Ph 205a "ADVANCED QUANTUM MECHANICS"

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I. Time-Dependent Perturbation Theory

Ph 205a ADVANCED QUANTUM MECHANICS

R.P. Feynman

I. Scattering

II. Solid State Physics

III. Relativistic Quantum Theory

Find a relativistically invariant S-equation. *

9/27/66

TIME-DEPENDENT PERTURBATION THEORY

A. FIRST-ORDER PERTURBATION THEORY

1) The time evolution of a state is given by

$$-\frac{1}{i}\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle \qquad (1)$$ ‡

Now suppose that somehow we can split up $H(t)$ into a constant part and a small time-varying part:

$$H(t) = H_0 + V(t) \qquad (2)$$

First consider the related problem for $V \equiv 0$

$$-\frac{1}{i}\frac{\partial}{\partial t}|\psi_0(t)\rangle = H_0|\psi_0(t)\rangle \qquad (3)$$

* all problems are denoted by ◀, and are to worked without reference to books.

‡ here $\hbar = c = 1$

Assume we can solve this by

$$|\psi_0(t)\rangle = \sum_n c_n(t)\, |\phi_n\rangle \tag{4}$$

where the $|\phi_n\rangle$ are defined by the eigenvalue problem

$$H_0|\phi_n\rangle = E_n|\phi_n\rangle \tag{5}$$

and

$$c_n(t) = \langle\phi_n|\psi_0(t)\rangle \tag{6}$$

If we plug our expansion (4) into (3) we find

$$-\frac{1}{i}\frac{dc_n}{dt} = E_n c_n(t)$$

or solving directly

$$c_n(t) = a_n e^{-iE_n t} \tag{7}$$

Since this worked for $V(t) = 0$, suppose we try it again for <u>$V(t)$ small</u>

$$-\frac{1}{i}\partial_t|\psi(t)\rangle = [H_0 + V(t)]\,|\psi(t)\rangle \tag{8}$$

and write again

$$\psi(t) = \sum_n c_n(t)\,|\phi_n\rangle \tag{9}$$

Substitute into (8)

$$\sum_n -\frac{1}{i}\dot{c}_n(t)|\phi_n\rangle = \sum_n c_n(t)\, H_0|\phi_n\rangle + \sum_n c_n(t) V(t)|\phi_n(t)\rangle \tag{10}$$

Take the scalar product with $\langle \psi_m |$ and use orthogonality to find

$$-\frac{1}{i}\dot{C}_m(t) = E_m C_m(t) + \sum_n C_n(t) \underbrace{\langle m|V(t)|n\rangle}_{V_{mn}(t)} \tag{11}$$

Now if $V(t)$ is small, try a solution like

$$C_m(t) = e^{-iE_m t}\,\gamma_m(t) \tag{12}$$

Note: $|C_m(t)|^2 = |\gamma_m(t)|^2 =$ prob. of being in state m at time t

i.e. $\gamma_m(t)$ differs from $C_m(t)$ by only a phase factor.

Plug this into (11)

$$-\frac{1}{i}\dot{\gamma}_m(t) = \sum_n \gamma_n(t) \underbrace{e^{i(E_m - E_n)t}\langle m|V(t)|n\rangle}_{\tilde{V}_{mn}(t)} \tag{13}$$

$$= \sum_n \tilde{V}_{mn}(t)\,\gamma_n(t) \tag{14}$$

This is still exact and is just a system of first order ODE's.
But far from solvable exactly.

Consider a special problem:

At $t=0$ we know we have state k. We want the amplitude at time T that we are in state ℓ, i.e.

$$\lambda_{\ell k} = \langle \ell | V(T) | k \rangle = \mathcal{F}\{\langle \phi_\ell | V | \phi_k \rangle\}$$

Claim: If we can solve this problem for given k & ℓ, we can solve it for any k, ℓ. ◀

Thus our initial condition becomes

$$t=0: \qquad \gamma_s(0) = \delta_{sk}$$

The idea is to use an iterative process, i.e. integrate (14) for $\gamma_m(t)$ and use various approximations to the integrand obtained from a lower order iteration. Thus in general

$$\gamma_m(t) = \gamma_m(0) - i\int_0^t \sum_n v_{mn}(t') \left[\gamma_n(0) - i\int_0^{t'} \sum_k v_{nk}(t'')\,\gamma_k(t'')\,dt''\right] dt'$$

$$= \gamma_m(0) - i\left(\int_0^t \sum_n v_{mn}(t')\,dt'\right)\gamma_n(0)$$

$$+ (-i)^2\left(\int_0^t dt' \int_0^{t'} dt'' \sum_n \sum_k v_{mn}(t')\,v_{nk}(t'')\right)\gamma_k(0)$$

$$+ (-i)^3 \int_0^t dt' \int_0^{t'} dt'' \int_0^{t''} dt''' \sum_n \sum_k \sum_\ell v_{mn}(t')\,v_{nk}(t'')\,v_{k\ell}(t''')\,\gamma_\ell(0)$$

$$+ \cdots$$

$$\cdots + (-i)^N \int_0^t dt' \cdots \int_0^{t^{[N-1]}} dt^{[N]} \sum_n \cdots \sum_N v_{mn}(t') \cdots v_{w-1,N}(t^{[N]})\, \gamma_N(0) + \cdots \quad (15)$$

Now using our i.c. $\gamma_s(0) = \delta_{sk}$ in our general "solution" for γ_m

$$\lambda_{lk} = \langle l | V(T) | k \rangle$$

$$= \gamma_l(T)$$

$$= \delta_{lk} + (-i) \int_0^T \sum_n v_{ln}(t')\, \delta_{nk}\, dt' + (-i)^2 \int_0^T dt' \int_0^{t'} dt'' \sum_n \sum_s v_{l,n} v_{ns}\, \delta_{sk} + \cdots$$

$$= \delta_{lk} + (-i) \int_0^T v_{lk}(t')\, dt' + (-i)^2 \int_0^T dt' \int_0^{t'} dt'' \sum_n v_{ln}(t') v_{nk}(t'') + \cdots \quad (16)$$

Now suppose our perturbation was <u>constant</u>, i.e. $V(t) = V$. Then

$$v_{mn}(t) = V_{mn} e^{i(E_m - E_n)t}$$

and from (16),

$$\lambda_{lk} = \delta_{lk} + (-i) \int_0^T V_{lk} e^{i(E_l - E_k)t}\, dt + \cdots$$

$$= \delta_{lk} - \frac{e^{i(E_l - E_k)t} - 1}{(E_l - E_k)} V_{lk} + \cdots \quad (17)$$

Thus

$$\left\{\begin{matrix}\text{prob. } k \to \ell \\ \text{for } k \neq \ell\end{matrix}\right\} = |\lambda_{\ell k}|^2$$

$$= 4 \frac{\sin^2 \frac{(E_\ell - E_k)T}{2}}{(E_\ell - E_k)^2} |V_{\ell k}|^2 + \cdots \qquad (18)$$

What is wrong with this? ◀

SUMMARY TO DATE

9/30/66 LECTURE

Problem: $-\frac{1}{i}\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$

Approach: Let $H(t) = H_0 + V(t)$

$$\Rightarrow \quad H_0|\phi_n\rangle = E_n|\phi_n\rangle$$

Write $|\psi(t)\rangle = \sum_n \gamma_n(t) e^{-iE_n t}|\phi_n\rangle$

Then find

$$i\dot{\gamma}_m(t) = \sum_n v_{mn}(t)\gamma_n(t)$$

where $v_{mn}(t) = e^{-iE_m t}\langle\phi_m|V(t)|\phi_n\rangle e^{iE_n t}$

$$= e^{i(E_n - E_m)t}\langle\phi_m|V(t)|\phi_n\rangle$$

Solution:

$$\gamma_m(t_f) = \sum_n \lambda_{mn}\gamma_n(t_i) \tag{19}$$

That is if $\gamma_n(t_i)$ is the coefficient γ_n at initial time, then the coefficient γ_m at final time is equal to the sum of each of the initial values $\gamma_n(t_i)$ times the amplitude that the state will go into $\gamma_m(t_f)$ at final time. Evidently $\lambda_{mn} = \lambda_{mn}(t_i, t_f)$. We found

$$\lambda_{mn}(t_i;t_f) = \delta_{mn} - i\int_{t_i}^{t_f} v_{mn}(t)dt + (-i)^2 \int_{t_i}^{t_f}\int_{t_i}^{t_1} \sum_k v_{mk}(t_1)v_{kn}(t_2)\,dt_1 dt_2 \qquad t_f > t_1 > t_2 > t_i$$

$$+ (-i)^3 \int_{t_i}^{t_f}\int_{t_i}^{t_1}\int_{t_i}^{t_2} \sum_k \sum_l v_{mk}(t_1)v_{kl}(t_2)v_{ln}(t_3)\,dt_1 dt_2 dt_3 \qquad t_f > t_1 > t_2 > t_3 > t_i \tag{20}$$

$$+ \cdots$$

This is a very important expression and is commonly referred to as the Born expansion.

Suggested Exercises

i.) play a few games with (20) until you understand it. Perhaps write it in a better notation.

ii.) Study its properties – run backwards in time, say given $\chi_m(t_f)$ and see what you can find out about $\chi_n(t_i)$

iii.) Check fact that total probability = 1. How does this affect λ_{mn}?

iv.) If $V(t) = V$, can we compare work to energy perturbation theory? (time integrals)

v.) make up several problems (masers, etc.) and work them

2.) The First Born Approximation

Now we will consider cases where just the first integral term in (20) is important. Later we will look into the higher order terms.

Return to the d.c. potential where

$$V_{mn}(t) = e^{i(E_m - E_n)t} V_{mn}$$

We find from (20)

$$\lambda_{mn} = \frac{e^{i(E_m - E_n)t_f} - e^{i(E_m - E_n)t_i}}{(E_m - E_n)} V_{mn} \qquad m \neq n$$

Last time we had

$t_i = 0$

$t_f = T$

Now setting $t_f - t_i = T$, we find

$$\text{Prob}_{n \to m} = |\lambda_{mn}|^2 = \frac{4 \sin^2 \frac{(E_m - E_n)}{2} T}{(E_m - E_n)^2} |V_{mn}|^2 \qquad (21)$$

Note this depends only on the relative time T, not on when we turn V on.

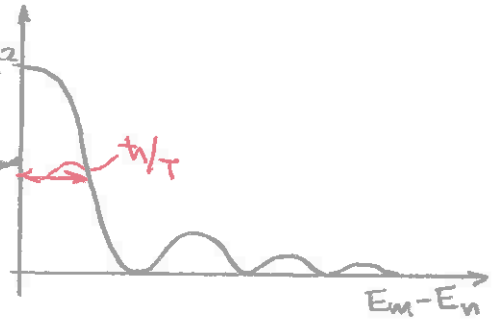
Of course we can see that if $E_m - E_n$ is very large, $\text{Prob}_{m\to n}$ is very small.

Note if $m = n$, we get a $\text{Prob} \sim T^2 |V_{mm}|^2$ dependence for small T. For larger T we need higher order terms.

To handle closely spaced levels, i.e. levels which in the limit form a continuum, we reason as follows. Our relation (21) for $\text{Prob}_{n\to m}$ gets into trouble since it is too "precise". We smear out our application of the final state a little and accept the probability of going into a range of states. Then

$$\text{Prob}_{n\to \leq m} = \sum_m \text{Prob}_{n\to m} = \sum_m \frac{4\sin^2\left(\frac{E_m - E_n}{2}\right)T}{(E_m - E_n)^2} |V_{mn}|^2$$

Now look at these terms. As T gets large, the details get squeezed in and don't matter very much, so we can take its value at $E_m = E_n$ by the limit $\sum \to \int$ and all of the contribution to the integral comes from near $E = E_n$:



$$\int_{\pi/T \to -\infty}^{\pi/T \to \infty} \frac{4\sin^2\frac{(E-E_n)T}{2}}{(E-E_n)^2} d(E-E_n) = 2T \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = 2\pi T$$

Thus we can interpret the individual probabilities and rates as

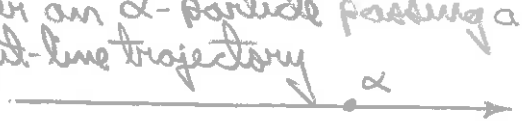
$$\underset{n\to m}{\text{Rate}} = P_{n\to m}/_{\text{sec}} = 2\pi \delta(E_m - E_n) |V_{mn}|^2 \qquad (22)$$

Fermi's Golden Rule

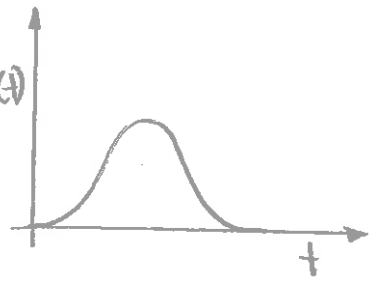
This doesn't always hold (but OK 99% of time). We can modify this to handle a continuum distribution of the initial states too.

EXAMPLE: Coulomb Excitation

Consider an α-particle passing a nucleus (assume a straight-line trajectory



The nucleus sees a time-dependent Coulomb potential $V(t)$ from the α. Sometimes this potential can excite the nucleus ("Coulomb excitation").



Consider $t_i = -\infty$ before collision

$t_f = +\infty$ after collision

[Now as $t_i \to -\infty$, $t_f \to +\infty$, the λ_{mn} is frequently denoted by S_{mn} in the literature. Thus the origin of <u>S-matrix terminology</u>.]

For $m \neq n$

$$S_{mn} = -i \int_{-\infty}^{\infty} e^{i(E_m - E_n)t} V_{mn}(t)\, dt \qquad \text{from eqn. (20)} \qquad (23)$$

where $\langle \varphi_m | V(t) | \varphi_n \rangle = V_{mn}(t)$

But recall the Fourier transform is defined by

$$\Phi(\omega) = \mathcal{F}\{f(t)\} = \int_{-\infty}^{\infty} e^{i\omega t} f(t)\, dt$$

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

We could define the Fourier transform of an operator

$$V^{FT}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} V(t)\, dt$$

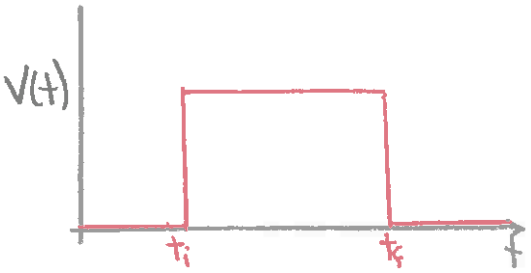
Thus

$$S_{mn} = -i \langle m | V^{FT}(\omega) | n \rangle \qquad (24)$$

$$\omega = E_m - E_n$$

Try to write series (20) for λ_{mn} or S_{mn} as Fourier transforms.

But suppose we try a V(t) as shown. Then



$$V^{FT}(\omega) = \frac{e^{i\omega T} - 1}{i\omega}$$

which is what we found earlier. Thus we can adapt the S-matrix to finite time intervals by inventing a V(t) which is turned on and off at finite times. If it makes the analytic work easier, we could smooth the square wave out.

Try to do the coulomb excitation calculation in detail (Pretty hard unless we assume straight trajectories).

3) Space-limited Central Potentials

What happens when a particle is deflected? We want the

$$\text{Prob}_{\vec{k}\to\vec{k}'}/\text{sec} = \text{Rate}_{\vec{k}\to\vec{k}'}$$

Here we write $$H = \frac{p^2}{2m} + V(r) = \underbrace{\frac{\hbar^2}{2m}\nabla^2}_{H_0} + \underbrace{V(r)}_{V}$$

Our unperturbed eigenfunctions satisfy the free-wave equation

$$H_0|\phi_n\rangle = \frac{\hbar^2}{2m}\nabla^2|\phi_n\rangle$$

Thus we identify $$|\phi_n\rangle = |\vec{k}\rangle$$

$$|\phi_m\rangle = |\vec{k}'\rangle$$

and in $\vec{r}$ representation

$$\langle\vec{r}|\vec{k}\rangle = \psi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\text{vol}}}$$

[Note we have used volume normalization of the plane wave $\psi_{\vec{k}}(\vec{r})$.]

$$\langle\vec{r}|\vec{k}'\rangle = \psi_{\vec{k}'}(\vec{r}) = \frac{e^{i\vec{k}'\cdot\vec{r}}}{\sqrt{\text{vol}}}$$

Then $$H_0|\vec{k}\rangle = \frac{k^2}{2m}|\vec{k}\rangle = E_n|\vec{k}\rangle$$

Now we can compute

$$V_{mn} = \langle m|V|n\rangle = \langle \vec{k}'|V|\vec{k}\rangle$$

$$= \int_{vol} \psi^*_{\vec{k}'}(\vec{r})\, V(r)\, \psi_{\vec{k}}(\vec{r})\, d^3\vec{r}$$

$$= \int_{vol} e^{-i\vec{k}'\cdot\vec{r}}\, V(r)\, e^{i\vec{k}\cdot\vec{r}}\, \frac{d^3\vec{r}}{(vol)}$$

But we can define a 3-dimensional Fourier transform by

$$V^{FT}(\vec{q}) = \int_{vol} e^{i\vec{q}\cdot\vec{r}}\, V(\vec{r})\, d^3\vec{r}$$

Thus

$$V_{mn} = \frac{V^{FT}(\vec{k}'-\vec{k})}{vol}$$

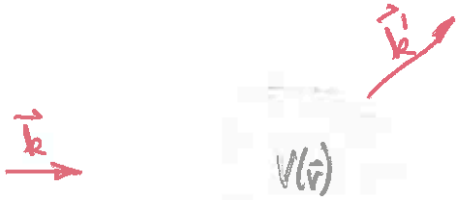
Try to plug this back into our work and finish the problem. Find the apparent scattering cross-section $\frac{d\sigma}{d\Omega}$ [not easy]

10/2/66 LECTURE

Recall we had found

$$\left\{\begin{array}{l}\text{Rate at which a system}\\ \text{is transferred from}\\ \text{state } n \text{ to } m \text{ by a}\\ \text{perturbation}\end{array}\right\} = 2\pi\,\delta(E_n - E_m)\,|\langle m|V|n\rangle|^2 \qquad (1)$$

We were considering scattering from a space-limited central potential $V(\vec{r})$



$$E_n = \frac{k^2}{2m} \qquad \varphi_n = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{vol}}$$

Thus our matrix elements are

$$V_{mn} = \frac{1}{vol}\int e^{-i\vec{k}'\cdot\vec{r}}\, e^{i\vec{k}\cdot\vec{r}}\, V(\vec{r})\, d^3\vec{r} = \frac{1}{vol}\, V^T(\vec{q}) \qquad (2)$$

$$\vec{q} = \vec{k}' - \vec{k}$$

EXAMPLE: Coulomb potential $V(\vec{r}) = \frac{Ze^2}{r}$ ∓

$$V^T(\vec{q}) = \iiint e^{i\vec{q}\cdot\vec{r}}\,\frac{Ze^2}{r}\,d^3\vec{r} = \frac{4\pi Ze^2}{q^2} \qquad (3)$$

∓ q_e is charge, $\frac{q_e^2}{4\pi\epsilon_0} = e^2$, $\frac{e^2}{\hbar c} = \frac{1}{137.0365}$

Thus using (1)

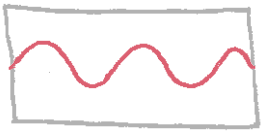
$$\text{Rate}_{\vec{k}\to\vec{k}'} = 2\pi\,\delta\left[\frac{k'^2}{2m} - \frac{k^2}{2m}\right] \frac{1}{(\text{vol})^2}\,|\tilde{V}(q)|^2$$

Note the δ-fcn implies $|\vec{k}| = |\vec{k}'| \Rightarrow$ conservation of energy. However we are actually interested in the probability of transition to some state in the neighborhood of $\vec{k}'$. Thus we need the state density about $\vec{k}'$ for a free particle.

We want to show

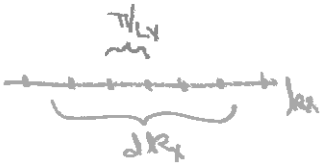
$$\text{No. of states having } \vec{k} \text{ in range } dk_x dk_y dk_z = \frac{d^3k\ (\text{vol})}{(2\pi)^3}$$

Consider a rectangular box and quantize the wave fcn as shown



$\sin k_x x \Rightarrow k_x L_x = n_x \pi$

L_x



$$\text{no. of states in } dk_x = \frac{dk_x}{\pi/L_x}$$

Thus

$$\text{no. of states in } d^3k = \frac{dk_x}{\pi/L_x}\,\frac{dk_y}{\pi/L_y}\,\frac{dk_z}{\pi/L_z} = \frac{d^3k\ (\text{vol})}{\pi^3}$$

But these are standing waves composed of two $e^{\pm ikx}$ waves which come from periodic b.c. Thus factors of $\frac{1}{2}$ give the required expression.

Thus

$$\underset{\vec{k}\to\vec{k}'}{\text{Rate}} = 2\pi\delta\left[\frac{k'^2}{2m} - \frac{k^2}{2m}\right] \frac{1}{\text{vol}} \frac{d^3k'}{(2\pi)^3} |V^T(q)|^2 \tag{4}$$

We are actually interested in scattering into a solid angle $d\Omega$. Thus we integrate (4) over k', using $d^3k' = k'^2 dk' d\Omega$.

Use

$$\int \delta[f(x)]\, \phi(x)\, dx = \frac{\phi(x_0)}{|f'(x_0)|} \tag{5}$$

where $f(x_0) = 0$

Note: if $f(x) = 0$ at several points x_i, we get a sum of terms.

$$\underset{\text{scattering into } d\Omega}{\text{Rate}} = \frac{2\pi}{\text{vol}} \frac{k^2}{2k/2m}\, d\Omega\, |V^T(q)|^2 \qquad \text{where } q \Rightarrow |\vec{k}'| = |\vec{k}|$$

We now introduce the concept of a cross-section: imagine an effective area which intersects the vol of $V(\vec{r})$. If we use

$\vec{k} \longrightarrow$ ||<- σ

$$v = \frac{dE}{dk} = \frac{k}{m}$$

in a time T, particle moves vT. Thus the effective volume is $\sigma v T$. But plane wave prob. in $cc = 1/\text{vol}$.

$$\therefore \text{Prob} = \frac{\sigma v T}{\text{vol}} \qquad \text{Rate} = \frac{\sigma v}{\text{vol}}$$

Thus

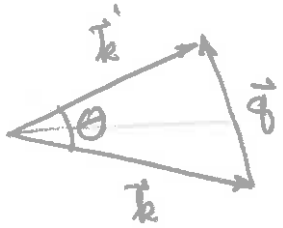
$$v\,d\sigma = \frac{mk}{4\pi^2}\,d\Omega\,|V^T(q)|^2$$

Note: the vol always cancels out. FORGET IT in the future and just normalize wave functions per unit vol.

Also E & k always appear with $\frac{1}{2\pi}$. Also $2\pi\,\delta(E_n - E_n)$, since δ-fcn involves $\frac{d}{dE}$.

EXAMPLE: Coulomb case.

$$V^T = \frac{4\pi Z e^2}{q^2}$$



$$q^2 = 4\sin^2\theta\,(2k^2)$$

$$= 2k^2(1-\cos\theta)$$

Thus

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2}\,\frac{mk}{\hbar}\,\frac{16\pi^2 Z^2 e^4}{16\left(\sin^4\theta/2\right)k^4}$$

This is Rutherford's law. Just a coincidence that this agrees with classical result. Accident & minus minus. But note:

classical works if slow, V large

first Born approx' if v high, V low

4.) Oscillating Perturbation

$$\underset{n\to m}{\text{Prob}} = \left| \int_{t_i}^{t_f} \langle m|v(t)|n\rangle \, dt \right|^2$$

Now take $V(t) = 2V_0 \cos\omega t$

Then

$$\langle m|v(t)|n\rangle = e^{-i(E_m - E_n)t} \, 2\cos\omega t \, \langle m|V_0|n\rangle$$

Upon integrating we find things like

$$\left[\frac{e^{-i(E_m - E_n - \omega)t_f} - e^{+i(E_m - E_n - \omega)t_i}}{E_m - E_n - \omega} + \frac{e^{-i(E_m - E_n + \omega)t_f} - e^{+i(E_n - E_n + \omega)t_i}}{E_m - E_n + \omega} \right]^2$$

For large T we can show cross-terms ~ 0 upon proper averaging. For continuum transitions

$$\underset{n\to m}{\text{Rate}} = 2\pi \delta(E_m - E_n - \hbar\omega) \, |(V_0)_{mn}|^2 + 2\pi\delta(E_m - E_n + \hbar\omega) \, |(V_0)_{mn}|^2$$

PROBLEM: Consider an H atom in the ground state. Consider the prob. of exciting this atom and emitting an electron when using an oscillating wave like field [disregard quantum nature of field -- assume it is very strong]. Do as detailed as you can. Various directions, etc.

10/3/66 LECTURE

Comment: Say we wish to compute the rate of transitions to a set of states m, e.g.

$$\underset{n\to(\text{set of } m)}{\text{Rate}} = \sum_m \underset{n\to m}{\text{Rate}} = \sum_m 2\pi\delta(E_m - E_n)\,|V_{mn}|^2$$

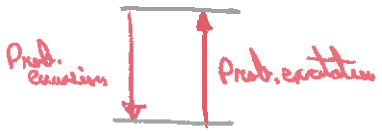
$$\to \int dE_m\, \rho(E_m)\, 2\pi\delta(E_m - E_n)\,|V_{mn}|^2 = 2\pi\,\rho(E_n)\,|V_{mn}|^2$$

which is the form of Fermi's golden rule to which we are more accustomed.

