\vec{r}'|\vec{p}')$ to calculate $(\vec{p}'|x|\vec{p}'')$ from $(\vec{r}'|x|\vec{r}'') = x'\delta(\vec{r}' - \vec{r}'')$.

2. Show that the trace (sum of diagonal elements) of the matrix of an observable is independent of representation, i.e., that

$$\sum_{\xi'}(\xi'|F|\xi') = \sum_{\eta'}(\eta'|F|\eta');$$

and that this sum is equal to the sum of the characteristic values F', weighted by their degeneracies (multiplicities).

3. Show that if F anticommutes with one of the complete set of observables $\xi$, i.e., if $F\xi_i + \xi_i F = 0$, with $\xi = (\xi_1, \ldots \xi_i, \ldots \xi_f)$ then

$$(\xi'|F|\xi'') = 0 \text{ unless } \xi_i' = -\xi_i''$$

4. Consider a set of m states $\Phi_{\xi ak}$, k = 1, ... m and a set of m states $\Phi_{\eta ak}$, k = 1, ... m related to the first set by a unitary transformation,

$$\Phi_{\eta ak} = \sum_{j=1}^{m} \Phi_{\xi aj}\,(\xi^{aj}|\eta^{ak})$$

Consider also a set of n states $\Phi_{\xi bk}$, k = 1, ... n, and another set of n states $\Phi_{\eta bk}$, k = 1, ... n, related to it by a unitary transformation. Show that

$$\sum_{i=1}^{m}\sum_{j=1}^{n} |(\xi^{ai}|F|\xi^{bj})|^2 = \sum_{i=1}^{m}\sum_{j=1}^{n} |(\eta^{ai}|F|\eta^{bj})|^2$$

('Principle of Spectroscopic Stability')

Assignment # 1
Problems 1–4

Paul Grant
DEAP – AP – 1G
P 251 b
3 – 12 – 61

3

1\. (1) Given: $\langle r'|x|r''\rangle = x'\,\delta(r'-r'')$ with the transformation functions $\langle r'|p'\rangle$ and $\langle p'|r'\rangle$

(2) Using the rules of fluency and matrix element multiplication, knowing that $r$ and $p$ have continuous eigenvalues, we can form the matrix element:

$$\langle p'|x|p''\rangle = \iint \langle p'|r'\rangle dr' \langle r'|x|r''\rangle dr'' \langle r''|p''\rangle$$

$$= \iint x'\langle p'|r'\rangle dr'\ \delta(r'-r'')\ dr''\ \langle r''|p''\rangle$$

$$= x' \int \langle p'|r'\rangle dr' \langle r'|p''\rangle \quad = \quad x'\langle p'|p''\rangle$$ X

You can't take $x'$ out from $\int dx'dy'dz'$ !!

(3) Now the following argument was given in lecture:

$\psi(r) \rightarrow \langle r'|\rangle$ ; $\psi(r) = \frac{1}{h^{3/2}}\int e^{ip\cdot r/\hbar}\ \varphi(p)\ dp$

$\varphi(p) \rightarrow \langle p'|\rangle$ : $\varphi(p) = 1/h^{3/2}\int e^{-ip\cdot r/\hbar}\ \psi(r)\ dr$

$\langle r'|\rangle = \int \langle r'|p'\rangle dp' \langle p'|\rangle$ ; $\therefore$ $\langle r'|p'\rangle = e^{ip'\cdot r'/\hbar}\cdot h^{-3/2}$

$\langle p'|\rangle = \int \langle p'|r'\rangle dr' \langle r'|\rangle$ ; $\therefore$ $\langle p'|r'\rangle = e^{-ip'\cdot r'/\hbar}\cdot h^{-3/2}$

$$\langle p'|p''\rangle = \int \langle p'|r'\rangle dr' \langle r'|p''\rangle$$

$$= \frac{1}{h^3}\int e^{i(p''-p')\cdot r'/\hbar}\ dr'$$

Let: $r' = \hbar s'$, $dr' = \hbar^3 ds'$

$$\therefore \langle p'|p''\rangle = \frac{1}{(2\pi)^3}\int e^{i(p''-p')\cdot s'}\ ds'$$

Now this is a definition of the Dirac $\delta$ function, therefore:

$$\langle p'|p''\rangle = \delta(p''-p') = \delta(p'-p'')$$

(4) $\therefore$ $\langle p'|x|p''\rangle = x'\,\delta(p'-p'')$ X

2. (1) We are given the matrix elements $\langle \xi' | F | \xi'' \rangle$ of the observable $F$. Consider the transformation of the trace of the $F$ matrix to some new representation, say that of $|\eta'\rangle$, defined by the transformation functions $\langle \eta' | \xi' \rangle$ and $\langle \xi' | \eta' \rangle$; and that $\delta_{\eta'\eta''} = \langle \eta' | \eta'' \rangle$:

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$$\text{Tr}\,F = \sum_{\xi'} \langle \xi' | F | \xi' \rangle = \sum_{\xi'\eta'\eta''} \langle \xi' | \eta' \rangle \langle \eta' | F | \eta'' \rangle \langle \eta'' | \xi' \rangle$$

$$= \sum_{\xi'\eta'\eta''} \langle \eta'' | \xi' \rangle \langle \xi' | \eta' \rangle \langle \eta' | F | \eta'' \rangle = \sum_{\eta'\eta''} \langle \eta'' | \eta' \rangle \langle \eta' | F | \eta'' \rangle$$

$$= \sum_{\eta'\eta''} \delta_{\eta''\eta'} \langle \eta' | F | \eta'' \rangle = \sum_{\eta'} \langle \eta' | F | \eta' \rangle$$

✓

so that the trace is invariant under an orthonormal transformation.

(2) Since $F$ is an observable, we can find its eigenvalues via the eigenvalue equation:

$$F | F' n_{F'} \rangle = F' | F' n_{F'} \rangle \quad , \quad \langle F' n_{F'} | F' n_{F'} \rangle = 1$$

where $|F' n_{F'}\rangle$ is an eigenket of $F$, the $n_{F'}$ indicating the <u>index</u> of degeneracy associated with the eigenvalue $F'$. Now, the observable $F$ can always be brought onto diagonal form by a principle axis transformation, which here would mean the use of the transformation function $\langle \xi' | F' n_{F'} \rangle$. Therefore, using the methods above:

$$\text{Tr}\,F = \sum_{\xi'} \langle \xi' | F | \xi' \rangle = \sum_{F'} \sum_{n_{F'}=1}^{g_{F'}} \langle F' n_{F'} | F | F' n_{F'} \rangle$$

where $g_{F'}$ indicates the <u>degree</u> of degeneracy associated with the eigenvalue $F'$. Now:

$$\text{Tr}\,F = \sum_{F'} \sum_{n_{F'}=1}^{g_{F'}} \langle F' n_{F'} | F' n_{F'} \rangle F' = \sum_{F'} \sum_{n_{F'}=1}^{g_{F'}} F'$$

$$= \sum_{F'} g_{F'} F' \quad , \quad \text{QED.}$$

✓

Assignment # 1
Continued

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3 - 12 - 61

3. (1) Given: A complete set of commuting observables

$$|\xi'\rangle = |\xi_1' \cdots \xi_i' \cdots \xi_f'\rangle$$

and that $F\xi_i + \xi_i F = 0$

(2) $\xi_i |\xi'\rangle = \xi_i' |\xi'\rangle$

$$\langle \xi' | \xi'' \rangle = \langle \xi_1' \cdots \xi_i' \cdots \xi_f' | \xi_1'' \cdots \xi_i'' \cdots \xi_f'' \rangle = \delta_{\xi_1''\xi_1'} \cdots \delta_{\xi_i''\xi_i'} \cdots \delta_{\xi_f''\xi_f'}$$

$= \delta_{\xi'\xi''}$ (Definition to make notation shorter)

(3) Consider the matrix element:

$$\langle \xi' | F\xi_i + \xi_i F | \xi'' \rangle = \langle \xi' | F\xi_i | \xi'' \rangle + \langle \xi' | \xi_i F | \xi'' \rangle = 0$$

Then; by matrix element multiplication:

$$\langle \xi' | F\xi_i + \xi_i F | \xi'' \rangle = \sum_{\xi'''} \{ \langle \xi' | F | \xi''' \rangle \langle \xi''' | \xi_i | \xi'' \rangle$$

$$+ \langle \xi' | \xi_i | \xi''' \rangle \langle \xi''' | F | \xi'' \rangle \}$$

$$= \sum_{\xi'''} \{ \langle \xi' | F | \xi''' \rangle \xi_i'' \delta_{\xi'''\xi''} + \xi_i''' \delta_{\xi'\xi'''} \langle \xi''' | F | \xi'' \rangle \}$$

$$= \langle \xi' | F | \xi'' \rangle \xi_i'' + \xi_i' \langle \xi' | F | \xi'' \rangle = 0$$

(4) $\therefore \quad (\xi_i'' + \xi_i') \langle \xi' | F | \xi'' \rangle = 0$

or $\langle \xi' | F | \xi'' \rangle = 0 \quad , \quad \xi_i'' \neq -\xi_i'$

5 4. (1) Given: two sets of $m$ states; $|\xi^{ak}\rangle, |\eta^{ak}\rangle$; $k = 1, 2, \dots m$, connected with each other by a unitary transformation:

No! Only true if states are complete!

$$|\eta^{ak}\rangle = \sum_{j=1}^{m} |\xi^{aj}\rangle\langle\xi^{aj}|\eta^{ak}\rangle$$

Also, two sets of $n$ states; $|\xi^{bk}\rangle, |\eta^{bk}\rangle$; $k = 1, 2, \dots n$, connected with each other by a unitary transformation:

$$|\eta^{bk}\rangle = \sum_{j=1}^{n} |\xi^{bj}\rangle\langle\xi^{bj}|\eta^{bk}\rangle$$

(2) Therefore, from (1) and the fact that the transformations are unitary:

$$\sum_{j=1}^{m} |\xi^{aj}\rangle\langle\xi^{aj}| = \sum_{j=1}^{m} |\eta^{aj}\rangle\langle\eta^{aj}| = \sum_{j=1}^{n} |\xi^{bj}\rangle\langle\xi^{bj}|$$

$$= \sum_{j=1}^{n} |\eta^{bj}\rangle\langle\eta^{bj}| = 1$$

(3) In what follows, we use fluency and matrix element multiplication. Consider the quantity:

$$\sum_{l=1}^{m}\sum_{j=1}^{n} |\langle\eta^{al}|F|\eta^{bj}\rangle|^2.$$ Now invoke equations (2):

(4)
$$\sum_{l=1}^{m}\sum_{j=1}^{n} |\langle\eta^{al}|F|\eta^{bj}\rangle|^2 = \sum_{l=1}^{m}\sum_{j=1}^{n} \langle\eta^{al}|F|\eta^{bj}\rangle\langle\eta^{bj}|F|\eta^{al}\rangle$$

$$= \sum_{l=1}^{m}\sum_{j=1}^{n}\sum_{p=1}^{m}\sum_{r=1}^{n}\sum_{s=1}^{n}\sum_{t=1}^{m} \Big\{ \langle\eta^{al}|\xi^{ap}\rangle\langle\xi^{ap}|F|\xi^{br}\rangle\langle\xi^{br}|\eta^{bj}\rangle\langle\eta^{bj}|\xi^{bs}\rangle \langle\xi^{bs}|F|\xi^{at}\rangle\langle\xi^{at}|\eta^{al}\rangle \Big\}$$

$$= \sum_{p=1}^{m}\sum_{r=1}^{n}\sum_{s=1}^{n}\sum_{t=1}^{m} \Big\{ \langle\xi^{at}|\xi^{ap}\rangle\langle\xi^{ap}|F|\xi^{br}\rangle\langle\xi^{br}|\xi^{bs}\rangle\langle\xi^{bs}|F|\xi^{at}\rangle \Big\}$$

$$= \sum_{p=1}^{m}\sum_{s=1}^{n} \Big\{ \langle\xi^{ap}|F|\xi^{bs}\rangle\langle\xi^{bs}|F|\xi^{ap}\rangle \Big\} = \sum_{p=1}^{m}\sum_{s=1}^{n} |\langle\xi^{ap}|F|\xi^{bs}\rangle|^2$$

$$= \sum_{l=1}^{m}\sum_{j=1}^{n} |\langle\xi^{al}|F|\xi^{bj}\rangle|^2$$, just changing the index of summation.

(5) $\therefore$
$$\sum_{l=1}^{m}\sum_{j=1}^{n} |\langle\eta^{al}|F|\eta^{bj}\rangle|^2 = \sum_{l=1}^{m}\sum_{j=1}^{n} |\langle\xi^{al}|F|\xi^{bj}\rangle|^2$$, QED.

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5. Show that when the method of partial waves is used, the formula

$$\sigma = \frac{4\pi}{k} \operatorname{Im} \big(f(0)\big)$$

gives the same result as was obtained in lecture by integrating the differential cross-section.

6. Show that f(0) is purely real in the first-order Born approximation, for a static force-field V(r). Obtain the result

$$\sigma = \frac{m^2}{\pi\hbar^4} \iint d\vec{r}\, d\vec{r}\,'\; V(r)V(r'). \;\frac{\sin^2 k\,|\vec{r}-\vec{r}\,'|}{k^2\,|\vec{r}-\vec{r}\,'|^2}$$

(a) by integrating the differential cross-section of the first-order Born approximation; Average over all directions of scatterings

(b) by using the second order of the Born approximation to calculate Im $\big(f(0)\big)$. Average over all directions of incidence.

7. For the case

$$V = 0,\; r > r_0; \quad V = V_0,\; r < r_0$$

$$|V_0| \ll E, \quad kr_0 \ll 1$$

calculate the total cross-section (a) by the method of partial waves; (b) by the Born approximation.

Average $= \frac{1}{4\pi}\int d\Omega \ldots$

$\sigma$ same for all directions since $V(r)$ spherically symmetric.

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5. Review of the Method of Partial Waves:

(1) $\psi \approx e^{ikz} + f(\vartheta)\dfrac{e^{ik\cdot r}}{r}$ ; $\psi \approx \psi_{free}(z) + f(\vartheta)\,\psi_{free}(r)$

(2) Consider the potential field of the scatterer to be spherically symmetric; $V(r)$, and that it fall off rapidly with r such that at some distance $r_0$, $V = 0$ for $r > r_0$. We can then write the asymptotic wave of (1) as a combination of the wave functions of the central field problem:

$$\psi = \sum_l B_l\, P_l(\cos\vartheta)\,\frac{v_l(r)}{r}$$

where $v_l(0) = 0$ ; $v_l'' + \left[k^2 - \dfrac{2mV}{\hbar^2} - \dfrac{l(l+1)}{r^2}\right] v_l = 0$

(3) For $\psi_{free}(z)$, a similar expansion holds:

$$\psi_{free}(z) = \sum_l c_l\, P_l(\cos\vartheta)\,\frac{u_l}{r}$$

where $u_l(0) = 0$, $u_l'' + \left(k^2 - \dfrac{l(l+1)}{r^2}\right) u_l = 0$ ; $k^2 = \dfrac{2mE}{\hbar^2}$

(4) $f(\vartheta)$ can be expanded in the Legendre orthogonal functions:

$$f(\vartheta) = \sum_l a_l\, P_l(\cos\vartheta)$$

(5) $\therefore$ $\displaystyle\sum_l B_l\, P_l(\cos\vartheta)\,\frac{v_l(r)}{r} = \sum_l c_l\, P_l(\cos\vartheta)\,\frac{u_l}{r}$

$$+ \sum_l a_l\, P_l(\cos\vartheta)\,\frac{e^{ik\cdot r}}{r}$$

(6) For $r \gg r_0$, $kr \gg l$ and the wave equations become:

$$v_l'' + k^2 v_l = 0 \quad : \quad v_l \sim \sin(kr + \epsilon_l + \delta_l)$$
$$u_l'' + k^2 u_l = 0 \quad : \quad u_l \sim \sin(kr + \epsilon_l)$$

where the phase factors $\epsilon_l$, $\delta_l$ are chosen so as to make $u_l(0)$, $v_l(0) = 0$.

(7) $\displaystyle\sum_l B_l\, P_l \left\{ \frac{e^{i(k\cdot r + \epsilon_l + \delta_l)} - e^{-i(k\cdot r + \epsilon_l + \delta_l)}}{2ir} \right\}$

$$= \sum_l c_l\, P_l \left\{ \frac{e^{i(k\cdot r + \epsilon_l)} - e^{-i(k\cdot r + \epsilon_l)}}{2ir} \right\}$$

$$+ \sum_l a_l\, P_l\, \frac{e^{ik\cdot r}}{r}$$

(8) Equating coefficients:

$$B_\ell = C_\ell e^{i\delta_\ell}$$

$$\frac{B_\ell e^{i(\epsilon_\ell+\delta_\ell)}}{2i} = \frac{C_\ell e^{i\epsilon_\ell}}{2i} + a_\ell$$

or $$\frac{C_\ell}{2i} e^{i(\epsilon_\ell+2\delta_\ell)} = \frac{C_\ell}{2i} e^{i\epsilon_\ell} + a_\ell$$

or $$a_\ell = C_\ell e^{i\epsilon_\ell} \frac{(e^{i2\delta_\ell}-1)}{2i} = C_\ell e^{i(\epsilon_\ell+\delta_\ell)} \sin\delta_\ell$$

(9) Now: $$\sum_\ell C_\ell P_\ell(\cos\vartheta) \frac{\sin(k\cdot r+\epsilon_\ell)}{r} = e^{ikr\cos\vartheta}$$

in the limit of $r \gg r_0$.

Using the orthogonality of Legendre functions:

$$C_\ell \frac{2}{2\ell+1} \frac{\sin(k\cdot r+\epsilon_\ell)}{r} = \int_{-1}^{1} e^{ikr\mu} P_\ell(\mu)\, d\mu$$

(10) $$\int_{-1}^{1} e^{ikr\mu} P_\ell(\mu)\, d\mu = \frac{1}{ikr}\left[e^{ikr\mu} P_\ell(\mu)\right]_{-1}^{1}$$

$$- \frac{1}{ikr}\int_{-1}^{1} e^{ikr\mu} P_\ell'(\mu)\, d\mu$$

$$= \frac{1}{ikr}\left[e^{ikr\mu} P_\ell(\mu)\right]_{-1}^{1} - \frac{1}{ikr}\left\{\frac{1}{ikr}\left[e^{ikr\mu} P_\ell'(\mu)\right]_{-1}^{1}\right.$$

$$\left. - \frac{1}{ikr}\int_{-1}^{1} e^{ikr\mu} P_\ell''(\mu)\, d\mu\right\}$$

Consider the identities: $P_\ell(-\mu) = (-1)^\ell P_\ell(\mu)$ ; $P_\ell(1) = 1$, $P_\ell'(\pm1) = 0$

$$\therefore \int_{-1}^{1} e^{ikr\mu} P_\ell(\mu)\, d\mu = \frac{1}{ikr}\left[e^{ikr\mu} P_\ell(\mu)\right]_{-1}^{1} = \frac{1}{ikr}\left[e^{ikr} - (-1)^\ell e^{-ikr}\right]$$

(11) $$C_\ell \sin(k\cdot r+\epsilon_\ell) = \frac{2\ell+1}{2ik}\left[e^{ikr} - (-1)^\ell e^{-ikr}\right]$$

$$= \frac{2\ell+1}{k}\begin{cases} \sin kr & \ell \text{ even} \\ \dfrac{\cos kr}{i} & \ell \text{ odd}\end{cases}$$

$$\therefore C_\ell = \frac{2\ell+1}{k}, \quad \ell \text{ even}, \quad \epsilon_\ell = 0$$

$$= \frac{2\ell+1}{ik}, \quad \ell \text{ odd}, \quad \epsilon_\ell = \pi/2$$

Then: $$C_\ell = \frac{2\ell+1}{k}(i)^\ell, \quad \epsilon_\ell = -\ell\pi/2$$

(12)

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(12) $\therefore \quad f(\vartheta) = \sum_l \frac{2l+1}{k} (i)^l \, e^{i(\delta_l - l\pi/2)} \sin\delta_l \; P_l(\cos\vartheta)$

$= \frac{1}{k} \sum_l (2l+1) \, e^{i\delta_l} \sin\delta_l \; P_l(\cos\vartheta)$

(13) $\sigma = \int \sigma(\vartheta) \, d\Omega = \int \sigma(\vartheta) \sin\vartheta \, d\vartheta \, d\varphi$

$= 2\pi \int f^*(\vartheta) f(\vartheta) \sin\vartheta \, d\vartheta = 2\pi \int_{-1}^{1} f^*(\mu) f(\mu) \, d\mu$

(14) $f^*(\mu) f(\mu) = \frac{1}{k^2} \sum_{ll'} (2l+1)(2l'+1) \, e^{i\delta_l} e^{-i\delta_{l'}} \sin\delta_l \sin\delta_{l'}$

$\cdot \; P_l(\mu) \, P_{l'}(\mu)$

Now $\int_{-1}^{1} P_l(\mu) P_{l'}(\mu) \, d\mu = \frac{2}{2l+1} \delta_{ll'}$

(15) $\therefore \quad \sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l$

(16) Now this same result can be had using the formula:

$\sigma = \frac{4\pi}{k} \, \mathrm{Im}\{f(0)\} = \frac{4\pi}{k} \, \mathrm{Im}\{ f(\vartheta)|_{\vartheta=0} \}$

(17) $f(0) = \frac{1}{k} \sum_l (2l+1) \, e^{i\delta_l} \sin\delta_l \; \underbrace{P_l(1)}_{1}$

(18) $\mathrm{Im}\, f(0) = \mathrm{Im} \left\{ \frac{1}{k} \sum_l (2l+1) (\cos\delta_l + i\sin\delta_l) \sin\delta_l \right\}$

$= \frac{1}{k} \sum_l (2l+1) \sin^2\delta_l$

(19) $\therefore \quad \sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l$ , as before.

✓

6. Review of Born Approximation:

(1) Scatterer; $H(q)\,u_m(q) = W_m\,u_m(q)$

$u_m(q)$ are the scatterer eigenfunctions, $W_m$ its eigenvalues, and $H(q)$ its Hamiltonian.

(2) Particle: assumed traveling with incident energy
$$T = \frac{\hbar^2 k_0^2}{2m}, \quad w_0 = e^{i\bar{k}_0\cdot\bar{r}}$$

$\therefore\ H_0 w_0 = T w_0$ or $\nabla^2 w_0 + k_0^2 w_0 = 0$

or: $\left\{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + k_0^2\right\} w_0 = 0$; $w_0 = e^{ik_{0x}x}e^{ik_{0y}y}e^{ik_{0z}z}$
$= e^{i\bar{k}_0\cdot\bar{r}}$ ; $k_0^2 = k_{0x}^2 + k_{0y}^2 + k_{0z}^2$

(3) Interaction Perturbation: $V(r,q)$

(4) The unperturbed wave function for the total system is taken as the product of the separate system wave functions:

$$u^{(0)} = e^{i\bar{k}_0\cdot\bar{r}}\,u_n(q),$$ where $n$ is the initial state of the scatterer.