Recall we had found

$$\underset{n\to m}{\text{Rate}} = 2\pi\delta(E_m - E_n - \hbar\omega)\,|V_{mn}|^2 + 2\pi\delta(E_m - E_n + \hbar\omega)\,|V_{mn}|^2$$

We can see the prob of excitation = prob of emission if the state populations are identical



EXAMPLE: Consider an atom in an electric field

$$V = (2\cos\omega t\ \mathcal{E}_0)\,z$$

What is prob. of being excited to 1st excited state?

$$\underset{0\to m}{\text{Rate}}_{\text{ground}\to\text{ex}} = 2\pi\,\delta(E_m - E_0 - \hbar\omega)\,|z_{mn}|^2\,\mathcal{E}_0^2$$

If we use white light, we must integrate. Use

$$\mathcal{I} \propto \langle \mathcal{E}^2 \rangle = 2\mathcal{E}_0^2 \qquad \text{intensity}$$

$$\text{Rate} = 2\pi \int \delta(E_m - E_n - \hbar\omega)\, |z_{mn}|^2\, \frac{\mathcal{I}(\omega)}{2}\, d\omega$$

$$= |z_{mn}|^2\, \mathcal{I}(\omega_m) \qquad \omega_m \equiv E_m - E_0$$

5.) Interaction with a Quantum Oscillator

We now consider the interaction of a system with a quantum mechanical oscillator (as distinct from a system being exposed to a classical perturbing field).

$$H = \underbrace{H_{atom} + H_{osc}}_{H_0} + \underbrace{\chi q}_{V}$$

χ operates involving atomic variables
q oscillator coordinate

$$H_{osc} = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 q^2$$

Use

$$\underset{m\to n}{\text{Rate}} = 2\pi\, \delta(E_m - E_n)\, |V_{mn}|^2$$

We want $H_0 |\phi_n\rangle = E_n |\phi_n\rangle$

Suppose we know

$$H_{atom} |\chi_a\rangle = \epsilon_a |\chi_a\rangle$$

We know

$$H_{osc}|u_N\rangle = \hbar\omega(N+\tfrac{1}{2})|u_N\rangle$$

Thus to find $|\phi_N\rangle$, use the non-interaction of H_{atom} & H_{osc} to write

$$|\phi_{a,N}\rangle = |\chi_a\rangle|u_N\rangle$$

$$E_{a,N} = \epsilon_a + \hbar\omega(N+\tfrac{1}{2})$$

Now plug into our expression

Rate $\{a,N\} \to \{b,M\}$ for atom in a to go to b while oscillator goes from N to M under

$$= 2\pi\,\delta(E_{N,a} - E_{M,b})\,|\langle\phi_{b,M}|\gamma_q|\phi_{a,N}\rangle|^2$$

$$= 2\pi\,\delta(\epsilon_a - \epsilon_b + \hbar\omega(N-M))\,|\langle b|\gamma|a\rangle|^2\,|\langle u_M|q|u_N\rangle|^2$$

To show this

$$\langle\phi_{b,M}|\gamma_q|\phi_{a,N}\rangle = \int \phi^*_{b,M}\,\gamma(\vec{r})\,q\,\phi_{a,N}\,d^3\vec{r}\,dq$$

$$= \int \chi^*_b(\vec{r})\,u^*_M(q)\,\gamma(\vec{r})\,q\,\chi_a(\vec{r})\,u_N(q)\,d^3\vec{r}\,dq$$

$$= \left[\int \chi^*_b(\vec{r})\,\gamma(\vec{r})\,\chi_a(\vec{r})\,d^3\vec{r}\right]\left[\int u^*_M\,q\,u_N\,dq\right]$$

$$= \langle\chi_b|\gamma|\chi_a\rangle\,\langle u_M|q|u_N\rangle$$

Now we can show

$$\langle N|q|N\rangle = 0 \quad \text{unless} \quad M = N \pm 1$$

$$\langle N+1|q|N\rangle = \sqrt{\frac{\hbar}{2\mu\omega}}\sqrt{N+1}$$

$$\langle N-1|q|N\rangle = \sqrt{\frac{\hbar}{2\mu\omega}}\sqrt{N}$$

Thus

$$\underset{\substack{a\to b\\ N\to N+1}}{\text{Rate}} = 2\pi\delta(\epsilon_a - \epsilon_b - \hbar\omega)\,|\gamma_{ba}|^2\,\frac{\hbar}{2\mu\omega}(N+1)$$

oscillator absorbs energy

$$\underset{\substack{a\to b\\ N\to N-1}}{\text{Rate}} = 2\pi\delta(\epsilon_a - \epsilon_b + \hbar\omega)\,|\gamma_{ba}|^2\,\frac{\hbar}{2\mu\omega}N$$

oscillator emits energy

Comparison with Classical Perturbation

Here $H = H_{atom} + \gamma q(t)$

$$q(t) = 2Q_0\cos\omega t$$

and

$$\underset{a\to b}{\text{Rate}} = 2\pi\delta(\epsilon_a - \epsilon_b - \hbar\omega)\,|\gamma_{ba}|^2 Q_0^2$$

$$\underset{a\to b}{\text{Rate}} = 2\pi\delta(\epsilon_a - \epsilon_b + \hbar\omega)\,|\gamma_{ba}|^2 Q_0^2$$

Suppose $\langle Q^2\rangle_{classical} = 2Q_0^2$. But for q.m. oscillator $\langle N|Q^2|N\rangle = \frac{\hbar}{\mu\omega}(N+\frac{1}{2})$

$\therefore$ classical: $\uparrow = \downarrow$ q.m: $\uparrow > \downarrow$

Try instead to compare with

$$\left\langle \mu \frac{\omega^2}{2} Q^2 \right\rangle_{cl} = \tfrac{1}{2} \text{ excitation energy in oscillator}$$

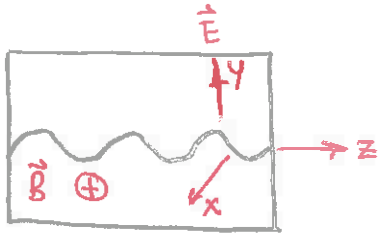
Then the q.m. oscillator gives

$$\underset{\substack{a\to b \\ \text{(atom emits)}}}{\text{Rate}} = 2\pi \delta(\epsilon_a - \epsilon_b - \hbar\omega) |V_{ba}|^2 \left[\tfrac{1}{2} \langle Q^2 \rangle_{\substack{cl \\ \text{excitation}}} + \frac{\hbar}{2\mu\omega} \right]$$

$$\underset{\substack{b\to a \\ \text{(atom abs)}}}{\text{Rate}} = 2\pi \delta(\epsilon_a - \epsilon_b + \hbar\omega) |V_{ba}|^2 \tfrac{1}{2} \langle Q^2 \rangle_{\substack{cl \\ \text{excitation}}}$$

Thus all but the $\frac{\hbar}{2\mu\omega}$ term can be handled by using a classical oscillating perturbation. Thus we have a certain added rate for moving downhill which would be there even for no excitation. This is the "spontaneous emission" rate. It is the difference between q.m. and classical fields.

PROBLEM: Consider a cavity with E.M. wave as shown.



Also a d.c. B_0 field in z direction. Interaction of atoms of

$$H = \mu_e g (\vec{J} \cdot \vec{B})$$

$$= \mu_e g J_z B_0 + \mu_e g J_x B_x$$

10/7/66 LECTURE

Recall we had been considering

$$H = H_{atom} + H_{osc} + \gamma q$$

EXAMPLE: Consider the nucleus of an atom in a solid as it vibrates as the quantized oscillator. We consider its interaction with an electron passing through a solid which is

$$U(\vec{r} - \vec{R}_{nucleus})$$

Locate the coordinate origin at the nucleus such that $\vec{R} = q\hat{e}_z$. Then we can linearize the interaction if q is small

$$U(\vec{r} - \vec{R}_{nucleus}) \sim U(\vec{r}_e) - \underbrace{\left(\frac{\partial U(\vec{r}_e)}{\partial z}\right)}_{\gamma} q$$

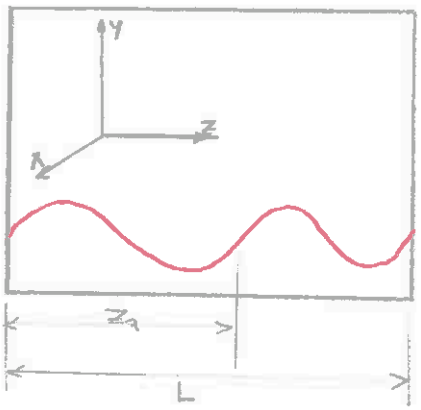
We had found for the quantized oscillator interaction

$$\underset{\substack{n \to m \\ N \to N+1}}{\text{Rate}} = 2\pi\, \delta(E_n - E_m - \hbar\omega)\, |\gamma_{mn}|^2\, \frac{\hbar}{2\mu\omega}(N+1)$$

[Note this assumes T is large, such that the states assume a continuum]

6. Nucleus in a Magnetic Field in a Cavity [NMR]

Let $\vec{B} = \underbrace{B_0 \hat{e}_z}_{\text{d.c.}} + \underbrace{B_x \hat{e}_x}_{\text{cavity mode}}$



Consider a typical cavity mode

$$\vec{A} = A_y \hat{e}_y = q(t) \sin kz \, \hat{e}_y \qquad kL = l\pi$$

$$\vec{E} = \frac{\partial \vec{A}}{\partial t} \Rightarrow E_y = \dot{q}(t) \sin kz$$

$$\vec{B} = \nabla \times \vec{A} \Rightarrow B_x = \frac{\partial A}{\partial z} = k q(t) \cos kz$$

Then

$$H = g\mu_N (\vec{J} \cdot \vec{B}) = \underbrace{g\mu_N J_z B_0}_{\text{Hatom}} + \underbrace{g\mu_N J_x (k \cos kz_a) q(t)}_{\gamma}$$

Now we know $J_z = m_z \qquad m_z = -j \cdots +j$

$$\epsilon_{m_z} = g\mu_N B_0 m_z$$

Thus we can calculate

$$\underset{\substack{m_z \to m_z' \\ N \to N+1}}{\text{Rate}} = 2\pi \, \delta\left[g\mu_N B_0 (m_z - m_z') - \hbar\omega\right] \frac{\pi}{2\mu\omega} (N+1) \left| \langle m_z | J_x | m_z' \rangle \right|^2 (g\mu_0 \cos kz_a)^2 \dot{q}(t)$$

Now we want to deal with the cavity in such a way that we can associate with it the quantum oscillators treated earlier in our analysis. We work by analogy. Classically

$$\text{Energy} = \frac{\epsilon_0}{2}\int (E^2 + c^2B^2)\, dVol = \frac{\epsilon_0 (Vol)}{2}\cdot\frac{1}{2}\left[\dot{q}^2 + k^2c^2q^2\right]$$

Now the usual simple harmonic oscillator obeys

$$\text{Energy} = \frac{\mu}{2}\dot{q}^2 + \frac{\mu\omega^2}{2}q^2$$

Thus we can identify $\omega = kc$ $\qquad [\mu\dot{q} = p]$

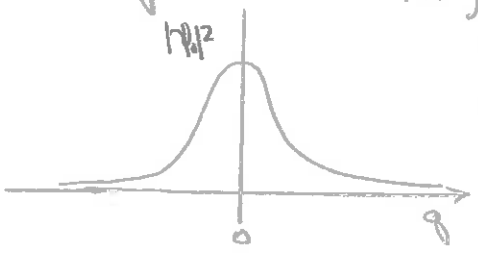
$$\mu = \frac{\epsilon_0 Vol}{2} = \epsilon_0 \int (\sin^2 kz)\, dVol$$

Assumption of Quantumelectrodynamics: The classical EM cavity oscillators become simple harmonic oscillators in the quantum theory treatment. Thus

$$H_{osc} = \frac{p^2}{2\mu} + \frac{\mu\omega^2 q^2}{2} = \frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2} + \frac{\mu\omega^2}{2}q^2$$

Note q is not a position variable, but merely a variable describing the excitation of the cavity.

EXAMPLE: $H_{osc}\psi = \lambda\psi$ creates the usual SHO wave functions. If we consider $|\psi_0|^2$, we can interpret it as meaning that if we measured $\vec{B}$ when the cavity was empty, there would be a certain probability of finding $\vec{B}$ non-zero



The energies are $\epsilon_N = \hbar\omega(N+1/2)$

We can either say that the cavity is in the 3rd excited state of the SHO or that we have 3 photons in the case of $N=3$. Thus photons ≡ oscillator excited states

Just remember however, ψ is not a position variable.

Now we also know

$$\langle m_z | J_x | m_z' \rangle = \sqrt{j(j+1) - m_z(m_z \pm 1)} \quad \text{for } m_z' = m_z \pm 1$$

$$= 0 \quad \text{otherwise}$$

Thus

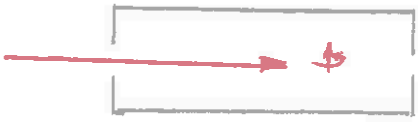
$$\underset{\substack{m_z \to m_z - 1 \\ N \to N+1}}{\text{Rate}} = 2\pi\delta(\omega_{B_0} - \omega)\frac{\hbar(N+1)}{2\left(\frac{\epsilon_{\text{cavity}}}{2}\right)\omega}\left(g_N \mu_N k_0 \cos kz_a\right)^2 [j(j+1) - m_z(m_z-1)]$$

$$\omega_{B_0} = g_N \mu_N B_0/\hbar$$

$$= \text{Larmor precession frequency}$$

Thus no nuclear transitions unless cavity ω is at the Larmor precession frequency, i.e. resonance [N.M.R].

Note if the atom has only been the the field for a time T, we must go back to eqn. (21) on p. 8.



7) Interaction with a System of Oscillators

We now want to extend the analysis for many modes. Not too useful for cavities, but for QED or phonons we need it.

$$H = \underbrace{H_{atom} + \sum_i H_{osc_i}}_{H_0} + \underbrace{\sum_i \gamma_i q_i}_{V}$$

Note we use the orthogonality of the q states to eliminate cross terms (use normal coordinates otherwise). Write

$$H_{osc_i} = \frac{p_i^2}{2\mu} + \frac{\omega_i^2 \mu}{2} q_i^2$$

$$V = \sum_i V_i$$

Now return to the general theory

Initial state n: atom in state a, 1st osc. in N_1, ...

$$|n\rangle = |{}^{a}_{N_1, N_2, N_3 \cdots}\rangle \qquad [\chi_a(\vec{r}) \phi_{N_1}(q_1) \phi_{N_2}(q_2) \cdots]$$

$$H_0 |n\rangle = [\epsilon_a + (N_1 + \tfrac{1}{2})\hbar\omega + (N_2 + \tfrac{1}{2})\hbar\omega + \cdots] |n\rangle$$

Final state m: atom b, N_1', N_2' ...

$$|m\rangle = |{}^{b}_{N_1', N_2', \cdots}\rangle$$

Now to calculate the matrix elements $\langle m|V|n\rangle$

$$\langle m|V|n\rangle = \sum_i \langle m|V_i|n\rangle$$

Now note

$$\langle m|V_j|n\rangle = \left\langle {}^{b}_{N_1'\cdots} \middle| \gamma_j(\hat{r}) q_{0_j} \middle| {}^{a}_{N_1 N_2 \cdots} \right\rangle$$

$$= 0 \quad \text{unless} \quad N_i = \underset{i\neq k}{N_i'}, \quad N_j' = N_j \pm 1$$

$$= \langle b|\gamma_j|a\rangle \frac{\hbar}{2\mu_j\omega_j}(N_j+1) \qquad N_j' = N_j \pm 1, \; N_i = \underset{i\neq j}{N_i'}$$

10/10/66 LECTURE

PROBLEM: Consider rotons in He such that the energy as a function of momentum is

$$\epsilon(p) = \Delta + \frac{1}{2m}(p-p_0)^2$$

where Δ & p_0 are constants. Now suppose

$$\Delta(p) = \Delta_0 + (p-p_0)d + O(p-p_0)^2$$

What is the prob. of emitting a phonon of momentum $\hbar k$

in terms of p_0, Δ_0, d, and c_s? [Assume only longitudinal sound waves, and if it helps, set $p_0 = 0$.]

PROBLEM: Make up a "significant" problem involving the second order term in our perturbation theory and work it out.

Last time we had

$$H = H_{atom} + \sum_i H_{i,osc} + \sum_i \gamma_i q_i$$

where $H_{i,osc} = \frac{p_i^2}{2\mu_i} + q_i^2 \frac{\omega_i^2 \mu_i}{2}$

Now we wanted the prob of $|N_1^a \dots\rangle \to |N_1^b \dots\rangle$

We found

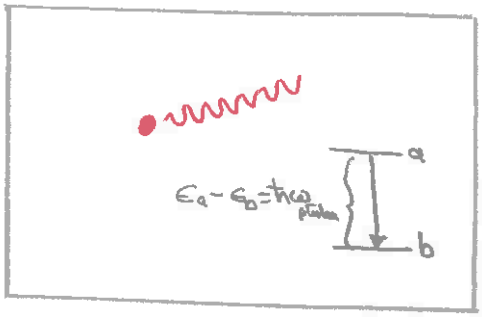
$$\underset{\substack{a\to b\\ N_j\to N_j+1}}{\text{Rate}} = 2\pi\,\delta(\epsilon_a-\epsilon_b-\hbar\omega_j)\,|\langle b|\gamma_j|a\rangle|^2\,\frac{(N_j+1)}{2\mu_j\omega_j}$$

$$\underset{\substack{a\to b\\ N_j\to N_j-1}}{\text{Rate}} = 2\pi\,\delta(\epsilon_a-\epsilon_b+\hbar\omega_j)\,|\langle b|\gamma_j|a\rangle|^2\,\frac{N_j}{2\mu_j\omega_j}$$

Thus each oscillator interacts independently with the system. If we wanted just the rate of transition, regardless of which oscillator was involved, we would merely sum over the class $N_j \to N_j \pm 1$ of the j oscillators.

8.) Atomic Transitions in a Cavity

EXAMPLE: We consider the probability that a one-electron atom radiates into an empty box. [Since we may take the box as arbitrarily large, this is just the problem of an excited atom interacting with the E&M field. It is our first real example of quantum electrodynamics -- although in the non-relativistic approximation.]



Assume when the atom is in state a, no photons in the box. When it falls into state b, a photon of energy $\hbar\omega$ photon is emitted. This may be interpreted as exciting a mode in a certain direction.

Now to quantize the field, first set up the classical field as a superposition of modes

$$\vec{A}(\vec{r},t) = Q_1(t)\sin k_z z\,\hat{e}_x + Q_2(t)\sin k_z z\,\hat{e}_y + Q_3(t)\sin k'_z z\,\hat{e}_x + \cdots$$

$k L_z = l_z \pi$

$$= \sum_{\vec{k},\vec{e}} \vec{e}\, Q_{\vec{k},\vec{e}}\, e^{i\vec{k}\cdot\vec{r}}$$

where $\vec{k}$ is the wave vector
$\vec{e}$ is the polarization vector

$\Rightarrow \vec{e}\cdot\vec{k} = 0$ (transverse modes)

Note: i.) we have chosen the scalar potential $\Phi \equiv 0$
ii.) we need a Re $\{\ \}$. This introduces a $\frac{1}{2}$ factor at the end.

Now to find the classical eqns, use Maxwells eqns to find

$$\nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = 0$$

Plug in (*) to find

$$-k^2 c^2 Q_{\vec{k},\vec{e}} - \ddot{Q}_{\vec{k},\vec{e}} = 0$$

(harmonic oscillator of $\omega_{\vec{k},\vec{e}} = kc$)

Now to get the qed, find

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t} = \sum_{\vec{k},\vec{e}} \vec{e}\, \dot{Q}_{\vec{k},\vec{e}}\, e^{i\vec{k}\cdot\vec{r}}$$

$$\vec{B} = \nabla \times \vec{A} = \sum_{\vec{k},\vec{e}} i(\vec{k} \times \vec{e}) Q_{\vec{k},\vec{e}} e^{i\vec{k}\cdot\vec{r}}$$

Then

$$\frac{\epsilon_0}{2}\int (E^2 + c^2 B^2)\, dVol = \frac{\epsilon_0}{2}\frac{Vol}{2} \sum_{\vec{k},\vec{e}} \left(\dot{Q}^2_{\vec{k},\vec{e}} + k^2 c^2 Q^2_{\vec{k},\vec{e}} \right)$$

$$\therefore \mu_{\vec{k},\vec{e}} = \frac{2}{\epsilon_0 Vol} = \mu$$

Now passing to q.e.d., use quantum oscillators

$$H(\text{free field}) = \frac{1}{2} \sum_{\vec{k},\vec{e}} \left[\frac{P^2_{\vec{k},\vec{e}}}{2\mu} + \mu \frac{(kc)^2}{2} Q^2_{\vec{k},\vec{e}} \right]$$

$$\mu = \frac{\epsilon_0 Vol}{2}$$

Now

$$H_{\substack{\text{atom in} \\ \text{a field}}} = \frac{1}{2m}(\vec{p} - q_e \vec{A})^2 + \frac{q_e^2 Z}{4\pi\epsilon_0 r} + \mu_e \vec{\sigma}\cdot\vec{B} + \underbrace{\cdots}_{\text{relativistic}}$$

$$= H_{atom} + \left[-\frac{q_e}{2m}\left(\vec{p}\cdot\vec{A}(\vec{r}_e) + \vec{A}(\vec{r}_e)\cdot\vec{p} \right) + \mu_e \vec{\sigma}\cdot(\nabla\times\vec{A}) \right]$$

$$+ \frac{q_e^2}{2\mu}\vec{A}(\vec{r}_e)\cdot\vec{A}(\vec{r}_e) + \cdots$$

Now if H_{int} is small, we drop the $\vec{A}\cdot\vec{A}$ term since it is 2nd order (and our perturbation theory is only to first order).

We find

$$H_{int} = \sum_{\vec{k},\vec{e}} \underbrace{\left\{ -\frac{q_e}{2m}\left[(\vec{p}\cdot\vec{e})e^{i\vec{k}\cdot\vec{r}} + e^{i\vec{k}\cdot\vec{r}}(\vec{p}\cdot\vec{e})\right] + \mu_e \vec{\sigma}\cdot(i\vec{k}\times\vec{e})e^{i\vec{k}\cdot\vec{r}} \right\}}_{\mathcal{V}_{\vec{k},\vec{e}}} Q_{\vec{k},\vec{e}}$$

We now want

Rate $a \to b$ vacuum $\to$ 1 photon of $\vec{k},\vec{e}$ (all $N_i = 0 \to$ all $N_i = 0$ except $N_{\vec{k},\vec{e}} = 1$)

$$= 2\pi\delta(\epsilon_a - \epsilon_b - \hbar kc)\,|\langle b|\mathcal{V}_{\vec{k},\vec{e}}|a\rangle|^2 \frac{N_j + 1}{2\epsilon_0 V_d \tfrac{1}{2}\omega}$$

$$= 2\pi\delta(\epsilon_a - \epsilon_b - \hbar kc)\,|\langle b|\mathcal{V}_{\vec{k},\vec{e}}|a\rangle|^2 \frac{1}{2\omega}\frac{1}{V_d\epsilon_0}$$

[taking into account $\frac{1}{2}$ factor from Re{ }]

Show $\vec{p}\,e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}}(\vec{p} + \vec{k})$ and then $[\vec{p}, \vec{A}] = 0$ ◀

Thus

Rate $a \to b$ emit photon with $\vec{k},\vec{e}$

$$= \frac{2\pi}{2\omega V_d}\,\delta(\epsilon_a - \epsilon_b - kc)\,4\pi e^2 \left|\langle b|\frac{(\vec{p}\cdot\vec{e})}{m}e^{i\vec{k}\cdot\vec{r}}|a\rangle\right|^2$$

using $\frac{q e^2}{4\pi\epsilon_0} = e^2$

and neglecting spin term.

Remember each time a photon couples with a system we get a $\sqrt{4\pi e^2}$ and $\frac{1}{2\omega}$ factor.

Now if we want the prob. of transition to $d^3\vec{k}$, we sum, passing in the limit to

$$\int [\quad] \frac{d^3\vec{k}}{(2\pi)^3} \text{ vol}$$

If we integrate over constant $|\vec{k}|$, we find

$$\underset{\substack{a \to b \\ \text{emit photon} \\ \text{in } d\Omega}}{\text{Rate}} = \frac{2\pi}{2\omega} \frac{k^2 d\Omega}{(2\pi)^3} 4\pi e^2 \left| \langle b | \frac{(\vec{p}\cdot\vec{e})}{m} e^{i\vec{k}\cdot\vec{r}} | a \rangle \right|^2$$

where $k = |\vec{k}| = \epsilon_a - \epsilon_b$

$c \equiv \hbar \equiv 1$

The Dipole Approximation

10/11/66 LECTURE

We had found

$$\left\{\begin{array}{l}\text{Rate of emission of}\\ \text{photon with } \vec{k},\vec{e},\\ \text{atom } a \to b\end{array}\right\} = 2\pi\,\delta(\epsilon_a-\epsilon_b-\hbar\omega)\,4\pi e^2\left|\langle b|\,\frac{\vec{p}\cdot\vec{e}}{m}\,e^{i\vec{k}\cdot\vec{r}}\,|a\rangle\right|^2\frac{d^3k_b}{2\omega(2\pi)^3}$$

The $e^{i\vec{k}\cdot\vec{r}}$ factor accounts for phase interference from different parts of the atom. Now for light radiated by atoms, typically $kr \sim \frac{r}{\lambda} << 1$. Thus we approximate

$$e^{i\vec{k}\cdot\vec{r}} \approx e^{i\vec{k}\cdot\vec{r}_{nucleus}}$$

Now $e^{i\vec{k}\cdot\vec{r}_{nucleus}}$ is no longer an operator, and can be removed from the matrix element. This is called the "electric dipole approximation." [Note: it frequently doesn't work!]

Thus we can find

$$\text{Rate into } d\Omega_{a\to b} = \frac{4\pi e^2}{2\omega}\,\frac{k^2\,d\Omega}{(2\pi)^3}\,\left|\langle b|\frac{\vec{p}\cdot\vec{e}}{m}|a\rangle\right|^2_{\omega=k=\epsilon_b-\epsilon_a}$$

Now if we consider $\vec{p}\cdot\vec{e} = p_z$, then

$$\langle b|\frac{p_z}{m}|a\rangle = \langle b|Hz - zH|a\rangle = \underbrace{(\epsilon_b-\epsilon_a)}_{\omega}\langle b|z|a\rangle$$

Thus

$$\text{Rate} = 2\omega^3 z^2\left|\langle b|\vec{r}\cdot\vec{e}|a\rangle\right|^2\frac{d\Omega}{4\pi}$$

Note all of this is exact within 1st order perturbation theory for non-relativistic theory.

Example: $2p \to 1s$

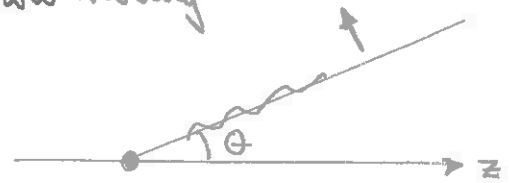
$l = 0 \quad (\cos\theta \sim z)$

$\langle b|x|a\rangle = 0$
$\langle b|y|a\rangle = 0$
$\langle b|z|a\rangle \neq 0$

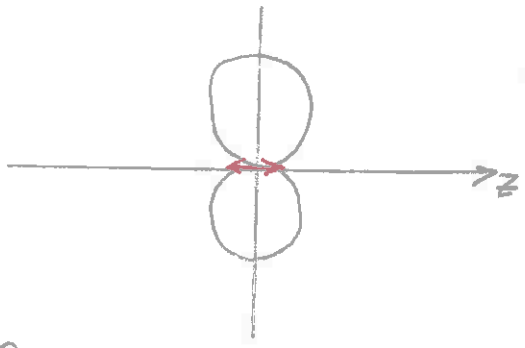
Then

$$\text{Rate} = 2\omega^3 e^2 |\langle b|z|a\rangle|^2 e_z^2 \frac{d\Omega}{4\pi}$$

Now noting



The polarization out of page will vanish



Now

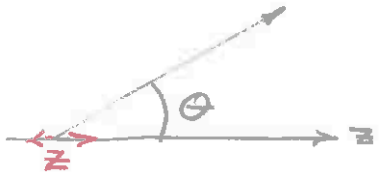
$$\text{Rate}_{a \to b} = \frac{4}{3}\frac{\omega^3 e^2}{\hbar c^3} |\langle b|\vec{r}|a\rangle|^2$$

any direction
any polarization

Then

$$\text{Energy loss rate} = \frac{4\omega^4}{3c^3} \overline{(\text{matrix element of dipole moment})^2}$$

We now compare this to a small classical oscillating dipole



$z = 2z_0 \cos\omega t$

Dipole moment $= 2ez_0 \cos\omega t$

$\overline{(\text{Dipole moment})^2} = 2(ez_0)^2$

$$\text{Energy radiated/sec} = \frac{2}{3}\frac{\omega^4}{c^3}\,\overline{(\text{Dipole moment})^2}$$

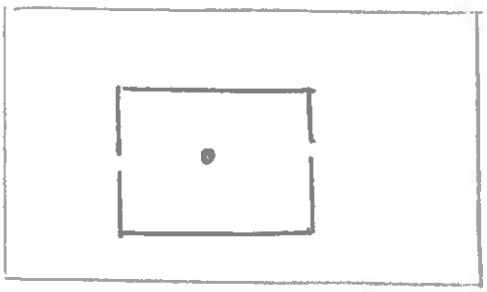
This is close to the quantum answer except for a factor 2. Thus an atom in empty space radiates as a dipole provided we use

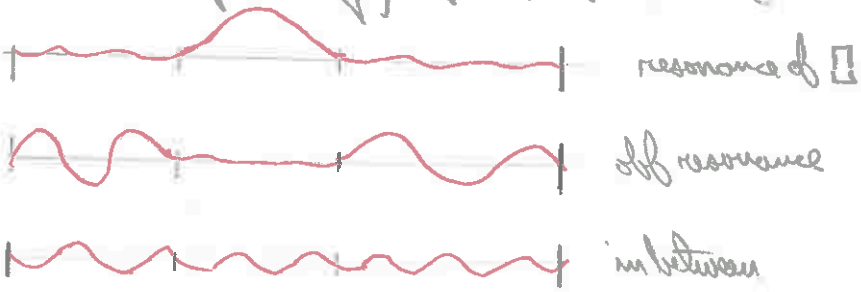
$$(\text{Dipole moment classical})^2 = 2\,|\text{Dipole matrix element} - \text{Q.M.}|^2$$

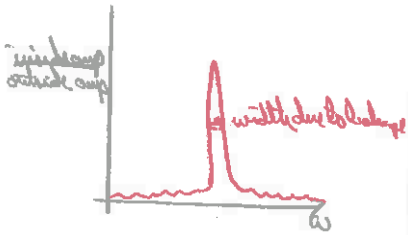
We will now prove that this rule holds for any cavity (even with holes and resistive walls).

We prove this for an atom radiating in a general cavity with holes in it [with perfect walls however].

Assume the atom dimensions $\ll$ size of cavity. Now surround the cavity by an enormous box. This has various modes [although very complicated, to be sure]. For the indicated geometry, the modes resemble







The superposition of these modes describe the leakage from the box. Thus a superposition of undamped modes yield a damped mode. If we take the box large enough, (several light years), we need not worry about reflection from the wall.

Suppose these modes are $Q_i(\vec{r})$. Then we use our result

$$\underset{a\to b}{\text{Rate}} = 2\pi\,\delta(\epsilon_a - \epsilon_b - \hbar\omega_i)\,|\langle b|P_i|a\rangle|^2 \frac{1}{2\mu_i\omega_i}$$

vacuum → photon

Now $H_{int} = \vec{j}\cdot\vec{A}(\vec{r}_0)$

Then expand $A(\vec{r}) = \sum_i Q_i(t)\,Q_i(\vec{r})$

Thus

$$\underset{a\to b}{\text{Rate}} = \sum_i 2\pi\,\delta(\epsilon_a - \epsilon_b - \hbar\omega_i)\,\frac{|Q_i(\vec{r}_0)|^2}{2\mu_i\omega_i}\,|j_{ab}|^2$$

We wish compare this to a classical problem

Classical: $\vec{J}(t)$ is the current in a dipole antenna located at $\vec{r}_0$. We have a coupling $\sim \vec{j}\cdot\vec{A}(\vec{r}_0)$. Now $\vec{A}$ satisfies

$$\frac{\partial^2\vec{A}}{\partial t^2} - \nabla^2\vec{A} = \vec{J}(\vec{r}) = \delta(\vec{r}-\vec{r}_0)\,\vec{j}$$

Now use $\vec{A} = \sum_i q_i(t)\,Q_i(\vec{r})$ and plug in to find

$$\sum_i (\ddot{q}_i + \omega_i^2 q_i)\,Q_i(\vec{r}) = \delta(\vec{r}-\vec{r}_0)\,j(t)$$

From orthogonality

$$\ddot{q}_i + \omega_i^2 q_i = \varphi_i(\vec{r}_0)\, j(t) \qquad (*)$$

If $j(t)$ varies as $e^{i\omega t}$ then the electric field varies as $E_\omega e^{i\omega t}$

$$E_\omega = Z(\omega)\, j_\omega$$

where $Z(\omega)$ is the impedance

Using $E_\omega = \sum q_i(t)\, \varphi_i(\vec{r}_0)$

we find, solving (*), that

$$E_\omega = \underbrace{i\omega \sum_i \frac{1}{\omega_i^2 - \omega}\, \varphi_i^2(\vec{r}_0)}_{Z(\omega)}\, j_\omega \qquad (1)$$

10/14/66 LECTURE

Now return to our q.m. model where we found

$$\underset{a\to b}{\text{Rate}} = 2\pi \sum_i \delta(\epsilon_a - \epsilon_b - \hbar\omega_i)\, |\langle b|j|a\rangle|^2\, |\varphi_i(\vec{r}_0)|^2 \frac{1}{2\mu_i\omega_i}$$

Claim: $\underset{a\to b}{\text{Rate}} = \frac{2}{\hbar\omega_{ab}} \left[\text{Re}\{Z(\omega_{ab})\}\right] |\langle b|j|a\rangle|^2$

Proof: If we return to (1),

$$Z(\omega) = i\omega \sum_i \frac{1}{\omega_i^2 - \omega} \varphi_i^2(\vec{r}_0) \qquad (1)$$

we realize we have no prescription for $\lim_{\omega \to \omega_i} Z(\omega)$.

If we use the analogy of a damped oscillator

$$\ddot{q} + \omega_0^2 q + \gamma \dot{q} = j_\omega e^{i\omega t}$$

or $$(-\omega^2 + \omega_0^2 + i\omega\gamma) q = j_\omega$$

$$q = \frac{j_\omega}{\omega_0^2 - \omega^2 + i\omega\gamma}$$

we see that we can apply the condition of causality and the initial condition of $q = 0$ for $t \leq 0^-$ to learn we should write (1) as

$$q_{i\omega} = \frac{1}{\omega_i^2 - (\omega - i\epsilon)^2} \varphi_i(\vec{r}_0)\, j_\omega$$

Thus we assume no free waves on i.c. before we turn on oscillator. We eventually take $\lim_{\epsilon \to 0}$. Note this is just like "turning off the interaction" at $|\vec{r}| \to \pm\infty$ in scattering problems.

Before continuing, we need a little more math first.

Detour

Cauchy Principal Values and Generalized Functions (a la Feynman)

It is convenient to take as a prescription

$$\lim_{\epsilon \to 0} \frac{1}{x+i\epsilon} = P.V.\left(\frac{1}{x}\right) - i\pi\delta(x) \qquad (3)$$

[Note we also might have specified

$$\lim_{\epsilon \to 0} \frac{1}{x+i\epsilon} = P.V.\left(\frac{1}{x}\right) + i\pi\delta(x)$$

or

$$\lim_{\epsilon \to 0} \frac{1}{x+i\epsilon} = P.V.\left(\frac{1}{x}\right)$$

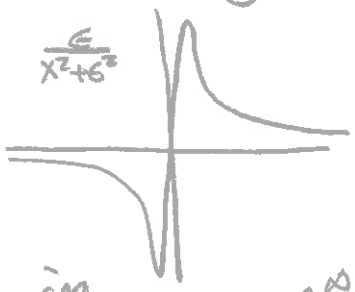
More generally

$$\lim_{\epsilon \to 0} \frac{1}{x+i\epsilon} = P.V.\left(\frac{1}{x}\right) + \lambda\,\delta(x) \;]$$

To "justify" (3), note

$$\frac{1}{x+i\epsilon} = \frac{x-i\epsilon}{x^2+\epsilon^2} = \underbrace{\frac{x}{x^2+\epsilon^2}}_{①} - i\underbrace{\frac{\epsilon}{x^2+\epsilon^2}}_{②}$$

The first term resembles

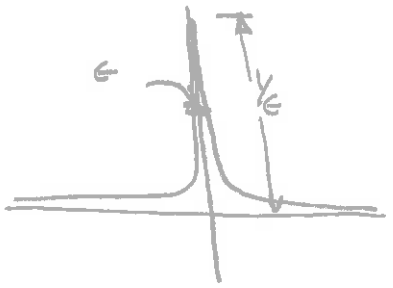


Now

$$P.V.\int_{-\infty}^{\infty}\left(\frac{1}{x}\right)f(x)\,dx = \int_{-\infty}^{-\eta}\frac{1}{x}f(x)\,dx + \int_{\eta}^{\infty}\frac{1}{x}f(x)\,dx$$

By keeping equal distances we get cancellation.

For the second term

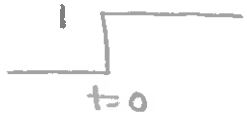


$$\int \frac{dx\,\epsilon}{x^2+\epsilon} = \pi$$

By definition $\int_{-\infty}^{\infty} \delta(x) f(x)\, dx = f(0)$

IMPORTANT POINT: We don't, however, make a rule to take P.V. for all physical problems. The trick is to leave it unspecified until we learn how to specify it.

EXAMPLE: Consider the Fourier transform of a step fcn



The usual $\mathcal{F}\{\ \}$ doesn't converge [at least in the usual sense. Consider instead

$$\int_0^\infty e^{-ixt}\, dt \text{ "}=\text{" } \lim_{\epsilon\to 0} \int_0^\infty e^{-ixt} e^{-\epsilon t}\, dt$$

$$= \lim_{\epsilon\to 0} \frac{1}{ix+\epsilon} = \lim_{\epsilon\to 0} \frac{-i}{x-i\epsilon}$$

Note that how we take our prescription effects the inverse transform.

Returning now to our problem, we find

$$\zeta(\omega) = i\omega \sum_i \frac{|\varphi_i|^2}{\omega_i^2 - \omega^2 + 2i\omega\epsilon}$$

$$= i\omega \sum_i \text{P.V.} \frac{1}{\omega_i^2 - \omega^2} |\varphi_i|^2 + i\omega \left(-i\pi \sum_i \delta(\omega_i^2 - \omega^2) |\varphi_i|^2\right)$$

Note this is very close to our q. m. result. When we take $\text{Re}\{\zeta(\omega)\}$ we get the result

$$\underset{a\to b}{\text{Rate}} = \frac{2}{\hbar\omega_{ab}} \left[\text{Re}\{\zeta(\omega)\}\right] |\langle b|j_\omega|a\rangle|^2$$

The difference of 2 between quantum and classical electrodynamics can be explained by noting that for q. m. we can have transitions both up and down

$$j_{\text{classical}} \to \langle a|j^2|a\rangle = \sum_c \langle a|j|c\rangle\langle c|j|a\rangle = \sum_c |\langle a|j|c\rangle|^2$$

$$= \underset{\text{up}}{|\langle a|j|b\rangle|^2} + \underset{\text{down}}{|\langle b|j|a\rangle|^2}$$

Comments from 10/18/66

We have now shown that the transition rate for an atom in an arbitrary cavity (with losses, resistance, etc.) is

$$\underset{a\to b}{\text{Rate}} = \frac{2}{\hbar\omega_{ab}} \operatorname{Re}\left\{Z(\omega_{ab})\right\} |\langle a|\vec{j}|b\rangle|^2$$

But for a perfect cavity the rate of transition with the energy going into the excitation of a well-defined mode ϕ_0

$$\underset{a\to b}{\text{Rate}} = 2\pi\delta(\omega_{ab}-\omega_0)\,|\langle a|\vec{j}|b\rangle|^2\,|\phi_0(\vec{r}_0)|\,\frac{\hbar}{2\mu\omega_0}$$

To reconcile these expressions, we merely realize that the impedance of a perfect mode is

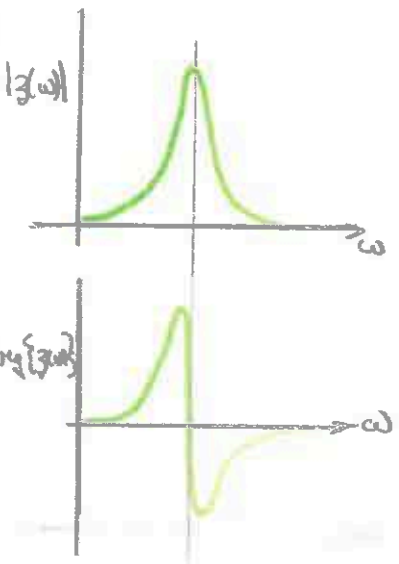
$$Z(\omega) = \lim_{\epsilon\to 0} \frac{i\omega}{\omega^2-\omega_0^2+i\epsilon\omega_0}\,|\phi_0(\vec{r}_0)|^2$$

$$= \omega\,\delta(\omega^2-\omega_0^2)\,|\phi_0(\vec{r}_0)|^2$$

For the more general case of a lossy cavity, the resonance broadens about $\omega = \omega_0 + \Delta\omega$

$$Z(\omega) = \frac{i\omega}{\omega^2-\omega_0^2+i\Gamma\omega}\,|\phi_0(\vec{r}_0)|^2 = \frac{i\omega}{2\omega_0(\Delta\omega)+i\Gamma\omega_0}$$

$$= \frac{\text{const.}}{(\omega-\omega_0)+i\frac{\Gamma}{2}}$$



Thus

$$\underset{a\to b}{\text{Rate}} = \frac{2\pi\left(\frac{\Gamma}{2}\right)^2}{(\omega-\omega_0)^2+\Gamma^2/4}\,|\langle a|\vec{j}|b\rangle|^2\,|\phi_0(\vec{r}_0)|^2\,\frac{\hbar}{2\mu\omega_0}$$

Claim: We now know quantum electrodynamics completely -- at least non-relativistically. The basic hypothesis: -- that every classical E&M mode of the field corresponds to a simple harmonic quantum oscillator -- was made prior to 1920. The next 20 years work consisted of putting this in relativistically covariant form. We will now examine how this was accomplished.

10) Recasting of Classical Electrodynamics

The basic equations are

$$\vec{B} = \nabla \times \vec{A} \tag{4}$$

$$\vec{E} = -\nabla\varphi + \frac{\partial \vec{A}}{\partial t} \tag{5}$$

$$\nabla \cdot \vec{E} = \rho/\epsilon_0 \tag{6}$$

$$\nabla \times \vec{B} = \mu_0 + \frac{\partial \vec{E}}{\partial t} \tag{7}$$

Now, of course, the gauge invariance is arbitrary, e.g.

$$\vec{A}' = \vec{A} + \nabla\chi$$

It was customary to take a Lorentz gauge

$$\nabla \cdot \vec{A} = \frac{\partial \varphi}{\partial t}$$

since it was thought this preserved relativistic covariance.

However any gauge preserves relativistic covariance -- the only difference is that the covariance is more obvious in Lorentz gauge, or as J. Schwinger would say, the equations are then "manifestly covariant".

Thus, because it doesn't hurt the relativity and may help us in making the transition to Q.E.D., we choose to work with the Coulomb gauge

$$\nabla \cdot \vec{A} = 0$$

[It took 20 years and a Nobel prize to get $\nabla \cdot \vec{A} = 0$ back to relativistic covariance.]

We now begin to manipulate to find, taking (5) in (6)

$$\nabla^2 \phi = \rho/\epsilon_0$$

Thus the scalar potential ϕ is always determined by electrostatics

$$\phi(1) = \int \frac{\rho(2)\, dV_2}{4\pi\epsilon_0 r_{12}} \qquad (8)$$

Thus using $\frac{e^2}{}$ is spot in the δ-eqn. All we need to know now is how to fill in the $\vec{A}$. But (8) $\Rightarrow$ disturbances propagate at infinite speed. Oh, well, "damn the torpedoes, full speed ahead!"

Use (4) in (7)

$$\nabla \times (\nabla \times \vec{A}) - \frac{\partial^2 \vec{A}}{\partial t^2} - \nabla \frac{\partial \phi}{\partial t} = \vec{j}/\epsilon_0$$

or

$$\nabla^2 \vec{A} - \frac{\partial^2 \vec{A}}{\partial t^2} = \vec{j}/\epsilon_0 - \nabla\left(\frac{\partial \phi}{\partial t}\right) \tag{9}$$

But $$\frac{\partial \phi}{\partial t} = \int \frac{\dot{\rho}(2)\, dV_2}{4\pi \epsilon_0 r_{12}}$$

Then

$$\nabla \cdot \vec{j} = \frac{\partial \rho}{\partial t} \Rightarrow \frac{\partial \phi}{\partial t} = \int \frac{\nabla \cdot J(2)\, dV_2}{4\pi \epsilon_0 r_{12}} \tag{10}$$

Thus $\vec{A}$ is completely determined by the current. This means we take into account the transverse part of the current so that $\nabla \cdot \vec{A} = 0$.

Now expand everything in plane waves

$$\vec{J}(\vec{r}, t) = \sum_{\vec{k}} \vec{J}(\vec{k}, t)\, e^{i \vec{k} \cdot \vec{r}}$$

$$A(\vec{r}, t) = \sum_{\vec{k}} \vec{A}(\vec{k}, t)\, e^{i \vec{k} \cdot \vec{r}} \tag{11}$$

Now then from (9), (10), (11)

$$\frac{d^2\vec{A}(k,t)}{dt^2} + k^2c^2\vec{A}(k,t) = \vec{J}_{transverse}(\vec{k},t) \qquad (12)$$

where $\vec{J}_{transverse} = \vec{J}(\vec{k},t) - \frac{(\vec{k}\cdot\vec{J})\vec{k}}{k^2}$

Equation (10)' is now the classical mode which we will quantize in passing to QED.

Comments from 10/18/66

Return to our formulation of classical electrodynamics using the Coulomb gauge $\nabla \cdot \vec{A} = 0$. We found the basic equations to then be

$$\nabla^2 \varphi(\vec{r},t) = \rho(\vec{r},t)/\epsilon_0$$

$$\nabla^2 \vec{A}(\vec{r},t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{A}(\vec{r},t) = \vec{j}/\epsilon_0 - \nabla\left(\frac{\partial \varphi}{\partial t}\right)$$

$$\nabla \cdot \vec{j} = -\frac{\partial \rho}{\partial t}$$

We solve immediately for

$$\varphi(\vec{r}_1,t) = \int \frac{\rho(\vec{r}_2,t)\, dV_2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}$$

This indicates one rule for quantization

i.) Use the instantaneous Coulomb potential $\sum_{i,j} \frac{e_i e_j}{r_{ij}}$ in the Schrödinger equation

In the non-relativistic limit this is all we need. However to be relativistically correct, we must add in the effect of $\vec{A}$. To find this classically, we use Fourier transforms (momentum space)

$$a(\vec{k},t) = \int e^{-i\vec{k}\cdot\vec{r}}\, \vec{A}(\vec{r},t)\, d^3\vec{r}$$

Also $\vec{J}(\vec{k},t) = \mathcal{F}\{\vec{j}(\vec{r},t)\}$

$\Phi(\vec{k},t) = \mathcal{F}\{\varphi(\vec{r},t)\}$

$P(\vec{k},t) = \mathcal{F}\{\rho(\vec{r},t)\}$

Transforming our equations, the gauge becomes

$$\vec{k}\cdot\vec{A}(\vec{k},t) = 0$$

while the other eqns are

$$k^2\Phi = P/\epsilon_0$$

$$\frac{\partial^2}{\partial t^2}\vec{A}(\vec{k},t) + k^2c^2\vec{A}(\vec{k},t) = \vec{J}/\epsilon_0 - i\vec{k}\left(\frac{\partial\Phi}{\partial t}\right)$$

$$i\vec{k}\cdot\vec{J} = -\frac{\partial P}{\partial t}$$

We can see $\frac{\partial\Phi}{\partial t} = \frac{1}{k^2\epsilon_0}\frac{\partial P}{\partial t} = -\frac{i\vec{k}\cdot\vec{J}}{k^2\epsilon_0}$

Thus we get

$$\frac{\partial^2\vec{A}}{\partial t^2} + k^2c^2\vec{A} = \frac{1}{\epsilon_0}\underbrace{\left(\vec{J} - \vec{k}\frac{(\vec{k}\cdot\vec{J})}{k^2}\right)}_{\vec{J}_{\text{transverse}}} \qquad (*)$$

We could expand $\vec{a}$ in two transverse polarization modes

$$\vec{a} = \hat{e}_1 \alpha_1(\vec{k},t) + \hat{e}_2 \alpha_2(\vec{k},t)$$

$$\hat{e}_1^* \cdot \hat{e}_2 = 0, \quad \hat{e}_1^* \cdot \hat{e}_1 = 1, \quad \hat{e} \cdot \vec{k} = 0$$

Plugging this into (*)

$$\hat{e}_1 \left(\frac{\partial^2}{\partial t^2} \alpha_1(\vec{k},t) + k^2 c^2 \alpha_1 \right) + \hat{e}_2 \left(\frac{\partial^2}{\partial t^2} \alpha_2(\vec{k},t) + k^2 c^2 \alpha_2 \right) = \frac{1}{\epsilon_0} \vec{J}_{\text{transverse}}$$

Now dot with $\hat{e}_i$ to find

$$\frac{\partial^2}{\partial t^2} \alpha_1(\vec{k},t) + k^2 c^2 \alpha_1(\vec{k},t) = \frac{\hat{e}_1 \cdot \vec{J}}{\epsilon_0}$$

$$\frac{\partial^2}{\partial t^2} \alpha_2(\vec{k},t) + k^2 c^2 \alpha_2(\vec{k},t) = \frac{\hat{e}_2 \cdot \vec{J}}{\epsilon_0} \qquad (**)$$

Thus the current along $\hat{e}_1$ feeds the α_1 mode, the $\hat{e}_2$ current feeds the α_2 mode. Here $\hat{e}_1 \cdot \vec{J}$ is the projection of the current in the shape of the mode -- like $(e^{i\vec{k}\cdot\vec{r}}, \vec{j}(\vec{r}))$

"This is the simplest form of electrodynamics that I could find."