(5) The total unperturbed wave equation is:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + H(q) - (W_n + T)\right\} u^{(0)} = 0$$

(6) We make the usual perturbation expansion of the complete wave function:

$$u = u^{(0)} + u^{(1)} + u^{(2)} + \cdots + u^{(\alpha)} + \cdots$$

We consider the perturbation $V(\bar{r},q)$ as a first order effect

(7) Then, to the first order:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + H(q) - (W_n + T)\right\} u^{(1)} = -V(r,q)\,u^{(0)}$$

or, to the $\alpha$ th order:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + H(q) - (W_n + T)\right\} u^{(\alpha)} = -V(r,q)\,u^{(\alpha-1)}$$

(8) Consider the $u^{(\alpha)}$ expanded in terms of the scatter wave functions:

$$u^{(\alpha)} = \sum_m v_m^{(\alpha)}(\bar{r})\,u_m(q)$$

Note that energy is conserved, viz, $W_m + T =$ constant

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(9) Definition: $\frac{2m}{\hbar^2}(W_n - W_m + T) \equiv k_{nm}^2$

Then:

$$\sum_m \left\{ \nabla^2 + k_{nm}^2 \right\} v_m^{(\alpha)}(\bar{r})\, u_m(q) = \frac{2m}{\hbar^2} V(\bar{r},q) \sum_m v_m^{(\alpha-1)}(\bar{r})\, u_m(q)$$

(10) Using the orthonormality of the $u_m$:

$$\left\{ \nabla^2 + k_{nm}^2 \right\} v_m^{(\alpha)}(\bar{r}) = \frac{2m}{\hbar^2} \sum_m v_m^{(\alpha-1)}(\bar{r}) \int u_m^*(q)\, V(r,q)\, u_n(q)\, dq$$

(11) Define the RHS of (10) as $h(r)$, then:

$$\left\{ \nabla^2 + k_{nm}^2 \right\} v^{(\alpha)}(\bar{r}) = h(\bar{r})$$

(12) We construct the solution through the use of Fourier transforms and the appropriate Green's function:

$$\bar{f}(\xi,\eta,\zeta) = \bar{f}(\bar{\rho}) = \iiint e^{-i(\xi x + \eta y + \zeta z)} f(x,y,z)\, dx\, dy\, dz$$

$$= \int e^{-i\bar{\rho}\cdot\bar{r}} f(\bar{r})\, d^3\bar{r}$$

$$f(x,y,z) = \frac{1}{8\pi^3} \iiint e^{i(\xi x + \eta y + \zeta z)} \bar{f}(\xi,\eta,\zeta)\, d\xi\, d\eta\, d\zeta$$

$$\text{or} \quad f(\bar{r}) = \frac{1}{8\pi^3} \int e^{i\bar{\rho}\cdot\bar{r}} \bar{f}(\bar{\rho})\, d^3\bar{\rho}$$

Transforming (11):

$$\bar{v}^{(\alpha)}(\bar{\rho}) = \frac{-\bar{h}(\xi,\eta,\zeta)}{\xi^2+\eta^2+\zeta^2 - k_{nm}^2} = \frac{-\bar{h}(\bar{\rho})}{\rho^2 - k_{nm}^2}$$

$$\therefore \quad v^{(\alpha)}(\bar{r}) = \frac{-1}{8\pi^3} \int \frac{e^{i\bar{\rho}\cdot\bar{r}}\, \bar{h}(\bar{\rho})}{\rho^2 - k_{nm}^2}\, d^3\bar{\rho}$$

$$= -\frac{1}{8\pi^3} \int \frac{e^{i\bar{\rho}\cdot(\bar{r}-\bar{r}')}}{\rho^2 - k_{nm}^2}\, d^3\bar{\rho} \int h(\bar{r}')\, d^3\bar{r}'$$

(13)
$$\int \frac{e^{i\bar{\rho}\cdot(\bar{r}-\bar{r}')}}{\rho^2 - k_{nm}^2}\, d^3\bar{\rho} = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \frac{e^{i\bar{\rho}\cdot(\bar{r}-\bar{r}')}}{\rho^2 - k_{nm}^2}\, d\rho\, \rho^2 \sin\varphi\, d\varphi\, d\theta$$

$$= -2\pi \int_0^{\pi}\int_0^{\infty} \frac{e^{i\rho|\bar{r}-\bar{r}'|\cos\varphi}}{\rho^2 - k_{nm}^2}\, \rho^2\, d\rho\, d(\cos\varphi)$$

$$= \frac{4\pi}{|\bar{r}-\bar{r}'|} \int_0^{\infty} \frac{\sin \rho|\bar{r}-\bar{r}'|}{\rho^2 - k_{nm}^2}\, \rho\, d\rho$$

(14) $$\int_0^\infty \frac{\sin \rho|\bar{r}-\bar{r}'|}{\rho^2 - k_{nm}^2}\,\rho\, d\rho = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\sin\rho|\bar{r}-\bar{r}'|\,\rho\, d\rho}{\rho^2 - k_{nm}^2}$$

$$\frac{\rho}{(\rho+k)(\rho-k)} = \frac{1/2}{\rho+k} + \frac{1/2}{\rho-k}$$

$$\therefore \int_0^\infty \frac{\sin\rho|\bar{r}-\bar{r}'|}{\rho^2-k_{nm}^2}\,\rho\, d\rho = \frac{1}{4}\left\{ \underset{①}{\int_{-\infty}^{\infty}\frac{\sin\rho|\bar{r}-\bar{r}'|\,d\rho}{\rho+k}} + \underset{②}{\int_{-\infty}^{\infty}\frac{\sin\rho|\bar{r}-\bar{r}'|\,d\rho}{\rho-k}} \right\}$$

① 



$$\int_{-\infty}^{\infty}\frac{e^{i\rho|\bar{r}-\bar{r}'|}}{\rho+k}\,d\rho$$
$$= i\pi\, e^{-ik|\bar{r}-\bar{r}'|}$$
$$= i\pi\,(\cos k|\,| - i\sin k|\,|)$$
$$① = \pi\cos k|\bar{r}-\bar{r}'|$$

② 

$$\int_{-\infty}^{\infty}\frac{e^{-i\rho|\bar{r}-\bar{r}'|}}{\rho-k}\,d\rho$$
$$= -i\pi\, e^{-ik|\bar{r}-\bar{r}'|}$$
$$= -i\pi\,(\cos k|\,| - i\sin k|\,|)$$
$$② = \pi\cos k|\bar{r}-\bar{r}'|$$

(15) $$\therefore \int \frac{e^{i\bar{\rho}\cdot(\bar{r}-\bar{r}')}}{\rho^2-k_{nm}^2}\,d^3\bar{\rho} = \frac{1}{2}\pi\cos k_{nm}|\bar{r}-\bar{r}'| \cdot \frac{4\pi}{|\bar{r}-\bar{r}'|} = \frac{2\pi^2\cos k_{nm}|\bar{r}-\bar{r}'|}{|\bar{r}-\bar{r}'|}$$

(16) Because we are interested only in the scattered wave, we throw out the negative exponential part of the cosine and obtain:

$$\int \frac{e^{i\bar{\rho}\cdot(\bar{r}-\bar{r}')}}{\rho^2-k_{nm}^2}\,d^3\bar{\rho} = 2\pi^2\,\frac{e^{ik_{nm}|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|}$$

as the appropriate Green's function.

(17) $$\therefore\ v^{(\alpha)}(\bar{r}) = -\frac{1}{4\pi}\int d\bar{r}'\, h(\bar{r}')\,\frac{e^{ik_{nm}|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|}$$

where $$h(\bar{r}) = \frac{2m}{\hbar^2}\sum_m v_m^{(\alpha-1)}(\bar{r})\int u_m^*(q)\,V(r,q)\,u_n(q)\,dq$$

(18) Now, if $V(\bar{r},q)$ depends only on $\bar{r}$, we have from the orthonormality of the $u_m$:

$$h(\bar{r}) = \frac{2m}{\hbar^2}\,V(r)\,v_n^{(\alpha-1)}(\bar{r})$$

and $$v_m^{(\alpha)}(\bar{r}) = -\frac{2m}{4\pi\hbar^2}\int d\bar{r}'\,V(r')\,v_n^{(\alpha-1)}(\bar{r}')\,\frac{e^{ik_n|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|}$$

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Problem 6
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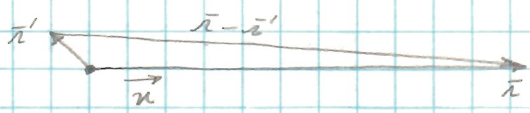
a. (1) In the first-order Born approximation:

$$v_n^{(\alpha-1)}(\bar{r}) = v^{(0)}(\bar{r}) = e^{i\bar{k}_0\cdot\bar{r}}$$

$$\therefore \quad v_n^{(1)}(\bar{r}) = -\frac{2m}{4\pi\hbar^2}\int d\bar{r}'\, V(\bar{r}')\, e^{i\bar{k}_0\cdot\bar{r}'}\,\frac{e^{ik_n|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|}$$

(2) We assume that $V(\bar{r}')$ falls off rapidly at large $\bar{r}'$ so that the contribution in this region is negligible. Therefore we have the situation:




$$\therefore \quad |\bar{r}-\bar{r}'| \simeq r - \bar{r}'\cdot\bar{n}$$

Neglecting $\bar{r}'\cdot\bar{n}$ in the denominator where it contributes less than in the exponential:

$$v_n^{(1)}(r) = \frac{-2m}{4\pi\hbar^2}\,\frac{e^{ik_n r}}{r}\int d\bar{r}'\, V(\bar{r}')\, e^{i(\bar{k}_0 - k\bar{n})\cdot\bar{r}'}$$

(3) The total wave is of the form:

$$\psi \sim u^{(0)} + u^{(1)} = e^{i\bar{k}_0\cdot r}\,u_n(\xi) + f_{el}\,\frac{e^{ikr}}{r}\,u_n(\xi)$$

so we see that the elastic scattering amplitude is:

$$f_{el}(\vartheta) = \frac{-2m}{4\pi\hbar^2}\int d\bar{r}'\, V(r')\, e^{i(\bar{k}_0-\bar{k})\cdot r'}$$

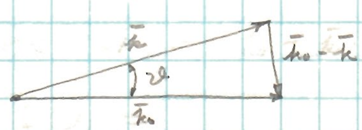
$$= \frac{2m}{4\pi\hbar^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} dr'\, r'^2\, d(\cos\vartheta)\, d\varphi\, V(r')\, e^{i|\bar{k}_0-\bar{k}|r\cos\vartheta}$$

$$= \frac{2m}{2\hbar^2}\int_0^{\infty} dr'\, r'^2\, V(r')\int_1^{-1} e^{i|\bar{k}_0-\bar{k}|r\mu}\, d\mu$$

$$= \frac{-2m}{\hbar^2|\bar{k}_0-\bar{k}|}\int_0^{\infty} dr'\, r'\, V(r')\, \sin|\bar{k}_0-\bar{k}|r'$$

Everything in the integrand is real, therefore the integral is real, and therefore $f_{el}$ is real.

(4)




$$|\bar{k}_0-\bar{k}| = 2k\sin\tfrac{1}{2}\vartheta$$

(5) ∴ $f_{el}(\vartheta) = -\frac{2m}{\hbar^2}\int_0^\infty dr'\, r'^2\, V(r')\, \frac{\sin\{2kr'\sin\frac{1}{2}\vartheta\}}{\{2kr'\sin\frac{1}{2}\vartheta\}}$

∴ $f_{el}(0) = -\frac{2m}{\hbar^2}\int_0^\infty dr'\, r'^2\, V(r')$

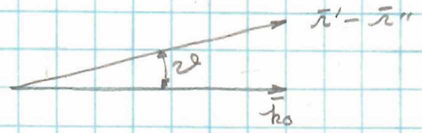
which is obviously real.

(6) Consider: $f_{el} = -\frac{2m}{4\pi\hbar^2}\int d\bar{r}'\, V(r')\, e^{i(\bar{k}_0-\bar{k})\cdot\bar{r}'}$

$f_{el}^* = \frac{-2m}{4\pi\hbar^2}\int d\bar{r}''\, V(r'')\, e^{-i(\bar{k}_0-\bar{k})\cdot\bar{r}''}$

$|f_{el}(\vartheta)|^2 = \frac{m^2}{4\pi^2\hbar^4}\iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, e^{i(\bar{k}_0-\bar{k})\cdot(\bar{r}'-\bar{r}'')}$

(7) Now average over all directions of incidence:




This can be done since all directions of incidence are equivalent due to $V(r)$

Thus we consider: $\frac{1}{4\pi}\int e^{i\bar{k}_0\cdot(\bar{r}'-\bar{r}'')}\, d\Omega$

$= -\frac{2\pi}{4\pi}\int_0^\pi e^{ik_0|\bar{r}'-\bar{r}''|\cos\vartheta}\, d(\cos\vartheta) = \frac{\sin k_0|\bar{r}'-\bar{r}''|}{k_0|\bar{r}'-\bar{r}''|}$

(8) $\sigma = \int |f_{el}(\vartheta)|^2_{av}\, d\Omega = -\frac{m^2}{2\pi\hbar^4}\iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, \frac{\sin k_0|\bar{r}'-\bar{r}''|}{k_0|\bar{r}'-\bar{r}''|}$

$\cdot\int_0^\pi e^{-ik|\bar{r}'-\bar{r}''|\cos\vartheta}\, d(\cos\vartheta)$

Now: $-\int_1^{-1} e^{-ik|\bar{r}'-\bar{r}''|\mu}\, d\mu = \int_{-1}^{1} e^{-ik|\bar{r}'-\bar{r}''|\mu}\, d\mu$

$= 2\,\frac{\sin k|\bar{r}'-\bar{r}''|}{k|\bar{r}'-\bar{r}''|}$

But since the scattering is elastic: $|\bar{k}_0| = |\bar{k}|$

Thus:

(9) $\sigma = \frac{m^2}{\pi\hbar^4}\iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, \frac{\sin^2 k|\bar{r}'-\bar{r}''|}{k^2|\bar{r}'-\bar{r}''|^2}$

ASSIGNMENT #2
Continued

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Problem 6
Continued

b. (1) Recall from lecture for elastic scattering:

$$\psi \sim e^{ikz} u_n(q) + f(\theta) \frac{e^{ikr}}{r} u_n(q)$$

Now proceed to the second order:

$$\psi \sim u^{(0)} + u^{(1)} + u^{(2)}$$

$$u^{(2)} = \sum_m v_m^{(2)}(r)\, u_m(q)$$

(2) From equation (18):

$$v_n^{(2)}(\bar{r}) = \frac{-2m}{4\pi\hbar^2} \int d\bar{r}'\, V(r')\, v_n^{(1)}(\bar{r}') \frac{e^{ik|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|}$$

$$v_n^{(1)}(\bar{r}) = \frac{-2m}{4\pi\hbar^2} \int d\bar{r}''\, V(r'')\, e^{i\bar{k}_0\cdot\bar{r}''} \frac{e^{ik|\bar{r}'-\bar{r}''|}}{|\bar{r}'-\bar{r}''|}$$

(3) $\therefore$ $$v_n^{(2)}(\bar{r}) = \frac{m^2}{4\pi^2\hbar^4} \iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, e^{i\bar{k}_0\cdot\bar{r}''} \frac{e^{ik|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|} \frac{e^{ik|\bar{r}'-\bar{r}''|}}{|\bar{r}'-\bar{r}''|}$$

(4) Making the same assumption about $|\bar{r}-\bar{r}'|$ as in a. (2), we have:

$$v_n^{(2)}(\bar{r}) = \frac{e^{ikr}}{r} \cdot \frac{m^2}{4\pi^2\hbar^2} \iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, e^{i\bar{k}_0\cdot\bar{r}''}\, e^{-i\bar{k}\cdot\bar{r}'} \frac{e^{ik|\bar{r}'-\bar{r}''|}}{|\bar{r}'-\bar{r}''|}$$

(5) $\therefore$ $$f(\theta) = \frac{m^2}{4\pi^2\hbar^4} \iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, e^{i(\bar{k}_0\cdot\bar{r}'' - \bar{k}\cdot\bar{r}')} \frac{e^{ik|\bar{r}'-\bar{r}''|}}{|\bar{r}'-\bar{r}''|}$$

(6) Now for $\theta = 0$, the scattered wave is in the same direction as the incident wave, e.i., $\bar{k}_0 = \bar{k}$.

$$\therefore f(0) = \frac{m^2}{4\pi^2\hbar^4} \iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'')\, e^{i\bar{k}_0\cdot(\bar{r}''-\bar{r}')} \frac{e^{ik|\bar{r}'-\bar{r}''|}}{|\bar{r}'-\bar{r}''|}$$

(7) Averaging over all directions of incidence (equivalent due to $V(r)$):

$$\frac{1}{4\pi} \int e^{-i\bar{k}_0\cdot(\bar{r}'-\bar{r}'')}\, d\Omega = \frac{1}{2} \int_{-1}^{1} e^{-ik_0|\bar{r}'-\bar{r}''|\mu}\, d\mu$$

$$= \frac{\sin k_0|\bar{r}'-\bar{r}''|}{k_0|\bar{r}'-\bar{r}''|} = \frac{\sin k|\bar{r}'-\bar{r}''|}{k|\bar{r}'-\bar{r}''|}, \quad \text{since } |\bar{k}_0| = |\bar{k}|$$

(8) $\therefore \quad f(0) = \frac{m^2}{4\pi^2 \hbar^4} \iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'') \frac{\sin k|\bar{r}'-\bar{r}''|}{k|\bar{r}'-\bar{r}''|^2} \quad e^{ik|\bar{r}'-\bar{r}''|}$

(9) Now: $\sigma = \frac{4\pi}{k} \operatorname{Im} f(0)$, therefore:

$$\sigma = \frac{m^2}{\pi \hbar^4} \iint d\bar{r}'\, d\bar{r}''\, V(r')\, V(r'') \frac{\sin^2 k|\bar{r}'-\bar{r}''|}{k^2 |\bar{r}'-\bar{r}''|^2}$$

Assignment #2
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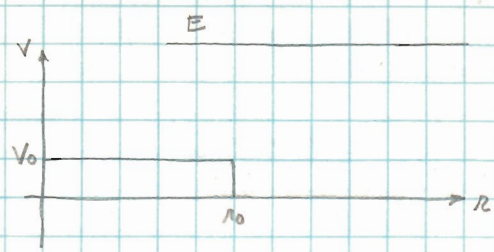
7.




Given: $|V_0| << E$ ; $k r_0 = 1$

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

a. (1) We have from problem 5: $\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l$

The problem is therefore to find $\delta_l$.

(2) For $r < r_0$: $v''(r) + \left\{ \frac{2m}{\hbar^2}(E - V_0) - \frac{l(l+1)}{r^2} \right\} v(r) = 0$

For $r > r_0$: $v''(r) + \left\{ \frac{2m}{\hbar^2} E - \frac{l(l+1)}{r^2} \right\} v(r) = 0$

where $v(r) = rR$, and $v(0) = 0$.

(3) for $|V_0| < E$ and $k r_0 << 1$, the particle at $r < r_0$ and for $r_0 < r < \frac{1}{k}$ sees principaly the centripetal potential and does not approach the scatterer. Both of equations (2) become the same and the phase difference between their solutions is almost zero and is negligible. However, for $l = 0$ there is no centripetal potential and the total and potential energy terms can no longer be neglected. We then get the following for (2):

$r < r_0$: $v''(r) + \kappa^2 v(r) = 0$

$r > r_0$: $v''(r) + k^2 v(r) = 0$

where $\kappa = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$ ; $k = \sqrt{\frac{2mE}{\hbar^2}}$

(4) For $r < r_0$, the solution that satisfies the boundary condition at $r = 0$ is:

$$v(r) = A \sin \kappa r$$

The general solution for $r > r_0$ is: $v(r) = B \sin(kr + \delta_0)$

(5) From the well-known continuity conditions of wave functions, we must have $\frac{v'}{v}$ continuous across $r = r_0$.

$$\therefore \quad \frac{\kappa \cos \kappa r_0}{\sin \kappa r_0} = \frac{k \cos(k r_0 + \delta_0)}{\sin(k r_0 + \delta_0)}$$

$$\text{or} \quad \frac{\tan \kappa r_0}{\kappa} = \frac{\tan(k r_0 + \delta_0)}{k}$$

(6) Since $|V_0| \ll E$, it follows that $\kappa \doteq k$ and thus $\delta_0$ must be small, as can be seen from the fact that the two solutions at the boundary must be equal. Therefore, it follows from this and the fact that $k r_0 \ll 1$, that we can expand the tan functions and consider their first few terms in $r_0$ to order $\delta_0$ and $(k r_0)^3$:

$$\frac{\kappa r_0 + \kappa^3 r_0^3/3 + \cdots}{\kappa} = \frac{(k r_0 + \delta_0) + \frac{(k r_0 + \delta_0)^3}{3} + \cdots}{k}$$

or: $$r_0 + \tfrac{1}{3}\kappa^2 r_0^3 = r_0 + \frac{\delta_0}{k} + \tfrac{1}{3} k^2 r_0^3$$

$$\therefore \quad \frac{\delta_0}{k} = \frac{1}{3}(\kappa^2 - k^2) r_0^3$$

or $$\delta_0 = \frac{k}{3}(\kappa^2 - k^2) r_0^3$$ : See note at end of problem!