Now to get QUANTUM ELECTRODYNAMICS

1.) use the instantaneous Coulomb potential $\sum_{i,j} \frac{e_i e_j}{r_{ij}}$ in the S-eqn.

2.) put (**) into the form of quantum oscillators

10/17/66 LECTURE

DETOUR: More Feynman quick and dirty methods.

Say we want to evaluate

$$\int e^{-i\vec{Q}\cdot\vec{r}}\,\varphi(\vec{r})\,dVol$$

We work backwards. Consider

$$\nabla^2\left(\frac{1}{r}\right) = 4\pi\,\delta(\vec{r})$$

If we take the $\mathcal{F}\left\{\nabla^2\left(\frac{1}{r}\right)\right\} = Q^2\,\mathcal{F}\left\{\frac{1}{r}\right\} = 4\pi\,\mathcal{F}\{\delta(\vec{r})\} = 4\pi$

$$\Rightarrow \int e^{-i\vec{Q}\cdot\vec{r}}\left(\frac{1}{r}\right)dVol = \frac{4\pi}{Q^2}$$

Now consider

$$(\nabla^2 - m^2)\,\varphi = 4\pi\,\delta(\vec{r})$$

From Yukawa, $\varphi \sim \frac{e^{-mr}}{r}$

Thus

$$\int e^{-\vec{q}\cdot\vec{r}}\,\frac{e^{-mr}}{r}\,d^3\vec{r} = \frac{4\pi}{q^2+m^2}$$

"Whatever I can remember are my axioms!"

PROBLEM 3: For a long time astrophysicists wondered about continuum radiation from various nebula. Some of this was due to synchrotron radiation. But not all. Consider an H atom (neglect spin)

2s ——— 2p ———

1s ———

Some gambling here, but neglect it if you wish

Now we know 2s → 1s transitions with one photon emitted are forbidden. However these transitions can be induced by collisions or an electric field. However in interstellar space collisions are effectively absent.

The alternative is the emission of 2 photons [although never seen in the lab]. The 2-photon emission explains the continuum spectrum.

Do as much as you can with this. Figure out the spectrum shape. Maybe even do the integrals by Simpson's rule. Just dump over the higher matrix elements, so approximations are needed.

[This problem was first solved by E. Teller. The opposite problem is of interest today by causing two lasers beams to interact in H gas.]

B.) Second-Order Time-Dependent Perturbation Theory

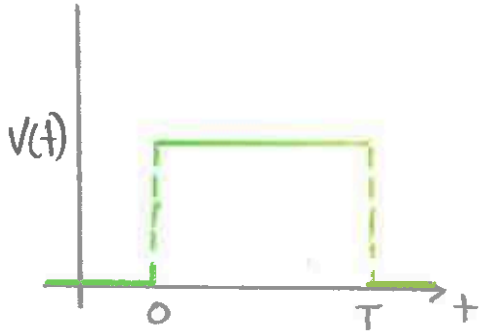
Recall we had

$$S_{mn} = \delta_{mn} - i\int V_{mn}(t)\,dt + (i)^2 \iint_{t_1>t_2} \sum_k V_{mk}(t_1) V_{kn}(t_2)\,dt_1\,dt_2 + \cdots \tag{1}$$

where $V_{mn}(t) = e^{-i(E_m - E_n)t} \underbrace{\langle \phi_m | V | \phi_n \rangle}_{V_{mn}}$

1.) Time-Independent Perturbation V

$$V(t) = 0 \qquad t < 0$$
$$= V \qquad 0 \le t \le T$$
$$= 0 \qquad T < t$$



A long calculation then finds

$$S_{mn} = \delta_{mn} - V_{mn}\left[\frac{e^{i(E_m - E_n)T} - 1}{(E_m - E_n)}\right] + \sum_{\substack{k \neq n \\ \neq m}} \frac{V_{mk}V_{kn}}{(E_k - E_n)}\left[\frac{e^{i(E_m - E_n)T} - 1}{(E_m - E_n)} - \frac{e^{i(E_m - E_k)T} - 1}{(E_m - E_k)}\right]$$

$$+ V_{mm}V_{mn}\left[\frac{e^{i(E_m - E_n)T} - 1}{(E_m - E_n)^2} - \frac{iT}{(E_m - E_n)}\right] + V_{mn}V_{nn}\left[\frac{[1 - i(E_m - E_n)T]e^{i(E_m - E_n)T} - 1}{(E_m - E_n)^2}\right]$$

We now calculate S_{mm}, the amplitude to remain in the same state as time goes on

$$S_{mm} = 1 - iTV_{mm} - \frac{T^2}{2}V_{mm}^2 - iT\sum_{k\neq m}\frac{V_{mk}V_{mm}}{(E_k - E_m)} + \sum_{k\neq m}\frac{(V_{mk})^2}{(E_k - E_m)^2}\left[e^{-i(E_m - E_m)T} - 1\right]$$

We could have used time-independent perturbation theory for this problem, however, to find

$$E_m' = E_m + \underbrace{V_{mm} + \sum_{k\neq m}\frac{V_{mk}V_{km}}{(E_k - E_m)}}_{\text{shift in level } m}$$

Now the state m varies in time as $e^{iE_m't}$. But our TDPT has taken out e^{-iE_mt}, e.g.

$$e^{-iE_m't}e^{iE_mt} = e^{-i(\underbrace{E_m' - E_m}_{\text{shift}})T}$$

If we plug this in and take into account that when turning on V we are still exactly in the right state, we get the above expression for S_{mm}.

10/21/66 LECTURE

Comment: This rather incoherent lecture was provided by one of the physics department substituting for Feynman

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Review: We were considering

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

We expand $|\psi\rangle$ in states of the unperturbed H_0, ϕ_n. Using the summation convention throughout

$$|\psi(t)\rangle = c_n|\phi_n\rangle$$

Now to put into "interaction picture", assume

$$c_n \sim e^{-i\omega_n t}\gamma_n$$

Then find

$$i\dot{\gamma}_n = v_{nm}\gamma_m \qquad \text{where } v_{nm} = V_{nm}(t)\,e^{i(\omega_n-\omega_m)t}$$

If we integrate this equation, we can expand

$$\underline{\gamma} = e^{-i\int \underline{\underline{v}}(t)\,dt} \qquad \text{using } \gamma_m(t) = S_{mn}\gamma_n(0)$$

to find

$$S_{mn} = \delta_{mn} - i\int v_{mn}\,dt + \iint_{t_1>t_2} v_{me}(t_1)\,v_{en}(t_2)\,dt_1\,dt_2 + \cdots$$

EXAMPLE: Consider tritium decay as example of $V = 0 \quad t < 0$

$= V_0 \quad t \geq 0$

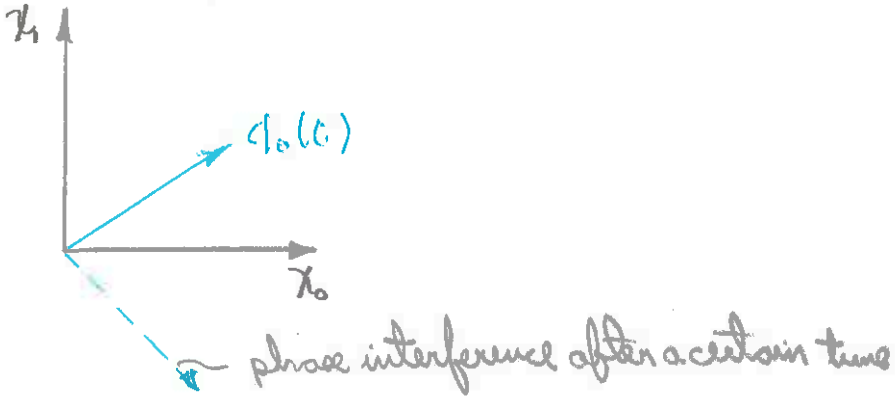
$t < 0$ $\qquad$ $t = 0^+$

H_0, ϕ_0 $\qquad$ H, χ

Also assume electron doesn't have time to adjust, so that $\psi(0^-) = \psi(0^+)$
What is the prob. for the electron to wind up in the s-state after the decay? Expand

$$\phi_0 = a_n \chi_n \qquad \text{where } |a_n|^2 \text{ is the prob.}$$

Consider a 2-state system



We can solve this problem by ~~stationary~~ perturbation theory.
Note:

Energy is conserved in T.I.P.T.
" " not " " T.D.P.T.

Now consider S_{mm}

$$S_{mm} = 1 - iTV_{mm} - \frac{T^2}{2} V_{mm}^2 - iT \sum_k \frac{V_{mk} V_{km}}{(E_k - E_m)} + \sum_k \frac{(V_{mk})^2}{(E_k - E_m)^2} \left[e^{-i(E_k - E_m)T} - 1 \right]$$

Note we can write this as

$$S_{mm} = \exp\left\{ -iT \left[V_{mm} - \sum_k \frac{(V_{mk})^2}{(E_k - E_m)^2} \right] \right\} \cdot \left\{ 1 + \sum_k \frac{|V_{mk}|^2}{(E_k - E_m)^2} \left[e^{i(E_m - E_k)T} - 1 \right] + \cdots \right\}$$

We can recognize the first term directly from TIPT. For the second term, just consider

$$|S_{mm}|^2 = 1 + 2\,\mathrm{Re}\left\{ \left[\sum_k \frac{|V_{mk}|^2}{(E_k - E_m)^2} \left[e^{i(E_m - E_k)T} - 1 \right] \right. \right.$$

$$= 1 - \sum_k \frac{4 \sin^2 (E_m - E_k) T/2}{(E_m - E_k)^2} |V_{mk}|^2$$

first order TDPT for transition prob.

2) Conservation of Probability (Unitarity)

$t=0$: $\gamma_n(0) = 1$, $\gamma_m = 0$ $\quad m \neq n$

$t = T$: $\gamma_m(t) = S_{mn}\gamma_n(0)$

Now for all t,

$$\sum_m |\gamma_m|^2 = 1$$

or $\quad \gamma_\ell^*(0) S_{m\ell}^* S_{mn} \gamma_n(0) = \gamma_n^*(t)\gamma_n(t)$

$$= \gamma_n^*(0)\gamma_n(0) \quad \text{postulate}$$

In matrix notation, this implies

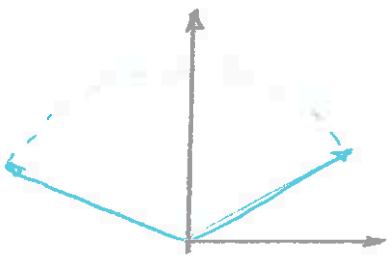
$$\gamma^* S^{*T} S \gamma = \gamma^* \gamma$$

$$\Rightarrow \quad S^{*T} S = 1$$

or $\quad S^\dagger S = 0$

Thus conservation of probability $\Rightarrow$ S is unitary ★

[In real vector space, $\Rightarrow$ S is orthogonal. Thus the S matrix is kind of a complex rotation, but it can't change length (by conservation of probability)



Thus is an extremely powerful principle. To apply it further, we define the T matrix by

$$S = 1 + 2iT$$

Thus we can find our new unitarity condition

$$S^\dagger S = (1 - 2iT^\dagger)(1 + 2iT) = 1$$

$$= 1 - 2i(T - T^\dagger) - (2i)^2 T^\dagger T = 1$$

$$\Rightarrow \quad \frac{T - T^\dagger}{2i} = T^\dagger T$$

APPLICATIONS:

a.) *Optical Theorem:*

Consider scattering $A + B \to A + B$ (1 to 1)
$\to C + D$ (2)
$\to C' + D' + E'$ (3)

To find the transition probability for forward elastic scattering, we look T_{11} (state 1 to state 1)

$$\frac{T_{11} - T_{11}^*}{2i} = T_{in}^\dagger T_{ni}$$

or

$$\text{Im}\{T_{11}\} = T_{ni} T_{ni}^* = \sum_n |T_{ni}|^2 = (\quad)\,\sigma_T$$

(kinematical factor)

Note how similar this looks to our TDPT.

Also note

$$|T_{11}| > \mathrm{Im}\{T_{11}\} > T_{11}T_{11}^* = |T_{11}|^2$$

b.) *Final State Theorem: (Watson)*

Known: $\pi^{(1)}N \to \pi^{(1)}N$ $\quad l=0$ (s-wave)

Want to examine $\gamma^{(2)}N \to \pi^{(1)}N$

From time reversal we know T is symmetric.

$$\therefore \mathrm{Im}\{T_{12}\} = T_{11}^* T_{12} + T_{12}^* T_{22}$$

If we assume ① intermediate state is dominant ($\pi\pi$ process is second order), then

$$\Rightarrow \text{phase}(T_{11}) = \text{phase}(T_{12})$$

10/25/66 LECTURE

3.) SCATTERING OF LIGHT FROM AN ATOM

Classically one develops Thomson scattering

By examining the terms in $\sum \frac{N_i}{\omega^2 - \omega^2}$ one eventually arrived at quantum mechanics. This kind of classical fiddling to obtain quantum results has its analogue in particle physics today.

We will develop the quantum theory more directly.

Part 1: The Student's Approach

We need a current density. Perhaps we could try

$$\vec{j}(\vec{r},t) = \psi^*\left(\frac{\hbar}{im}\nabla\psi\right) + \left(\frac{\hbar}{im}\nabla\psi\right)^*\psi$$

and then use

$$\Box^2\vec{A} = \vec{j}(\vec{r},t)$$

But look at the special case when the incident light is turned off. If $\psi = \psi(\vec{r},t)$, we expand

$$\psi(\vec{r},t) = \sum_n c_n \phi_n(\vec{r}) e^{-iE_n t}$$

Then

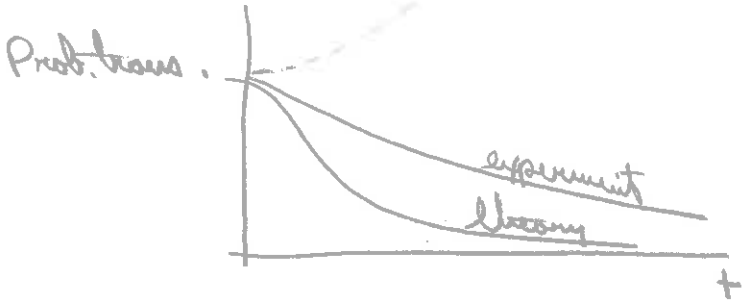
$$\vec{J}(\vec{r},t) = \sum_{n,m} C_n C_m^* e^{i(E_m - E_n)t} \left[\phi_n^*(\vec{r}) \left(\frac{\hbar}{i m} \nabla \phi_m \right) + \left(\frac{\hbar}{i m} \nabla \phi_n \right)^* \phi_m \right]$$

But if ψ is an eigenstate, $\psi = C_n \phi_n$ and $\vec{j} \neq \vec{j}(t)$. Also look at

Energy radiated into $(E_m - E_n) = |C_n C_m^*|^2 = |C_n|^2 |C_m|^2$

joint probability

Thus if $C_n = 0$, all in the n-state so no spontaneous emission.



Point: if we think like other people we frequently go down the same drains

We might try to disregard the bad treatment of spontaneous emission and plow ahead. Solve

$$\frac{\partial \psi}{\partial t} = (H_0 + V)\psi$$

We can do it if we use <u>both</u> incoming and outgoing waves (advanced and retarded potentials)

The problem is that we have been dealing with the EM field classically. The N+1 ; N difference is needed for spontaneous emission.

How is one photon changed into another? Regard the atom as kind of a weak spring between the modes. Write

$$\vec{A} = \sum_{\vec{k},\hat{e}} Q_{\vec{k},\hat{e}}\, e^{i\vec{k}\cdot\vec{r}}\,\hat{e}$$

Find $$H = \sum_i \left(\frac{1}{2\mu_i} P_i^2 + \frac{\mu_i}{2} Q_i^2\right) + C_{ij} Q_i Q_j$$

Use

$$H_{atom} = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)\cdot\left(\vec{p} - \frac{e}{c}\vec{A}\right) + eV$$

$$= \frac{1}{2m}p^2 - \frac{\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}}{2m} + \frac{\vec{A}\cdot\vec{A}}{2\mu} + eV$$

Try

$$\frac{1}{2m}\vec{A}(\vec{r})\cdot\vec{A}(\vec{r}) = \frac{1}{2m}\sum_{\vec{k}',\hat{e}'}\sum_{\vec{k}'',\hat{e}''} Q_{\vec{k}'\hat{e}'}\, Q_{\vec{k}''\hat{e}''}\,\hat{e}'\cdot\hat{e}''\, e^{i(\vec{k}'+\vec{k}'')\cdot\vec{r}}$$

Thus we suspect

$$\text{Rate} = 2\pi\,\delta(\epsilon_a + \omega_1 - \epsilon_b - \omega_2)\,|M_{ij}|^2$$

$$|M_{ij}| = \sum_i \sum_j \langle b, \vec{k}_2 | Q_i Q_j C_{ij}(\vec{r}) | a, \vec{k}_1 \rangle$$

$$= \frac{\hat{e}_1\cdot\hat{e}_2}{2m}\langle b | e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}} | a\rangle \sqrt{\frac{\pi}{2\mu\omega_1}}\sqrt{\frac{\pi}{2\mu\omega_2}}$$

Note if $\hat{e}_1\cdot\hat{e}_2 = 0$, no scattering.

Part 2: Feynman's Approach

10/28/66 LECTURE

We were considering the scattering of photons off of atoms

initial state $|$atom in a, one photon of $\vec{k}_1, \hat{e}_1\rangle$ energy $\epsilon_a + \omega_1$

final state $|$atom in b, one photon of $\vec{k}_2, \hat{e}_2\rangle$ energy $\epsilon_b + \omega_2$

We had suggested that the scattering rate could be represented by

$$\text{Rate} = 2\pi\, \delta(E_f - E_i)\, |\langle f|M|i\rangle|^2$$

We will show later that

$$\langle f|M|i\rangle = -i\left[\langle f|V|i\rangle + \sum_k \frac{\langle f|V|k\rangle\langle k|V|i\rangle}{E_i - E_k \pm i\eta} + \cdots\right]$$

Study this series, calculate higher terms, and interpret it.

Now

$$H = \frac{p^2}{2m} + V(\vec{r}) - \underbrace{q_{el}\left(\frac{\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}}{2m}\right) + q_{el}^2 \frac{\vec{A}\cdot\vec{A}}{2m}}_{H_{interaction}} + H_{field}$$

Now we expand

$$\vec{A} = \sum_{\vec{k},\hat{e}} Q_{\vec{k},\hat{e}}\, \hat{e}\, e^{i\vec{k}\cdot\vec{r}}$$

[Note we have two quantizations -- that of the classical field modes and the true quantization of each of these field modes. Sometimes called second quantization]

Now we had only been considering the $\vec{A}\cdot\vec{A}$ term since it gave rise to a direct coupling between photon k_1 and photon k_2. We found

$$\langle f|M|i\rangle = \frac{\hat{e}_1\cdot\hat{e}_2}{\sqrt{2\mu\omega_1}\sqrt{2\mu_4\omega_2}}\langle b|e^{i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}}|a\rangle$$

But classically we found terms like $\sum \frac{q_i}{\omega^2-\omega_i^2}$. Why don't we get this by our q. m.?

We forgot that indirect coupling of photons through intermediate states is also second order like $\vec{A}\cdot\vec{A}$. We must then consider the probability that a photon interacts with the atom by $\vec{p}\cdot\vec{A}$ and then the atom re-admits a new photon again by $\vec{p}\cdot\vec{A}$. This will involve the

$$\sum_k \frac{\langle f|V|k\rangle\langle k|V|i\rangle}{E_i - E_k + i\eta} \qquad (*)$$

Now our V is

$$V = \sum_{k,\hat{e}} q_{el}\frac{\vec{p}\cdot\hat{e}\,e^{i\vec{k}\cdot\vec{r}}}{m}Q_{\vec{k},\hat{e}}$$

Now what intermediate states are possible? Certainly not all. Only those states for which $\langle k|V|i\rangle$ exist contribute to $(*)$. Thus one must see where one can get from initial state via the perturbation. Only one Q in Hint, so one photon processes are all that are possible.

		Energy
initial state	atom in a, all oscillators zero except $\vec{k}_1, \hat{e}_1$	$\epsilon_a + \omega_1$
possible intermediate states	① atom in c, all oscillators zero	ϵ_c
	② atom in c, 1 photon in $\vec{k}_3$, 1 photon in $\vec{k}_1$	$\epsilon_c + \omega_3 + \omega_1$
	③ atom in c, 2 photons in $\vec{k}_1$	$\epsilon_c + 2\omega_1$

Now try to calculate the matrix elements $\langle k|V|i\rangle$ using the dumb approach [don't consider $\langle f|V|k\rangle$ yet]

$$\langle k|V|i\rangle_{①} = q_{el}\langle c|\frac{\vec{p}\cdot\hat{e}_1}{m}e^{i\vec{k}_1\cdot\vec{r}}|a\rangle\frac{1}{\sqrt{2\mu_1\omega_1}}$$

$$\langle k|V|i\rangle_{②} = q_{el}\langle d|\frac{\vec{p}\cdot\hat{e}_3}{m}e^{-i\vec{k}_3\cdot\vec{r}}|a\rangle\frac{1}{\sqrt{2\mu_3\omega_3}}$$

$$\langle k|V|i\rangle_{③} = q_{el}\langle c|\frac{\vec{p}\cdot\hat{e}_1}{m}e^{-i\vec{k}_1\cdot\vec{r}}|a\rangle\frac{1}{\sqrt{2\mu_1\omega_1}}$$

Note that when a photon is eaten, $e^{+i\vec{k}\cdot\vec{r}}$, and when it is spit out, $e^{-i\vec{k}\cdot\vec{r}}$. Now for $\langle f|V|k\rangle$

$$\langle f|V|k\rangle_{①} = q_{el}\langle b|\frac{\vec{p}\cdot\hat{e}_2}{m}e^{-i\vec{k}_2\cdot\vec{r}}|c\rangle\frac{1}{\sqrt{2\mu_2\omega_2}}$$

$$\langle f|V|k\rangle_{②} = q_{el}\langle b|\frac{\vec{p}\cdot\hat{e}_1}{m}e^{i\vec{k}_1\cdot\vec{r}}|c\rangle\frac{1}{\sqrt{2\mu_1\omega_1}} \qquad [\text{note } \vec{k}_3 \text{ must be } \vec{k}_2]$$

$\langle f|V|k\rangle_{③} = 0$ unless $\vec{k}_2 = \vec{k}_1$, but we won't consider forward scattering [do it yourself]

Thus we find finally

$$\langle f|M|i\rangle = i\left\{ \frac{\hat{e}_1\cdot\hat{e}_2}{\sqrt{2\mu_1\omega_1}\sqrt{2\mu_2\omega_2}} \langle b| e^{i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}} |a\rangle \right.$$

$$+ \sum_c \frac{q_{el}^2}{\sqrt{2\mu_1\omega_1}\sqrt{2\mu_2\omega_2}} \frac{\langle b|\frac{\vec{p}\cdot\hat{e}_2}{m} e^{-i\vec{k}_2\cdot\vec{r}}|c\rangle\langle c|\frac{\vec{p}\cdot\hat{e}_1}{m} e^{+i\vec{k}_1\cdot\vec{r}}|a\rangle}{\epsilon_a+\omega_1-\epsilon_c+i\eta}$$

$$\left. + \sum_c \frac{q_{el}^2}{\sqrt{2\mu_1\omega_1}\sqrt{2\mu_1\omega_1}} \frac{\langle b|\frac{\vec{p}\cdot\hat{e}_1}{m} e^{+i\vec{k}_1\cdot\vec{r}}|c\rangle\langle c|\frac{\vec{p}\cdot\hat{e}_2}{m} e^{-i\vec{k}_2\cdot\vec{r}}|a\rangle}{\epsilon_a+\omega_1-\epsilon_c-\omega_1-\omega_2+i\eta} \right\}$$

Now up to this point the analysis has been of a very general type. You will run into this quite frequently [phonon-roton scattering, etc.]

We will now make a few comments of specific interest in photon scattering

1.) violation of energy conservation ["Them that violate energy conservation the most is the least contributors."]

How to explain violation of energy conservation in barrier penetration to inquisitive students: must use experiments to measure the effect and then uncertainty principle fouls you up.

[If you don't like this explanation, just ask them to invent a physical experiment which shows a paradox.]

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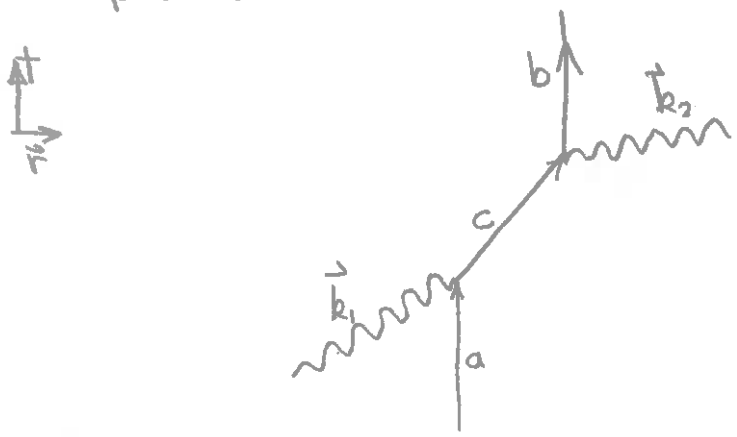
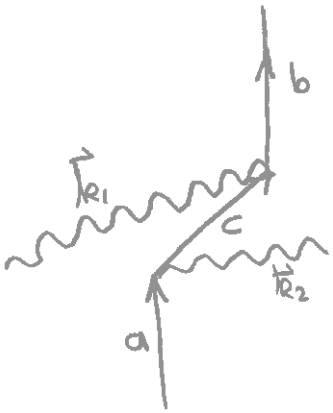
ii.) The atom may emit a photon before it absorbs the incident photon.

We can show this with Feynman diagrams [or as the master says, "me"-diagrams]

normal process



pair emission



10/31/66 LECTURE

Problem: Derive a more elegant theory for the S-matrix (Use matrix algebra or such) – derivation, more terms, etc. Maybe just properties of S-matrix (time reversal).

Special Properties of Light Scattering:

We had found

$$\text{Rate} = c\sigma = 2\pi\delta(\epsilon_a + \omega_{in} - \epsilon_b - \omega_{out}) \frac{d^3\vec{k}_{out}}{(2\pi)^3} \frac{(4\pi e^2)^2}{2\omega_{in} 2\omega_{out}} |M|^2$$

Note for each photon coupling $(4\pi e^2)$. Also

$$M = \sum_c \frac{\langle b | \frac{\vec{p}\cdot\vec{e}_1}{m} e^{-i\vec{k}_2\cdot\vec{r}} | c\rangle\langle c | \frac{\vec{p}\cdot\vec{e}_1}{m} e^{i\vec{k}\cdot\vec{r}} | a\rangle}{\epsilon_c - \epsilon_a - \omega_1 + i\eta}$$

$$+ \sum_c \frac{\langle b | \frac{\vec{p}\cdot\hat{e}_1}{m} e^{+i\vec{k}_1\cdot\vec{r}} | c\rangle\langle c | \frac{\vec{p}\cdot\hat{e}_2}{m} e^{-i\vec{k}_2\cdot\vec{r}} | a\rangle}{\epsilon_c - \epsilon_a + \omega_2 + i\eta}$$

$$+ \frac{1}{m}\langle b | e^{i(\vec{k}_1 - \vec{k}_2)\cdot\vec{r}} | a\rangle (\hat{e}_1\cdot\hat{e}_2)$$

See what the rules are for example $\hat{e}_1, \hat{e}_2$ (circularly polarized light.

Consider atomic systems with more than one electron. Include spin

Note that the outgoing photon may have a shifted frequency ω, and thus the atom is excited. In oxygen, the electronic levels are largely spaced. However molecular levels are close, thus some scattering [Rahman scattering -- made Rahman the hero of India and Indian science known to the world]

We consider now elastic scattering from H-atom

$$\epsilon_a + \vec{k}_1 \rightarrow \epsilon_a + \vec{k}_2$$

[Of course, we should really deal with 2 particle system because of finite nuclear mass. Do this yourself for a problem.]

Assume wavelength >> size of atom. [Ordinary light scattering] Then in matrix elements we can take

$$\vec{k}\cdot\vec{r} \rightarrow 0$$

and find

$$M = \sum_c \frac{\langle a|\frac{\vec{p}\cdot\hat{e}_2}{m}|c\rangle\langle c|\frac{p\cdot\hat{e}_1}{m}|a\rangle}{\epsilon_c - \epsilon_a - \omega + i\eta}$$

$$+ \sum_c \frac{\langle a|\frac{\vec{p}\cdot\hat{e}_1}{m}|c\rangle\langle c|\frac{\vec{p}\cdot\hat{e}_2}{m}|a\rangle}{\epsilon_c - \epsilon_a + \omega + i\eta}$$

$$+ \frac{1}{m}\langle a|1|a\rangle(\hat{e}_1\cdot\hat{e}_2)$$

Note

we find resonant scattering for ω ~ level energy difference and we can see a very large scattering.

Now we have seen $\frac{\vec{p}}{m} = \dot{\vec{x}} = i(H\vec{x} - \vec{x}H)$

Thus

$$\langle c|\frac{\vec{p}}{m}|d\rangle = i\langle c|H\vec{x} - \vec{x}H|d\rangle$$

$$= i(\epsilon_c - \epsilon_d)\langle c|\vec{x}|d\rangle$$

Then

$$M_1 = \sum_c \frac{i(\epsilon_a - \epsilon_c)\langle a|\vec{x}\cdot\hat{e}_2|c\rangle\langle c|\frac{\vec{p}\cdot\hat{e}_1}{m}|a\rangle}{\epsilon_c - \epsilon_a - \omega}$$

$$- \sum_c \frac{i(\epsilon_a - \epsilon_c)\langle a|\frac{\vec{p}\cdot\hat{e}_1}{m}|c\rangle\langle c|\vec{x}\cdot\vec{e}_2|a\rangle}{\epsilon_c - \epsilon_a + \omega}$$

$$+ \frac{1}{m}\langle a|a\rangle(\hat{e}_1\cdot\hat{e}_2)$$

$$= -i\omega\sum_c\left\{\frac{\langle a|\vec{x}\cdot\hat{e}_2|c\rangle\langle c|\frac{\vec{p}\cdot\hat{e}_1}{m}|a\rangle}{\epsilon_c - \epsilon_a - \omega} + \frac{\langle a|\frac{\vec{p}\cdot\vec{e}_1}{m}|c\rangle\langle c|\vec{x}\cdot\hat{e}_2|a\rangle}{\epsilon_c - \epsilon_a + \omega}\right\} \quad (*)$$

$$- i\sum_c\left\{\langle a|\vec{x}\cdot\hat{e}_2|c\rangle\langle c|\frac{\vec{p}\cdot\hat{e}_1}{m}|a\rangle - \langle a|\frac{\vec{p}\cdot\vec{e}_1}{m}|c\rangle\langle c|\vec{x}\cdot\hat{e}_2|a\rangle\right\}$$

$$+ \frac{1}{m}\langle a|a\rangle(\hat{e}_1\cdot\hat{e}_2)$$

Now use the matrix product

$$\sum_c \langle a|A|c\rangle\langle c|B|b\rangle = \langle a|AB|b\rangle$$

Our second term becomes

$$-i\left\{\langle a|(\vec{x}\cdot\hat{e}_2)\left(\frac{\vec{p}\cdot\hat{e}_1}{m}\right)|a\rangle - \langle a|\left(\frac{\vec{p}\cdot\hat{e}_1}{m}\right)(\vec{x}\cdot\hat{e}_2)|a\rangle\right\}$$

Now $\quad pq - qp = \frac{\hbar}{i}$

$$= -\frac{1}{m}\langle a|a\rangle(\hat{e}_1\cdot\hat{e}_2)$$

and cancels the third term.

Talks some about sum rules

$$\sum_k |X_{nk}|^2 (E_n - E_k) \stackrel{?}{=} \frac{\hbar}{m}$$

If we had also done the $\langle c|\frac{\vec{p}\cdot\hat{e}}{m}|a\rangle$ we would have arrived

$$\sum_c (\epsilon_c - \epsilon_a)\left|\langle a|\vec{x}_1|c\rangle\right|^2 = \frac{1}{m}$$

Now in the first term in (*), we see that for small ω, $\epsilon_c - \epsilon_a - \omega$, are ~ const. Then we can do sum.
Thus sum rules are very useful.

11/1/66 LECTURE

4.) ROTON EXCITATION PROBLEM:

$$\epsilon(p) = \Delta + \frac{1}{2\mu}(p-p_0)^2$$

roton energy

If we allow the density to vary,

$$\epsilon(p) = \Delta + \frac{1}{2\mu}(p-p_0)^2 + d(\rho-\rho_0)$$

If density varies in space, roton energy also varies. This interaction is our perturbation

The amplitude for finding the roton at $\vec{r}$ can be taken to be

$$\psi(\vec{r}) = e^{i\vec{p}\cdot\vec{r}}$$

$$\therefore \psi(\vec{r}, \text{inter}) \sim e^{i\vec{p}\cdot\vec{r}}\,\Phi(\text{inter})$$

Thus we take

initial state: roton $\vec{p}$

final state: roton $\vec{p}'$, phonon $\vec{k}$

Phonons are to sound what photons are to light. Expect sound modes

Classical

Displacement $\vec{u}$

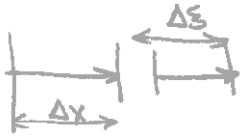
$$\vec{u}(x,t) = \sum_{\vec{k}} Q_{\vec{k}}(t) e^{i\vec{k}\cdot\vec{r}} \frac{\vec{k}}{k}$$

Kinetic energy

$$T = \int \tfrac{1}{2} \rho \left(\frac{\partial \vec{u}}{\partial t}\right)^2 dVol \simeq \frac{1}{2}\rho_0 \sum_{\vec{k}} \left(\dot{Q}_{\vec{k}}\right)^2$$

Potential energy

$$V = \frac{\lambda}{2}(\rho - \rho_0)^2$$



$$\Delta\xi = \Delta x + u(x,t) - u(x+\Delta x, t)$$

$$= \Delta x + \Delta x \frac{\partial u}{\partial x}$$

$$\rho \Delta\xi = \rho_0 \Delta x$$

$$\frac{\rho_0}{\rho} = 1 + \nabla\cdot\vec{u} \quad \Rightarrow \quad \rho_0 \simeq \rho + \rho_0 \nabla\cdot\vec{u}$$

$$V \simeq \frac{\lambda}{2}\left[\rho_0 \nabla\cdot\vec{u}\right]^2 = \frac{\lambda}{2}\rho_0^2 \sum_{k} Q_k^2 k^2$$

Total energy

$$E = \sum_{k} \frac{\rho_0}{2}\left(\dot{Q}_k^2 + \lambda \rho_0 k^2 Q_k^2\right)$$

Now $\omega = kc_s$ $\quad \therefore \lambda = \frac{c_s^2}{\rho_0}$

Quantum:

Set Q_k become quantum oscillators

$$H_{phonon} = \sum_k \left(\frac{P_k^2}{2\rho_0} + \frac{\rho_0 \omega_k^2}{2} Q_k^2 \right)$$

Thus

$$H = H_{electrons} + H_{phonon} + H_{int}$$

$$= \epsilon(p) + \sum_{\vec{k}} \left(\frac{P_k^2}{2\rho_0} + \frac{\rho_0 \omega_k^2}{2} Q_k^2 \right) + d(\rho(\vec{r}) - \rho_0)$$

$$H_{int} = di\rho_0 \sum_k k Q_k e^{i\vec{k}\cdot\vec{r}}$$

Then

$$\text{Rate}_{\vec{p} \to \vec{p}', \vec{k}} = 2\pi \delta(\epsilon(p') + \hbar k c_s - \epsilon(p)) \, |M|^2 \frac{d^3\vec{k}}{(2\pi)^3}$$

Now

$$M = \langle \vec{p}', \vec{k} | di\rho_0 k Q_k e^{i\vec{k}\cdot\vec{r}} | \vec{p}, 0 \rangle$$

$$= \frac{di\rho_0 k}{\sqrt{2\rho_0 \omega_k}} \langle \vec{p}' | e^{i\vec{k}\cdot\vec{r}} | \vec{p} \rangle$$

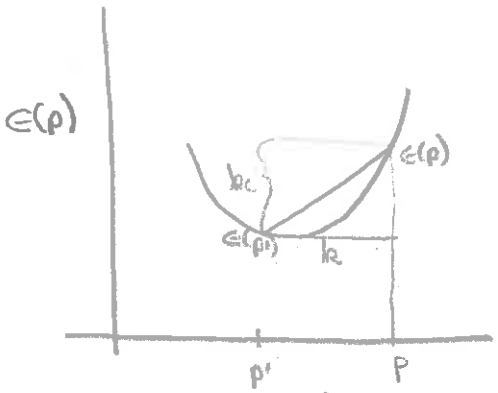
$$\langle \vec{p}' | e^{i\vec{k}\cdot\vec{r}} | \vec{p} \rangle = \int e^{-i\vec{p}'\cdot\vec{r}} e^{-i\vec{k}\cdot\vec{r}} e^{i\vec{p}\cdot\vec{r}} d^3\vec{r}$$

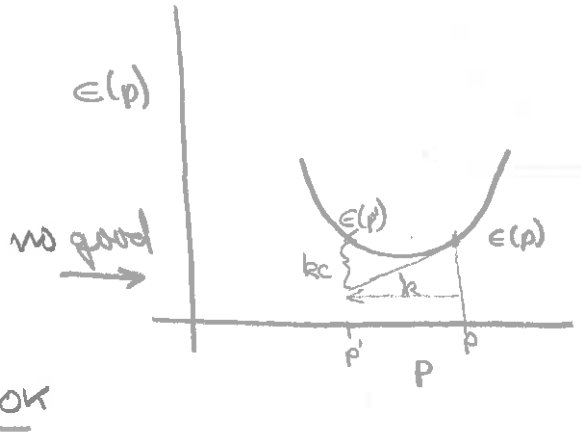
$$= \delta(\vec{p}' - (\vec{p} - \vec{k}))$$

conservation of momentum

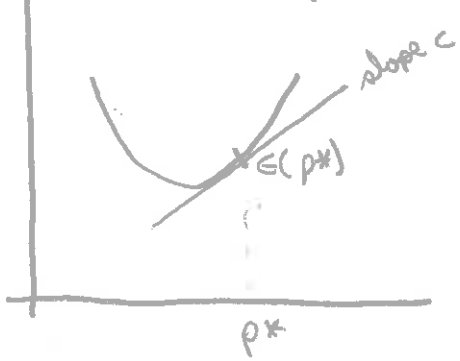
$$\underset{\vec{p} \to \vec{p}', \vec{k}}{\text{Rate}} = 2\pi \delta(\epsilon(p') + \hbar c k - \epsilon(p)) \frac{d^2k^2 e_a^2}{2\rho_0 \hbar c} \frac{k^2 dk d\Omega}{(2\pi)^3}$$

Consider first forward emission





Thus a critical p^* below which we cannot emit phonons



$$\left.\frac{d\epsilon(p)}{dp}\right|_{p^*} = c_s$$

In any system with $\epsilon = \epsilon(p)$

$$\frac{d\epsilon}{dp} = v_{group}$$

Proof: $\Delta\epsilon = F\,\Delta x$ $\qquad F = \frac{\Delta p}{\Delta t}$

$$\frac{\Delta\epsilon}{\Delta t} = \frac{\Delta p}{\Delta t} v$$

$$\frac{\Delta\epsilon}{\Delta p} = v$$

Thus velocity of return must exceed speed of sound c_s to have phonon emission [same as Cerenkov radiation]

5.) Some Improvements to our Theory

11/4/66 LECTURE

We had found things like

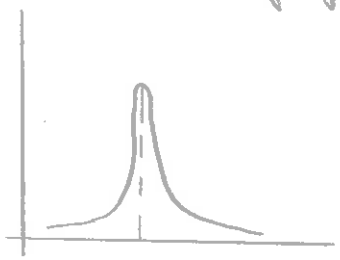
$$\sigma \sim \sum_c \frac{\langle b|\hat{O}_1|c\rangle\langle c|\hat{O}_2|a\rangle}{\epsilon_c - \epsilon_a - \omega_1}$$

But results like this are very similar to classical physics in which the atom is treated as a classical harmonic oscillator

$$m(\ddot{x} + \gamma\dot{x} + \omega_0^2 x) = E$$

$$\therefore x \sim \frac{1}{\omega_0^2 - \omega^2 + i\omega\gamma} \sim \frac{1}{2\omega_0(\omega - \omega_0 + i\frac{\gamma}{2})} \quad \text{near resonance}$$

This gives a broadening of the resonance.



We can reverse this argument to obtain absorption lines in solar spectra

Now we would like to get such a line width into our quantum theory for very close to resonance (when we aren't close, our new theory would be quite right).

The trouble with the old theory arises from a degeneracy, e.g. a level n is degenerate with a class of states in the continuum

We will find the state n then has a finite lifetime and will eventually decay into the continuum states.

Recall we began our treatment of time-dependent perturbation theory by trying to calculate $\gamma_m(t)$, the amplitude that we will find the system in state m at time t. We found

$$i\dot{\gamma}_m(t) = \sum_n v_{mn}(t)\,\gamma_n(t)$$

$$= \sum_n V_{mn} e^{i(E_n - E_m)t}\,\gamma_n(t) \qquad (1)$$

Now let our system (say, an atom) be in a state n and let state k be in a continuum [e.g. scattering of light from a particle that can disintegrate]. Then (1) becomes

$$i\dot{\gamma}_n(t) = \left(\begin{array}{c}\text{terms relating}\\ \text{states other than}\\ \text{the continuum}\end{array}\right) + \int_k V_{nk} e^{i(E_k - E_n)t}\,b_k(t) \qquad (2)$$

If we assume k interacts only with n, we can write

$$i\dot{b}_k(t) = V_{kn} e^{i(E_n - E_k)t}\,\gamma_n(t) \qquad (3)$$

We want to include the effects of k close to n, thus we assume V_{nk} are very small (so the system has at least a reasonable lifetime). Then we integrate (3) directly

$$b_k(t) = -i \int_0^t V_{kn} e^{i(E_n - E_k)t'}\gamma_n(t')\,dt'$$

Substitute this into (2) to find

$$i\dot{\gamma}_n(t) = (\text{other terms}) - i \int_k \int_0^t dt' \,|V_{kn}|^2 e^{-i(E_n - E_k)(t-t')}\gamma_n(t') \qquad (4)$$

We now have an equation in terms of the γ_n's alone. We have removed details of the b_k. We only retain its effect on the actual process we are interested in.

Now assume the γ_n's vary slowly and

$$\gamma_n(t) \sim \gamma_n(t')$$

If we also consider time-independent perturbations and note

$$\int_0^\infty du\, e^{-i(E_n - E_k)u} e^{-\epsilon u} = \frac{1}{\epsilon + i(E_n - E_k)}$$

we can write (4) as

$$i\dot{\gamma}_n(t) = (\text{other terms}) - \left[\sum_k \frac{|V_{kn}|^2}{E_n - E_k - i\epsilon} \right] \gamma_n(t) \tag{5}$$

Now define

$$\lim_{\epsilon \to 0} \sum_k \frac{|V_{kn}|^2}{E_n - E_k - i\epsilon} = \Delta_n + i\frac{\Gamma_n}{2} \tag{6}$$

so that (5) becomes

$$i\dot{\gamma}_n(t) = (\text{other terms}) - \left(\Delta_n + i\frac{\Gamma_n}{2}\right)\gamma_n(t) \tag{7}$$

Special Case: Solve (7) neglecting (other terms)

$$\gamma_n(t) = \gamma_n(0)\, e^{\left(\Delta_n + i\frac{\Gamma}{2}\right)t}$$

But recall $\gamma_n(t) = C_n(t)\, e^{iE_n t}$

Thus $$C_n(t) = e^{-i(E_n - \Delta_n)t} e^{-\frac{\Gamma_n}{2}t}$$

We can see from this special case that the continuum interaction shifts the levels by Δ_n [for example, all levels of the S-eqn for atoms should be shifted because atoms can radiate into a continuum].

Also note

$$|C_n|^2 = e^{-\Gamma_n t}$$

Thus the probability of remaining in the state n decays with a mean life $1/\Gamma_n$.

In the remainder of our analysis we will forget the small shift corrections Δ_n for a bit. The important physical effect for us is Γ_n, the line width.

We now return to calculating Γ_n and Δ_n from (6).

Recall

$$\lim_{\epsilon \to 0} \frac{1}{x + i\epsilon} \simeq \text{P.V.}\left(\frac{1}{x}\right) - i\pi\delta(x)$$

We then find

$$\Delta_n = \text{P.V.} \sum_k \frac{|V_{kn}|^2}{E_n - E_k}$$

[similar to 2nd order perturbation theory result]

$$\Gamma_n = 2\pi \sum_k |V_{kn}|^2 \delta(E_n - E_n)$$

rate to go from state n to anything (all k)

[decays with $\frac{dP_n}{dt} = -\Gamma_n P_n$]

To generalize these results we recognize that we get a Γ_i for each type of continuum (α decay, β decay, etc -- each decay "channel").

EXAMPLE: Light emission by an atom which itself can disintegrate

n ——— m ——— both n and m can disintegrate

Let the atom initially be in state n, i.e. $a_n(0) = 1$
The analogue to (5) becomes

$$\dot{a}_n(t) = -i V_{nm}(t) a_m(t) - \frac{\Gamma_n}{2} a_n(t) \tag{7a}$$

$$\dot{a}_m(t) = -i V_{mn}(t) a_n(t) - \frac{\Gamma_m}{2} a_m(t) \tag{7b}$$

where we have ignored Δ_n and Δ_m. Ignoring V_{nn} in (7a), we can solve directly for

$$a_n(t) = e^{-\frac{\Gamma_n}{2}t}$$

We can then substitute this into (7b) to find

$$a_m(t) = e^{-\frac{\Gamma_m}{2}t} \int_0^t \left(-i V_{mn}(t')\right) e^{-\frac{\Gamma_m}{2}t'} e^{+\frac{\Gamma_n}{2}t'} dt$$

Let $V = \text{const}$, $V_{nm} = V_{nm} e^{-i(E_n - E_m)t'}$

Thus

$$a_m(t) = \frac{V_{nm}}{i\left(\frac{\Gamma_m - \Gamma_n}{2}\right) + (E_n - E_m)} \left[e^{-\frac{\Gamma_n}{2}t} e^{-i(E_n - E_m)t} - e^{-\frac{\Gamma_m}{2}t} \right]$$

$$\therefore P_n(t) = \frac{|V_{nm}|^2}{(E_n-E_m)^2 + \frac{(\Gamma_n-\Gamma_m)^2}{4}} \left[e^{-\Gamma_n t} + e^{-\Gamma_m t} - 2\cos(E_n-E_m)t\, e^{-\frac{\Gamma_n}{2}t} e^{-\frac{\Gamma_m}{2}t} \right]$$

Suppose

state n: atom in a

state m: atom in b, photon ω

If we use $\int_0^\infty \frac{dx}{x^2+\Gamma^2/4} = \frac{\pi}{\Gamma}$ $\int_0^\infty \frac{dx}{x^2+\frac{\Gamma^2}{4}} \cos xt = \frac{\pi}{\Gamma} e^{-|\Gamma|t}$

we can find

$$\sum_n P_n(t) = \rho(E_m)|V_{nm}|^2 \frac{\pi}{\Gamma_n-\Gamma_m} \left[e^{-\Gamma_n t} + e^{-\Gamma_m t} - 2e^{-\left(\frac{\Gamma_n-\Gamma_m}{2}\right)t} e^{-\frac{\Gamma_n}{2}t} e^{-\frac{\Gamma_m}{2}t} \right]$$

$$= \rho(E_m)|V_{nm}|^2 \frac{\pi}{\Gamma_n-\Gamma_m} \left[e^{-\Gamma_n t} - e^{-\Gamma_m t} \right]$$

We can liken this to the following problems ("leaky barrels")

_____ $P_n(t)$ $\quad \dot{P}_n(t) = -\Gamma_n P_n(t)$

_____ $P_m(t)$ $\quad \dot{P}_m(t) = r P_n(t) - \Gamma_m P_m(t)$

11/7/66 LECTURE

PROBLEM: In strong interactions, Gell-Mann cooked up a quantity S called strangeness ∋ $\Delta S = 0$.

Ex:

$$\pi^- + p \rightarrow \Lambda^0 + K^0$$
$$S=0 \quad S=0 \quad S=-1 \quad S=+1$$

or

$$\pi^- + p \rightarrow p + K^- + \bar{K}^0$$
$$S=0 \quad S=0 \quad S=0 \quad S=+1 \quad S=-1$$

To distinguish, we note that in matter,

$$\bar{K}^0 + p \rightarrow \Lambda^0 + \pi^+$$

$$K^0 + p \not\rightarrow \Lambda^0 + \pi^+$$

Now the K's decay by weak interactions (slow) in which $\Delta S = \pm 1$ (or 0)

Ex: $K^0 \rightarrow \pi^+ + \pi^-$ $\quad 10^{-10}$ sec (mean life of decay)
$S=+1 \quad S=0 \quad S=0$

and

$\bar{K}^0 \rightarrow \pi^+ + \pi^-$
$S=-1$

thus matrix elements of these reactions are equal

Try to work from this to see what you can find out. Note we are just dealing with disintegration into a continuum of states. Gell-Mann and Pais found that for two states decaying into same continuum, the prob. of finding a K decays not-exponentially. Find out how it does decay, and see how one could measure the effect. [Feynman observed that this proves the principle of superposition of amplitudes.]

If you want to go further, you might like to see

$$K^0 \longrightarrow \pi^- + \mu^+ + \nu$$

rate = 1/500 of 2π decay

$$\overline{K^0} \longrightarrow \pi^+ + \mu^- + \bar{\nu}$$

which makes a more realistic problem (will need CP $\Rightarrow$ $\langle\ \rangle = \langle\ \rangle$)

We return to our perturbation theory of states which can decay into something you are not interested in. Since the state doesn't have an infinite lifetime due to the decay, we know qualitatively from the uncertainty principle that it cannot have a definite energy, but must be regarded as an interaction with a continuum of states, one of which was our earlier definite energy state. This kind of a degenerate perturbation theory.