(7) Now: $$\kappa^2 - k^2 = \frac{2m}{\hbar^2}(E - V_0) - \frac{2m}{\hbar^2}E = -\frac{2m}{\hbar^2}V_0$$

or: $$\delta_0 = \frac{-2mk V_0 r_0^3}{3\hbar^2} = -\frac{2m}{3\hbar^2}(k r_0)^3\left(\frac{V_0}{k^2}\right)$$

(8) $$\sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}\sin^2\delta_0$$

Note that: $$\delta_0 = \frac{-2m}{3\hbar^2}(k r_0)^3\left(\frac{V_0}{\frac{2mE}{\hbar^2}}\right) = -\frac{1}{3}(k r_0)^3\left(\frac{V_0}{E}\right)$$

which is truly $\ll 1$, so that $\sin^2\delta_0 \doteq \delta_0^2$

$$\therefore \quad \sigma = \frac{4\pi}{9k^2}(k r_0)^6\left(\frac{V_0}{E}\right)^2 = \frac{16\pi m^2 V_0^2 r_0^6}{9\hbar^4}$$

Note that, under the conditions of the problem, the sign of $V_0$ does not affect the result.

b. (1) From the results of lecture and considerations in problem 6; we have for the coefficient of scattering in a spherically symmetric field; under the Born approximation:

$$f(\vartheta) = \frac{m}{2\pi\hbar^2}\int d\bar{r}'\, e^{i(\bar{k}_0 - \bar{k})\cdot\bar{r}}\, V(r')$$

which reduces to under the use of spherical coordinates as shown in problem 6:

$$f(\vartheta) = -\frac{2m}{\hbar^2}\int_0^\infty \frac{dr'\, r'\, V(r')\, \sin|\bar{k}_0 - \bar{k}|r'}{|\bar{k}_0 - \bar{k}|}$$

Assignment #2
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Problem 7
Continued:

b. (2) For $V = V_0$, $r < r_0$; $V = 0$, $r > r_0$:

$$f(\vartheta) = \frac{-2m V_0}{\hbar^2 |\bar{k}_0 - \bar{k}|} \int_0^{r_0} dr'\, r' \sin |\bar{k}_0 - \bar{k}| r'$$

(3) $\int_0^{r_0} dr'\, r' \sin|\bar{k}_0 - \bar{k}| r'$

Let $u = r'$ $\quad dv = \sin|\bar{k}_0 - \bar{k}| r'$

$du = dr'$ $\quad v = \frac{-1}{|\bar{k}_0 - \bar{k}|} \cos |\bar{k}_0 - \bar{k}| r'$

$$= \left. \frac{-r'}{|\bar{k}_0 - \bar{k}|} \cos|\bar{k}_0 - \bar{k}| r' \right]_0^{r_0} + \frac{1}{|\bar{k}_0 - \bar{k}|} \int_0^{r_0} \cos|\bar{k}_0 - \bar{k}| r'\, dr'$$

$$= \frac{-r_0}{|\bar{k}_0 - \bar{k}|} \cos|\bar{k}_0 - \bar{k}| r_0 + \frac{\sin|\bar{k}_0 - \bar{k}| r_0}{|\bar{k}_0 - \bar{k}|^2}$$

(4) Consider the relation between the $k$ vectors of the incident and scattered waves:


Since the scattering is elastic, $|k_0| = |k|$, $|k_0 - k|$ is just the cord of an arc and we have from the usual formula:

$$|\bar{k}_0 - \bar{k}| = 2k \sin \tfrac{1}{2}\vartheta$$

(5) $\therefore$ $$f(\vartheta) = \frac{-2m V_0 r_0^3}{\hbar^2} \left\{ \frac{\sin(2kr_0 \sin\frac{1}{2}\vartheta) - (2kr_0 \sin\frac{1}{2}\vartheta)\cos(2kr_0\sin\frac{1}{2}\vartheta)}{(2kr_0 \sin\frac{1}{2}\vartheta)^3} \right\}$$

(6) $$\sigma = \int |f(\vartheta)|^2 d\Omega = \int_0^{2\pi}\int_0^{\pi} |f(\vartheta)|^2 d\vartheta \sin\vartheta\, d\varphi$$

$$= 2\pi \int_0^{\pi} |f(\vartheta)|^2 \sin\vartheta\, d\vartheta = 2\pi \int_0^{\pi} |f(2kr_0 \sin\tfrac{1}{2}\vartheta)|^2 \sin\vartheta\, d\vartheta$$

(7) Let $u = 2kr_0 \sin\frac{1}{2}\vartheta$

$$du = kr_0 \cos\tfrac{1}{2}\vartheta\, d\vartheta = \frac{kr_0 \sin\vartheta\, d\vartheta}{2\sin\frac{1}{2}\vartheta}$$

or $$\sin\vartheta\, d\vartheta = \frac{u\, du}{(kr_0)^2}$$

(8) $\therefore \quad \sigma = \dfrac{2\pi}{(k r_0)^2} \displaystyle\int_0^{2kr_0} |f(u)|^2 \, u \, du$

$$= \frac{2\pi}{(kr_0)^2} \left\{ \frac{2m V_0 r_0^3}{\hbar^2} \right\}^2 \int_0^{2kr_0} \left( \frac{\sin^2 u - 2u \sin u \cos u + u^2 \cos^2 u}{u^5} \right) du$$

Now, after some manipulation:

$$\int_0^{2kr_0} (\;\;) \, du = \frac{1}{4} \left\{ 1 - \frac{1}{(2kr_0)^2} + \frac{\sin 4kr_0}{(2kr_0)^3} - \frac{\sin^2 2kr_0}{(2kr_0)^4} \right\}$$

(9) Consider:

$$\frac{1}{x^2} - \frac{1}{x^4} + \frac{\sin 2x}{x^5} - \frac{\sin^2 x}{x^6}$$

where $x \to 0$, $x$ denoting $2kr_0$ which satisfies $kr_0 \ll 1$:

$$\frac{1}{x^2} - \frac{1}{x^4} + \frac{2x - \frac{(2x)^3}{6} + \frac{(2x)^5}{120}}{x^5} - \frac{\left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!}\right)\left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!}\right)}{x^6}$$

$$= \frac{1}{x^2} - \frac{1}{x^4} + \frac{2}{x^4} - \frac{4}{3x^2} + \frac{32}{120} - \left( \frac{1}{x^5} - \frac{1}{3!\,x^3} + \frac{1}{5!\,x} \right)\left( x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \right)$$

$$= \frac{1}{x^2} - \frac{1}{x^4} + \frac{2}{x^4} - \frac{4}{3x^2} + \frac{4}{15} - \frac{1}{x^4} + \frac{1}{6x^2} - \frac{1}{120} + \frac{1}{6x^2} - \frac{1}{36} - \frac{1}{120}$$

$$= \frac{32}{120} - \frac{2}{120} - \frac{1}{36} = \frac{1}{4} - \frac{1}{36} = \frac{8}{36} = \frac{2}{9}$$

(10) $\therefore \quad \sigma = 2\pi \left( \dfrac{4m^2 V_0^2 r_0^6}{\hbar^4} \right) \dfrac{1}{4} \cdot \dfrac{2}{9} \cdot 4 = \dfrac{16 \pi m^2 V_0^2 r_0^6}{9 \hbar^4}$ ✓

Which is the same as for the method of partial waves.

NB: In part a, equation (6), the reason terms like $(kr_0)^2 \delta_0$ and $kr_0 \delta_0^2$ can be neglected with respect to $(kr_0)^3$ is the following: Since $|V_0| \ll E$, we have:

$\kappa r_0 \simeq k r_0$ and equation a.(5) becomes:

$$\tan \kappa r_0 \sim \tan(kr_0 + \delta_0)$$

So for this to be true, we must have $\delta_0 \ll kr_0$, so that $\delta_0^2 kr_0$ and $(kr_0)^2 \delta_0$ are much less than $(kr_0)^3$.

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8. Beginning with $\psi_{j_{max}, m_{max}}$ and using ladder operators and orthogonalization, construct all the $\psi_{jm}$ in terms of the products $u_{m_1} v_{m_2}$ for the case $j_1 = \frac{3}{2}$, $j_2 = 1$.

9. Using the relations for infinitesimal rotation operators,

$$E_z x = -y, \quad E_z y = x, \text{ etc.}$$

and the fact that these are essentially operators of differentiation, so that

$$E_k uv = uE_k v + vE_k u$$

show that when we start with the function xy just four more functions are required to express all effects of the operators $E_k$ within the set of functions.

Write the 5-rowed matrices $\|E_k\|$ that express the effects of the rotations on the one-column matrix $\begin{pmatrix} a \\ \vdots \\ e \end{pmatrix}$ of the coefficients in the expression

$$axy + byz + czx + d(x^2 - y^2) + e(z^2 - x^2).$$

Find the products $\|E_x\| \cdot \|E_y\|$, $\|E_y\| \cdot \|E_x\|$, $\|E_y\| \cdot \|E_z\|$, etc., and verify that the values of the commutators are those required by the identification

$$E_k = \frac{i}{\hbar} M_k \quad .$$

10. A system with j = 2 has been previously found to have magnetic quantum number $m_o$ with respect to the $z_o$ - axis. Find the probabilities of the various results $m\hbar$, if the component of angular momentum along the z-axis (angle $\theta$ with $z_o$-axis) is measured:

(a) For $m_o = 0$, $\theta = 45^\circ$

(b) For $m_o = 1$, $\theta = 90^\circ$

(c) For $m_o = 2$, $\theta = 90^\circ$

Which of these results shows most clearly (by itself) that a measurement of the component of angular momentum along an axis in general disturbs the value along another axis?

11. The component of the spin angular momentum of an electron along the $z_o$-axis has been previously found. Find the probability that the value of the component along the z-axis will be found to be the same, and the probability for it to be opposite, for angle $\theta$ between these axes:

(a) By the matrix method used in Problem 10.

(b) By using the operator for a finite rotation as found in class.

8. Beginning with $\psi_{j_{max}\, m_{max}}$ and using ladder operators and orthogonalization, construct all the $\psi_{jm}$ in terms of the products $u_{m_1} v_{m_2}$ for the case $j_1 = \frac{3}{2}$, $j_2 = 1$.

9. Using the relations for infinitesimal rotation operators

$$\Xi_z x = -y, \quad \Xi_z y = x, \text{ etc.}$$

and the fact that these are essentially operators of differentiation, so that

$$\Xi_k uv = u\Xi_k v + v\Xi_k u$$

show that when we start with the function xy just four more functions are required to express all effects of the operators $\Xi_k$ within the set of functions.

Write the 5-rowed matrices $[\Xi_k]$ that express the effects of the rotations on the one-column matrix $\begin{pmatrix} a \\ \vdots \\ e \end{pmatrix}$ of the coefficients in the expression

$$axy + byz + czx + d(x^2 - y^2) + e(z^2 - x^2).$$

Find the products $[\Xi_x]\cdot[\Xi_y]$, $[\Xi_y]\cdot[\Xi_x]$, $[\Xi_y]\cdot[\Xi_z]$, etc., and verify that the values of the commutators are those required by the identification

10. A system with $j = 2$ has been previously found to have magnetic quantum number $m_0$ with respect to the $z_0$ - axis. Find the probabilities of the various results $m$'s, if the component of angular momentum along the z-axis (angle $\Theta$ with $z_0$-axis) is measured:

(a) For $m_0 = 0$, $\Theta = 45°$

(b) For $m_0 = 1$, $\Theta = 90°$

(c) For $m_0 = 2$, $\Theta = 90°$

Which of these results shows most clearly (by itself) that a measurement of the component of angular momentum along an axis in general disturbs the value along another axis?

11. The component of the spin angular momentum of an electron along the $z_0$-axis has been previously found. Find the probability that the value of the component along the z-axis will be found to be the same, and the probability for it to be opposite, for angle $\Theta$ between these axes:

(a) By the matrix method used in Problem 10.

(b) By using the operator for a finite rotation as found in class.

Assignment # 3
Problems 8-11

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8. (1) Given $j_1$ and $j_2$ and $u_{m_1}, v_{m_2}$ we wish to find the linear combinations that form:

$$|j_1 j_2 j m\rangle = \sum_{m_1, m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 m j\rangle$$

where $j = j_1 + j_2, \; j_1 + j_2 - 1, \ldots |j_1 - j_2|$ ; $m = m_1 + m_2$

$$|j_1 j_2 j m\rangle = \psi_{jm}$$
$$|j_1 j_2 m_1 m_2\rangle = u_{m_1} v_{m_2}$$
$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 m j\rangle = a_{m_1 m_2}$$

$$\therefore \quad \psi_{jm} = \sum_{\substack{m_1, m_2 \\ (m_1 + m_2 = m)}} a_{m_1 m_2} u_{m_1} v_{m_2}$$

(2) $|m| \leq j$ ; $j_{max} = j_1 + j_2$ ; $m_{max} = j_1 + j_2 = (m_1 + m_2)_{max} = m_{1\,max} + m_{2\,max}$

$$\psi_{j_{max}\, m_{max}} = u_{m_1\,max}\, v_{m_2\,max}$$
$$= u_{j_1} v_{j_2}$$

choosing the arbitrary constant for normality

We will generate orthogonal sets with the step down operator:

$$\frac{M_-}{\hbar} \psi_{jm} = \left\{(j+m)(j-m+1)\right\}^{1/2} \psi_{j, m-1}$$

(3) Consider $j_1 = \frac{3}{2}$, $j_2 = 1$ : Available products:

| $m$ | $5/2$ | $3/2$ | $1/2$ | $-1/2$ | $-3/2$ | $-5/2$ |
|---|---|---|---|---|---|---|
| | $u_{3/2} v_1$ | $u_{1/2} v_1$ | $u_{3/2} v_{-1}$ | $u_{-3/2} v_1$ | $u_{-1/2} v_{-1}$ | $u_{-3/2} v_{-1}$ |
| | | $u_{3/2} v_0$ | $u_{1/2} v_0$ | $u_{-1/2} v_0$ | $u_{-3/2} v_0$ | |
| | | | $u_{-1/2} v_1$ | $u_{1/2} v_{-1}$ | | |

$u_{3/2}, u_{1/2}, u_{-1/2}, u_{-3/2}, v_1, v_0, v_{-1}$

(4) Begin with $\psi_{5/2\, 5/2} = u_{3/2} v_1$ :

$$\sqrt{5 \cdot 1}\, \psi_{5/2\, 3/2} = \sqrt{3 \cdot 1}\, u_{1/2} v_1 + \sqrt{2 \cdot 1}\, u_{3/2} v_0$$

$$\psi_{5/2\, 3/2} = \sqrt{\frac{3}{5}}\, u_{1/2} v_1 + \sqrt{\frac{2}{5}}\, u_{3/2} v_0$$

(5) $$\sqrt{4 \cdot 2}\, \psi_{5/2\, 1/2} = \sqrt{\frac{3}{5}} \left( \sqrt{2 \cdot 2}\, u_{-1/2} v_1 + \sqrt{2 \cdot 1}\, u_{1/2} v_0 \right)$$
$$+ \sqrt{\frac{2}{5}} \left( \sqrt{3 \cdot 1}\, u_{1/2} v_0 + \sqrt{1 \cdot 2}\, u_{3/2} v_{-1} \right)$$
$$= \sqrt{\frac{12}{5}}\, u_{-1/2} v_1 + \sqrt{\frac{24}{5}}\, u_{1/2} v_0 + \sqrt{\frac{4}{5}}\, u_{3/2} v_{-1}$$

(5) $$\psi_{5/2\ 1/2} = \sqrt{\tfrac{3}{10}}\, u_{-1/2} v_1 + \sqrt{\tfrac{6}{10}}\, u_{1/2} v_0 + \sqrt{\tfrac{1}{10}}\, u_{3/2} v_{-1}$$

(6) $$\sqrt{3\cdot 3}\ \psi_{5/2\ -1/2} = \sqrt{\tfrac{3}{10}}\left(\sqrt{1\cdot 3}\, u_{-3/2} v_1 + \sqrt{2\cdot 1}\, u_{-1/2} v_0\right)$$

$$+ \sqrt{\tfrac{6}{10}}\left(\sqrt{2\cdot 2}\, u_{-1/2} v_0 + \sqrt{1\cdot 2}\, u_{1/2} v_{-1}\right) + \sqrt{\tfrac{1}{10}}\left(\sqrt{3\cdot 1}\, u_{1/2} v_{-1}\right)$$

$$= \sqrt{\tfrac{9}{10}}\, u_{-3/2} v_1 + 3\sqrt{\tfrac{6}{10}}\, u_{-1/2} v_0 + 3\sqrt{\tfrac{3}{10}}\, u_{1/2} v_{-1}$$

or $$\psi_{5/2\ -1/2} = \sqrt{\tfrac{1}{10}}\, u_{-3/2} v_1 + \sqrt{\tfrac{6}{10}}\, u_{-1/2} v_0 + \sqrt{\tfrac{3}{10}}\, u_{1/2} v_{-1}$$

(7) Similarly: $$\psi_{5/2\ -3/2} = \sqrt{\tfrac{3}{5}}\, u_{-1/2} v_{-1} + \sqrt{\tfrac{2}{5}}\, u_{-3/2} v_0$$

$$\psi_{5/2\ -5/2} = u_{-3/2} v_{-1}$$

(8) We construct $\psi_{3/2\ 3/2}$ orthogonal to $\psi_{5/2\ 3/2}$:

$$\psi_{3/2\ 3/2} = a\, u_{1/2} v_1 + b\, u_{3/2} v_0$$

$$\left.\begin{aligned} a^2 &= 1 - 3/5 = 2/5 \\ b^2 &= 1 - 2/5 = 3/5 \end{aligned}\right\}\ \text{choose } b \text{ negative}$$

$$\therefore\ \psi_{3/2\ 3/2} = \sqrt{\tfrac{2}{5}}\, u_{1/2} v_1 - \sqrt{\tfrac{3}{5}}\, u_{3/2} v_0$$

(9) $$\sqrt{3\cdot 1}\ \psi_{3/2\ 1/2} = \sqrt{\tfrac{2}{5}}\left(\sqrt{2\cdot 2}\, u_{-1/2} v_1 + \sqrt{2\cdot 1}\, u_{1/2} v_0\right)$$

$$- \sqrt{\tfrac{3}{5}}\left(\sqrt{3\cdot 1}\, u_{1/2} v_0 + \sqrt{1\cdot 2}\, u_{3/2} v_{-1}\right)$$

$$= \sqrt{\tfrac{8}{5}}\, u_{-1/2} v_1 - \sqrt{\tfrac{1}{5}}\, u_{1/2} v_0 - \sqrt{\tfrac{6}{5}}\, u_{3/2} v_{-1}$$

$$\therefore\ \psi_{3/2\ 1/2} = \sqrt{\tfrac{8}{15}}\, u_{-1/2} v_1 - \sqrt{\tfrac{1}{15}}\, u_{1/2} v_0 - \sqrt{\tfrac{6}{15}}\, u_{3/2} v_{-1}$$

(10) Similarly: $$\psi_{3/2\ -1/2} = \sqrt{\tfrac{8}{15}}\, u_{1/2} v_{-1} - \sqrt{\tfrac{1}{15}}\, u_{-1/2} v_0 - \sqrt{\tfrac{6}{15}}\, u_{-3/2} v_1$$

$$\psi_{3/2\ -3/2} = \sqrt{\tfrac{2}{5}}\, u_{-1/2} v_{-1} - \sqrt{\tfrac{3}{5}}\, u_{-3/2} v_0$$

Assignment #3
Continued

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Problem 8
Continued:

(11) $\psi_{1/2\,1/2} = a\, u_{-1/2} v_1 + b\, u_{1/2} v_0 + c\, u_{3/2} v_{-1}$

$$a^2 = 1 - \frac{3}{10} - \frac{8}{15} = \frac{30-9-16}{30} = 1/6 = 1/6$$

$$b^2 = 1 - \frac{6}{10} - \frac{1}{15} = \frac{30-18-2}{30} = 1/3 = 2/6$$

$$c^2 = 1 - \frac{1}{10} - \frac{6}{15} = \frac{30-3-12}{30} = 1/2 = 3/6$$

To find the proper sign, examine:

$$\sqrt{\frac{3}{60}} \qquad 2\sqrt{\frac{3}{60}} \qquad \sqrt{\frac{3}{60}}$$

$$2\sqrt{\frac{2}{90}} \qquad -\sqrt{\frac{2}{90}} \qquad -3\sqrt{\frac{2}{90}}$$

By Inspection:

$$\psi_{1/2\,1/2} = \sqrt{\frac{1}{6}}\, u_{-1/2} v_1 - \sqrt{\frac{2}{6}}\, u_{1/2} v_0 + \sqrt{\frac{3}{6}}\, u_{3/2} v_{-1}$$

(12) By symmetry: $\psi_{1/2\,-1/2} = \sqrt{\frac{1}{6}}\, u_{1/2} v_{-1} - \sqrt{\frac{2}{6}}\, u_{-1/2} v_0 + \sqrt{\frac{3}{6}}\, u_{-3/2} v_1$

Recapitulation:

$j = 5/2$:

$$\psi_{5/2\,5/2} = u_{3/2} v_1$$
$$\psi_{5/2\,3/2} = \sqrt{\frac{3}{5}}\, u_{1/2} v_1 + \sqrt{\frac{2}{5}}\, u_{3/2} v_0$$
$$\psi_{5/2\,1/2} = \sqrt{\frac{3}{10}}\, u_{-1/2} v_1 + \sqrt{\frac{6}{10}}\, u_{1/2} v_0 + \sqrt{\frac{1}{10}}\, u_{3/2} v_{-1}$$
$$\psi_{5/2\,-1/2} = \sqrt{\frac{3}{10}}\, u_{1/2} v_{-1} + \sqrt{\frac{6}{10}}\, u_{-1/2} v_0 + \sqrt{\frac{1}{10}}\, u_{-3/2} v_1$$
$$\psi_{5/2\,-3/2} = \sqrt{\frac{3}{5}}\, u_{-1/2} v_{-1} + \sqrt{\frac{2}{5}}\, u_{-3/2} v_0$$
$$\psi_{5/2\,-5/2} = u_{-3/2} v_{-1}$$

$j = 3/2$:

$$\psi_{3/2\,3/2} = \sqrt{\frac{2}{5}}\, u_{1/2} v_1 - \sqrt{\frac{3}{5}}\, u_{3/2} v_0$$
$$\psi_{3/2\,1/2} = \sqrt{\frac{8}{15}}\, u_{-1/2} v_1 - \sqrt{\frac{1}{15}}\, u_{1/2} v_0 - \sqrt{\frac{6}{15}}\, u_{3/2} v_{-1}$$
$$\psi_{3/2\,-1/2} = \sqrt{\frac{8}{15}}\, u_{1/2} v_{-1} - \sqrt{\frac{1}{15}}\, u_{-1/2} v_0 - \sqrt{\frac{6}{15}}\, u_{-3/2} v_1$$
$$\psi_{3/2\,-3/2} = \sqrt{\frac{2}{5}}\, u_{-1/2} v_{-1} - \sqrt{\frac{3}{5}}\, u_{-3/2} v_0$$

$j = 1/2$:

$$\psi_{1/2\,1/2} = \sqrt{\frac{1}{6}}\, u_{-1/2} v_1 - \sqrt{\frac{2}{6}}\, u_{1/2} v_0 + \sqrt{\frac{3}{6}}\, u_{3/2} v_{-1}$$
$$\psi_{1/2\,-1/2} = \sqrt{\frac{1}{6}}\, u_{1/2} v_{-1} - \sqrt{\frac{2}{6}}\, u_{-1/2} v_0 + \sqrt{\frac{3}{6}}\, u_{-3/2} v_1$$

Assignment #3
Continued

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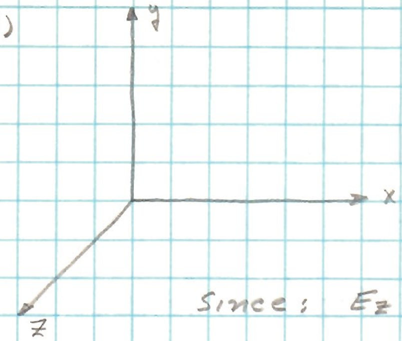
9. (1)




We define the class of infinitesimal clockwise rotations:

$E_z x = -y \qquad E_y x = z \qquad E_x x = 0$
$E_z y = x \qquad E_y y = 0 \qquad E_x y = -z$
$E_z z = 0 \qquad E_y z = -x \qquad E_x z = y$

Since: $E_z = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}$ ; $E_y = z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}$ ; $E_x = y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}$

(2) We generate, using $E_k uv = u E_k v + v E_k u$, the following expressions for future use:

$E_z xy = x^2 - y^2 \qquad E_z yz = zx \qquad E_z zx = -zy$
$E_y xy = yz \qquad E_y yz = -yx \qquad E_y zx = z^2 - x^2$
$E_x xy = -xz \qquad E_x yz = y^2 - z^2 \qquad E_x zx = xy$

$E_z x^2 = -2xy \qquad E_z y^2 = 2yx \qquad E_z z^2 = 0$
$E_y x^2 = 2xz \qquad E_y y^2 = 0 \qquad E_y z^2 = -2zx$
$E_x x^2 = 0 \qquad E_x y^2 = -2yz \qquad E_x z^2 = 2zy$

$E_z (x^2-y^2) = -4xy \qquad E_z (y^2-z^2) = 2xy \qquad E_z (z^2-x^2) = 2xy$
$E_y (x^2-y^2) = 2zx \qquad E_y (y^2-z^2) = 2zx \qquad E_y (z^2-x^2) = -4zx$
$E_x (x^2-y^2) = 2yz \qquad E_x (y^2-z^2) = -4yz \qquad E_x (z^2-x^2) = 2yz$

(3) From the above tables, we see that if we start with the operations of the class on $xy$ and repetitively operate with each element, that is:

$E_z xy = x^2 - y^2 \qquad E_x E_z xy = 2yz \qquad E_y E_x E_z xy = -2xy$
$E_y xy = yz \qquad E_z E_y xy = zx \qquad E_x E_z E_y xy = xy$
$E_x xy = -zx \qquad E_y E_x xy = -(z^2 - x^2) \qquad E_z E_y E_x xy = -2xy$

it is then clear that the functions $xy$, $yz$, $zx$, $(x^2-y^2)$, $(z^2-x^2)$ form a basis for the representation of the class which is consistent. The last four functions are the new ones.