We had introduced these concepts by writing

$$i\dot{a}_n = \sum_m V_{nm}(t) a_m(t) + \sum_k M_{nk} b_k(t) e^{i(E_n - E_k)t}$$

$$i\dot{b}_k = \sum_m M_{km} e^{+i(E_n - E_k)t} a_m(t)$$

We want to ignore the details of the b_k's and worry only about the a_n's. We found

$$\dot{a}_n = -i \sum_m V_{nm}(t) a_m(t) - \sum_k \int_0^t |M_{kn}|^2 e^{-i(E_n - E_k)(t-t')} a_n(t')\, dt'$$

$$+ \sum_m \int_0^t M_{nk} M_{km} e^{-i(E_n - E_k)t} e^{+(E_m - E_k)t'} a_m(t')\, dt'$$

We are not interested in the last term since it won't affect us very much (no "secular" or resonance effects), so we will ignore it.

If we assume constant perturbations and $a_n(t') \sim a_n(t)$ we could integrate to find

$$\dot{a}_n = -i \sum_m V_{nm}(t) a_m(t) - i \left(\Delta_n - i\frac{\Gamma_n}{2}\right) a_n(t)$$

where $$\Delta_n - i\frac{\Gamma_n}{2} = \sum_k \frac{|M_{kn}|^2}{E_n - E_k + i\epsilon}$$

$$\Gamma_n = 2\pi \sum_k \delta(E_k - E_n) |M_{kn}|^2$$

If we ignore the shift Δ_n, we find

$$\dot{a}_n = -i \sum_m V_{nm}(t) a_m(t) - \frac{\Gamma_n}{2} a_n(t)$$

Now prob. to be in some discrete state from n state is

$$P_{(n)dis} = \sum_k b_k^* b_k$$

Can show.

$$\dot{P}_{(n)dis} = \Gamma_n |a_n(t)|^2$$

[Show it]

Last time we were considering an example

——— a, Γ_a m state: atomic, no photon

n state: atomic, photon ω

——— b, Γ_b

$$\dot{a}_m = -i V_{mn} e^{i(E_m - E_n)t} a_n(t) - \frac{\Gamma_m}{2} a_m(t)$$

$$\dot{a}_n = -\frac{\Gamma_n}{2} a_n(t)$$

Can do this only to first order, by first solving

$$a_n(t) = a_n(0) e^{-\frac{\Gamma_n}{2}t} = e^{-\frac{\Gamma_n}{2}t} \qquad a_n(0) \equiv 1$$

Can then find

$$a_m(t) = -V_{mn} \left\{ \frac{e^{i(E_m - E_n)t - \Gamma_n t/2} - e^{-\Gamma_m t/2}}{E_m - E_n - i\left(\frac{\Gamma_m - \Gamma_n}{2}\right)} \right\}$$

$$P_m = |a_m(t)|^2 = |V_{mn}|^2 \left\{ \frac{e^{-\Gamma_n t} + e^{-\Gamma_m t} - 2e^{-\frac{\Gamma_m + \Gamma_n}{2}t} \cos(E_m - E_n)t}{(E_m - E_n)^2 + \left(\frac{\Gamma_m - \Gamma_n}{2}\right)^2} \right\}$$

Now $E_m - E_n = \epsilon_b + \omega - \epsilon_a = \omega - \omega_{ab} = \nu$ frequency difference from energy level distance

$\Gamma_m = \Gamma_b$, $\Gamma_n = \Gamma_a$

But we want prob. of finding photon of ν and don't want to worry about what happened to state b.

$$P_\nu(t) = P_m + P_{b\,\text{decays}}$$

and

$$\dot{P}_{b\,\text{decays}} = \Gamma_b P_m \qquad (1)$$

11/8/66 LECTURE

Recall

P_m = probability of photoemission of frequency $\omega_0 + \nu = \omega$ and atom in b

$P_{b\,\text{decays}}$ = probability that atom in b decays (photon still there)

P_ν = probability that some photon of ν is present

Thus

$$P_\nu(t) = P_m(t) + P_{b\,\text{decays}}(t)$$

Look at $P_\nu(\infty) = P_m(\infty) + P_{b\,\text{decays}}(\infty)$

now $P_m(\infty) = 0$ [atom certainly has decayed by $t = \infty$]

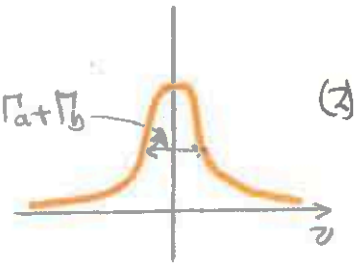
$$P_{b\,\text{decays}} = \Gamma_b \int_0^\infty P_m(t)\,dt' \qquad \text{from (1)}$$

Thus

$$P_\nu(\infty) = \Gamma_b |V_{mn}|^2 \frac{1}{\nu^2 + \left(\frac{\Gamma_a - \Gamma_b}{2}\right)^2} \left[\frac{1}{\Gamma_a} + \frac{1}{\Gamma_b} - \frac{2\left(\frac{\Gamma_a + \Gamma_b}{2}\right)}{\nu^2 + \left(\frac{\Gamma_a + \Gamma_b}{2}\right)^2}\right]$$

Thus

$$P_\nu(t) = \frac{|V_{mn}|^2}{\Gamma_a} \frac{(\Gamma_a+\Gamma_b)}{\left[\nu^2+\left(\frac{\Gamma_a+\Gamma_b}{2}\right)^2\right]} \qquad (2)$$



"Lorentzian" or "Breit-Wigner" line shape

Note: if our instruments aren't very accurate, this looks like

$$P_\nu(t) \sim 2\pi \frac{|V_{mn}|^2}{\Gamma_a} \delta(\nu) \qquad (3)$$

Thus the probability of any photon of any ν can be found by summing over m (or integrating (3) over ν)

$$P = \sum_m P_\nu(t) \sim \int P_\nu(t)\, d\nu = \frac{2\pi |V_{mn}|^2 \rho(\eta)}{\Gamma_a}$$

Comment: We might arrive at (3) using a different argument

$$\text{Rate of emission of photon/sec} = 2\pi |V_{mn}|^2 \delta(\nu) \underbrace{[\text{Prob to be in upper state}]}_{e^{-\Gamma_a t}}$$

$$\therefore \quad \text{Total prob. of emission} = \int \text{Rate}\, dt = \frac{2\pi |V_{mn}|^2 \delta(\nu)}{\Gamma_a}$$

Note that if we replace $\delta(\nu) \to \frac{\Gamma_a+\Gamma_b}{2\pi\left[\nu^2+\left(\frac{\Gamma_a+\Gamma_b}{2}\right)^2\right]}$ we come back to (3).

Quite a few people use (3) to say that the line shape obeys $\delta(\nu)$ or Lorentzian but decays as $e^{-\Gamma_a t}$. However this is incorrect as we can see by considering a special case of

Γ_a

transitions to a stable state b

$\Gamma_b = 0$

$$P_2(t) = P_m = |V_m|^2 \frac{1 + e^{-\Gamma_a t} - e^{-\Gamma_a t/2}\cos\nu t}{\nu^2 + \left(\frac{\Gamma_a}{2}\right)^2}$$

$$\neq |V_{mm}|^2 \frac{1 - e^{-\Gamma_a t}}{\nu^2 + \left(\frac{\Gamma_a}{2}\right)^2}$$ as we would have expected from (3)

Thus the line shape changes with time if we have decay. This has been verified by using Mössbauer effect with X-rays.

Now return to our light scattering problem. Consider only elastic scattering from a stable state a

c

a $\Gamma_a = 0$

i initial state
f final state
k intermediate state

We can then set up the "Wigner-Weisskopf" equations

$$\dot{a}_i = -i V_{ik} a_k(t) e^{-i(E_k - E_i)t} - \frac{\Gamma_i a_i}{2}$$

$$\dot{a}_j = -i V_{jk} a_k(t) e^{-i(E_k - E_j)t} - \frac{\Gamma_j a_j}{2}$$

$$\dot{a}_k = -i V_{ki} a_i(t) e^{+i(E_k - E_i)t} - \frac{\Gamma_k}{2} a_k$$

Zero-order: $a_i = 1$

First order: $a_k = -i e^{-\frac{\Gamma_k t}{2}} \int_0^t V_{ki} e^{i(E_k - E_i)t} e^{\frac{\Gamma_k t}{2}} dt$

$$= -V_{ki}\left[\frac{e^{i(E_k - E_i)t} - e^{-\Gamma_k t/2}}{E_k - E_i - i\Gamma_k/2}\right]$$

We then find

$$a_j = \frac{-i V_{jk} V_{ki}}{E_k - E_i - i\frac{\Gamma_k}{2}} \int_0^t \left[e^{-i(E_k - E_j)t'} e^{+i(E_k - E_i)t'} - \underbrace{e^{-\Gamma_k t/2} e^{-i(E_k - E_j)t'}}_{\text{disappears for long scattering times}}\right] dt'$$

Thus we find

$$a_j(T) = \underbrace{\left\{V_{ji} + \sum_k \left(\frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Gamma_k}{2}}\right)\right\}}_{M_{ji}} \underbrace{\int_0^T e^{i(E_j - E_i)t} dt}_{\frac{e^{i(E_j - E_i)T} - 1}{E_j - E_i}}$$

Thus

$$\text{Prob}_{i \to j} = |M_{ji}|^2 \frac{\sin^2 (E_j - E_i) T/2}{(E_j - E_i)^2}$$

$$\text{Rate}_{i \to j} = 2\pi \delta(E_i - E_j) |M_{ji}|^2$$

where $M_{ji} = V_{ji} + \sum_k \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Gamma_k}{2}}$

↖ replaces ϵ in our light scattering

[This corresponds to complex index of refraction (absorption) for resonant scattering.]

This is the desired correction to our second-order perturbation theory. Since all real states have finite lifetimes, we always have a Γ (like resistance in circuit theory).

Long ago we found

$$\mathcal{T}_{\substack{\text{imp} \\ n \to m}} = \sum_k \frac{V_{mk} V_{kn}}{E_k - E_n} \left(\frac{e^{i(E_m - E_n)T} - 1}{E_m - E_n} - \frac{e^{i(E_m - E_k)T} - 1}{E_m - E_k} \right)$$

Look in Hilbrand Feynman, p. 154 to get

$$\sum_k \frac{V_{mk} V_{kn}}{E_k - E_n - i\epsilon}$$

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Tricks & Sum Rules

$$\sum_k \epsilon_k \langle a|x|k\rangle\langle k|x|b\rangle = \langle a|xHx|b\rangle$$

$$\sum_k \frac{\langle a|x|k\rangle\langle k|x|b\rangle}{\epsilon_k + \Omega} = \langle a|x \underbrace{\frac{1}{H+\Omega}} x|b\rangle$$

very hard to invert however

Hints to get back $\hbar$'s c

$$e^2/\hbar c = \frac{1}{137}$$ [all theoretical physicists knew before 137]

Length & time are equivalent units

$$\text{Lifetime} = \frac{\text{length}}{c}$$

$$\frac{1}{\text{length}} = \frac{1}{\text{time}} = \text{energy} = \text{momentum} = \text{mass}$$

Now $\frac{\hbar}{\text{time}} = \text{energy}$

$$\therefore \text{mass} = \frac{\hbar/c^2}{\text{lifetime}}$$

C. ALTERNATIVE FORMULATIONS 11/14/66 LECTURE

Today we write the perturbation theory in different forms (not important, but necessary to read literature)

1.) Evolution Operator

We should be able to write

$$|\psi(t_b)\rangle = U(t_b, t_a)\,|\psi(t_a)\rangle$$

where $U(t_b, t_a)$ is a linear operator. Now we have

$$i\frac{\partial|\psi(t_a)\rangle}{\partial t_a} = H(t_a)|\psi(t_a)\rangle$$

Thus

$$i\frac{\partial U(t_b, t_a)}{\partial t_b} = H(t_b)U(t_b, t_a)$$

$$\text{subject to } U(t_a, t_a) \equiv 1$$

Sometimes we use

$$S = \text{"}\lim_{\substack{t_a\to-\infty \\ t_b\to\infty}} U(t_b, t_a)\text{"}$$

although, strictly speaking, the limit doesn't exist.

More trouble than it is worth, however.

Suppose H is independent of time

$$U(t_b, t_a) = e^{-iH(t_b - t_a)} = e^{-iHT} \qquad T = t_b - t_a$$

What is e^{operator}? Several possible (and equivalent) definitions

i.) if $H|\phi\rangle = E|\phi\rangle$, then

$$e^{-iHT}|\phi\rangle \equiv e^{-iET}|\phi\rangle$$

ii.) power series expansion of e^{-iHT}
iii.) define by differential equation

If ϕ_n are base states of $H|\phi_n\rangle = E_n|\phi_n\rangle$, then

$$\langle\phi_m|U|\phi_n\rangle = \langle\phi_m|e^{-iHT}|\phi_n\rangle$$

$$= \langle\phi_m|\phi_n\rangle e^{-iE_nT} = \delta_{mn} e^{iE_nT}$$

Can now return and write

$$U = \sum_{m,n} |\phi_m\rangle\langle\phi_m|U|\phi_n\rangle\langle\phi_n|$$

$$= \sum_n |\phi_n\rangle e^{-iE_n(t_b - t_a)} \langle\phi_n|$$

useful if we can find $|\phi_n\rangle$.

2.) Integral Formulations

We can now write U in other representations, say x-representation

$$\langle x'|U(t_b,t_a)|x\rangle = K(x',x';t_b,t_a)$$

= propagation function

If H is constant

$$K(x';x,T) = \sum_n \varphi_n(x')\,\varphi_n^*(x)\,e^{-iE_nT}$$

Thus

$$\psi(x',t_b) = \int K(x',x;T)\,\psi(x,t_a)\,d^n_x$$

For many cases $K(x',x;T)$ can be found [free particle gives

$$K(x',x;T) = \sqrt{\frac{2\pi i m}{\hbar T}}\; e^{-\frac{mi(x'-x)^2}{2\hbar T}}$$

[= the diffusion kernel]]

Can sum for anything that has p or q only up to quadratic order.

3.) Some properties of U

$$U(t_b, t_a) = U(t_b, t_c)\, U(t_c, t_a) \qquad t_a < t_c < t_b \quad (*)$$

[U is a relation in Hilbert space, so obvious]

$$U(t_N, t_0) = \prod_{i=0}^{N} U(t_{i+1}, t_i)$$

but not relativistic complete

Phys. Rev. 84, 108 (1951) also an ordering rider

$$U(t_N, t_0) = \prod_{i=0}^{N} U_{i+1,\, i}(t_{i+1}, t_i)$$

where U_{i+1} U_i

Thus if you want BA, write $A_2 B_1$ or $B_1 A_2$.
Frees us from ordering.

Ex: old: $\nabla \times (U \times V)$

new: $\nabla_1 \times (U_2 \times V_3)$ (? ?)

Now using

$$U(t+\Delta t, t) = e^{-i H(t) \Delta t}$$

we find

$$U(t_b,t_a) = \lim_{\substack{\Delta t\to 0\\ N\to\infty\\ N\Delta t\to t_b-t_a}} e^{-i H(t_N)\Delta t}\, e^{-i H(t_{N-1})\Delta t} \cdots e^{-i H(t_0)\Delta t}$$

$$= \lim_{\substack{\Delta t\to 0\\ N\to\infty\\ N\Delta t\to t_b-t_a}} e^{-i \sum H(t_i)\Delta t}$$

$$= e^{-i\int_{t_a}^{t_b} H(t)\,dt}$$

But wrong because order hasn't been preserved

Instead use

$$U(t_b,t_a) = e^{-\int_{t_a}^{t_b} H_t(t)\,dt}$$

[Haggit found a good use for this yet, but feels it will come in handy somewhere.]

Now from conservation of probability and causality

$$\left[U(t_b,t_a)\right]^\dagger U(t_b,t_a) = 1$$

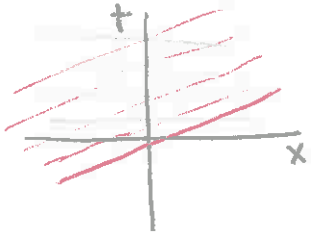
$\Rightarrow$ U is a unitary operator

Try to extend definition of U such that

$$U(t_b,t_a) = U(t_b,t_c)\,U(t_c,t_a) \qquad t_c \notin [t_a,t_b]$$

Suppose things in future can affect past, then U is not unitary and (*) doesn't work. However we can fix (*) up with some new variables. Maybe causality isn't correct.

Ex: EM field can be thrown out leaving only particle variables. Use both retarded and advanced interactions. Feynman got stuck 3/4 through. Threw out differential equation approach (he did get a "prize" for it however). D.E.'s are not useful relativistically.



All he did was not consider

$$H = (H_+^{(1)} + H_+^{(2)}) + \text{constant}$$

in $\quad U = e^{-i\int H_+\,dt} = e^{-i\int (H_+^{(1)}+H_+^{(2)})dt} + e^{-i\iint \frac{e^2\,\delta(t_1,t_2-r)}{|r_1t_1 - r_2t_2|}\,dt_1\,dt_2}$

$$\left(1 - \frac{\vec{r}_{1t_1}\cdot\vec{r}_{2t_2}}{c^2}\right)$$

Doesn't quite work.

Recall we had defined

$U(t_b, t_a)$: $\quad i\frac{\partial U}{\partial t_b} = H(t_b)\,U$ $\qquad$ 11/15/66 LECTURE

$U(t_a, t_a) = 1$ $\qquad$ (1)

If H independent of time,

$$U(t_b, t_a) = e^{-iH(t_b - t_a)}$$

$$= \sum_n |\varphi_n\rangle e^{-iE_n(t_b - t_a)} \langle\varphi_n|$$

4.) *Neumann Series*

If we can write $H = H_0 + V$, we can set up a perturbation scheme. No physical significance of V (not "interaction" or such -- whatever is convenient)

Suppose

$$i\frac{\partial}{\partial t_b} U_0 = H_0(t_b)\, U_0(t_b, t_a) \qquad (2)$$

We can integrate (1) and use (2) to write

$$U(t_b, t_a) = U_0(t_a, t_a) - i\int_{t_a}^{t_b} U_0(t_b, t)\, V(t)\, U(t, t_a)\, dt \qquad (3)$$

By iteration we can set up the Neumann series

$$U(t_b, t_a) = U_0(t_b, t_a) - i\int U_0(t_a, t) V(t) U_0(t, t_a) dt \qquad (4)$$

$$+ (-i)^2 \iint_{t_a < t_2 < t_1 < t_b} U_0(t_a, t_1)\, V(t_1)\, U_0(t_1, t_2)\, V(t_2)\, U_0(t_2, t_a)\, dt_2\, dt_1$$

$$+ \cdots$$

One can prove the convergence of this series, but who cares? "If it don't converge, it don't work, and we don't use it?"

Now let H_0 be our old and simple example so we know

$$H_0|\phi_n\rangle = E_n|\phi_n\rangle$$

Thus

$$U_0(t_b, t_a) = e^{-iH_0(t_b - t_a)}$$

We can plug this in (4) to find

$$U(t_b, t_a) = e^{-iH_0(t_b-t_a)} - i\int e^{-iH_0(t_b-t_1)} e^{-iH_0(t_1-t_a)} dt_1 + \cdots$$

Now consider $\langle m|U|n\rangle$. Note

$$e^{-iH_0 t}|n\rangle = e^{-iE_n t}|n\rangle$$

Thus our series becomes

$$\langle m|U|n\rangle = \delta_{mn} e^{-iE_n(t_b-t_a)} - i\int e^{-iE_m(t_b-t_1)}\langle m|V(t)|n\rangle e^{-iE_n(t_1-t_a)} dt_1$$

$$+ (i)^2 \iint e^{-iE_m(t_b-t_1)} \langle m|V(t_1) e^{-iH_0(t_1-t_2)} V(t_2)|n\rangle \cdot$$

$$\cdot e^{-iE_n(t_2-t_1)} dt_1 dt_2$$

Use $\langle m|AB|n\rangle = \sum_k \langle m|A|k\rangle\langle k|B|n\rangle$

Thus write

$$\langle m|V(t_1)e^{-iH_0(t_1-t_2)}V(t_2)|n\rangle = \sum_{k,\ell}\langle m|V(t_1)|k\rangle\underbrace{\langle k|e^{-iH_0(t_1-t_2)}|\ell\rangle}_{e^{-iE_k(t_1-t_2)}\delta_{k\ell}}\langle \ell|V(t_2)|n\rangle$$

Thus the 3rd term becomes

$$(-i)^2\iint\sum_k e^{-iE_m(t_0-t_1)}\langle m|V(t_1)|k\rangle e^{-iE_k(t_1-t_2)}\langle k|V(t_2)|n\rangle e^{-iE_n(t_2-t_0)}\,dt_2\,dt_1$$

Now back long ago we calculated

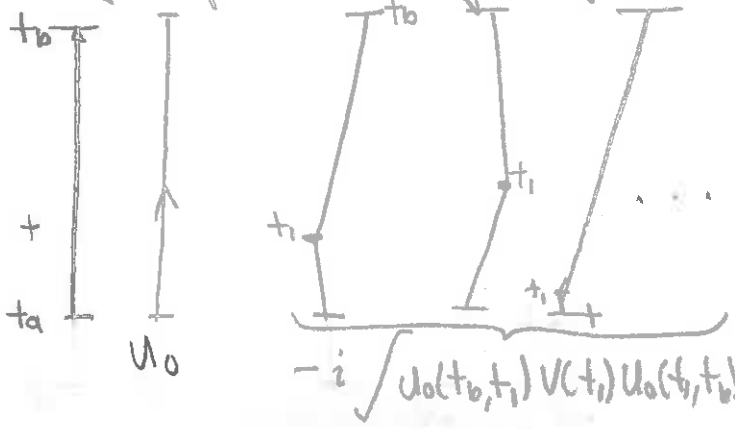
$e^{iE_m t_0}e^{-iE_n t_0}\langle m|U|n\rangle$. Realizing this, we can recognize our earlier series.

Frequently people refer to using

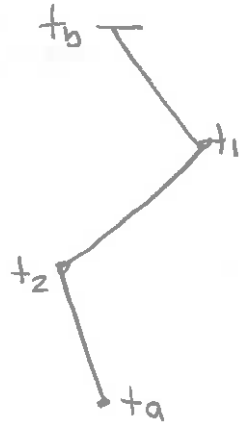
$$v(t) = e^{i(E_b-E_a)t}V(t)$$

as the "interaction representation". Only a matter of convenience ["one-up-manship"].

5.) Interpretation by Feynman Diagrams



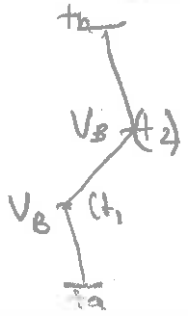
Disturbance V can act on system any number of times [each time scatters]. Amplitude to be scattered at t is dt is $-iV(t)$. Thus an interpretation of $V(t)$ is the scattering amplitude for t. We can see how these amplitudes add up



$$(-i)^2 \iint_{t_b>t_1>t_2>t_a} U_0(t_b,t_1)V(t_1)U_0(t_1,t_2)V(t_2)U_0(t_2,t_a)\,dt_1\,dt_2$$

Sometimes some people call U_0 the propagator. Feynman just calls V the scatterer

EXAMPLE: Consider two V's, V_A & V_B. But only interested in first order in V_A, first order in V_B.



$$\iint_{t_1<t_2} U_0(b,2)V_B(2)U_0(2,1)V_A(1)U_0(1,a)\,dt_1\,dt_2$$

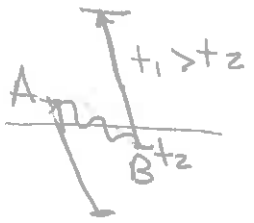
Can we have ↓ ?

wrong

Instead reverse B & A to pick up a second term

$$(-i)^2 \iint_{t_1>t_2} U_0(b,1)\, V_A(1)\, U_0(1,2)\, V_B(2)\, U_0(2,a)\, dt_1\, dt_2$$

Actually this scheme isn't really dead in relativistic theory. Thus represents pair production, for instance. Need a new type of perturbation integral however. Need a more general definition



Comments:

① Must add all terms together -- find phase interference.

② To define U_0 for negative time,

$$U_0(t_2, t_1) = 0 \qquad t_2 < t_1$$

Then restrictions on integrations are automatic.

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$$U(t_b,t_a) = U_0(t_b,t_a) - i\int U_0(t_b,t_1)V(t_1)U_0(t_1,t_a)\,dt_1$$

$$+ (-i)^2 \iint U_0(t_b,t_2)V(t_2)U(t_2,t_1)V(t_1)U(t_1,t_a)\,dt_1\,dt_2$$

$U_0(t_1,t_2)$ propagator
$-iV(t_i)$ scattering amplitude per unit time

$$U_{mn}e^{i(E_m t_b - E_n t_a)} = \delta_{mn} - i\int e^{-i(E_m-E_n)t}V_{mn}\,dt$$

$$+ (-i)^2 \int e^{-i(E_m-E_k)t_1}V_{mk}e^{-i(E_k-E_n)t_2}V_{kn}\,dt_1\,dt_2$$

---

6) *Physics of V:* $H = H_0 + V$

Is this only a mathematical convenience? It is not unique. But what is physics anyway. Can think of V connecting H_0 to the real world. H_0 is very simple & solvable. H is dependent on an infinite number of variables. V connects the two.

We can't describe the world exactly. Can't get it out of

$$H = \sum_{j=1}^{10^{23}} \frac{\hbar^2}{2m_e}\nabla_j^2 + \sum_{i<j} V(r_{ij})$$

We don't want the general solution. We want a specific solution for specific conditions.

The physics is the approximation we make to solve the problem. We can thus consider V as the correction to our approximation. In this sense it is physical. "Everything is approximate".

—o—

To understand bound states, V operates again and again. Thus we need the infinite series. Thus should attempt to analyze H atom by consider free p + e with V = coulomb interaction. Once we group bound states in H_0, then we can apply perturbation of $O(e^2)$ for EM interactions.

The $e^2 = \frac{1}{137}$ makes the treatment of QED feasible by this series. For mesons, $g^2 = 10$, and series doesn't converge. [Field theory means perturbation theory]. Could try expansion in $1/g^2$. People don't know where to make zero approximation. Note love enough to experience.

Problems may look the same, but have different numbers such that the same methods won't work for both. Dif. between a bad and good theoretical physicist is between a guy who uses someone's method and between a guy who thinks for himself. Design methods from physics -- not vice-versa.

[Don't conclude we don't understand superconductivity because BCS theory doesn't apply to nuclear structure.]

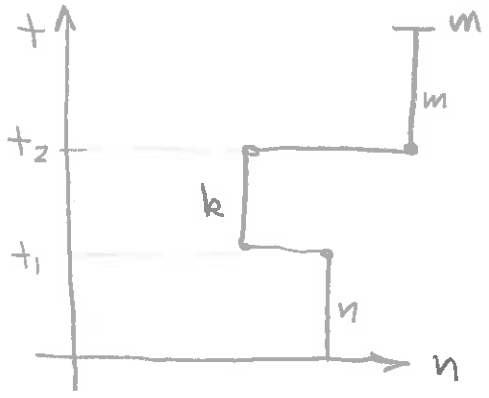
DON'T COPY METHODS. THINK FIRST
Decide what approximations will work for your problem, then think up a method.

EXAMPLES:

Propagator in state of energy E_n is $e^{-iE_k(t_2-t_1)}$

Scattering amplitude $= -iV_{mn}$
Y sec to scatt from $m \to n$

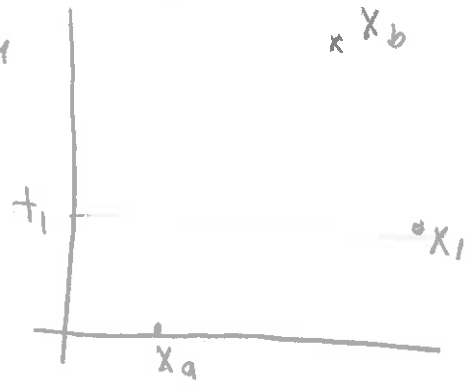
To find second order term:



$$(-i)^2 \iint_{t_1<t_2} e^{-iE_m(t_b-t_2)} V_{mk} e^{-iE_k(t_2-t_1)} V_{kn} e^{-iE_n(t_1-t_a)} dt_1 dt_2$$

There is also a space representation
Look for first order, say

$$-i\int K_0(x_b,x_1;t_b-t_1)\, V(x_1)\, K_0(x_1,x_a;t_1-t_a)\, dx_1$$



Still a third method [interaction representation]

Prop. n is $\delta_{mn} = 1$

Scatt. amplitude $= -i V_{mk}(t)\, e^{i(E_m - E_k)t}$

Now recall

$$U_{mn} e^{i(E_m t_b - E_n t_a)} = \delta_{mn} - i \int_0^T e^{-i(E_m - E_n)t} V_{mn}\, dt$$

$$+ (-i)^2 \iint e^{-i(E_m - E_k)t_1} V_{mk} e^{-i(E_k - E_n)t_2} V_{kn}\, dt_1 dt_2$$

$+ \cdots$

We can use a shortcut by integrating over the difference assuming it is effective only over a finite time. Then we are left with

$$\delta_{mn} + (-i) \int_0^T e^{-i(E_m - E_n)t} dt \Big[\overbrace{V_{mn} + V_{mk} \frac{1}{E_n - E_k - i\epsilon} V_{kn}}^{T_{mn}} + V_{mk} \frac{1}{E_n - E_k - i\epsilon} V_{kl} \frac{1}{E_n - E_l - i\epsilon} V_{ln} + \cdots \Big]$$

Thus

$$\underset{m \to n}{\text{Rate}} = 2\pi \delta(E_m - E_n) \, |T_{mn}|^2$$

7.) T-MATRIX

We have found

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$$\underset{m\to n}{\text{Rate}} = 2\pi\,\delta(E_m - E_n)\,|T_{mn}|^2 \qquad \text{Golden Rule \#2} \qquad (1)$$

$$T_{mn} = V_{mn} + \sum_k V_{mk}\frac{1}{E_n - E_k \pm i\epsilon}V_{kn} + \sum_{k,l} V_{mk}\frac{1}{E_n - E_k \pm i\epsilon}V_{kl}\frac{1}{E_n - E_l \pm i\epsilon}V_{ln} \qquad (2)$$

Golden Rule #1

These can again be written in different forms. First note for $E = E_n$,

$$T = V + V\frac{1}{E - H_0 \pm i\epsilon}V + V\frac{1}{E - H_0 \pm i\epsilon}V\frac{1}{E - H_0 \pm i\epsilon}V + \cdots \qquad (3)$$

where we have defined $f(H_0)|\phi_k\rangle = f(E_k)|\phi_k\rangle$

$$\left[f(H_0)\right]_{lk} = f(E_k)\,\delta_{lk}$$

Note we actually only want $[T(E_n)]_{mn}$ however. $T(E)$ is "off the energy shell". Some people like to play with this, but not really very useful.

If A and B are operators

$$\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A}B\frac{1}{A} + \frac{1}{A}B\frac{1}{A}B\frac{1}{A} - \cdots$$

Proof: Set $X = \frac{1}{A+B}$ Show $(A+B)X = 1$

$$AX = 1 - B\frac{1}{A} + B\frac{1}{A}B\frac{1}{A} - \cdots = 1 - B\left(\frac{1}{A} - \frac{1}{A}B\frac{1}{A}\right)\cdots$$

$$= 1 - BX \quad \Rightarrow \quad (A+B)X = 1$$

Now write

$$T = V + V\,W(E)\,V$$

where $W(E) = \frac{1}{E_\cdot - H_0 + i\epsilon} + \frac{1}{E-H_0+i\epsilon} V \frac{1}{E-H_0+i\epsilon} V + \cdots$

$$= \frac{1}{E - H_0 - V + i\epsilon} = \frac{1}{E - H + i\epsilon}$$

$$\therefore \quad T(E) = V + V \frac{1}{E-H+i\epsilon} V$$

$$= (H - H_0) + (H - H_0) \frac{1}{E-H+i\epsilon} (H - H_0)$$

Now suppose we want to study $\frac{1}{Q}$. This means

$$\frac{1}{Q}|\chi_n\rangle = \frac{1}{q_n}|\chi_n\rangle$$

or $$\frac{1}{Q} = \sum_n |\chi_n\rangle \frac{1}{q_n} \langle\chi_n|$$

Thus $$\frac{1}{E-H+i\epsilon} = \sum_N |\chi_N\rangle \frac{1}{E-E_N+i\epsilon} \langle\chi_N|$$

where $H|\chi_N\rangle = E_N|\chi_N\rangle$

Back where we started from.

Also mentions $e^A e^B \neq e^{A+B}$

Now in a system where $H \neq H(t)$,

$$U(T) = e^{-iHT}$$

Now consider the Fourier transform

$$\int_0^\infty e^{iET} U(T)\, dT = iW(E)$$

But note

$$-i\int_0^\infty e^{i(E-H)T}\, dT = \frac{1}{E-H+i\varepsilon} = W(E)$$

Thus $W(E) = \mathcal{F}\{U(T)\}$

We have been considering $H = H_0 + V$. But now consider

EXAMPLE: $A + B \to C + D$, e.g. $\underbrace{He^+}_{x} + \underbrace{H}_{4} \to p + He$

Write

$$H = \frac{P_x^2}{2m_x} + \frac{P_y^2}{2m_y} + \frac{e_1 e_x}{r_{1x}} + \frac{e_2 e_x}{r_{2x}} + \frac{e_1 e_y}{r_{1y}} + \frac{e_2 e_y}{r_{2y}} + \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + \frac{e_x e_y}{r_{xy}} + \frac{e_1 e_2}{r_{12}}$$

incoming $H = H_{0_I} + V_I$

$$H_{0_I} = \frac{P_x^2}{2m_x} + \frac{P_1^2}{2m_1} + \frac{e_1 e_x}{r_{1x}}$$

$$V = \frac{e_{2x}}{r_{2x}} + \frac{e_{1y}}{r_{1y}} + \frac{e_x e_y}{r_{xy}} + \frac{e_1 e_2}{r_{12}} + \frac{P_y^2}{2m_y} + \frac{P_2^2}{2m_2} + \frac{e_2 e_y}{r_{1y}}$$

outgoing $H = H_{0II} + V_{II}$

$$H_{0I} = \left(\frac{p_y^2}{2m_y}\right) + \left(\frac{p_x^2}{2m_x} + \frac{e_x e_1}{r_{1x}} + \frac{e_x e_2}{r_{2x}} + \frac{e_1 e_2}{r_{12}}\right)$$

$$V_{II} = \frac{e_y e_1}{r_{1y}} + \frac{e_y e_2}{r_{2y}} + \frac{e_x e_y}{r_{xy}}$$

Which V do we use in our formula? In

$$T(E) = (H-H_0) + (H-H_0)\frac{1}{E-H+i\epsilon}(H-E_I)$$

$$= (H-E_I) + (H-E_{II})\frac{1}{E-H+i\epsilon}(H-E_I)$$

It makes no difference.

On the energy shell

$$T_{\text{on shell}} = V_I + V_{II}\frac{1}{E_I-H+i\epsilon}V_I$$

$E_I = E_{II}$

Now

$$_{M_{II}}T_{N_I} = \langle M_{II}|V_I|N_I\rangle \stackrel{?}{=} \langle M_{II}|V_{II}|N_I\rangle$$

$$= \langle M_{II}|H-H_0|N_I\rangle \stackrel{?}{=} \langle M_{II}|H-H_{II}|N_I\rangle$$

Chemists

8) $K^0, \bar{K}^0$ Decay Problem

11/22/66 LECTURE

$K^0 \to \pi^+ + \pi^-$ amp

$\bar{K}^0 \to \pi^+ + \pi^-$ amp

$$i\dot{a}_{K^0} = E_0 a_{K^0} + \sum_{\pi} M_{K^0,\pi\pi} b_{\pi\pi}$$

$$i\dot{a}_{\bar{K}^0} = E_0 a_{\bar{K}^0} + \sum_{\pi} M^*_{K^0,\pi\pi} b_{\pi\pi}$$

$$i\dot{b}_{\pi\pi} = \mathcal{E}_{\pi\pi} b_{\pi\pi} + M^*_{K^0,\pi\pi} a_{K^0} + M^*_{\bar{K}^0,\pi\pi} a_{\bar{K}^0}$$

Write $$b_{\pi\pi}(t) = \int_0^t e^{i(\mathcal{E}_{\pi\pi} - E_0)t} M^* \left[a_K(t') + a_{\bar{K}^0}(t')\right] dt'$$

Then

$$i\dot{a}_{K^0} = \sum_{\pi} \int_0^t e^{i(\mathcal{E}_{\pi\pi} - E_0)(t-t')} M M^*_{\pi} \left[a_{\bar{K}^0}(t') + a_{K^0}(t')\right] dt'$$

$$i\dot{a}_{K^0} \approx \left(\Delta - i\frac{\Gamma}{2}\right)\left[a_{K^0}(t) + a_{\bar{K}^0}(t)\right]$$

$$i\dot{a}_{\bar{K}^0} \approx \left(\Delta - i\frac{\Gamma}{2}\right)\left[a_{K^0}(t) + a_{\bar{K}^0}(t)\right]$$

Solving

$$a_{K^0} + a_{\bar{K}^0} = C e^{-i\Delta t} e^{-\Gamma t/2}$$

$$a_{K^0} - a_{\bar{K}^0} = D$$

Try $a_{K^0} = 1 \quad a_{\bar{K}^0} = 0$

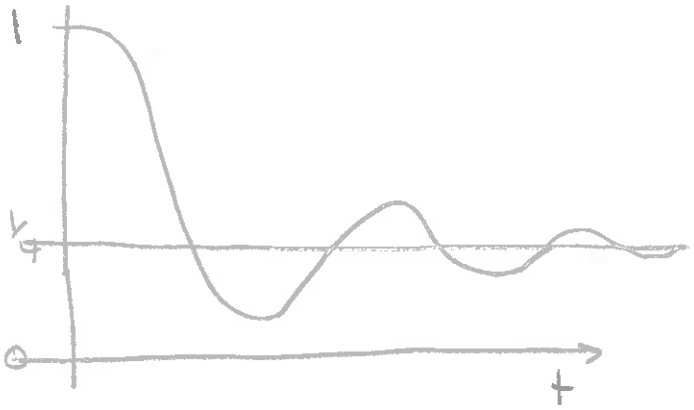
$$a_{K^0} = \tfrac{1}{2}\left[1 + e^{-\Gamma t/2} e^{-i\Delta t}\right]$$

$$a_{\bar{K}^0} = \tfrac{1}{2}\left[1 - e^{-\Gamma t/2} e^{-i\Delta t}\right]$$

Thus $|a_{K_0}|^2 = \frac{1}{4}\left[1 + 2\cos(\Delta t)\, e^{-\Gamma t/2} + e^{-\Gamma t}\right]$

$|a_{\bar{K}_0}|^2 = \frac{1}{4}\left[1 - 2\cos(\Delta t)\, e^{-\Gamma t/2} + e^{-\Gamma t}\right]$

Thus production of Λ in a shot



This general effect is true for any system with two states. K_0, K_0

$$|K_1\rangle = \frac{1}{\sqrt{2}}\left(|K_0\rangle + |\bar{K}_0\rangle\right) \qquad a_{K_1} = \frac{1}{\sqrt{2}}\left(a_{K_0} + a_{\bar{K}_0}\right)$$

$$|K_2\rangle = \frac{1}{\sqrt{2}}\left(|K_0\rangle - |\bar{K}_0\rangle\right) \qquad a_{K_2} = \frac{1}{\sqrt{2}}\left(a_{K_0} - a_{\bar{K}_0}\right)$$

Thus in our problem, K_2 cannot decay into $\pi^+ + \pi^-$
Thus $|K_1\rangle$ & $|K_2\rangle$ are best states to work with.
Δ is mass difference between K_1 & K_2, $\Delta = .48\,\Gamma$
$\sim 5\text{-}6$ eV.

Use this to argue against negative mass theory of antimatter.

But it is found K_2 does decay into π^+, π^- at large times. This $\Rightarrow M_{K^0} \neq M_{\bar{K}^0} \Rightarrow$ CP is not conserved. One of the best understood problems today. Must break CP.

Mentions "fifth force" theory. Maybe universe is asymmetrical. Theories explain this experiment, but predict weird things in other areas.

Thinks this is "irrelevant for this generation".

ANGULAR MOMENTUM

11/28/66 LECTURE

PROBLEM: Extend this weeks work on angular momentum as far as you can. (Lorentz transformations).

A. ROTATION GROUPS

Most of what we do can be generalized to other groups than rotations. Also directly of interest.

1.) Rotation of States

Consider our isolated system described by a state $|\psi\rangle$. Now rotate the apparatus which prepares $|\psi\rangle$. Then we produce a new rotated state $|R\psi\rangle$ which would have been $|\psi\rangle$ if we had not rotated the apparatus.

[If we assume we rotate the observer instead we merely get sign changes.]

Now by superposition of states, we expand in base states,

$$|\psi\rangle = \sum_i c_i |i\rangle$$

$$|R\psi\rangle = \sum_j D_j |j\rangle$$

But if R is linear,

$$|R\psi\rangle = \sum_i c_i |Ri\rangle$$

Now we can also expand

$$|Ri\rangle = D^R_{ji} |j\rangle$$

to find

$$D_j = \sum_i D^R_{ji} c_i$$

To every rotation there is associated a matrix D^R

Rotations form a "group" since

i.) first R_1, second R_2 = R_3 where $R_3 = R_2 R_1$

ii.) identity rotation

iii.) $C(BA) = (CB)A$

It is called a "continuous group" since continuum of rotations corresponding to different angles. Actually a 3-parameter group.

Now note i.) means

$$|R_3 \varphi_i\rangle = |R_2(R_1 \varphi_i)\rangle = \sum_j |R_2 \varphi_j\rangle D^R_{ji}$$

$$= \sum_{j,k} D^{R_2}_{kj} D^{R_1}_{ji} |\varphi_k\rangle$$

Thus

$$D^{R_3}_{ki} = \sum_j D^{R_2}_{kj} D^{R_1}_{ji}$$

or as a matrix product

$$D^{R_3} = D^{R_2} D^{R_1}$$

to within a phase which can be appropriately chosen

To find how angles combine during rotations is a question of geometry. Feynman's way

α about x axis

$$x' = x$$
$$y' = y\cos\alpha + z\sin\alpha$$
$$z' = z\cos\alpha - y\sin\alpha$$

α' about y axis

$$y'' = y'$$
$$x'' = x'\cos\alpha' - z'\sin\alpha'$$
$$z'' = z'\cos\alpha' + x'\sin\alpha'$$

Substitute in and use general transformations to do this. Also note

$$x_i' = \sum_j L_{ij}^R x_j \qquad L^{R_3} = L^{R_2} L^{R_1}$$

an example with 3x3 matrices

2.) Construction of Angular Momentum Operators (Generators)

We can now find our matrices by considering these infinitesimal rotations.

Take ϵ about z axis. Then D^ϵ. Now for α about z, use

$$\underbrace{D^\epsilon D^\epsilon \cdots D^\epsilon}_{\alpha/\epsilon \text{ terms}}$$

Only need to know D to order ϵ

Thus write

$$D^\epsilon = 1 + i\left(\frac{J_z}{\hbar}\right)\epsilon$$

where J_z is as yet unknown

Thus

$$|\text{Rot}_{\epsilon \text{ about } z}\,\psi\rangle = |\psi\rangle + \frac{i\epsilon}{\hbar} J_z |\psi\rangle$$

J_z is called the "generator of the rotation".

Now rotation of α about z

$$\mathcal{D}^\alpha = \left(1 + \frac{i\epsilon}{\hbar} J_z\right)\left(1 + \frac{i\epsilon}{\hbar} J_z\right) \cdots \left(1 + \frac{i\epsilon}{\hbar} J_z\right)$$

$$= \left(1 + \frac{i\epsilon}{\hbar} J_z\right)^{\alpha/\epsilon}$$

$$= 1 + i\alpha J_z + \frac{(i\alpha)^2}{2!} J_z^2 + \frac{(i\alpha)^3}{3!} J_z^3 + \cdots$$

$$= e^{i\alpha J_z}$$

Thus to find $\mathcal{D}^\alpha$, we only need the generator J_z.

Now suppose state is unchanged by rotation

$$|\text{Rot}_\alpha\,\psi\rangle = e^{i\delta(\alpha)}|\psi\rangle$$

But $\text{Rot}_{\alpha_2}\text{Rot}_{\alpha_1} = \text{Rot}_{\alpha_3 = \alpha_1 + \alpha_3}$

$$\Rightarrow \quad \delta(\alpha_1 + \alpha_2) = \delta(\alpha_1) + \delta(\alpha_2)$$

$$\Rightarrow \quad \delta = m\alpha \qquad m \text{ constant of proportionality}$$

$\hbar m \equiv$ angular momentum about z axis

Now suppose

$$J_z|\psi\rangle = m|\psi\rangle$$

Then

$$|R_\alpha \psi\rangle = \mathcal{D}^\alpha|\psi\rangle = e^{i\alpha J_z}|\psi\rangle = e^{i\alpha m}|\psi\rangle$$

Why is m called angular momentum? Merely convenience since if we suppose a particle rotating in a track

$e^{ip \cdot \text{arc distance}/\hbar} = e^{ip a\theta/\hbar}$

$\therefore m \longrightarrow \frac{pa}{\hbar}$

But pa = angular momentum

Thus m corresponds to classical angular momentum.

Suppose $|\psi\rangle$: $f(x,y,z)$

$$|Rot_\epsilon \psi\rangle = f(x',y',z') = f(x+\epsilon y, y-\epsilon x, z)$$

$$= f(x,y,z) + \epsilon\left(y\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial y}\right)$$

Thus identify $J_z = \frac{\hbar}{i}\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) = yP_x - xP_y$

3) Restrictions on Eigenvalues of J 11/29/66 LECTURE

We had found

$$|R\psi\rangle = |\psi\rangle + i\epsilon J_z|\psi\rangle$$

We noted if $J_z|\psi\rangle = m|\psi\rangle$ then $e^{im\alpha}$ phase change. Also found if our state is a function, then define $J_z \to L_z$ where

$$L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Note we found this purely by rotations, not by correspondence with classical mechanics.

Now if we have

$$L_z|\psi\rangle = m|\psi\rangle$$

then

$$L_z f(x,y,z) = m f(x,y,z) \Rightarrow L_z = \frac{1}{i}\frac{\partial}{\partial\phi}$$

$$\therefore f(r,\theta,\phi) = F(r,\theta)\, e^{im\phi}$$

[Note this specific example concerns orbital angular momentum, i.e. ang. mom. due to position (x,y,z)

What values do m have to have? For 2-dimensional groups m's arbitrary! This is so because we can get state back by properly defining our phase.

Need to go to 3-dimension.

Three-dimensions

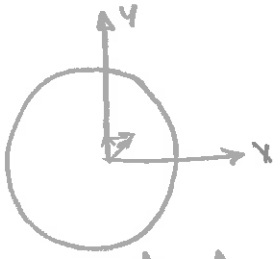
$$|R_z\psi\rangle = |\psi\rangle + i\epsilon J_z|\psi\rangle$$

$$|R_x\psi\rangle = |\psi\rangle + i\eta J_x|\psi\rangle$$

What about

$$|\text{Rot}_{\eta \text{ about axis } \vec{v}}\,\psi\rangle = |\psi\rangle + i\eta J_v|\psi\rangle$$

Note $(\eta V_x \text{ about } x)(\eta V_y \text{ about } y)(\eta V_z \text{ about } z) = (\eta \text{ about } V)$ if η is very small



Thus we can write this rotation as

$$(1 + i\eta V_z J_z)(1 + i\eta V_y J_y)(1 + i\eta V_x J_x)|\psi\rangle$$

The order makes no difference to $O(\eta)$.

$$= 1 + i\eta(V_z J_z + V_y J_y + V_x J_x)$$

Thus the generator for infinitesimal rotation about V is

$$\underline{J}_V = V_x \underline{J}_x + V_y \underline{J}_y + V_z \underline{J}_z = \vec{V} \cdot \vec{\underline{J}}$$

[Note $\vec{\underline{J}}$ is both a vector and an operator]

Now we must make sure that

$$\text{if} \quad \text{first } R_1, \text{ second } R_2 \to R_3$$

$$\Rightarrow \quad \mathcal{D}^{R_2}\mathcal{D}^{R_1} = \mathcal{D}^{R_3} \qquad (*)$$

What properties must the J's have so this holds. Lie studied continuous groups and found if we could get (*) to work to second order, it will work for any order. Can see this

$$\underbrace{(\mathcal{D}^{\epsilon V_2}\mathcal{D}^{\epsilon V_2}\mathcal{D}^{\epsilon V_2}\cdots\mathcal{D}^{\epsilon V_2})}_{\alpha_2/\epsilon}\underbrace{(\mathcal{D}^{\epsilon V_1}\mathcal{D}^{\epsilon V_1}\cdots\mathcal{D}^{\epsilon V_1})}_{\alpha_1/\epsilon} = \underbrace{(\mathcal{D}^{\epsilon V_3}\cdots\mathcal{D}^{\epsilon V_3})}_{O(V_{\epsilon^2})}$$

Note rotations do not commute

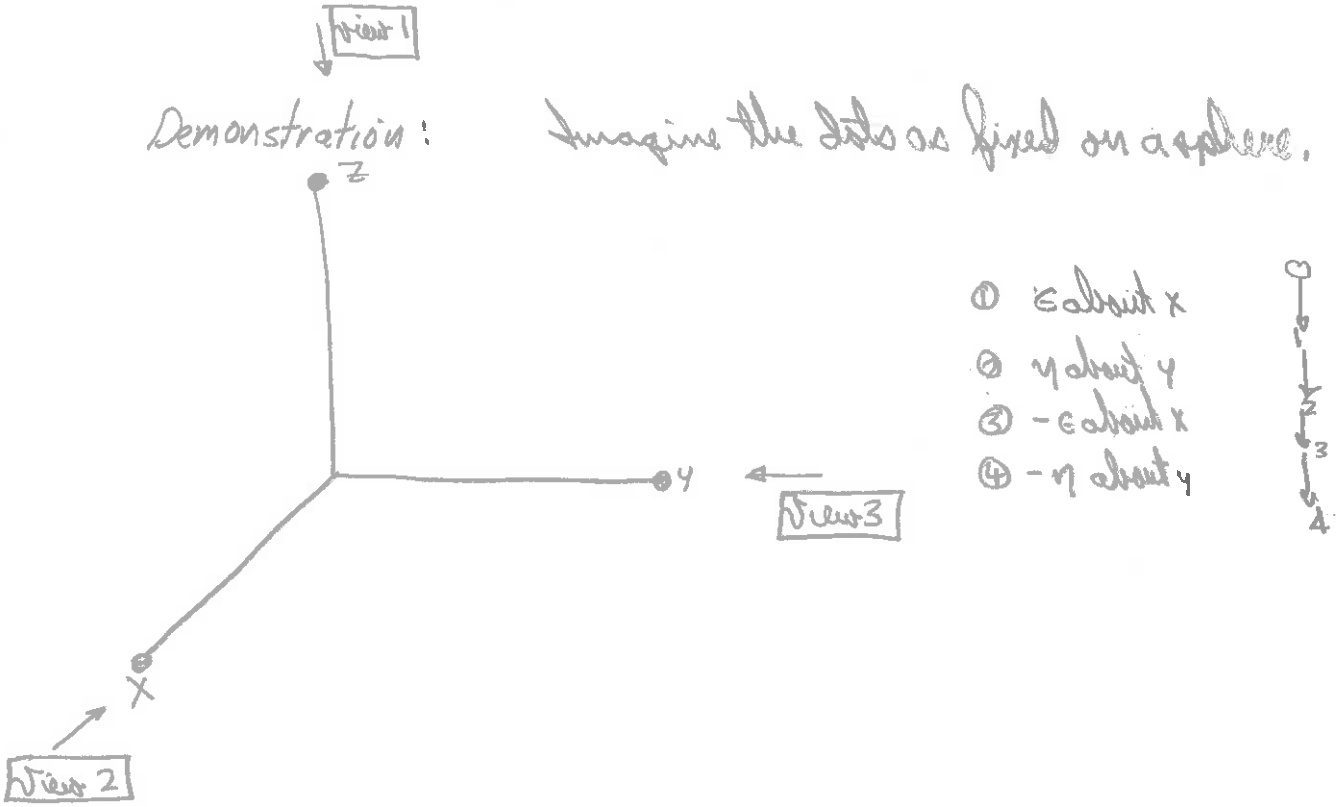
$$(1^{st} \ \epsilon \text{ about } x)\ (2^{nd}\ \eta \text{ about } y) \neq (1^{st}\ \eta \text{ about } y)(2^{nd}\ \epsilon \text{ about } x)$$