Note that $y^2 - z^2$ is not an independent basis function since $y^2 - z^2 = -\{(x^2-y^2) + (z^2-x^2)\}$

and it is a linear combination of two other previously defined basis functions.

(4) Consider the expression $a\,xy + b\,yz + c\,zx + d(x^2-y^2) + e(z^2-x^2) = F$ upon which we operate with each of the elements of the class:

$$E_x F = a(-zx) + b(y^2-z^2) + c(xy) + d(2yz) + e(2yz)$$

$$= c\,xy + (2e+2d)\,yz - a\,zx - b(x^2-y^2) - b(z^2-x^2)$$

$$E_y F = a(yz) + b(-xy) + c(z^2-x^2) + d(2zx) + e(-4zx)$$

$$= -b\,xy + a\,yz + (2d-4e)\,zx + (0)(x^2-y^2) + c(z^2-x^2)$$

$$E_z F = a(x^2-y^2) + b(zx) + c(-zy) + d(-4xy) + e(2xy)$$

$$= (2e-4d)\,xy - c\,yz + b\,zx + a(x^2-y^2) + (0)(z^2-x^2)$$

(5) We can express the operations on $F$ as matrices operating on the coefficients of the basis functions in $F$. We write the matrices by inspection:

$$\|E_x\| \cdot \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} c \\ 2e+2d \\ -a \\ -b \\ -b \end{pmatrix}$$

$$\|E_y\| \cdot \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -4 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} -b \\ a \\ 2d-4e \\ 0 \\ c \end{pmatrix}$$

$$\|E_z\| \cdot \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -4 & 2 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} 2e-4d \\ -c \\ b \\ a \\ 0 \end{pmatrix}$$

(6) We now form the products of the matrices:

$$\|E_x\| \cdot \|E_y\| = \begin{pmatrix} 0 & 0 & 0 & 2 & -4 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \end{pmatrix} ; \quad \|E_y\| \cdot \|E_x\| = \begin{pmatrix} 0 & 0 & 0 & -2 & -2 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\|E_x\| \cdot \|E_y\| - \|E_y\| \cdot \|E_x\| = \begin{pmatrix} 0 & 0 & 0 & 4 & -2 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = -\|E_z\|$$

Assignment #3
Continued

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Problem 9
Continued:

(7)

$$\|E_x\|\cdot\|E_z\| = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & -2 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} ; \quad \|E_z\|\cdot\|E_x\| = \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\|E_x\|\cdot\|E_z\| - \|E_z\|\cdot\|E_x\| = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -4 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} = \|E_y\|$$

(8)

$$\|E_y\|\cdot\|E_z\| = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -4 & 2 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} ; \quad \|E_z\|\cdot\|E_y\| = \begin{pmatrix} 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & -2 & 4 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\|E_y\|\cdot\|E_z\| - \|E_z\|\cdot\|E_y\| = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -2 & -2 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} = -\|E_x\|$$

(9) Dropping the matrix notation, we see we can write in general:

$$[E_j, E_k] = -\epsilon_{jkl} E_l \quad , \text{where } \epsilon_{jkl} = \begin{cases} 1, & jkl = xyz,\ yzx,\ zxy \\ 0, & jkl \text{ not different} \\ -1, & jkl = xzy,\ yxz,\ zyx \end{cases}$$

(10) We have from lecture:

$$[M_j, M_k] = i\hbar\, \epsilon_{jkl} M_l \quad , \text{where } \epsilon_{jkl} \text{ is the same as above.}$$

(11) If we make the identification $E_k = \frac{i}{\hbar} M_k$ and substitute in (9), we have:

$$-\frac{1}{\hbar^2}[M_j, M_k] = -\frac{i}{\hbar}\epsilon_{jkl} M_l$$

$$\text{or} \quad [M_j, M_k] = i\hbar\, \epsilon_{jkl} M_l$$

thus justifying the identification.

Assignment #3
Continued

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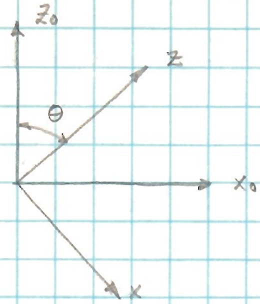
10. (1)




Consider that with constant $j$ the states of the different components of angular momentum are expressible as linear combinations of each other, that is:

$$|m_0\rangle = \sum_m |m\rangle\langle m|m_0\rangle$$

(2) Now: $M_{z0}|m_0\rangle = m_0\hbar\,|m_0\rangle$

$$M_{z0} = M_z\cos\theta - M_x\sin\theta$$

$$= M_z\cos\theta - M_+\frac{\sin\theta}{2} - M_-\frac{\sin\theta}{2}$$

(3) $\dfrac{M_+}{\hbar} = \dfrac{M_x + iM_y}{\hbar}$ : $\dfrac{M_+}{\hbar}|m\rangle = \{(j-m)(j+m-1)\}^{1/2}|m+1\rangle$

$\dfrac{M_-}{\hbar} = \dfrac{M_x - iM_y}{\hbar}$ : $\dfrac{M_-}{\hbar}|m\rangle = \{(j+m)(j-m+1)\}^{1/2}|m-1\rangle$

(4) $\dfrac{M_{z0}}{\hbar}|m_0\rangle = m_0|m_0\rangle = \sum_m \Big\{ m\cos\theta\,|m\rangle - \sqrt{(j-m)(j+m+1)}\,\dfrac{\sin\theta}{2}|m+1\rangle$

$- \sqrt{(j+m)(j-m+1)}\,\dfrac{\sin\theta}{2}|m-1\rangle\Big\}\langle m|m_0\rangle = \sum_m m_0|m\rangle\langle m|m_0\rangle$

(5) $\sum_m |m\rangle\Big\{(m\cos\theta - m_0)\langle m|m_0\rangle - \sqrt{(j-m+1)(j+m)}\,\dfrac{\sin\theta}{2}\langle m-1|m_0\rangle$

$- \sqrt{(j+m+1)(j-m)}\,\langle m+1|m_0\rangle\Big\} = 0$

(6)

$\sqrt{(j-m+1)(j+m)}\,\dfrac{\sin\theta}{2}\langle m-1|m_0\rangle - (m\cos\theta - m_0)\langle m|m_0\rangle$

$+ \dfrac{\sin\theta}{2}\sqrt{(j+m+1)(j-m)}\,\langle m+1|m_0\rangle = 0$

(7) Take $j=2$, $m=2$:

$\sin\theta\,\langle 1|m_0\rangle - (2\cos\theta - m_0)\langle 2|m_0\rangle = 0$

$j=2$, $m=-2$:

$(2\cos\theta + m_0)\langle -2|m_0\rangle + \sin\theta\,\langle -1|m_0\rangle = 0$

(8) $j = 2,\ m = 1$ :

$$\sqrt{6}\ \frac{\sin\theta}{2}\ \langle 0|m_0\rangle - (\cos\theta - m_0)\langle 1|m_0\rangle + \sin\theta\ \langle 2|m_0\rangle = 0$$

$j = 2$ : $m = -1$ :

$$\sin\theta\ \langle -2|m_0\rangle + (\cos\theta + m_0)\langle -1|m_0\rangle + \sqrt{6}\ \frac{\sin\theta}{2}\ \langle 0|m_0\rangle = 0$$

$j = 2$ ; $m = 0$ :

$$\sqrt{6}\ \frac{\sin\theta}{2}\langle -1|m_0\rangle + m_0\ \langle 0|m_0\rangle + \sqrt{6}\ \frac{\sin\theta}{2}\ \langle 1|m_0\rangle = 0$$

(9)

| | $\langle -2\|m_0\rangle$ | $\langle -1\|m_0\rangle$ | $\langle 0\|m_0\rangle$ | $\langle 1\|m_0\rangle$ | $\langle 2\|m_0\rangle$ |
|---|---|---|---|---|---|
| $m = 2$ | 0 | 0 | 0 | $\sin\theta$ | $m_0 - 2\cos\theta$ |
| $m = -2$ | $m_0 + 2\cos\theta$ | $\sin\theta$ | 0 | 0 | 0 |
| $m = 1$ | 0 | 0 | $\sqrt{6}\ \frac{\sin\theta}{2}$ | $m_0 - \cos\theta$ | $\sin\theta$ |
| $m = -1$ | $\sin\theta$ | $m_0 + \cos\theta$ | $\sqrt{6}\ \frac{\sin\theta}{2}$ | 0 | 0 |
| $m = 0$ | 0 | $\sqrt{6}\ \frac{\sin\theta}{2}$ | $m_0$ | $\sqrt{6}\ \frac{\sin\theta}{2}$ | 0 |

$= 0$

(10)

| | $\langle -2\|m_0\rangle$ | $\langle -1\|m_0\rangle$ | $\langle 0\|m_0\rangle$ | $\langle 1\|m_0\rangle$ | $\langle 2\|m_0\rangle$ |
|---|---|---|---|---|---|
| $m = 2$ | 0 | 0 | 0 | $\sin\theta$ | $m_0 - 2\cos\theta$ |
| $m = 1$ | 0 | 0 | $\sqrt{6}\ \frac{\sin\theta}{2}$ | $m_0 - \cos\theta$ | $\sin\theta$ |
| $m = 0$ | 0 | $\sqrt{6}\ \frac{\sin\theta}{2}$ | $m_0$ | $\sqrt{6}\ \frac{\sin\theta}{2}$ | 0 |
| $m = -1$ | $\sin\theta$ | $m_0 + \cos\theta$ | $\sqrt{6}\ \frac{\sin\theta}{2}$ | 0 | 0 |
| $m = -2$ | $m_0 + 2\cos\theta$ | $\sin\theta$ | 0 | 0 | 0 |

$= 0$

(11) $|m_0\rangle = \sum_m |m\rangle\langle m|m_0\rangle$ ; $\langle m_0| = \sum_{m'} \langle m_0|m'\rangle\langle m'|$

$\therefore\ \langle m_0|m_0\rangle = 1 = \sum_{mm'} \langle m_0|m'\rangle\langle m'|m\rangle\langle m|m_0\rangle$

$\therefore\ \sum_m |\langle m|m_0\rangle|^2 = 1$

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Assignment #3
Continued

Problem 10
Continued:

(12) Consider $m_0 = 0$, $\theta = \pi/4$

$$\begin{vmatrix} \langle -2|0\rangle & \langle -1|0\rangle & \langle 0|0\rangle & \langle 1|0\rangle & \langle 2|0\rangle \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} & -\sqrt{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{3}}{2} & 0 & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \sqrt{2} & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{vmatrix} = 0$$

(13) Since we have a set of homogeneous equations, we solve in the usual manner:

$$\langle -2|0\rangle = k \begin{vmatrix} 0 & 0 & \sqrt{2}/2 & -\sqrt{2} \\ 0 & \sqrt{3}/2 & -\sqrt{2}/2 & \sqrt{2}/2 \\ \sqrt{3}/2 & 0 & 0 & 0 \\ \sqrt{2}/2 & \sqrt{3}/2 & 0 & 0 \end{vmatrix} = \sqrt{3}/2\, k \begin{vmatrix} 0 & \sqrt{2}/2 & -\sqrt{2} \\ \sqrt{3}/2 & -\sqrt{2}/2 & \sqrt{2}/2 \\ \sqrt{3}/2 & 0 & 0 \end{vmatrix}$$

$$= \frac{3}{4} k \left(\frac{1}{2} - 1\right) = -\frac{3}{8} k$$

$$\therefore\ |\langle -2|0\rangle|^2 = \frac{9}{64} k^2$$

$$\langle -1|0\rangle = -k \begin{vmatrix} 0 & 0 & \sqrt{2}/2 & -\sqrt{2} \\ 0 & \sqrt{3}/2 & -\sqrt{2}/2 & \sqrt{2}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \\ \sqrt{2}/2 & \sqrt{3}/2 & 0 & 0 \end{vmatrix} = -\frac{\sqrt{2}}{2} k \cdot -\frac{\sqrt{3}}{2} \cdot \frac{\sqrt{6}}{2} = -\frac{3}{4} k$$

$$|\langle -1|0\rangle|^2 = \frac{9}{16} k^2$$

$$\langle 0|0\rangle = k \begin{vmatrix} 0 & 0 & \sqrt{2}/2 & -\sqrt{2} \\ 0 & 0 & -\sqrt{2}/2 & \sqrt{2}/2 \\ 0 & \sqrt{3}/2 & \sqrt{3}/2 & 0 \\ \sqrt{2}/2 & \sqrt{2}/2 & 0 & 0 \end{vmatrix} = -\frac{\sqrt{2}}{2} k \cdot \frac{\sqrt{3}}{2} \left(\frac{1}{2} - 1\right) = \frac{\sqrt{6}}{8} k$$

$$|\langle 0|0\rangle|^2 = \frac{6}{64} k^2 = \frac{3}{32} k^2$$

$$\langle 1|0\rangle = -k \begin{vmatrix} 0 & 0 & 0 & -\sqrt{2} \\ 0 & 0 & \sqrt{3}/2 & \sqrt{2}/2 \\ 0 & \sqrt{3}/2 & 0 & 0 \\ \sqrt{2}/2 & \sqrt{2}/2 & \sqrt{3}/2 & 0 \end{vmatrix} = -\frac{\sqrt{2}}{2} k \cdot \frac{\sqrt{3}}{2} \cdot \frac{\sqrt{6}}{2} = +\frac{3}{4} k$$

$$|\langle 1|0\rangle|^2 = \frac{9}{16} k^2$$

(13) $\langle 2|0\rangle = k \begin{vmatrix} 0 & 0 & 0 & \sqrt{2}/2 \\ 0 & 0 & \sqrt{3}/2 & -\sqrt{2}/2 \\ 0 & \sqrt{3}/2 & 0 & \sqrt{3}/2 \\ \sqrt{2}/2 & \sqrt{2}/2 & \sqrt{3}/2 & 0 \end{vmatrix} = -\frac{\sqrt{2}}{2} k \cdot \frac{\sqrt{2}}{2} \cdot -\frac{3}{4} = \frac{3}{8} k$

$|\langle 2|0\rangle|^2 = \frac{9}{64} k^2$

(14) $\sum_{m=-2}^{2} |\langle m|0\rangle|^2 = 2\left\{ \frac{9}{64} + \frac{36}{64} \right\} k^2 + \frac{3}{32} k^2 = \frac{48}{32} k^2$

$= \frac{3}{2} k^2 = 1 \quad ; \quad k^2 = \frac{2}{3}$

(15) $|\langle -2|0\rangle|^2 = |\langle 2|0\rangle|^2 = \frac{3}{32}$

$|\langle -1|0\rangle|^2 = |\langle 1|0\rangle|^2 = \frac{3}{8}$

$|\langle 0|0\rangle|^2 = \frac{1}{16}$

(16) Consider $m_0 = 1$, $\theta = \pi/2$

$$\begin{matrix} \langle -2|1\rangle & \langle -1|1\rangle & \langle 0|1\rangle & \langle 1|1\rangle & \langle 2|1\rangle \end{matrix}$$

$$\begin{vmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & \sqrt{6}/2 & 1 & 1 \\ 0 & \sqrt{6}/2 & 1 & \sqrt{6}/2 & 0 \\ 1 & 1 & \sqrt{6}/2 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{vmatrix} = 0$$

(17) $\langle 2|1\rangle = k \begin{vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & \sqrt{6}/2 & 1 \\ 0 & \sqrt{6}/2 & 1 & \sqrt{6}/2 \\ 1 & 1 & \sqrt{6}/2 & 0 \end{vmatrix} = -\frac{\sqrt{6}}{2} k \cdot -\frac{\sqrt{6}}{2} = \frac{3}{2} k \; ; \; |\langle 2|1\rangle|^2 = \frac{9}{4} k^2$

$\langle 1|1\rangle = -k \begin{vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & \sqrt{6}/2 & 1 \\ 0 & \sqrt{6}/2 & 1 & 0 \\ 1 & 1 & \sqrt{6}/2 & 0 \end{vmatrix} = -\frac{\sqrt{6}}{2} k \cdot -\frac{\sqrt{6}}{2} = -\frac{3}{2} k \; ; \; |\langle 1|1\rangle|^2 = \frac{9}{4} k^2$

$\langle 0|1\rangle = k \begin{vmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & \sqrt{6}/2 & \sqrt{6}/2 & 0 \\ 1 & 1 & 0 & 0 \end{vmatrix} = 0 \; ; \; |\langle 0|1\rangle|^2 = 0$

$\langle -1|1\rangle = -k \begin{vmatrix} 0 & 0 & 1 & 1 \\ 0 & \sqrt{6}/2 & 1 & 1 \\ 0 & 1 & \sqrt{6}/2 & 0 \\ 1 & \sqrt{6}/2 & 0 & 0 \end{vmatrix} = -k \cdot -\frac{\sqrt{6}}{2} \cdot -\frac{\sqrt{6}}{2} = +\frac{3}{2} k \; ; \; |\langle -1|1\rangle|^2 = \frac{9}{4} k^2$

$\langle -2|1\rangle = k \begin{vmatrix} 0 & \sqrt{6}/2 & 1 & 1 \\ \sqrt{6}/2 & 1 & \sqrt{6}/2 & 0 \\ 1 & \sqrt{6}/2 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{vmatrix} = \frac{\sqrt{6}}{2} k \cdot -\frac{\sqrt{6}}{2} = -\frac{3}{2} k \; ; \; |\langle -2|1\rangle|^2 = \frac{9}{4} k^2$

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Assignment #3
Continued

Problem # 10
Continued

(18) $\sum_{m=-2}^{2} |\langle m|1\rangle|^2 = 4 \cdot \frac{9}{4} k^2 = 1 \; ; \quad k^2 = 1/9$

(19) $|\langle -2|1\rangle|^2 = |\langle -1|1\rangle|^2 = |\langle 1|1\rangle|^2 = |\langle 2|1\rangle|^2 = 1/4$

$|\langle 0|1\rangle|^2 = 0$

(20) Consider: $m_0 = 2 \; ; \quad \theta = \pi/2$

$$\begin{array}{ccccc} \langle -2|2\rangle & \langle -1|2\rangle & \langle 0|2\rangle & \langle 1|2\rangle & \langle 2|2\rangle \end{array}$$

$$\begin{vmatrix} 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & \sqrt{6}/2 & 2 & 1 \\ 0 & \sqrt{6}/2 & 2 & \sqrt{6}/2 & 0 \\ 1 & 2 & \sqrt{6}/2 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 \end{vmatrix} = 0$$

(21) $$\langle 2|2\rangle = k \begin{vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & \sqrt{6}/2 & 2 \\ 0 & \sqrt{6}/2 & 2 & \sqrt{6}/2 \\ 1 & 2 & \sqrt{6}/2 & 0 \end{vmatrix} = -k \cdot \frac{\sqrt{6}}{2} \cdot -\frac{\sqrt{6}}{2} = \frac{3}{2} k \; ; \quad |\langle 2|2\rangle|^2 = \frac{9}{4} k^2$$

$$\langle 1|2\rangle = -k \begin{vmatrix} 0 & 0 & 0 & 2 \\ 0 & 0 & \sqrt{6}/2 & 1 \\ 0 & \sqrt{6}/2 & 2 & 0 \\ 1 & 2 & \sqrt{6}/2 & 0 \end{vmatrix} = +\frac{\sqrt{6}}{2} k \cdot -\sqrt{6} = -3k \; ; \quad |\langle 1|2\rangle|^2 = 9 k^2$$

$$\langle 0|2\rangle = k \begin{vmatrix} 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & 1 \\ 0 & \sqrt{6}/2 & \sqrt{6}/2 & 0 \\ 1 & 2 & 0 & 0 \end{vmatrix} = -\frac{\sqrt{6}}{2} k \cdot -3 = \frac{3\sqrt{6}}{2} k \; ; \quad |\langle 0|2\rangle|^2 = \frac{27}{2} k^2$$

$$\langle -1|2\rangle = -k \begin{vmatrix} 0 & 0 & 1 & 2 \\ 0 & \sqrt{6}/2 & 2 & 1 \\ 0 & 2 & \sqrt{6}/2 & 0 \\ 1 & \sqrt{6}/2 & 0 & 0 \end{vmatrix} = +2k \cdot -3 + \frac{\sqrt{6}}{2} k \cdot +\sqrt{6} = -3k \; ; \quad |\langle -1|2\rangle|^2 = 9k^2$$

$$\langle -2|2\rangle = k \begin{vmatrix} 0 & \sqrt{6}/2 & 2 & 1 \\ \sqrt{6}/2 & 2 & \sqrt{6}/2 & 0 \\ 2 & \sqrt{6}/2 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{vmatrix} = -\frac{\sqrt{6}}{2} k \cdot -\frac{\sqrt{6}}{2} = \frac{3}{2} k \; ; \quad |\langle -2|2\rangle|^2 = \frac{9}{4} k^2$$

(22) $$\sum_{m=-2}^{2} |\langle m|2\rangle|^2 = 2 \left\{ \frac{9}{4} + \frac{36}{4} \right\} k^2 + \frac{27}{2} k^2 = 36 k^2 = 1 \; ; \quad k^2 = \frac{1}{36}$$

(23) $|\langle -2|2\rangle|^2 = |\langle 2|2\rangle|^2 = \frac{1}{16}$

$|\langle -1|2\rangle|^2 = |\langle 1|2\rangle|^2 = \frac{1}{4}$

$|\langle 0|2\rangle|^2 = \frac{3}{8}$

(24) Consider $m_0 = 1$; $\theta = \pi/2$; and $|\langle 0|1\rangle|^2$, the probability of having $m = 0$ along an axis 90° from $z_0$. That is, we have made one measurement along $z_0$ and have found $m_0 = 1$. However, we have now disturbed the system. Thus, when we make a subsequent measurement along $m$, we should have a finite probability of having $m=0$. However, $|\langle 0|1\rangle|^2 = 0$. Thus, when we make a measurement on the system and find it to have had $m_0 = 1$ along $z_0$, it destroys any chance the system had to have $m = 0$ along $z$ 90° away.

Assignment # 3
Continued

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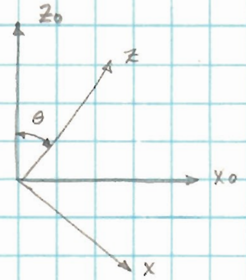
11\. a. (1) For the sake of experience, we derive a method of relating spin probabilities along the lines of problem 10 as follows:

(2)




$$|m_{s0}\rangle = \sum_{m_s} |m_s\rangle\langle m_s|m_{s0}\rangle$$

$$S_{z0}|m_{s0}\rangle = m_{s0}\hbar|m_{s0}\rangle$$

$$S_{z0} = S_z\cos\theta - S_x\sin\theta$$

(3) From results derived in class:

$$|1/2\rangle = \begin{pmatrix}1\\0\end{pmatrix} \; ; \; |-1/2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$S_+ = S_x + iS_y = \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix}$$

$$S_- = S_x - iS_y = \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix}$$

$$S_x = \frac{S_+ + S_-}{2}$$

$$\therefore \; S_{z0} = S_z\cos\theta - S_+\frac{\sin\theta}{2} - S_-\frac{\sin\theta}{2}$$

(4)
$$S_+|1/2\rangle = \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$$

$$S_+|-1/2\rangle = \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \hbar\begin{pmatrix}1\\0\end{pmatrix} = \hbar|1/2\rangle$$

$$S_-|1/2\rangle = \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \hbar\begin{pmatrix}0\\1\end{pmatrix} = \hbar|-1/2\rangle$$

$$S_-|-1/2\rangle = \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0$$

$$\therefore \; S_+|m_s\rangle = \hbar|m_s+1\rangle\,\delta_{m_s,-1/2}$$

$$S_-|m_s\rangle = \hbar|m_s-1\rangle\,\delta_{m_s,1/2}$$

(5)
$$\therefore \; \frac{S_{z0}}{\hbar}|m_{s0}\rangle = m_{s0}|m_{s0}\rangle = \sum_{m_s} m_{s0}|m_s\rangle\langle m_s|m_{s0}\rangle$$

$$= \sum_{m_s}\left\{ m_s\cos\theta\,|m_s\rangle - \frac{\sin\theta}{2}|m_s+1\rangle\,\delta_{m_s,-1/2} - \frac{\sin\theta}{2}|m_s-1\rangle\,\delta_{m_s,1/2}\right\}\langle m_s|m_{s0}\rangle$$

(6) $$\sum_{m_s} |m_s\rangle \Big\{ (m_s \cos\theta - m_{so}) \langle m_s | m_{so}\rangle - \frac{\sin\theta}{2} \langle m_s - 1 | m_{so}\rangle \, \delta_{m_s-1,\,-1/2}$$

$$- \frac{\sin\theta}{2} \langle m_s + 1 | m_{so}\rangle \, \delta_{m_s+1,\,1/2} \Big\} = 0$$

(7) $m_s = 1/2$ : $\left(m_{so} - \frac{\cos\theta}{2}\right) \langle \tfrac{1}{2} | m_{so}\rangle + \frac{\sin\theta}{2} \langle -1/2 | m_{so}\rangle = 0$

$m_s = -1/2$ : $\left(m_{so} + \frac{\cos\theta}{2}\right) \langle -\tfrac{1}{2} | m_{so}\rangle + \frac{\sin\theta}{2} \langle \tfrac{1}{2} | m_{so}\rangle = 0$

or:

$$\begin{array}{cc} \langle -\frac{1}{2} | m_{so}\rangle & \langle \frac{1}{2} | m_{so}\rangle \end{array}$$
$$\begin{vmatrix} \frac{\sin\theta}{2} & m_{so} - \frac{\cos\theta}{2} \\ m_{so} + \frac{\cos\theta}{2} & \frac{\sin\theta}{2} \end{vmatrix} = 0$$

(8) Now: $\sum_{m_s} |\langle m_s | m_{so}\rangle|^2 = |\langle -\tfrac{1}{2} | m_{so}\rangle|^2 + |\langle \tfrac{1}{2} | m_{so}\rangle|^2 = 1$

(9) $$\langle -\tfrac{1}{2} | m_{so}\rangle = \frac{\cos\theta - 2 m_{so}}{\sin\theta} \langle \tfrac{1}{2} | m_{so}\rangle$$

$$|\langle -\tfrac{1}{2} | m_{so}\rangle|^2 = \frac{\cos^2\theta - 4 m_{so} \cos\theta + 4 m_{so}^2}{\sin^2\theta} |\langle \tfrac{1}{2} | m_{so}\rangle|^2$$

(10) Plugging in (8), we have:

$$|\langle \tfrac{1}{2} | m_{so}\rangle|^2 = \frac{\sin^2\theta}{1 - 4 m_{so} \cos\theta + 4 m_{so}^2}$$

(11) $m_{so} = 1/2$ : $|\langle \tfrac{1}{2} | \tfrac{1}{2}\rangle|^2 = \frac{1}{2} \left\{ \frac{\sin^2\theta}{1 - \cos\theta} \right\} = \frac{1}{2} \{ 1 + \cos\theta \} = \cos^2\frac{\theta}{2}$

$m_{so} = -1/2$ : $|\langle \tfrac{1}{2} | -\tfrac{1}{2}\rangle|^2 = \frac{1}{2} \left\{ \frac{\sin^2\theta}{1 + \cos\theta} \right\} = \frac{1}{2} \{ 1 - \cos\theta \} = \sin^2\frac{\theta}{2}$

(12) The same result can be achieved using equation (6) of Problem 10 and taking $j = 1/2$, and $m_s = \pm 1/2$, which will give directly equations (7).

Assignment #3
Continued

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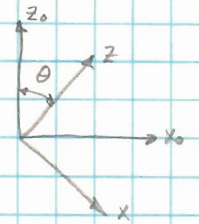
Problem 11
Continued:

11. b. (1) Recall from lecture the definition of the spinor rotation operator:

$$|m_s\rangle = e^{i\frac{\theta}{2}\bar{u}\cdot\bar{\sigma}}\,|m_{s0}\rangle$$

(2) For rotation about the y-axis:




$$\bar{u}\cdot\bar{\sigma} = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

(3) $$e^{i\theta/2\,\sigma_y} = \cos\frac{\theta}{2}\sigma_y + i\sin\frac{\theta}{2}\sigma_y$$

$$\sigma_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \therefore \quad \sigma_y^{2n} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma_y^3 = \sigma_y \;; \quad \therefore \; \sigma_y^{2n+1} = \sigma_y$$

$$\therefore \; e^{i\theta/2\,\sigma_y} = \cos\frac{\theta}{2} + i\sigma_y \sin\frac{\theta}{2}$$

$$= \begin{pmatrix} \cos\theta/2 & 0 \\ 0 & \cos\theta/2 \end{pmatrix} + \begin{pmatrix} 0 & \sin\theta/2 \\ -\sin\theta/2 & 0 \end{pmatrix} = \begin{pmatrix} \cos\theta/2 & \sin\theta/2 \\ -\sin\theta/2 & \cos\theta/2 \end{pmatrix}$$

(4) Choose $|m_{s0}\rangle = |1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$:

$$|m_s\rangle = e^{i\theta/2\,\sigma_y}\,|1/2\rangle = \begin{pmatrix} \cos\theta/2 \\ -\sin\theta/2 \end{pmatrix}$$

$$= \cos\theta/2\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \sin\theta/2\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \cos\theta/2\,|1/2\rangle - \sin\theta/2\,|-1/2\rangle$$

$$= |1/2\rangle\langle 1/2|m_s\rangle + |-1/2\rangle\langle -1/2|m_s\rangle$$

(5) Now, the probability that $m_s = 1/2$ from the measurement is:

$$\cos^2\theta/2 = |\langle 1/2|1/2\rangle|^2$$

and the probability that the measurement will give $m_s = -1/2$ is:

$$|\langle \tfrac{1}{2}|-1/2\rangle|^2 = \sin^2\theta/2$$

(6) We could also write, taking the transpose:

$$|m_{s0}\rangle = \begin{pmatrix} \cos\theta/2 & -\sin\theta/2 \\ \sin\theta/2 & \cos\theta/2 \end{pmatrix} |m_s\rangle$$

Take $|m_s\rangle = |1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\therefore\ |m_s\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix}$$

which gives the same result as before, as expected from the theorem of reciprocity (Dirac).

(7) Another way to approach the problem is to begin with $|m_{s0}\rangle$ unprepared, that is:

$$|m_{s0}\rangle = \begin{pmatrix} \psi_{0\,1/2} \\ \psi_{0\,-1/2} \end{pmatrix}, \text{ where } |\psi_{0\,1/2}|^2 = \text{prob. of spin} \uparrow$$

$$|\psi_{0\,-1/2}|^2 = \text{prob of spin} \downarrow$$

(8) From (6):

$$\begin{pmatrix} \psi_{0\,1/2} \\ \psi_{0\,-1/2} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\theta/2 \\ \sin\theta/2 & \cos\theta/2 \end{pmatrix} \begin{pmatrix} \psi_{1/2} \\ \psi_{-1/2} \end{pmatrix}$$

$$= \begin{matrix} \cos\frac{\theta}{2}\,\psi_{1/2} - \sin\theta/2\,\psi_{-1/2} \\ \sin\frac{\theta}{2}\,\psi_{1/2} + \cos\frac{\theta}{2}\,\psi_{-1/2} \end{matrix}$$

or $$\psi_{0\,1/2} = \underbrace{\cos\frac{\theta}{2}}_{\langle 1/2|1/2\rangle}\,\psi_{1/2} - \underbrace{\sin\theta/2}_{\langle -1/2|1/2\rangle}\,\psi_{-1/2}$$

$$\psi_{0\,-1/2} = \underbrace{\sin\frac{\theta}{2}}_{\langle 1/2|-1/2\rangle}\,\psi_{1/2} + \underbrace{\cos\theta/2}_{\langle 1/2|1/2\rangle}\,\psi_{-1/2}$$

which leads to the same results for the probabilities as before.

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# Physics 251b Problems, 1961

12. Enumerate the possible values of $m_{\ell a}$, $m_{sa}$ $(a=1,2,3)$ for a system of three equivalent p electrons, $(np)^3$ ('possible' means consistent with antisymmetrization of the wave functions). Determine the spectral terms that can arise from this configuration.

13. Prove Ehrenfest's theorem for the case of a particle in an electromagnetic field; i.e., from

$$\frac{d}{dt}\overline{\underline{F}} \underset{\text{(definition)}}{=} \overline{\dot{\underline{F}}} = \frac{i}{\hbar}\overline{[\underline{H}, \underline{F}]} + \overline{\frac{\partial}{\partial t}\underline{F}}$$

$$\underline{H} = \frac{1}{2m}\vec{\pi}\cdot\vec{\pi} + e\varphi, \quad \vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}$$

show that

$$\frac{d}{dt}\overline{\vec{r}} = \frac{1}{m}\overline{\vec{\pi}}$$

$$\frac{d}{dt}\overline{\vec{\pi}} = \overline{\text{(Lorentz force)}}$$

14. Consider the case of a uniform magnetic field $(0, 0, \mathcal{H})$ imposed on a spherically symmetric electric field $\varphi = \varphi(r)$. Take the vector potential to be

$$\vec{A} = \tfrac{1}{2}\mathcal{H}(\hat{k} \times \vec{r}), \text{ or } A_k = \tfrac{1}{2}\mathcal{H}\epsilon_{k3\ell}x_\ell ,$$

and define the orbital angular momentum operator as

$$\vec{\underline{L}} = \vec{r}\times\vec{p}, \text{ or } \underline{L}_k = \epsilon_{k\ell m}x_\ell p_m .$$

a) Calculate the commutators $(\underline{H}, \underline{L}_k)$, and show that

1) $\underline{L}_z$ is an exact constant of the motion.

2) The terms linear in $\mathcal{H}$ in the time derivatives of $\underline{L}_x$ and $\underline{L}_y$ are in agreement with the classical picture of the Larmor precession.

b) Show that, if terms in $\mathcal{H}^2$ are neglected, $\underline{L}^2$ is a constant of the motion.

c) The unperturbed state of an atom is that with $\mathcal{H} = 0$,

$\frac{\langle a | H^{(1)} | d \rangle}{\Delta E} \sim \frac{\langle | [H, L^2] | \rangle}{\Delta E \, \Delta L^2}$



and $\underline{L}^2$ exactly quantized. For the action of the perturbing magnetic field, the following order-of-magnitude relations hold:

$$(\text{Element of } [H, \underline{L}^2]) \sim (\text{off-diagonal element of } H) \cdot (\Delta L^2)$$

$$\Delta L^2 \sim \hbar^2$$

$$(\Delta E)\,(\mathcal{H} = 0,\ \Delta L \neq 0) \sim \frac{me^4}{\hbar^2}$$

$$\overline{x_k} \sim a_o, \quad \overline{x_k x_\ell} \sim a_o^2 \ ; \quad a_o = \frac{\hbar^2}{me^2}$$

Find the order of magnitude of the coefficient with which a wave-function of <u>different</u> $L^2$ is combined with the unperturbed wave-function. Evaluate numerically for field of 10,000 gauss.

15. For the atom in the presence of the magnetic field used in Problem 14, calculate the magnetic moment from the formula

$$\vec{\mu} = \frac{1}{2c} \int (\vec{r} \times \vec{j}) \, d\tau$$

(Here $\vec{j}$ is the 'electric current' --- probability current multiplied by charge $\underline{e}$). Express result as two terms, both involving mean values (no other integrals): one term is the value for $\mathcal{H} = 0$, the other a term proportional to $\mathcal{H}$.

Assignment #4

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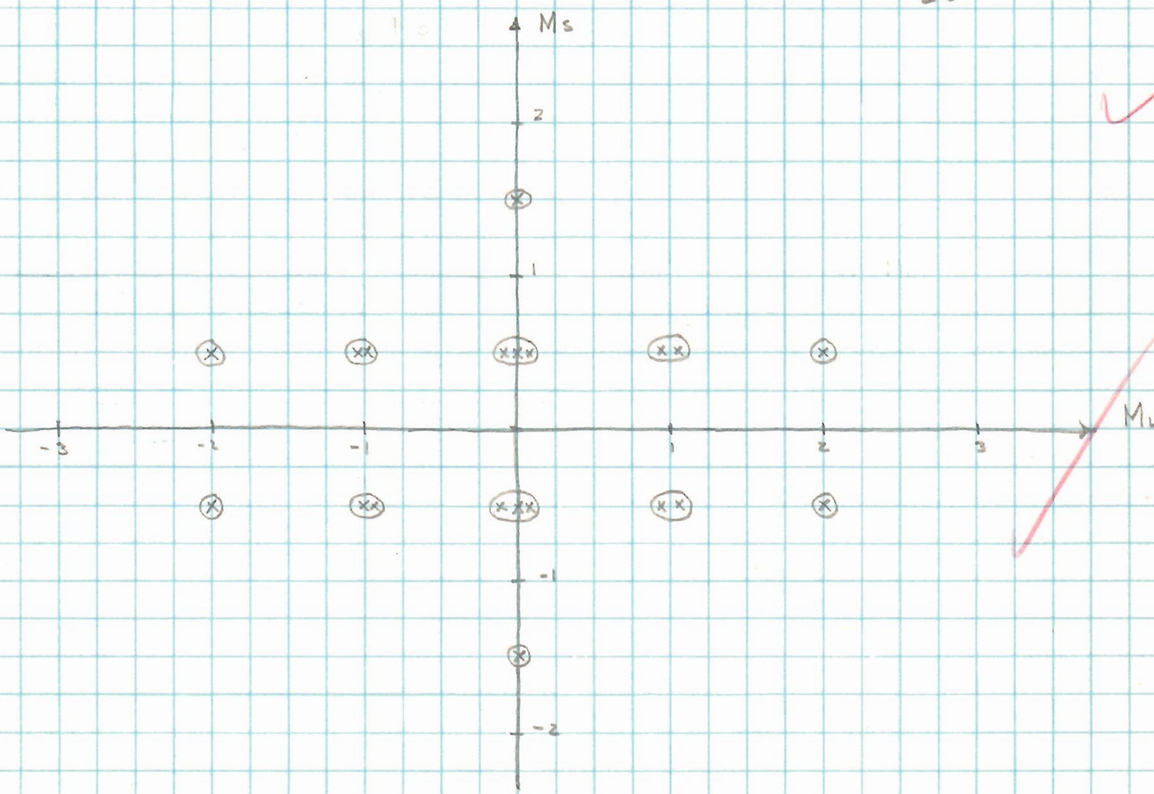
12. (1) We form antisymmetric wave functions with the use of the following table; for 3 equivalent p electrons $(np)^3$ : $M_L = 2,1,0,-1,2,3$ ; $M_S = \pm 3/2, \pm 1/2$

| $m_{l1}$ | $m_{s1}$ | $m_{l2}$ | $m_{s2}$ | $m_{l3}$ | $m_{s3}$ | Number | $M_L$ | $M_S$ |
|---|---|---|---|---|---|---|---|---|
| 1 | + | 1 | − | 0 | ± | 2 | 2 | $1/2, -1/2$ |
| 1 | + | 1 | − | −1 | ± | 2 | 1 | $1/2, -1/2$ |
| 1 | ± | 0 | − | 0 | + | 2 | 1 | $1/2, -1/2$ |
| −1 | ± | 0 | − | 0 | + | 2 | −1 | $1/2, -1/2$ |
| −1 | ± | 0 | ± | 1 | ± | 8 | 0 | $3/2, -3/2, \pm 1/2, \pm 1/2, \pm 1/2$ |
| −1 | ± | −1 | − | 0 | ± | 2 | −2 | $1/2, -1/2$ |
| −1 | ± | −1 | + | 1 | − | 2 | −1 | $1/2, -1/2$ |
| | | | | | | 20 | | |

(2)




(3) D term : $L = 2$ , $M_L = \pm 2, \pm 1, 0$ ; Multiplicity = 2 ; $^2D$
P term : $L = 1$ , $M_L = \pm 1, 0$ ; Multiplicity = 2 ; $^2P$
S term : $L = 0$ , $M_L = 0$ ; Multiplicity = 4 ; $^4S$
} Spectral terms

(4) ∴ $^2D$ ; $^2P$ ; $^4S$ are the spectral terms arising from the configuration.

Assignment #4
Continued

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13. a. (1) We have by definition:

$$\frac{d}{dt}\overline{F} = \frac{i}{\hbar}\overline{[H,F]} + \frac{\partial}{\partial t}\overline{F}$$

where $H = \frac{1}{2m}\vec{\pi}\cdot\vec{\pi} + e\varphi$ ; $\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}$

(2) $\therefore$ $H = \frac{1}{2m}\vec{p}\cdot\vec{p} - \frac{e}{2mc}\left\{\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right\} + \frac{1}{2m}\left(\frac{e}{c}\right)^2\vec{A}\cdot\vec{A} + e\varphi$

(3) In tensor notation:

$$H = \sum_i \left[\frac{p_i^2}{2m} - \frac{e}{2mc}\left\{p_iA_i + A_ip_i\right\} + \frac{\left(\frac{e}{c}\right)^2}{2m}A_i^2\right] + e\varphi$$

(4) We assume implicit time independence in all quantities:

$$\frac{\partial}{\partial t}\vec{r} = \frac{\partial}{\partial t}\vec{p} = \frac{\partial}{\partial t}\vec{A} = \frac{\partial}{\partial t}\vec{\pi} = \frac{\partial}{\partial t}\varphi = 0$$

with $A_i$ and $\varphi$ functions of position.

(5) $[p_i, x_j] = -i\hbar\,\delta_{ij}$ ; $[A_i, x_j] = 0$ ; $[\varphi, x_i] = 0$ ; $[p_i, p_i] = [x_i, x_i] = 0$

$[\varphi, A_i] = 0$

(6) $$\frac{dx_j}{dt} = \frac{i}{\hbar}[H, x_j] = \frac{i}{\hbar}\sum_i\left[\frac{[p_i^2, x_j]}{2m} - \frac{e}{2mc}\left\{[p_iA_i, x_j] + [A_ip_i, x_j]\right\}\right]$$

(7) $[p_i^2, x_j] = [p_i, x_j]p_i + p_i[p_i, x_j] = -2i\hbar\,p_i\,\delta_{ij}$

$[p_iA_i, x_j] = [p_i, x_j]A_i + p_i[A_i, x_j] = -i\hbar\,A_i\,\delta_{ij}$

$[A_ip_i, x_j] = [A_i, x_j]p_i + A_i[p_i, x_j] = -i\hbar\,A_i\,\delta_{ij}$

(8) $\therefore$ $$\frac{dx_j}{dt} = \frac{p_j}{m} - \frac{e}{c}\frac{A_j}{m} = \frac{\pi_j}{m}$$

(9) $\therefore$ $$\boxed{\frac{d}{dt}\overline{\vec{r}} = \frac{\overline{\vec{\pi}}}{m}}$$

✓

b. (1) $$\frac{d\Pi_j}{dt} = \frac{i}{\hbar}[H, \Pi_j] = \frac{i}{\hbar}\left[H, p_j - \frac{e}{c}A_j\right]$$

$$= \frac{i}{\hbar}\sum_i\left[-\frac{e}{2mc}\left\{[p_i A_i, p_j] + [A_i p_i, p_j] - \frac{e}{c}\left([p_i A_i, A_j] + [A_i p_i, A_j]\right)\right\} + \frac{1}{2m}\left(\frac{e}{c}\right)^2[A_i^2, p_j] - \frac{1}{2mc}\frac{e}{c}[p_i^2, A_j] + e[\varphi, p_j]\right]$$

(2) $$\frac{d\Pi_j}{dt} = \frac{i}{\hbar}\left[\sum_i\left[-\frac{e}{2mc}\left\{\underbrace{[p_i A_i, p_j]}_{p_i[A_i,p_j]} + \underbrace{[A_i p_i, p_j]}_{[A_i,p_j]p_i} + \underbrace{[p_i^2, A_j]}_{[p_i,A_j]p_i + p_i[p_i,A_j]} - \frac{e}{c}\left(\underbrace{[p_i A_i, A_j]}_{[p_i,A_j]A_i} + \underbrace{[A_i p_i, A_j]}_{A_i[p_i,A_j]} + \underbrace{[A_i^2, p_j]}_{[A_i,p_j]A_i + A_i[A_i,p_j]}\right)\right\}\right] + e[\varphi, p_j]\right]$$

$$= \frac{i}{\hbar}\left[\sum_i\left[-\frac{e}{2mc}\left\{p_i - \frac{e}{c}A_i\right\}\left\{\underbrace{[A_i,p_j]}_{-\frac{\hbar}{i}\frac{\partial A_i}{\partial x_j}} + \underbrace{[p_i,A_j]}_{\frac{\hbar}{i}\frac{\partial A_j}{\partial x_i}}\right\} - \frac{e}{2mc}\left\{\underbrace{[A_i,p_j]}_{-\frac{\hbar}{i}\frac{\partial A_i}{\partial x_j}} + \underbrace{[p_i,A_j]}_{\frac{\hbar}{i}\frac{\partial A_j}{\partial x_i}}\right\}\left\{p_i - \frac{e}{c}A_i\right\}\right] + e\underbrace{[\varphi,p_j]}_{-\frac{\hbar}{i}\frac{\partial\varphi}{\partial x_j}}\right]$$

$$= \frac{e}{2mc}\sum_i\left[\underbrace{\left\{p_i - \frac{e}{c}A_i\right\}}_{A}\underbrace{\left\{\frac{\partial A_i}{\partial x_j} - \frac{\partial A_j}{\partial x_i}\right\}}_{B} + \left\{\frac{\partial A_i}{\partial x_j} - \frac{\partial A_j}{\partial x_i}\right\}\left\{p_i - \frac{e}{c}A_i\right\}\right] - e\frac{\partial\varphi}{\partial x_j}$$

where use has been made of the fact that the $p$'s are differential operators. Take the mean with respect to some ket $|\xi\rangle$ and bra $\langle\xi|$:

(3) $$\frac{d\overline{\Pi_j}}{dt} = \frac{d}{dt}\langle\xi|\Pi_j|\xi\rangle = \frac{e}{mc}\sum_i\left[\langle\xi|\frac{AB + BA}{2}|\xi\rangle\right]_{i,j} - e\langle\xi|\frac{\partial\varphi}{\partial x_j}|\xi\rangle$$

(4) It is now important to determine if $\frac{AB+BA}{2}$ is Hermitian. A Hermitean operator can be written as: $\frac{AB + (AB)^+}{2}$. $(AB)^+ = B^+A^+$, so that here $A$ and $B$ must be Hermitean. $A$ is obviously Hermitian since it contains the momentum operator and a function of the coordinates $A_i$. Now: $B = \frac{\partial A_i}{\partial x_j} - \frac{\partial A_j}{\partial x_i}$ which is Hermitean as $B$ is a function of the coordinates only and real. Hence $\frac{AB+BA}{2}$ is Hermitean and its average value corresponds to the classical product $AB$, or what Schiff calls the symmetric average.

(5) Since $\vec{H} = \text{curl}\,\vec{A}$:
$$\boxed{\frac{d\overline{\vec{\Pi}}}{dt} = \frac{e}{mc}\left\{\frac{\overline{(\vec{p} - \frac{e}{c}\vec{A})\times\vec{H} - \vec{H}\times(\vec{p} - \frac{e}{c}\vec{A})}}{2}\right\} - e\,\overline{\text{grad}\,\varphi}}$$ ✓

which corresponds under the conditions stated above as to Hermiticity to:

$$\frac{d\vec{p}}{dt} = \frac{e}{c}\vec{v}\times\vec{H} + e\vec{E} \quad \text{, classically}$$ ✓

where $\frac{e}{c}\vec{v}\times\vec{H} + eE$ is the Lorentz force.

Assignment # 4
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14. a. (1) $\mathcal{H} = (0\,0\,\mathcal{H})$ ; $\varphi = \varphi(r)$ ; $\vec{A} = \frac{1}{2}\mathcal{H}(\vec{k}\times\vec{r})$ or $A_k = \frac{1}{2}\mathcal{H}\epsilon_{k3l}\,x_l$

and $\vec{L} = \vec{r}\times\vec{p}$ or $L_k = \epsilon_{klm}\,x_l\,p_m$ (sum implied on $l, m$)

where $\epsilon_{klm} = 0$ unless $klm$ all different

$1$   123, 231, 312

$-1$   132, 321, 213

(2) $$H = \sum_k \left[\frac{p_k^2}{2m} - \frac{e}{2mc}\left(p_k A_k + A_k p_k\right) + \frac{\left(\frac{e}{c}\right)^2}{2m} A_k^2\right] + e\varphi$$

(3) $$H = \sum_l \sum_k \left[\frac{p_k^2}{2m} - \frac{e}{2mc}\left(\frac{1}{2}\mathcal{H}\epsilon_{k3l}\,p_k x_l + \frac{1}{2}\mathcal{H}\epsilon_{k3l}\,x_l p_k\right)\right.$$

$$\left. + \frac{\left(\frac{e}{c}\right)^2}{2m}\cdot\frac{1}{4}\mathcal{H}^2\left(\epsilon_{k3l}x_l\right)^2\right] + e\varphi$$

$$= \sum_k \left[\frac{p_k^2}{2m} - \sum_l \frac{e\mathcal{H}}{4mc}\epsilon_{k3l}\left\{p_k x_l + x_l p_k\right\} + \sum_l \frac{\left(\frac{e}{c}\right)^2}{4m}\mathcal{H}^2\left(\epsilon_{k3l}x_l\right)^2\right]$$
$$+ e\varphi$$

(4) Now: $$L_r = \sum_s \sum_t \epsilon_{rst}\,x_s\,p_t$$

$$\therefore \left[H, L_r\right] = \sum_k \sum_s \sum_t \left[\frac{1}{2m}\epsilon_{rst}\left[p_k^2, x_s p_t\right] - \sum_l \frac{e\mathcal{H}}{4mc}\epsilon_{k3l}\epsilon_{rst}\left\{\left[p_k x_l, x_s p_t\right]\right.\right.$$

$$\left.\left. + \left[x_l p_k, x_s p_t\right]\right\} + \sum_l \frac{\left(\frac{e}{c}\right)^2\mathcal{H}^2}{4m}\epsilon_{rst}\left(\epsilon_{k3l}\right)^2\left[x_l^2, x_s p_t\right]\right] + \sum_{st} e\,\epsilon_{rst}\left[\varphi, x_s p_t\right]$$

(5) $$\left[p_k^2, x_s p_t\right] = \left[p_k^2, x_s\right]p_t = \left[p_k, x_s\right]p_k p_t + p_k\left[p_k, x_s\right]p_t$$

$$= -2i\hbar\,p_k p_t\,\delta_{ks}$$

(6) $$\left[p_k x_l, x_s p_t\right] = \left[p_k, x_s p_t\right]x_l + p_k\left[x_l, x_s p_t\right]$$

$$= \left[p_k, x_s\right]p_t x_l + p_k x_s\left[x_l, p_t\right] = -i\hbar\,p_t x_l\,\delta_{ks} + i\hbar\,p_k x_s\,\delta_{lt}$$

(7) $$\left[x_l p_k, x_s p_t\right] = \left[x_l, x_s p_t\right]p_k + x_l\left[p_k, x_s p_t\right]$$

$$= x_s\left[x_l, p_t\right]p_k + x_l\left[p_k, x_s\right]p_t = i\hbar\,x_s p_k\,\delta_{lt} - i\hbar\,x_l p_t\,\delta_{ks}$$

(8) $$\left[x_l^2, x_s p_t\right] = x_s\left[x_l^2, p_t\right] = x_s\left[x_l, p_t\right]x_l + x_s x_l\left[x_l, p_t\right] = 2i\hbar\,x_s x_l\,\delta_{lt}$$

(9) $$\left[\varphi, x_s p_t\right] = x_s\left[\varphi, p_t\right]$$

(10) $[H, L_r] = \sum_s \sum_t -\frac{i\hbar}{m} \epsilon_{rst}\, p_s p_t - \sum_l \sum_s \sum_t \frac{i\hbar e \mathcal{H}}{4mc} \epsilon_{s3l} \epsilon_{rst} \left(-p_t x_l - x_l p_t\right)$

$- \sum_k \sum_s \sum_t \frac{i\hbar e \mathcal{H}}{4mc} \epsilon_{k3t} \epsilon_{rst} \left(p_k x_s + x_s p_k\right) + \sum_k \sum_s \sum_t \frac{2i\hbar \left(\frac{e}{c}\right)^2 \mathcal{H}^2}{4m} \epsilon_{rst} \left(\epsilon_{k3t}\right)^2 x_s x_t$

$+ \sum_s \sum_t e\, x_s [\varphi, p_t]\, \epsilon_{rst}$

(11) $(x\,y\,z) \rightarrow (1\,2\,3)$

$\therefore [H, L_x] = -\frac{i\hbar}{m} \sum_s \sum_t \epsilon_{1st} p_s p_t + \frac{i\hbar e \mathcal{H}}{4mc} \sum_l \sum_s \sum_t \epsilon_{s3l} \epsilon_{1st} \left(p_t x_l + x_l p_t\right)$

$- \sum_k \sum_s \sum_t \frac{i\hbar e \mathcal{H}}{4mc} \epsilon_{k3t} \epsilon_{1st} \left(p_k x_s + x_s p_k\right) + \sum_k \sum_s \sum_t \frac{2i\hbar \left(\frac{e}{c}\right)^2 \mathcal{H}^2}{4m} \epsilon_{1st} \left(\epsilon_{k3t}\right)^2 x_s x_t$

$+ \sum_s \sum_t e\, \epsilon_{1st}\, x_s [\varphi, p_t]$

(12) $\sum_s \sum_t \epsilon_{1st} p_s p_t = p_2 p_3 - p_3 p_2 = 0$

More generally: $\sum_s \sum_t \epsilon_{rst} p_s p_t = 0$

(13) $\sum_l \sum_s \sum_t \epsilon_{s3l} \epsilon_{1st} \left(p_t x_l + x_l p_t\right)$ :

$s=1:\ 0$
$s=2:$ $\quad \sum_l \sum_t \epsilon_{23l} \epsilon_{12t} \left(p_t x_l + x_l p_t\right)$
$s=3:\ 0$

$\quad l=1: \sum_t \epsilon_{12t} \left(p_t x_1 + x_1 p_t\right)$ $\quad (p_3 x_1 + x_1 p_3) = 2 x_1 p_3$

$\quad l=2,3:\ 0$

(14) $\sum_k \sum_s \sum_t \epsilon_{k3t} \epsilon_{1st} \left(p_k x_s + x_s p_k\right)$ :

$t=1:\ 0$
$t=2:$ $\quad \sum_k \sum_s \epsilon_{k32} \epsilon_{1s2} \left(p_k x_s + x_s p_k\right)$
$t=3:\ 0$

$\quad k=1: \sum_s -\epsilon_{1s2} \left(p_1 x_s + x_s p_1\right) = \left(p_1 x_3 + x_3 p_1\right) = 2 x_3 p_1$

$\quad k=2,3:\ 0$

(15) $\sum_k \sum_s \sum_t \epsilon_{1st} \left(\epsilon_{k3t}\right)^2 x_s x_t$

$t=1:\ 0$
$t=2:$ $\quad \sum_k \sum_s \epsilon_{1s2} \left(\epsilon_{k32}\right)^2 x_s x_2$
$t=3:\ 0$

$\quad k=1 \quad \sum_s \epsilon_{1s2}\, x_s x_2 = -x_3 x_2$

$\quad k=2,3:\ 0$

(16) $\sum_s \sum_t e\, \epsilon_{1st}\, x_s [\varphi, p_t]$

$s=1:\ 0$
$s=2:$ $\quad e\, x_2 [\varphi, p_3] - e\, x_3 [\varphi, p_2]$
$s=3:$ $\quad = e \left\{ x_2 \varphi p_3 - x_2 p_3 \varphi - x_3 \varphi p_2 + x_3 p_2 \varphi \right\}$

$\quad = e \left\{ -x_2 p_3 \varphi + x_3 p_2 \varphi \right\} = e \left(x_3 p_2 - x_2 p_3\right) \varphi$

Assignment #4
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Problem 14
Continued

a. (17) $\therefore [H, L_x] = \frac{i\hbar e\mathcal{H}}{4mc}(2x_1 p_3 - 2x_3 p_1)$

$+ \frac{2i\hbar(\frac{e}{c})^2\mathcal{H}^2}{4m}(-x_3 x_2) + e(x_3 p_2 - x_2 p_3)\varphi$

$[H, L_x] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{x p_z - z p_x - \frac{e\mathcal{H}}{c} zy\right\} + e(z p_y - y p_z)\varphi$

(18) $[H, L_z] = \frac{i\hbar e\mathcal{H}}{4mc}\sum_l\sum_s\sum_t \epsilon_{s3l}\epsilon_{3st}(p_t x_l + x_l p_t)$

$- \sum_k\sum_s\sum_t \frac{i\hbar e\mathcal{H}}{4mc}\epsilon_{k3t}\epsilon_{3st}(p_k x_s + x_s p_k) + \sum_k\sum_s\sum_t \frac{i\hbar(\frac{e}{c})^2\mathcal{H}^2}{2m}\epsilon_{3st}(\epsilon_{k3t})^2 x_s x_t$

$+ \sum_s\sum_t e\,\epsilon_{3st}\, x_s[\varphi, p_t]$

(19) $\sum_l\sum_s\sum_t \epsilon_{s3l}\epsilon_{3st}(p_t x_l + x_l p_t)$

$s = 1, 2$; $s = 3 : 0$ $\Big\}$ $\sum_l\sum_t(\epsilon_{13l}\epsilon_{31t} + \epsilon_{23l}\epsilon_{32t})(p_t x_l + x_l p_t)$

$l = 1 : \quad \sum_t \epsilon_{32t}(p_t x_1 + x_1 p_t) = -(p_1 x_1 + x_1 p_1)$

$l = 2 : \quad \sum_t -\epsilon_{31t}(p_t x_2 + x_2 p_t) = -(p_2 x_2 + x_2 p_2)$

$l = 3 : 0$

(20) $\sum_k\sum_s\sum_t \epsilon_{k3t}\epsilon_{3st}(p_k x_s + x_s p_k)$

$t = 1, 2$ :; $t = 3 : 0$ $\quad \sum_k\sum_s(\epsilon_{k31}\epsilon_{3s1} + \epsilon_{k32}\epsilon_{3s2})(p_k x_s + x_s p_k)$

$s = 1 : \quad \sum_k \epsilon_{k32}(p_k x_1 + x_1 p_k) = -(p_1 x_1 + x_1 p_1)$

$s = 2 : \quad \sum_k -\epsilon_{k31}(p_k x_2 + x_2 p_k) = -(p_2 x_2 + x_2 p_2)$

$s = 3 : 0$

(21) $\sum_k\sum_s\sum_t \epsilon_{3st}(\epsilon_{k3t})^2 x_s x_t$

$t = 1, 2$ :; $t = 3 : 0$ $\quad \sum_k\sum_s\left\{\epsilon_{3s1}(\epsilon_{k31})^2 x_s x_1 + \epsilon_{3s2}(\epsilon_{k32})^2 x_s x_2\right\}$

$s = 1 : \quad \sum_k\left\{(\epsilon_{k32})^2 x_1 x_2\right\} = x_1 x_2$

$s = 2 : \quad \sum_k\left\{-(\epsilon_{k31})^2 x_2 x_1\right\} = -x_2 x_1$

(22) $\sum_s\sum_t e\,\epsilon_{3st}\, x_s[\varphi, p_t] = e\sum_t\left\{\epsilon_{31t}\, x_1[\varphi, p_t] + \epsilon_{32t}\, x_2[\varphi, p_t]\right\}$

$= e\left\{x_1[\varphi, p_2] - x_2[\varphi, p_1]\right\} = e(x_2 p_1 - x_1 p_2)\varphi$

(23) $\therefore \ [H, L_z] = e\,(y\,p_x - x\,p_y)\,\varphi$

(24) $$[H, L_y] = +\frac{i\hbar e\mathcal{H}}{4mc}\sum_l \sum_s \sum_t \epsilon_{s3l}\,\epsilon_{2st}\,(p_t x_l + x_l p_t)$$

$$-\sum_k \sum_s \sum_t \frac{i\hbar e\mathcal{H}}{4mc}\,\epsilon_{k3t}\,\epsilon_{2st}\,(p_k x_s + x_s p_k) + \sum_k \sum_s \sum_t \frac{i\hbar\left(\frac{e}{c}\right)^2\mathcal{H}^2}{4m}\,\epsilon_{2st}\,(\epsilon_{k3t})^2\,x_s x_t$$

$$+\sum_s \sum_t e\,x_s\,[\varphi, p_t]\,\epsilon_{2st}$$

(25) $\sum_l \sum_s \sum_t \epsilon_{s3l}\,\epsilon_{2st}\,(p_t x_l + x_l p_t)$ :

$s = 1$ : $\sum_l \sum_t \epsilon_{13l}\,\epsilon_{21t}\,(p_t x_l + x_l p_t)$

$s = 2, 3$ : $0$ $\qquad t = 1, 2$ : $0$

$t = 3$ : $\sum_l -\epsilon_{13l}\,(p_3 x_l + x_l p_3) = 2\,x_2\,p_3$

(26) $\sum_k \sum_s \sum_t \epsilon_{k3t}\,\epsilon_{2st}\,(p_k x_s + x_s p_k)$

$t = 1$ : $\sum_k \sum_s \epsilon_{k31}\,\epsilon_{2s1}\,(p_k x_s + x_s p_k)$

$t = 2, 3$ : $0$ $\qquad s = 1, 2$ : $0$

$s = 3$ $\quad \sum_k \epsilon_{k31}\,(p_k x_3 + x_3 p_k) = 2\,x_3\,p_2$

(27) $\sum_k \sum_s \sum_t \epsilon_{2st}\,(\epsilon_{k3t})^2\,x_s x_t$

$t = 1$ : $\sum_k \sum_s \epsilon_{2s1}\,(\epsilon_{k31})^2\,x_s x_1$

$t = 2, 3$ : $0$ $\qquad s = 1, 2$ : $0$

$s = 3$ : $\sum_k (\epsilon_{k31})^2\,x_3 x_1 = x_3 x_1$

(28) $$\sum_s \sum_t e\,\epsilon_{2st}\,x_s\,[\varphi, p_t] = e\sum_s \left\{\epsilon_{2s1}\,x_s\,[\varphi, p_1] + \epsilon_{2s3}\,x_s\,[\varphi, p_3]\right\}$$

$$= e\left\{x_3\,[\varphi, p_1] - x_1\,[\varphi, p_3]\right\} = e\left\{x_1 p_3 - x_3 p_1\right\}\varphi$$

(29) $$[H, L_y] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{y\,p_z - z\,p_y + \frac{e\mathcal{H}}{c}\,zx\right\} + e\left\{x\,p_z - z\,p_x\right\}\varphi$$

(30) Now: since $\varphi = \varphi(r) = \varphi\left(r = \sqrt{x^2+y^2+z^2}\right)$

$$p_x\,\varphi = \frac{\hbar}{i}\frac{\partial}{\partial x}\varphi = \frac{\hbar\,x}{i\,r}\,\varphi' \ ; \quad z\,p_x = \frac{\hbar}{i}\,\frac{zx}{r}\,\varphi'$$

$$p_z\,\varphi = \frac{\hbar}{i}\,\frac{z}{r}\,\varphi' \ ; \quad x\,p_z\,\varphi = \frac{\hbar}{i}\,\frac{xz}{r}\,\varphi' \ , \text{ etc.}$$

Thus, since the potential is spherical, the last potential term vanishes in each case:

(31)
$$[H, L_x] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{x\,p_z - z\,p_x - \frac{e\mathcal{H}}{c}\,zy\right\}$$
$$[H, L_y] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{y\,p_z - z\,p_y + \frac{e\mathcal{H}}{c}\,zx\right\}$$
$$[H, L_z] = 0$$

Assignment #4
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Problem 14
Continued: Check on part (a):

(1) Use the identity $\sum_{\ell} \epsilon_{j k \ell} \epsilon_{\ell m n} = \delta_{mj}\delta_{nk} - \delta_{nj}\delta_{mk}$ in a.(10); knowing that the first and last terms always vanish:

$$\frac{i\hbar e\mathcal{H}}{4mc}\left\{\sum_{\ell}\sum_{s}\sum_{t} \epsilon_{3\ell s}\epsilon_{st r}(p_t x_\ell + x_\ell p_t)\right.$$

$$\left. - \sum_{k}\sum_{s}\sum_{t}\epsilon_{k3t}\epsilon_{trs}(p_k x_s + x_s p_k) + \frac{2e\mathcal{H}}{c}\sum_{k}\sum_{s}\sum_{t}\epsilon_{rst}\epsilon_{tk3}\epsilon_{k3}\, x_s x_t\right\}$$

(2) $$\sum_{\ell}\sum_{t}(\delta_{3t}\delta_{\ell r} - \delta_{\ell t}\delta_{r3})(p_t x_\ell + x_\ell p_t)$$

$$= p_3 x_r + x_r p_3 - \delta_{r3}\sum_{\ell}(p_\ell x_\ell + x_\ell p_\ell)$$

(3) $$\sum_{k}\sum_{s}(\delta_{kr}\delta_{3s} - \delta_{3r}\delta_{ks})(p_k x_s + x_s p_k)$$

$$= p_r x_3 + x_3 p_r - \delta_{r3}\sum_{k}(p_k x_k + x_k p_k)$$

(4) $$\sum_{k}\sum_{s}\sum_{t}\epsilon_{rst}\epsilon_{3tk}\epsilon_{k3t}\, x_s x_t$$

$$= \sum_{s}\sum_{t}\epsilon_{rst}(\delta_{33}\delta_{tt} - \delta_{3t}\delta_{3t})\, x_s x_t$$

$$= \sum_{s}\sum_{t}\epsilon_{rst}\, x_s x_t - \sum_{s}\sum_{t}\delta_{3t}\epsilon_{rst}\, x_s x_t$$

$$= -\sum_{s}\epsilon_{rs3}\, x_s x_3 = -\left\{\epsilon_{r13}\, x_1 x_3 + \epsilon_{r23}\, x_2 x_3\right\}$$

$$= -\left\{\delta_{r2}\, x_1 x_3 + \delta_{r1}\, x_2 x_3\right\}$$

(5) $\therefore$ $$\boxed{[H, L_r] = \frac{i\hbar e\mathcal{H}}{4mc}\left\{(p_3 x_r + x_r p_3) - (p_r x_3 + x_3 p_r) + \frac{2e\mathcal{H}}{c}(\delta_{r2}\, x_1 x_3 - \delta_{r1}\, x_2 x_3)\right\}}$$

(6) $$[H, L_x] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{p_z x - z p_x - \frac{e\mathcal{H}}{c} y z\right\}$$

$$[H, L_y] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{y p_z - z p_y + \frac{e\mathcal{H}}{c} x z\right\}$$

$$[H, L_z] = 0$$

Assignment #4
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Problem 14
Continued

a. (32) Since $\dot{L}_z = \frac{i}{\hbar}[H, L_z] + \frac{\partial L_z}{\partial t}$ ; $\frac{\partial L_z}{\partial t} = 0$,

$$\boxed{\dot{L}_z = \frac{i}{\hbar}[H, L_z] = 0}$$ and hence is a constant of the motion.

(33) The classical equation of Larmour precession is:

$$\frac{d\vec{L}}{dt} = \vec{T} = \vec{\mu} \times \vec{\mathcal{H}} = \frac{e}{2mc}\vec{L} \times \vec{\mathcal{H}} = \frac{e}{2mc}(\vec{r} \times \vec{p}) \times \vec{\mathcal{H}}$$

$$\frac{d\vec{L}}{dt} = \frac{-e}{2mc}\vec{\mathcal{H}} \times (\vec{r} \times \vec{p}) = \frac{-e}{2mc}\left\{(\vec{\mathcal{H}} \cdot \vec{p})\vec{r} - (\vec{\mathcal{H}} \cdot \vec{r})\vec{p}\right\}$$

(34) $$\frac{d\vec{L}}{dt} = \frac{-e\mathcal{H}}{2mc}\left\{p_z \vec{r} - z\vec{p}\right\}$$

$$\frac{dL_x}{dt} = \frac{-e\mathcal{H}}{2mc}\left\{x p_z - z p_x\right\} = \frac{e\mathcal{H}}{2mc}\left\{z p_x - x p_z\right\}$$

$$\frac{dL_y}{dt} = \frac{-e\mathcal{H}}{2mc}\left\{y p_z - z p_y\right\} = \frac{e\mathcal{H}}{2mc}\left\{z p_y - y p_z\right\}$$

$$\frac{dL_z}{dt} = \frac{-e\mathcal{H}}{2mc}\left\{z p_z - z p_z\right\} = 0$$

(35) Quantum mechanically, we have:

$$\frac{dL_x}{dt} = \frac{i}{\hbar}[H, L_x] = \frac{e\mathcal{H}}{2mc}\left\{z p_x - x p_z + \frac{e\mathcal{H}}{c} z y\right\}$$

$$\frac{dL_y}{dt} = \frac{i}{\hbar}[H, L_y] = \frac{e\mathcal{H}}{2mc}\left\{z p_y - y p_z - \frac{e\mathcal{H}}{c} z x\right\}$$

which is the same as the classical motions for linear terms in $\mathcal{H}$.

---

b. (1) Now: $L^2 = L_x^2 + L_y^2 + L_z^2$

and $[H, L^2] = [H, L_x^2] + [H, L_y^2] + [H, L_z^2]$

(2) Since $[L_j, L_k] = \epsilon_{jkl} L_l$,

$$[H, L^2] = [H, L_x]L_x + L_x[H, L_x] + \cdots$$

b. (3) Since $[H, L_z] = 0$:

$$[H, L^2] = [H, L_x]L_x + L_x[H, L_x] + [H, L_y]L_y + L_y[H, L_y]$$

(4) $$[H, L_x]L_x = \frac{i\hbar e\mathcal{H}}{2mc}\left\{xp_z - zp_x - \frac{e\mathcal{H}}{c}zy\right\}\left\{yp_z - zp_y\right\}$$

$$= \frac{i\hbar e\mathcal{H}}{2mc}\left\{xp_z\,yp_z - xp_z\,zp_y - zp_x\,yp_z + zp_x\,zp_y - \frac{e\mathcal{H}}{c}\left(zy^2p_z - zy\,zp_y\right)\right\}$$

(5) $$L_x[H, L_x] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{yp_z\,xp_z - zp_y\,xp_z - yp_z\,zp_x + zp_y\,zp_x\right\} - \frac{e\mathcal{H}}{c}\left(yp_z\,zy - zp_y\,zy\right)$$

(6) $$[H, L_y]L_y = \frac{i\hbar e\mathcal{H}}{2mc}\left\{yp_z - zp_y + \frac{e\mathcal{H}}{c}zx\right\}\left\{zp_x - xp_z\right\}$$

$$= \frac{i\hbar e\mathcal{H}}{2mc}\left\{yp_z\,zp_x - yp_z\,xp_z - zp_y\,zp_x + zp_y\,xp_z - \frac{e\mathcal{H}}{c}\left(zx\,zp_x - zx\,xp_z\right)\right\}$$

(7) $$L_y[H, L_y] = \frac{i\hbar e\mathcal{H}}{2mc}\left\{zp_x\,yp_z - xp_z\,yp_z - zp_x\,zp_y + xp_z\,zp_y - \frac{e\mathcal{H}}{c}\left(zp_x\,zx - xp_z\,zx\right)\right\}$$

(8) $$[H, L^2] = \frac{i\hbar e\mathcal{H}}{2mc}\Big\{(xp_z\,yp_z - \underbrace{yp_z\,xp_z}_{xp_z\,yp_z}) + (-xp_z\,zp_y + zp_y\,xp_z)$$

$$+ (-zp_x\,yp_z + yp_z\,zp_x) + (zp_x\,zp_y - \underbrace{zp_y\,zp_x}_{zp_x\,zp_y}) + (yp_z\,xp_z - \underbrace{xp_z\,yp_z}_{yp_z\,xp_z})$$

$$+ (-zp_y\,xp_z + xp_z\,zp_y) + (-yp_z\,zp_x + zp_x\,yp_z) + (zp_y\,zp_x - \underbrace{zp_x\,zp_y}_{zp_y\,zp_x})$$

$$- \frac{e\mathcal{H}}{c}\Big[(zy\,yp_z + \underbrace{yp_z\,zy}_{p_z\,yyz}) + (-\underbrace{zp_y\,zy}_{p_y\,zzy} - \underbrace{zy\,zp_y}_{yzzp_y}) + (\underbrace{zx\,zp_x}_{xzzp_x} + \underbrace{zp_x\,zx}_{p_x\,zzx})$$

$$+ (-\underbrace{zxxp_z}_{zxxp_z} - \underbrace{xp_z\,zx}_{p_z\,xxz})\Big]\Big\}$$

(9) $$\therefore\ [H, L^2] = \frac{-i\hbar\left(\frac{e}{c}\right)^2\mathcal{H}^2}{2m}\left[\{zy, yp_z\} - \{p_yz, zy\} + \{xz, zp_x\} - \{zx, xp_z\}\right]$$

(10) Since $\frac{d}{dt}L^2 = \frac{i}{\hbar}[H, L^2]$ and $\frac{\partial}{\partial t}L^2 = 0$;

$L^2$ is a constant of the motion if terms in $\mathcal{H}^2$ are neglected.

✓

Assignment #4
Continued

Paul Grant
DEAP - AP - 16
P 2516
5-7-61

Problem 14
Continued:

c. (1) The appropriate coefficient is of the form:

$$\frac{\langle i | H^{(1)} | j \rangle}{\Delta E}$$

(2) Note that $\langle i | H | j \rangle = \langle i | H^{(0)} | j \rangle + \langle i | H^{(1)} | j \rangle$

$$= \langle i | H^{(1)} | j \rangle$$

since $\langle i |, | j \rangle$ represent states of the unperturbed system

(3) From the statement of the problem:

$$\frac{\langle i | H^{(1)} | j \rangle}{\Delta E} \sim \frac{\langle | [H, L^2] | \rangle}{\Delta E \ (\Delta L^2)}$$

(4) Now: $\langle | [H, L^2] | \rangle = \frac{-i\hbar \left(\frac{e}{c}\right)^2 \mathcal{H}^2}{2m} \left[ \overline{\{zy, yp_z\}} - \overline{\{p_y z, zy\}} + \overline{\{xz, zp_x\}} - \overline{\{zx, xp_z\}} \right]$

(5) $[H, L^2]$ may be better written:

$$[H, L^2] = \frac{-i\hbar \left(\frac{e}{c}\right)^2 \mathcal{H}^2}{2m} \left[ \{zy, L_x\} + \{zx, L_y\} \right]$$

$$\langle | [H, L^2] | \rangle = \frac{i\hbar \left(\frac{e}{c}\right)^2 \mathcal{H}^2}{2m} \left[ \overline{\{zy, L_x\}} + \overline{\{zx, L_y\}} \right]$$

(6) Taking as orders of magnitude: $L_k \sim \hbar$ ; $\overline{x_k x_l} \sim a_0^2$
$\Delta L^2 \sim \hbar^2$, $\Delta E(\mathcal{H} = 0, \Delta L \neq 0) \sim \frac{me^4}{\hbar^2}$ ; $a_0 = \hbar^2 / me^2$

$$\langle | [H, L^2] | \rangle \sim \frac{\hbar \left(\frac{e}{c}\right)^2 \mathcal{H}^2}{m} a_0^2 \hbar = \frac{\hbar^2 \left(\frac{e}{c}\right)^2 \mathcal{H}^2 a_0^2}{m}$$

(7) $$\frac{\langle i | H^{(1)} | j \rangle}{\Delta E} \sim \frac{\hbar^2 \left(\frac{e}{c}\right)^2 \mathcal{H}^2 a_0^2}{m \hbar^2 \frac{e^2}{a_0}} = \frac{\mathcal{H}^2 a_0^3}{mc^2}$$

$$\frac{\langle i | H^{(1)} | j \rangle}{\Delta E} \sim \frac{\mathcal{H}^2 a_0^3}{mc^2}$$

(8) $mc^2 \sim 10^{-6}$ erg ; $a_0^3 \sim 10^{-25}$ cm$^3$ ; $\mathcal{H}^2 \sim 10^8$

$\therefore \frac{\langle i | H^{(1)} | j \rangle}{\Delta E} \sim 10^{-11} \to 10^{-12}$, gives very small contribution to new wave function.

✓

Assignment #4
Continued

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10

15. (1) $\overline{\mu} = \frac{1}{2c} \int (\vec{r} \times \vec{J})\, d\tau$

(2) From Lecture: $\vec{J} = -\frac{i\hbar e}{2m}\left\{\psi^* \nabla \psi - \psi \nabla \psi^*\right\} - \frac{e^2}{mc}\vec{A}\,\psi^*\psi$

$= \frac{e}{2m}\left\{\psi^* \vec{p}\,\psi - \psi\,\vec{p}\,\psi^*\right\} - \frac{e^2}{mc}\vec{A}\,\psi^*\psi$

(3) $\vec{r} \times \vec{J} = \frac{e}{2m}\left\{\psi^* \vec{r}\times\vec{p}\,\psi - \psi\,\vec{r}\times\vec{p}\,\psi^*\right\} - \frac{e^2}{mc}\vec{r}\times\vec{A}\;\psi^*\psi$

$= \frac{e}{2m}\left\{\psi^* \vec{L}\,\psi - \psi \vec{L}\,\psi^*\right\} - \frac{e^2}{mc}\vec{r}\times\vec{A}\;\psi^*\psi$

(4) Now: taking components: $L_k = \sum_l \sum_m \epsilon_{klm} x_l p_m$

$(\vec{r}\times\vec{A})_k = \sum_l \sum_m \epsilon_{klm} x_l A_m$

$A_m = \frac{1}{2}\mathcal{H} \sum_s \epsilon_{m3s} x_s$

$\therefore\ (\vec{r}\times\vec{A})_k = \frac{1}{2}\mathcal{H} \sum_l \sum_m \sum_s \epsilon_{klm}\epsilon_{m3s} x_l x_s$

(5) $\therefore\ \overline{\mu}_k = \frac{e}{2c}\sum_l\sum_m\left[\frac{\epsilon_{klm}}{2m}\int \psi^* x_l p_m \psi\, d\tau - \frac{\epsilon_{klm}}{2m}\int \psi x_l p_m \psi^*\, d\tau \right.$

$\left. - \frac{e}{mc}\cdot\frac{1}{2}\mathcal{H}\sum_s \epsilon_{klm}\epsilon_{m3s}\int x_l x_s \psi^*\psi\, d\tau\right]$

(6) $\overline{\mu}_k = \frac{e}{4mc}\sum_l\sum_m \epsilon_{klm}\left[\left\{\int \psi^* x_l p_m \psi\, d\tau - \int \psi x_l p_m \psi^*\, d\tau\right\} \right.$

$\left. - \frac{e\mathcal{H}}{c}\sum_s \epsilon_{m3s}\int \psi^* x_l x_s \psi\, d\tau\right]$

(7) Consider $\int \psi x_l p_m \psi^*\, d\tau$ ; $l \neq m$

or $\frac{\hbar}{i}\int \psi \frac{\partial}{\partial x_m}(x_l \psi^*)\, d\tau = \frac{\hbar}{i}\psi x_l \psi\Big]_\tau - \frac{\hbar}{i}\int x_l \psi^* \frac{\partial \psi}{\partial x_m}\, d\tau$

$u = \psi$ $\quad dv = \frac{\partial}{\partial x_m}(x_l\psi^*)\, d\tau$

$du = \frac{\partial \psi}{\partial x_m}\, d\tau$ $\quad v = x_l \psi^*$

$= -\int \psi^* x_l p_m \psi\, d\tau$ , taking the appropriate BC.

(8) $\therefore \quad \overline{\mu_k} = \frac{e}{2mc} \sum_l \sum_m \epsilon_{klm} \left[ \int \psi^* x_l p_m \psi \, d\tau - \frac{e\mathcal{H}}{2c} \sum_s \epsilon_{m3s} \int \psi^* x_l x_s \psi \, d\tau \right]$

(9) Using $(x\,y\,z) \rightarrow (1\,2\,3)$

$$\overline{\mu_1} = \frac{e}{2mc} \sum_l \sum_m \epsilon_{1lm} \left[ \int \psi^* x_l p_m \psi \, d\tau - \frac{e\mathcal{H}}{2c} \sum_s \epsilon_{m3s} \int \psi^* x_l x_s \psi \, d\tau \right]$$

$$\sum_l \sum_m \epsilon_{1lm} \int \psi^* x_l p_m \psi \, d\tau = \sum_l \sum_m \epsilon_{1lm} \overline{x_l p_m} = \overline{L_1} = \overline{x_2 p_3} - \overline{x_3 p_2}$$

$$\sum_l \sum_m \sum_s \epsilon_{1lm} \epsilon_{m3s} \overline{x_l x_s}$$

$m = 1, 3 : 0$

$m = 2 : \quad \sum_l \sum_s \epsilon_{1l2} \epsilon_{23s} \overline{x_l x_s} = -\overline{x_3 x_1}$

or $\overline{\mu_x} = \frac{e}{2mc} \left[ \overline{L_x} + \frac{e\mathcal{H}}{2c} \overline{zx} \right]$

(10) $\sum_l \sum_m \epsilon_{2lm} \overline{x_l p_m} = \overline{L_2} = \overline{x_3 p_1} - \overline{x_1 p_3}$

$$\sum_l \sum_m \sum_s \epsilon_{2lm} \epsilon_{m3s} \overline{x_l x_s}$$

$m = 2, 3 : 0$

$m = 1 : \quad \sum_l \sum_s \epsilon_{2l1} \epsilon_{13s} \overline{x_l x_s} = -\overline{x_3 x_2}$

or $\overline{\mu_y} = \frac{e}{2mc} \left[ \overline{L_y} + \frac{e\mathcal{H}}{2c} \overline{zy} \right]$

(11) $\sum_l \sum_m \epsilon_{3lm} \overline{x_l p_m} = \overline{L_3} = \overline{x_1 p_2} - \overline{x_2 p_1}$

$$\sum_l \sum_m \sum_s \epsilon_{3lm} \epsilon_{m3s} \overline{x_l x_s}$$

$m = 3 : 0 \qquad \sum_l \sum_s \epsilon_{3l1} \epsilon_{13s} \overline{x_l x_s} = \overline{x_2^2}$

$m = 1, 2 : \qquad \sum_l \sum_s \epsilon_{3l2} \epsilon_{23s} \overline{x_l x_s} = \overline{x_1^2}$

or $\overline{\mu_z} = \frac{e}{2mc} \left[ \overline{L_z} - \frac{e\mathcal{H}}{2c} \left( \overline{y^2} + \overline{x^2} \right) \right]$

(12) $\therefore \quad \overline{\mu_k} = \frac{e}{2mc} \left[ \overline{L_k} - \frac{e\mathcal{H}}{2c} \left( \delta_{k3} \sum_l \overline{x_l^2} - \overline{x_3 x_k} \right) \right]$

or: $\overline{\vec{\mu}} = \frac{e}{2mc} \left[ \overline{\vec{L}} - \frac{e\mathcal{H}}{2c} \overline{\vec{r} \times (\vec{k} \times \vec{r})} \right]$

or: $\overline{\vec{\mu}} = \frac{e}{2mc} \left[ \int \psi^* \vec{L} \psi \, d\tau - \frac{e\mathcal{H}}{2c} \int \psi^* \vec{r} \times (\vec{k} \times \vec{r}) \psi \, d\tau \right]$

in the form requested.

10/10 ✓

P 251-b Homework

(1) $\langle \vec{p}\,| x | \vec{p}\,'' \rangle = \int \langle \vec{p}\,' | \vec{r}\,' \rangle \, d\vec{r}\,' \, \langle \vec{r}\,' | x | \vec{r}\,'' \rangle \, d\vec{r}\,'' \, \langle \vec{r}\,'' | \vec{p}\,'' \rangle$

$$= \frac{1}{h^3} \int d\vec{r}\,' d\vec{r}\,'' \, \delta(\vec{r}\,' - \vec{r}\,'') \, x' \, e^{-i\vec{p}\,'\cdot\vec{r}\,'/\hbar} \, e^{i\vec{p}\,''\cdot\vec{r}\,''/\hbar}$$

$$= \frac{1}{h^3} \int d\vec{r}\,' \, x' \, e^{-i(\vec{p}\,' - \vec{p}\,'')\cdot\vec{r}\,'/\hbar}$$

$$= -\frac{\hbar}{i} \frac{\partial}{\partial p_x'} \left\{ \frac{1}{h^3} \int d\vec{r}\,' \, e^{-i(\vec{p}\,' - \vec{p}\,'')\cdot\vec{r}\,'/\hbar} \right.$$

$$= -\frac{\hbar}{i} \frac{\partial}{\partial p_x'} \, \delta(\vec{p}\,' - \vec{p}\,'')$$

---

(2) (a) $\sum_{\xi'} \langle \xi' | F | \xi' \rangle = \sum_{\eta'\eta''} \sum_{\xi'} \langle \xi' | \eta' \rangle \langle \eta' | F | \eta'' \rangle \langle \eta'' | \xi' \rangle$

$$= \sum_{\eta'\eta''} \sum_{\xi'} \langle \eta' | F | \eta'' \rangle \langle \eta'' | \xi' \rangle \langle \xi' | \eta' \rangle$$

$$= \sum_{\eta'\eta''} \langle \eta' | F | \eta'' \rangle \, \delta_{\eta'\eta''} = \sum_{\eta'} \langle \eta' | F | \eta' \rangle$$

(b) Let $F$ be one of a complete set of mutually commuting observables $F, \alpha$. Then from part (a):

$$\sum_{\xi'} \langle \xi' | F | \xi' \rangle = \sum_{F',\alpha'} \langle F',\alpha' | F | F',\alpha' \rangle = \sum_{F'} \sum_{\alpha'} \langle F',\alpha' | F',\alpha' \rangle F'$$

$$= \sum_{F'} F' \, g(F')$$

where $g(F') \equiv \sum_{\alpha'} \langle F'\alpha' | F'\alpha' \rangle = \sum_{\alpha'} 1$ is the number of states for which the eigenvalue of $F$ is $F'$; that is, the degeneracy of $F'$.

(3) $F\xi_2 + \xi_2 F = 0$

$$0 = \langle \xi' | F\xi_2 + \xi_2 F | \xi'' \rangle = \langle \xi' | F | \xi'' \rangle (\xi_2'' + \xi_2')$$

since $\langle \xi' | \xi_2 = \xi_2' \langle \xi' |$ ; $\xi_2 | \xi'' \rangle = \xi_2'' | \xi'' \rangle$.

Hence $\langle \xi' | F | \xi'' \rangle = 0$ unless $\xi_2'' = -\xi_2'$

---

(4) $|\xi^{aj}\rangle$, $|\eta^{ak}\rangle$ are complete sets of states, related by a unitary transformation, $\langle \xi^{aj} | \eta^{ak} \rangle$. They are not necessarily orthonormal. Note that $j, k$ can take on any value. We are given two sets of $m$ states $\Phi_{\xi a k}$ ; $\Phi_{\eta a k}$ connected by the $m \times m$ unitary transformation $\langle \xi^{aj} | \eta^{ak} \rangle$ ($j, k = 1, 2, \ldots, m$). Since this is unitary:

$$\sum_{j=1}^{m} \langle \eta^{ak} | \xi^{aj} \rangle \langle \xi^{aj} | \eta^{ar} \rangle = \begin{cases} \delta_{kr} & k, r = 1, 2, \ldots, m \\ 0 & \text{otherwise} \end{cases}$$

Similarly, the second part of the hypotheses implies:

$$\sum_{j=1}^{n} \langle \eta^{bl} | \xi^{bj} \rangle \langle \xi^{bj} | \eta^{bs} \rangle = \begin{cases} \delta_{ls} & l, s = 1, 2, \ldots, n \\ 0 & \text{otherwise} \end{cases}$$

The theorem holds for any operator $F$, not necessarily Hermitean, and any value of $m$ and $n$. The completeness relation is:

$\sum_{\text{all } k} |\eta^{ak}\rangle \langle \eta^{ak}| = 1$ ; it is clear that

$\sum_{k=1}^{m} |\eta^{ak}\rangle \langle \eta^{ak}|$ is <u>not</u> the unit operator as the $m$ states are not complete.

④ The problem itself is relatively trivial:

$$\sum_{i=1}^{m}\sum_{j=1}^{n} |\langle \xi^{ai}|F|\xi^{bj}\rangle|^2 = \sum_{i=1}^{m}\sum_{j=1}^{n} \langle \xi^{ai}|F|\xi^{bj}\rangle\langle \xi^{bj}|F^{\dagger}|\xi^{ai}\rangle$$

$$= \sum_{k,l=1}^{\infty}\sum_{r,s=1}^{\infty}\sum_{i=1}^{m}\sum_{j=1}^{n} \langle \xi^{ai}|\eta^{ak}\rangle\langle \eta^{ak}|F|\eta^{bl}\rangle\langle \eta^{bl}|\xi^{bj}\rangle$$

$$\cdot \langle \xi^{bj}|\eta^{bs}\rangle\langle \eta^{bs}|F^{\dagger}|\eta^{ar}\rangle\langle \eta^{ar}|\xi^{ai}\rangle$$

$$= \sum_{k,r=1}^{m}\sum_{l,s=1}^{n} \delta_{kr}\,\delta_{ls}\,\langle \eta^{ak}|F|\eta^{bl}\rangle\langle \eta^{bs}|F^{\dagger}|\eta^{ar}\rangle$$

$$= \sum_{k=1}^{m}\sum_{l=1}^{n} \langle \eta^{ak}|F|\eta^{bl}\rangle\langle \eta^{ak}|F|\eta^{bl}\rangle^{*}$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{n} |\langle \eta^{ai}|F|\eta^{bj}\rangle|^2$$

---

⑤ From class: $f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l}\sin\delta_l\,P_l(\cos\theta)$; $P_l(1)=1$

Then $\sigma = \frac{4\pi}{k}\,\mathrm{Im}\,f(0) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$

---

⑥ Born's Approximation:

$$u^{(1)} \sim -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{i(\vec{k}_0-\vec{k})\cdot\vec{r}\,'}\,V(\vec{r}\,')\,d\tau' \quad \text{where } \vec{k} = k\hat{n}$$

Then: $f^{(1)}(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{ik_0(\hat{n}_0-\hat{n})\cdot\vec{r}\,'}\,V(\vec{r}\,')\,d\tau'$

Clearly, $f^{(1)}(0) = -\frac{m}{2\pi\hbar^2}\int V(r')\,d\tau'$ is real.

Take spherical polar coordinates $\alpha', \beta'$, the axis $\alpha'=0$ being taken in the direction of $(\hat{n}_0-\hat{n})$:

$$f^{(1)}(\theta) = -\frac{m}{2\pi\hbar^2}\int_0^{2\pi}d\beta'\int_{-1}^{1}d(\cos\alpha')\int_0^{\infty}r'^2\,dr'\,e^{ik_0|\hat{n}_0-\hat{n}|\,r'\cos\alpha'}\,V(r')$$

$$= -\frac{2m}{\hbar^2}\int_0^{\infty}\frac{\sin N k_0 r'}{N k_0 r'}\,V(r')\,r'^2\,dr' \quad \text{since } |\hat{n}_0-\hat{n}| = 2\sin\tfrac{1}{2}\theta = N$$

(6) Then: $f^{(1)}(0) = -\frac{2m}{\hbar^2}\int_0^\infty V(r')\, r'^2\, dr'$ is purely real, as is $f^{(1)}(\theta)$ for any $\theta$.

(a) $|f^{(1)}(\theta)|^2 = \frac{m^2}{4\pi^2\hbar^4}\iint d\tau' d\tau''\, V(r')V(r'')\, e^{ik_0(\hat{n}_0-\hat{n})\cdot(\vec{r}'-\vec{r}'')}$

$\sigma = \int |f^{(1)}(\theta)|^2 d\Omega = \frac{m^2}{4\pi^2\hbar^4}\iiint d\Omega\, d\tau' d\tau''\, V(r')V(r'')$

$\cdot\, e^{ik_0\hat{n}_0\cdot(\vec{r}'-\vec{r}'')}\, e^{-ik_0\hat{n}\cdot(\vec{r}'-\vec{r}'')}$

$d\Omega = d(\cos\alpha)\,d\beta$ ; $d\tau' = r'^2 dr'\, d(\cos\alpha')\, d\beta'$ ; take $\alpha = 0$ in the direction of $\vec{r}''-\vec{r}'$.

$$\sigma = \frac{m^2}{\pi\hbar^4}\iint d\tau' d\tau''\, V(r')V(r'')\, e^{ik_0\hat{n}_0\cdot(\vec{r}'-\vec{r}'')}\,\frac{\sin k_0|\vec{r}'-\vec{r}''|}{k_0|\vec{r}'-\vec{r}''|}$$

Let $\vec{r}' \equiv \rho + \vec{r}''$ ; $d\tau' = d\vec{\rho} = \rho^2 d\rho\, d(\cos\gamma)\, d\eta$ ; take $\gamma = 0$ in direction of $\hat{n}_0$.

$$\sigma = \frac{4m^2}{\hbar^4}\int d\tau''\, V(r'')\int_{-r''}^{\infty} V(|\vec{\rho}+\vec{r}''|)\,\frac{\sin^2 k_0\rho}{k_0^2\rho^2}$$

$$= \frac{4m^2}{\hbar^4}\int d\tau''\, V(r'')\int_0^\infty V(r')\,\frac{\sin^2 k_0|\vec{r}'-\vec{r}''|}{k_0^2|\vec{r}'-\vec{r}''|}\, dr'$$

$$= \frac{m^2}{\pi\hbar^4}\iint d\tau' d\tau''\, V(r')V(r'')\,\frac{\sin^2 k_0|\vec{r}'-\vec{r}''|}{k_0^2|\vec{r}'-\vec{r}''|}$$

using $\frac{1}{4\pi}\int_0^{2\pi} d\beta' \int_{-1}^{1} d(\cos\alpha') = 1$.

(b) $u^{(2)} \sim \frac{m^2}{4\pi^2\hbar^4}\frac{e^{ik_0 r}}{r}\iint d\tau' d\tau''\, V(r')V(r'')\,\frac{e^{ik_0|\vec{r}'-\vec{r}''|}}{|\vec{r}'-\vec{r}''|}$

$\cdot\, e^{-ik_0(\hat{n}\cdot\vec{r}' - \hat{n}_0\cdot\vec{r}'')}$

$f^{(2)}(0) \sim \frac{m^2}{4\pi^2\hbar^4}\iint d\tau' d\tau''\, V(r')V(r'')\,\frac{e^{ik_0|\vec{r}'-\vec{r}''|}}{|\vec{r}'-\vec{r}''|}\, e^{-ik_0\hat{n}_0\cdot(\vec{r}'-\vec{r}'')}$

$\sim \frac{m^2}{\pi\hbar^4}\int d\tau''\, V(r'')\int_{-r''}^{\infty} V(|\vec{\rho}+\vec{r}''|)\,\frac{e^{ik_0\rho}}{\rho}\,\frac{\sin k_0\rho}{k_0\rho}$

$\sim \frac{m^2}{4\pi^2\hbar^4}\iint d\tau'\, d\tau''\, V(r')V(r'')\,\frac{e^{ik_0|\vec{r}'-\vec{r}''|}}{|\vec{r}'-\vec{r}''|}\,\frac{\sin k_0|\vec{r}'-\vec{r}''|}{k_0|\vec{r}'-\vec{r}''|}$

$\sigma = \frac{4\pi}{k_0}\,\mathrm{Im}\{f^{(2)}(0)\} \sim \frac{m^2}{\pi\hbar^4}\iint d\tau' d\tau''\, V(r')V(r'')\,\frac{\sin^2 k_0|\vec{r}'-\vec{r}''|}{k_0^2|\vec{r}'-\vec{r}''|^2}$

(7) (a) Since $kr_0 \ll 1$, only $l=0$ need be considered. $\sigma = \frac{4\pi}{k^2}\sin^2\delta_0$.

Let $R_0(r) = \frac{v_0(r)}{r}$. Then $-\frac{\hbar^2}{2m} v_0'' + V_0 v_0 = E v_0 \quad (r<r_0)$

$$-\frac{\hbar^2}{2m} v_0'' = E v_0 \quad (r>r_0)$$

$r<r_0$: $v_0(r) = A\sin k'r + B\cos k'r$ where $k'^2 = \frac{2m(E-V_0)}{\hbar^2}$

" $k^2 = \frac{2mE}{\hbar^2}$

Since $R_0$ is finite at $r=0$, $B=0$. Continuity of $\frac{R'}{R}$ at $r=r_0$ gives

$r<r_0$: $R' = A\frac{k'\cos k'r}{r} - A\frac{\sin k'r}{r^2}$

$r>r_0$: $R' = C\frac{k\cos(kr+\delta_0)}{r} - C\frac{\sin(kr+\delta_0)}{r^2}$

$$\left(\frac{R'}{R}\right)_{r=r_0} = k'\cot k'r_0 - \frac{1}{r_0} = k\cot(kr_0+\delta_0) - \frac{1}{r_0}$$

$$\tan(kr_0+\delta_0) = \frac{k}{k'}\tan k'r_0$$

$$\delta_0 = -kr_0 + \tan^{-1}\left(\frac{k}{k'}\tan k'r_0\right)$$

$$= -kr_0 + \tan^{-1}\left[{}^{k}/_{k'}\tan {}^{k'}/_{k}(kr_0)\right]$$

$$\approx -kr_0 + \tan^{-1}\left\{kr_0 + {}^1/_3\, {}^{k'^2}/_{k^2}(kr_0)^3\right\}$$

But $\frac{k'^2}{k^2} = 1 - \frac{V_0}{E}$; thus:

$$\delta_0 \approx -kr_0 + \tan^{-1}\left\{kr_0 + \tfrac{1}{3}\left(1-\tfrac{V_0}{E}\right)(kr_0)^3\right\}$$

$$\approx -{}^1/_3\, {}^{V_0}/_E\,(kr_0)^3 \approx -{}^1/_3\,\frac{2mV_0}{\hbar^2}\,k r_0^3$$

$$\sigma \approx \frac{4\pi}{k^2}\delta_0^2 = \frac{16\pi m^2 V_0^2 r_0^6}{9\hbar^4}$$

(b) From problem 6: $\sigma = \frac{m^2}{\pi\hbar^4}\iint d\vec r\, d\vec r'\, V(r)V(r')\,\frac{\sin^2 k|\vec r-\vec r'|}{k^2|\vec r-\vec r'|^2}$

$$= \frac{16\pi m^2}{\hbar^4}\int_0^{r_0}\!\!\int_0^{r_0} r^2\,dr\, r'^2\,dr'\, V_0^2\,\frac{\sin^2 k|\vec r-\vec r'|}{k^2|\vec r-\vec r'|^2}$$

$$\approx \frac{16\pi m^2}{\hbar^4}\int_0^{r_0}\!\!\int_0^{r_0} r^2\,dr\, r'^2\,dr'\, V_0^2 \approx \frac{16\pi m^2 V_0^2 r_0^6}{9\hbar^4}$$

(8) $j_1 = 3/2$ ; $j_2 = 1$ : $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$. To construct $\varphi_{j,m}$.

Begin with $\varphi_{5/2,5/2} = u_{3/2} v_1$. Apply:

$M_- \varphi_{jm} = \sqrt{(j+m)(j-m+1)}\, \varphi_{j,m-1}$ and $M_- = M_{1-} + M_{2-}$

Then: get same answers as we did in homework.

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(9) $E_i \vec{r} = \hat{I}_i \times \vec{r}$ where $\hat{I}_i$ is a unit vector in the $i$ direction: Let:

$f_1 = xy$, $f_2 = yz$, $f_3 = zx$, $f_4 = (x^2 - y^2)$; $f_5 = (z^2 - x^2)$

We easily find:

| | $f_1$ | $f_2$ | $f_3$ | $f_4$ | $f_5$ |
|---|---|---|---|---|---|
| $E_x$ | $-f_3$ | $-f_4 - f_5$ | $f_1$ | $2f_2$ | $2f_2$ |
| $E_y$ | $f_2$ | $-f_1$ | $f_5$ | $2f_3$ | $-4f_3$ |
| $E_z$ | $f_4$ | $f_3$ | $-f_2$ | $-4f_1$ | $2f_1$ |

proving the set is closed. The matrix representation of $\vec{E}$ is now clearly:

$$\| E_x \| = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \end{pmatrix} ; \quad \| E_y \| = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} ; \quad \| E_z \| = \begin{pmatrix} 0 & 0 & 0 & -4 & 2 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

By direct matrix multiplication we find:

$$[E_i, E_j] = -\epsilon_{ijk} E_k$$

Letting $E_k = \frac{i}{\hbar} M_k$, we find the angular momentum commutation relations: $\vec{M} \times \vec{M} = i\hbar \vec{M}$

(10) My method is probably better. The incompatibility of measurements is probably shown most clearly in (c) where we obtain a finite probability for $M_z = 2\hbar$ in the $z$ direction, despite the fact that we knew $M_{z_0} = 2\hbar$ in the (perpendicular) $z_0$ direction, and the magnitude of the angular momentum vector must be $\sqrt{6}\,\hbar$.

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(11) $j = 1/2$ ; $m_s = \pm 1/2$

(a) $$\frac{\sin\alpha}{2}\left\{\left(\tfrac{3}{2}-m\right)\left(\tfrac{1}{2}+m\right)\right\}^{1/2}\langle m-1|m_0\rangle + (m_0 - m\cos\alpha)\langle m|m_0\rangle$$
$$+ \frac{\sin\alpha}{2}\left\{\left(\tfrac{3}{2}-m\right)\left(\tfrac{1}{2}-m\right)\right\}^{1/2}\langle m+1|m_0\rangle = 0$$

Get: $$|\langle -\tfrac{1}{2}|\pm\tfrac{1}{2}\rangle|^2 = \frac{(1\mp\cos\alpha)^2}{\sin^2\alpha}\,|\langle\tfrac{1}{2}|\pm 1/2\rangle|^2$$

Normalizing: $$|\langle\tfrac{1}{2}|\pm\tfrac{1}{2}\rangle|^2 = \frac{1\mp\cos\alpha}{2} = \begin{cases}\sin^2\frac{\alpha}{2}\\ \cos^2\frac{\alpha}{2}\end{cases}$$

(b) From class:

$$\psi' = \begin{pmatrix}\cos\frac{\alpha}{2} + i\,\mathcal{M}_z\sin\frac{\alpha}{2} & (i\mathcal{M}_x + \mathcal{M}_y)\sin\frac{\alpha}{2}\\ (i\mathcal{M}_x - \mathcal{M}_y)\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} - i\,\mathcal{M}_z\sin\frac{\alpha}{2}\end{pmatrix}\psi$$

Rotating through $\alpha$ about the $y$ axis:

$$\psi' = \begin{pmatrix}\cos\frac{\alpha}{2} & \sin\frac{\alpha}{2}\\ -\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2}\end{pmatrix}\psi$$

For $\psi = \begin{pmatrix}1\\0\end{pmatrix}$ : $\psi' = \begin{pmatrix}\cos\frac{\alpha}{2}\\ -\sin\frac{\alpha}{2}\end{pmatrix}$ : $|\langle\tfrac{1}{2}|\pm\tfrac{1}{2}\rangle|^2 = \begin{cases}\cos^2\frac{\alpha}{2}\\ \sin^2\frac{\alpha}{2}\end{cases}$

For $\psi = \begin{pmatrix}0\\1\end{pmatrix}$ : $\psi' = \begin{pmatrix}\sin\frac{\alpha}{2}\\ \cos\frac{\alpha}{2}\end{pmatrix}$ : $|\langle -\tfrac{1}{2}|\pm\tfrac{1}{2}\rangle|^2 = \begin{cases}\sin^2\frac{\alpha}{2}\\ \cos^2\frac{\alpha}{2}\end{cases}$

Physics 251b : Problem Set # 4

12. Same as own work

13. a. $[H, r_k] = \frac{1}{2m}[\pi_j\pi_j, r_k] + e[\varphi, r_k] = \frac{1}{2m}\{\pi_j[\pi_j, r_k] + [\pi_j, r_k]\pi_j\}$

$[\pi_j, r_k] = [p_j, r_k] = \frac{\hbar}{i}\delta_{jk}$

$[H, r_k] = \frac{\hbar}{mi}\pi_k \quad , \therefore \frac{d}{dt}\vec{r} = \frac{i}{\hbar}\overline{[H, \vec{r}]} = \frac{1}{m}\vec{\pi}$

b. $[H, \pi_k] = \frac{1}{2m}[\pi_j\pi_j, \pi_k] + e[\varphi, \pi_k]$

$= \frac{1}{2m}\{\pi_j[\pi_j, \pi_k] + [\pi_j, \pi_k]\pi_j\} + e\underbrace{[\varphi, p_k]}_{i\hbar\partial_k\varphi}$

$[\pi_j, \pi_k] = \frac{e}{c}\{[p_k, A_j] - [p_j, A_k]\} = \frac{e\hbar}{ic}(\partial_k A_j - \partial_j A_k)$

$[H, \pi_k] = \frac{e\hbar}{2imc}\{[\vec{\pi}\times(\nabla\times\vec{A})]_k - [(\nabla\times\vec{A})\times\vec{\pi}]_k\} - \frac{e\hbar}{i}\partial_k\varphi$

since $\vec{v} = \frac{\vec{\pi}}{m}$ ; $\vec{\mathcal{H}} = \nabla\times\vec{A}$ ; $\vec{\mathcal{E}} = -\nabla\varphi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t}$

$\therefore \frac{d}{dt}\vec{\pi} = \frac{i}{\hbar}\overline{[H, \vec{\pi}]} - \frac{e}{c}\frac{\partial\vec{A}}{\partial t}$

$= \overline{e\vec{\mathcal{E}} + \frac{e}{2c}[\vec{v}\times\vec{\mathcal{H}} - \vec{\mathcal{H}}\times\vec{v}]}$ = Lorentz Force

14. a. $H = \frac{1}{2m}p_j p_j - \frac{e\mathcal{H}}{2mc}L_z + \frac{e^2\mathcal{H}^2}{8mc^2}(x^2+y^2) + e\varphi$

$[H, L_x] = \frac{1}{2m}[p^2, L_x] - \frac{e\mathcal{H}}{2mc}\underbrace{[L_z, L_x]}_{i\hbar L_y} + \frac{e^2\mathcal{H}^2}{8mc^2}\underbrace{[y^2, L_x]}_{-2i\hbar yz}$

$= \frac{e\hbar\mathcal{H}}{2imc}L_y + \frac{e^2\hbar\mathcal{H}^2}{4imc^2}yz$

14. $[H, L_y] = \frac{-e\hbar\mathcal{H}}{2imc} L_x - \frac{e^2\hbar\mathcal{H}^2}{4imc^2} xz$

$[H, L_z] = \frac{e^2\mathcal{H}^2}{8mc^2}\left[(x^2+y^2), L_z\right] = \frac{e^2\mathcal{H}^2}{8mc^2}\left[\frac{\hbar}{i}2xy - \frac{\hbar}{i}2xy\right] = 0$

$\therefore$ $L_z$ is an exact constant of the motion.

$\dot{L}_x \sim \frac{e\mathcal{H}}{2mc} L_y = \omega_L L_y$

$\dot{L}_y \sim -\frac{e\mathcal{H}}{2mc} L_x = -\omega_L L_x$

$\dot{L}_z = 0$

(b) To first order in $\mathcal{H}$:

$[H, L^2] = [H, L_x^2] + [H, L_y^2] = \frac{e\hbar\mathcal{H}}{2imc}\{L_x, L_y\}$

$- \frac{e\hbar\mathcal{H}}{2imc}\{L_x, L_y\} = 0$

(c) Let $C_{ba} = \frac{H_{ba}}{E_a - E_b}$

$\langle b|[H, L^2]|a\rangle = \langle b|HL^2 - L^2H|a\rangle = \Delta L^2 H_{ba} \sim \hbar^2 H_{ba}$

$[H, L^2]_{ba} \sim \frac{\hbar\alpha^2}{m}\overline{2r_e}\,\hbar \sim \frac{\hbar^2\alpha^2 a_0^2}{m}$

$E_a - E_b \sim \frac{e^2}{a_0} = \frac{me^4}{\hbar^2}$

$\therefore C_{ba} \sim \frac{\alpha^2 a_0^3}{me^2} = \frac{a_0^3 r_0}{4\alpha\hbar c}\mathcal{H}^2 \sim 10^{-11}$

15. $$\vec{j} = \frac{e\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{e^2}{mc}\vec{A}\,\psi^*\psi$$

$$\vec{r}\times\vec{j} = \frac{e}{2m}\left\{\psi^*(\vec{r}\times\vec{p})\psi + \psi(\vec{r}\times\vec{p})^*\psi^*\right\}$$

$$- \frac{e^2\mathcal{H}}{2mc}\left[r^2\vec{\mathcal{H}} - (\vec{r}\cdot\vec{\mathcal{H}})\vec{r}\right]\psi^*\psi$$

$$\vec{\mu} = \frac{1}{2c}\int(\vec{r}\times\vec{j})\,d\tau$$

$$= \frac{e}{4mc}\left\{\int\psi^*\vec{L}\psi\,d\tau + \left[\int\psi^*\vec{L}\psi\,d\tau\right]^*\right\} - \frac{e^2\mathcal{H}}{4mc^2}\int\psi^*(r^2\vec{h} - z\vec{r})\psi\,d\tau$$

$$= \frac{e}{2mc}\langle\vec{L}\rangle - \frac{e^2\mathcal{H}}{4mc^2}\left\{\langle r^2\rangle\vec{h} - \langle z\vec{r}\rangle\right\}$$