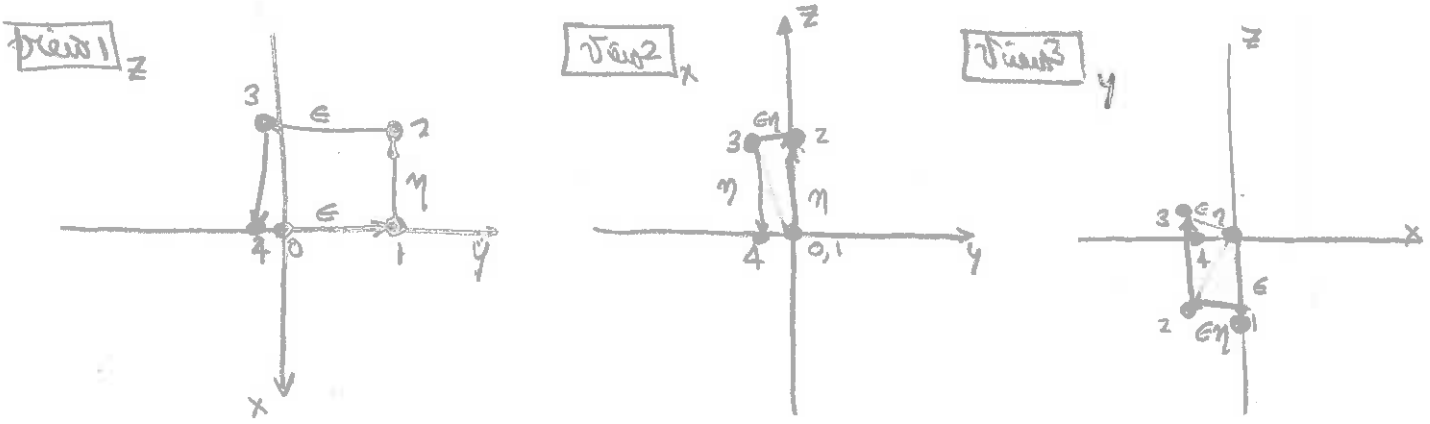
Try to undo it by applying them

$$(3^{rd} - \epsilon \text{ about } x)(4^{th} - \eta \text{ about } y)$$

This gives $(1)(2)(3)(4) = (\epsilon\eta \text{ about } z)$

This is a fact of geometry, not g.m. [We as humans only understand 2-dimensional commutative groups. Bird and fish understand 3-dimensional " "]





We can see that on rotation of $\epsilon\eta$ about z is necessary to return to the original o.

Thus we have found to second order

$$\left(1 - i\eta J_y - \frac{\eta^2}{2} J_y^2\right)\left(1 - i\epsilon J_x - \frac{\epsilon^2}{2} J_x^2\right)\left(1 + i\eta J_y - \frac{\eta^2}{2} J_y^2\right)\left(1 + i\epsilon J_x - \frac{\epsilon^2}{2} J_x^2\right)$$

$$= \left(1 + i\epsilon\eta J_z\right)$$

by expanding

4 ones | 3 ones

$$1 + (i\epsilon J_x + i\eta J_y - i\epsilon J_x - i\eta J_y - \epsilon^2 J_x^2 - \eta^2 J_y^2)$$

2 ones

$$+ (-\epsilon\eta J_y J_x + \epsilon^2 J_x^2 + \epsilon\eta J_x J_y + \epsilon\eta J_y J_x + \eta^2 J_y^2 - \epsilon\eta J_y J_x)$$

Thus

$$1 + \epsilon\eta(J_x J_y - J_y J_x) = 1 + i\epsilon\eta J_z$$

Therefore

$$J_x J_y - J_y J_x = i J_z$$

must be obeyed by the generators of the group if $D^{R_2} D^{R_1} = D^{R_3}$.

[This is a much more logical formulation than the more elementary one from classical mechanics.]

We could also find

$$J_y J_z - J_z J_y = i J_x$$

$$J_z J_x - J_x J_z = i J_y$$

Thus $\mathcal{D}^{R_2}\mathcal{D}^{R_1} = \mathcal{D}^{R_3} \Rightarrow$

i) $\underline{J}_v = \vec{v} \cdot \vec{\underline{J}}$

ii) $J_x J_y - J_y J_x = i J_z$

$J_y J_z - J_z J_y = i J_x$

$J_z J_x - J_x J_z = i J_y$

These handle any angles or rotations

We now could use algebra to generate the e.v. and e.f. of the J's. Define

$$J_\pm = J_x \pm i J_y$$

Then using $[K, J_i] = 0$ where $\underline{K} = J_x^2 + J_y^2 + J_z^2$ we consider

$$J_z |m\rangle = m |m\rangle$$

$$\underline{K} |m\rangle = k |m\rangle$$

Our commutation rules become

$$J_z J_+ - J_+ J_z = J_+$$

$$J_z J_- - J_- J_z = -J_-$$

$$J_+ J_- = J_x^2 + J_y^2 + J_z = \underline{K} - J_z(J_z - 1)$$

$$J_- J_+ = \underline{K} - J_z(J_z + 1)$$

Thus $J_\pm J_\mp |m\rangle = [\ell(\ell+1) - m(m\mp 1)]\,|m\rangle$

Applying

$$J_z(J_+|m\rangle) = J_+|m\rangle + J_+ J_z|m\rangle$$

$$= (m+1)(J_+|m\rangle)$$

Thus

$$J_+|m\rangle = C_m\,|m+1\rangle \qquad \langle n|J_+|m\rangle = C_m \delta_{n,m+1}$$

Also

$$J_-|m+1\rangle = C_m^*\,|m\rangle \qquad \langle m|J_-|m\rangle = C_m^* \delta_{m,m+1}$$

Now

$$J_- J_+ |m\rangle = C_m C_m^*\,|m\rangle$$

$$\Rightarrow |C_m|^2 = \ell(\ell+1) - m(m+1)$$

12/2/66 LECTURE

$$J_x J_y - J_y J_x = i J_z$$
$$J_y J_z - J_z J_y = i J_x$$
$$J_z J_x - J_x J_z = i J_y$$

$$\vec{J} \times \vec{J} = i \vec{J}$$

$$[J_x, J_y] = i J_z \quad \text{etc.}$$

We had found $J_z |m\rangle = m|m\rangle$ by commutative algebra.

$$\vec{J} \cdot \vec{J} |m\rangle = j(j+1)|m\rangle$$

m goes from $-j$ to $+j$ in integer steps
$\Rightarrow$ j is a half integer

Also

$$\langle m' | J_+ | m \rangle = \delta_{m+1,m} \sqrt{j(j+1) - mm'} \qquad m' = m+1$$

$$\langle m' | J_- | m \rangle = \delta_{m-1,m} \sqrt{j(j+1) - mm'} \qquad m' = m-1$$

where $J_\pm = J_x \pm i J_y$

We can then deduce

$$\langle m' | J_x | m \rangle = \delta_{m\pm1,m} \tfrac{1}{2} \sqrt{j(j+1) - m(m\pm1)}$$

$$\langle m' | J_z | m \rangle = \delta_{m,m} \, m$$

Thus the $|m\rangle$ states provide a representation for the group of rotations, so that

$$\langle m' | \mathcal{D}^R | m \rangle = D^R_{m'm}$$

(might try to work them out)

Other forms since

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

Thus

$$\langle m|J_\pm|m\rangle = \sqrt{(j+m_>)(j-m_<)}$$

5) Could study these for special j's

$j=0$: $m=0$ $\quad J_\pm|m\rangle = 0 \quad J_{x,y,z}|m\rangle = 0$

A rotation of any kind produces the same state $|R\psi\rangle = |\psi\rangle$

$j=\frac{1}{2}$: $m=+\frac{1}{2} \quad |+\rangle = |\alpha\rangle$

$m=-\frac{1}{2} \quad |-\rangle = |\beta\rangle$

Call $\vec{J}=\vec{S}$ for this special case.

$$S_z|+\rangle = \tfrac{\hbar}{2}|+\rangle \qquad S_z|-\rangle = -\tfrac{\hbar}{2}|-\rangle$$

$$S_x|+\rangle = \tfrac{\hbar}{2}|-\rangle \qquad S_x|-\rangle = \tfrac{\hbar}{2}|+\rangle$$

$$S_y|+\rangle = -i\tfrac{\hbar}{2}|-\rangle \qquad S_y|-\rangle = i\tfrac{\hbar}{2}|+\rangle$$

Sometimes one uses Pauli matrices $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

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

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1 \qquad \sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z$$

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

Since these 3 matrices and $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ can represent any $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, they are used quite frequently in 2-state systems.

[In the beginning, only integral j were allowed since if we use S-eqn, $j = \frac{2n+1}{2}$ yield the negative of the state ($e^{im\theta}$) after rotating 360°. Thus Pauli used his matrices to handle 2 wave fcns, ψ_+, ψ_-. Why can't we have spin $\frac{1}{3}$

$$|m\rangle \rightarrow e^{i\frac{1}{3}2\pi}|m\rangle = e^{i\delta}|m\rangle$$

Why must 2 rotations around 360° restore state to original value, while one rotation doesn't have to.

—o—

Consider restoring rotations (path of successive rotations which restore coordinate systems) ≡ turns.

Consider 2 turns infinitesimally close to each other. We suppose these turns are in the same class.

Let 0 turns have phase 0. Then consider class of turns infinitesimal from 0. Assume these turns have phase 0. Then class of turns have some phase. Will show

$720°_z$ . . . . . $0°_z$

$360°_z$ . . . . . $0°_z$ not possible

Will show class 720° has phase 0, class 360° has phase ±1. Thus 720° is different than 360° from a geometrical standpoint.

To prove this, he demonstrates that a loop containing both 720° and 0° exists.

$720°_z$ ... $360°_z$ / $360°_{-z}$ ... $10°_z$ / $-10°_z$ ... $0°_z$

He shows you can't do this for 360°. A curious property of 3 dimensional rotations.

$J=1$: $|+\rangle, |0\rangle, |-\rangle$ now $\vec{J} \to \vec{\ell}$

$$\ell_+|+\rangle = 0 \quad \ell_+|0\rangle = \sqrt{2}|+\rangle \quad \ell_+|-\rangle = \sqrt{2}|0\rangle$$

$$\ell_-|+\rangle = \sqrt{2}|0\rangle \quad \ell_-|0\rangle = \sqrt{2}|-\rangle \quad \ell_-|-\rangle = 0$$

If we rotate coordinate systems $|x\rangle$ $|y\rangle$ $|z\rangle$

$$|+\rangle = \frac{1}{\sqrt{2}}(|x\rangle - i|y\rangle)$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle)$$

$$|0\rangle = |z\rangle$$

A particle of spin 1 is called a vector particle in field theory since it behaves as a vector.

B. Combination of Angular Momenta

12/5/66 Lectures

Problem:

i) anything you want

ii.) find the paradox in letting

$$J_z = \frac{1}{i}\left[v_x \frac{\partial}{\partial v_y} - v_y \frac{\partial}{\partial v_x}\right] + \gamma_z(v_x, v_y, v_z)$$

$$J_y = \frac{1}{i}\left[v_x \frac{\partial}{\partial v_z} - v_z \frac{\partial}{\partial v_x}\right] + \gamma_x(v_x, v_y, v_z)$$

$$J_x = \frac{1}{i}\left[v_z \frac{\partial}{\partial v_y} - v_y \frac{\partial}{\partial v_z}\right] + \gamma_y(v_x, v_y, v_z)$$

Let

$$\gamma_z = \lambda v_z$$

$$\gamma_x = -\lambda v_y \phi \qquad \phi = \tan^{-1}\frac{v_x}{v_y}$$

$$\gamma_y = \lambda v_x \phi$$

[Show it commutes correctly]

Claim: Total ang. mom. needn't be an integer.

iii.) Consider two canceled objects (nucleus & electron) with j_a, j_b. Assume neither object is excited. Assume

$$H = A \frac{\vec{J}}{j_a} \cdot \frac{\vec{J}}{j_b} + B_z\left(\frac{\mu_a}{j_a}\left(\frac{\vec{J}}{j_a}\right)_z + \frac{\mu_b}{j_b}\left(\frac{\vec{J}}{j_b}\right)_z\right)$$

a. In general, for very small B find the energy levels of the combined system and find formulae for magnetic moment

b. For special values of j_a, j_b find energy w.r.B for arbitrary B

1.) Introduction

Consider a system composed of two parts a & b

a: $|\psi_a\rangle$ any j_a $\quad 2j_a+1$ states
$m_a = -j_a$ to j_a

b: $|\psi_b\rangle$ any j_b $\quad 2j_b+1$ states
$m_b = -j_b$ to j_b

Now try to represent the base states of the combined system

$$|\psi\rangle = |\psi_a\rangle|\psi_b\rangle = |m_a\rangle_a |m_b\rangle_b$$

Thus $(2j_a+1)(2j_b+1)$ states.

EXAMPLE: $j_a = 1 \quad j_b = 1/2$

$|+1\rangle|\tfrac{1}{2}\rangle, |0\rangle|\tfrac{1}{2}\rangle, |-1\rangle|\tfrac{1}{2}\rangle, |+1\rangle|-\tfrac{1}{2}\rangle, |0\rangle|-\tfrac{1}{2}\rangle, |-1\rangle|-\tfrac{1}{2}\rangle$

Suppose we want to form from these states, new states of definite total angular momentum J, M. What do we mean?

$$\mathcal{D}^R|\psi\rangle = \mathcal{D}_a^R|\psi_a\rangle\mathcal{D}_b^R|\psi_b\rangle = \left(\mathcal{D}_a^R \otimes \mathcal{D}_b^R\right)|\psi_a\rangle|\psi_b\rangle$$

Let $R = \epsilon$ about z

$$|\psi\rangle + i\epsilon J_z|\psi\rangle = \left(1 + i\epsilon J_z^a\right)|\psi_a\rangle\left(1 + i\epsilon J_z^b\right)|\psi_b\rangle$$

$$\Rightarrow \quad J_z|\psi\rangle = \left(J_z^a 1^b + J_z^b 1^a\right)|\psi_a\rangle|\psi_b\rangle$$

$$\Rightarrow \quad \vec{J} = \vec{J}^a 1^b + \vec{J}^b 1^a$$

Try to find

$$J_z|\psi\rangle = M|\psi\rangle = \left(J_z^a + J_z^b\right)|m_a\rangle_a |m_b\rangle_b$$

$$= (m_a + m_b)|m_a\rangle_a |m_b\rangle_b$$

[For our example, max. $M = 3/2 \Rightarrow J = 3/2$
$\therefore M = +3/2, +1/2, -1/2, -3/2$
$+1/2, -1/2$ left over $\Rightarrow J = 1/2$ state
Thus don't get a definite J in general.]

In general, a possible $J = j_a + j_b$. Also can reason another possibility $J = j_a + j_b - 1$, $J = j_a + j_b - 2$
Lowest J is $J = j_a - j_b$. Thus

$$|j_a - j_b| \leq J \leq j_a + j_b \qquad \text{(triangle rule)}$$

$2J+1$ states for each J.

Now what are these states, e.g. $|J, M\rangle = |3/2, +3/2\rangle$?
For the highest J

$$|3/2, 3/2\rangle = |+1\rangle_a |+1/2\rangle_b$$

But for

$$|3/2, +1/2\rangle = a|0\rangle_a |1/2\rangle_b + b|1\rangle_a |-1/2\rangle_b$$

What combination will work? Find a & b. These are Clebsch-Gordan coefficients.

2) Method 1: Look in a table.

3.) Method 2: Use

$$J_- = J_-^a + J_-^b$$

We can start from the highest state, and work down.
[For any Lie group, just work up or down from a known state]

$$J_- |\tfrac{3}{2}, \tfrac{3}{2}\rangle = \sqrt{3}\,|\tfrac{3}{2}, \tfrac{1}{2}\rangle = (J_-^a + J_-^b)\,|+1\rangle|+\tfrac{1}{2}\rangle$$

$$\sqrt{3}\,|\tfrac{3}{2}, \tfrac{1}{2}\rangle = \sqrt{2}\,|0\rangle|\tfrac{1}{2}\rangle + |+1\rangle|-\tfrac{1}{2}\rangle$$

$$\Rightarrow \quad a = \sqrt{2/3}\,, \quad b = \frac{1}{\sqrt{3}}$$

J_-

$+\frac{1}{2}$	1	$3/2$	2
$\downarrow$	0	$\downarrow$	1
$-\frac{1}{2}$	$\downarrow$	$-\frac{1}{2}$	$\downarrow$
	-1	$\downarrow$	0
		$-3/2$	$\downarrow$
			-1
			$\downarrow$
			-2
$j = \frac{1}{2}$	$j = 1$	$j = 3/2$	$j = 2$

How do we reduce J now? Try to get $|\frac{1}{2}, \frac{1}{2}\rangle$.

$$|\tfrac{1}{2}, \tfrac{1}{2}\rangle = -\tfrac{1}{\sqrt{3}}|0\rangle_a|\tfrac{1}{2}\rangle_b - \sqrt{\tfrac{2}{3}}|+1\rangle_a|-\tfrac{1}{2}\rangle_b$$ use orthogonality

General method: ① get J_{max}, and use J_- to get $|J, m\rangle$
② use orthog to get next $|J-1, m\rangle$

4.) Method 3: Straight Forward Method 12/6/66 LECTURE

The best way to generate C-G coefficients is to play with $J_\pm$. However to evaluate one in the middle. Say we want

$$|2,1\rangle = a|2\rangle_a|-1\rangle_b + b|+1\rangle_a|0\rangle_b + c|0\rangle_a|+1\rangle_b \qquad (1)$$

Want $J=2$, $M=1$, i.e.

$$(J_{az} + J_{bz})\,|2,+1\rangle = +1\,|2,+1\rangle \qquad \text{gives (1)}$$

$$\vec{J}\cdot\vec{J}\,|2,1\rangle = J(J+1)\,|2,1\rangle = 6\,|2,1\rangle$$

Now

$$\vec{J}\cdot\vec{J} = (\vec{J}_a+\vec{J}_b)\cdot(\vec{J}_a+\vec{J}_b) = \vec{J}_a\cdot\vec{J}_a + \vec{J}_b\cdot\vec{J}_b + 2\vec{J}_a\cdot\vec{J}_b$$

Thus

$$\vec{J}\cdot\vec{J}\,|J,M\rangle = \underset{6}{j_a(j_a+1)} + \underset{2}{j_b(j_b+1)} + 2J_{az}J_{bz} + J_{a+}J_{b-} + J_{a-}J_{b+}$$

or

$$\left[8 + 2J_{az}J_{bz} + J_{a+}J_{b-} + J_{a-}J_{b+}\right]\left[a|+2\rangle|-1\rangle + b|+1\rangle|0\rangle + c|0\rangle|+1\rangle\right]$$

$$[8a + (-2a)]\,|+2\rangle|-1\rangle + 0 + 2\sqrt{2}\,a\,|+1\rangle_a|0\rangle_b$$
$$+ [8b + 0b]\,|+1\rangle|0\rangle + 2\sqrt{2}\,b\,|+2\rangle|-1\rangle + \sqrt{6}\sqrt{2}\,b|0\rangle|+1\rangle$$
$$[8c + \quad]\,|0\rangle|1\rangle + \sqrt{6}\sqrt{2}|+1\rangle|0\rangle$$

$$= 6\,a|2\rangle|-1\rangle + 6b|1\rangle|0\rangle + 6c|0\rangle|+\rangle$$

$|+2\rangle|-1\rangle$: $4a + 2\sqrt{2}b = 6a \Rightarrow a = \sqrt{2} \quad b = 1$

$|+1\rangle|0\rangle$: $2\sqrt{2}a + 8b + \sqrt{2}\sqrt{6}c = 6b$

$|0\rangle|+1\rangle$: $\sqrt{6}\sqrt{2}b + 8c = 6c \qquad c = -\sqrt{3}$

These methods are much more simple than using the general formulas that can be obtained for the Clebsch-Gordan coefficients.

C. Another Example of Group Ideas

1.) Isotopic Spin

Consider nucleons that can be in 2 states. If we transform all the nucleons in a nucleus.

$$|p\rangle = \alpha|p\rangle + \beta|n\rangle$$

$$|n\rangle = \beta^*|p\rangle - \alpha^*|n\rangle$$

such that $|\alpha|^2 + |\beta|^2 = 1$

This group now depends continuously on α & β. α, β are parameters of the group. Now still have

$$D^G|\psi\rangle = |\psi'\rangle$$

Again find $D^{G_3} = D^{G_2} D^{G_1}$

Can follow our work on angular momentum since there are Lie groups. Take

$\beta = \epsilon$	$\alpha = 1$	G_X
$\beta = i\epsilon$	$\alpha = 1$	G_4
$\beta = 0$	$\alpha = 1 + i\epsilon_1$	G_Z

Again $D^G = 1 + i\epsilon_1 M_1$ etc.

It turns out this group is similar to groups for spin ½ objects. Thus we introduce isotopic spin, so we can use the work on ½ spin objects. Let

M	T_3	(J_z)
J	T_+, T_-	(J_+, J_-)

Just a matter of convenience.

7.) The Eightfold Way

PROBLEM: Consider a system of 3 objects

$$|p\rangle = \alpha|p\rangle + \beta|n\rangle + \gamma|\lambda\rangle$$

$$|n\rangle = \alpha'|p\rangle + \beta'|n\rangle + \gamma'|\lambda\rangle$$

$$|\lambda\rangle = \alpha''|p\rangle + \beta''|n\rangle + \gamma''|\lambda\rangle$$

Use ON. system of states.

8 independent numbers [8 parameter group]

Not analogous to rotation groups anymore, but use same procedure. Representations

① singlet
③ triplet ½ $\bar{③}$
⑥ ⑥
⑧ etc.

This is called "8-fold way" in high energy physics.

$N, P, \Lambda, \Sigma^+, \Sigma^0, \Sigma^-, \Xi^-, \Xi^0$

If we consider only strong interactions, they all the objects have same energy. But nature is not invariant with this group. This group is called SU_6. Think now that all particles can be represented by such groups

SU_2	2 states
SU_6	3 states
SU_{12}	6 states

Actually π mesons correspond to isotopic spin $T=1$ π^-, π^0, π^+. Λ $T=0$

(3)(3) are like integer + $\frac{1}{2}$ integer in angular momentum. Haven't seen any (3) yet.

People have tried to combine angular momentum with quality and found

$$SU_6 \otimes SU_2 = SU_{12}$$

Don't really know much about it yet. Some regularities appear, but may be coincidence. SU_{12} has 6 states.

Special Case: spin $j = 1/2$ 12/9/66 LECTURE

Suppose we want

$\langle 1/2|x|1/2\rangle$ $\langle 1/2|y|1/2\rangle$ $\langle 1/2|z|1/2\rangle$

$\langle -1/2|x|1/2\rangle$ . . . etc

We are calculating matrix elements between two $|s\rangle$ states that differ only by the value of m_z -- $j = 1/2$ remains fixed. Thus same internal state, differs only by m_z.

Recall any matrix for spin $1/2$ can be written with spinors

$$\underline{\underline{M}} = \alpha \underline{\underline{I}} + a_x \underline{\underline{\sigma_x}} + a_y \underline{\underline{\sigma_y}} + a_z \underline{\underline{\sigma_z}}$$

We can then write our matrix elements as

$$\langle m_2|x|m_1\rangle = \xi_{m_1,m_2} \quad (\xi \text{ takes on 4 values})$$

Then

$$X = \xi_0 I + \xi_x \sigma_x + \xi_y \sigma_y + \xi_z \sigma_z$$

$$Y = \eta_0 I + \cdots$$

$$Z = \gamma_0 I + \cdots$$

Now since x, y, z are components of a vector, the matrices must transform (rotate) like a vector. We are saying

$$\langle m_2|\vec{R}|m_1\rangle \propto \langle m_2|\vec{\sigma}|m_1\rangle \begin{pmatrix} \xi_{++} & \xi_{+-} \\ \xi_{-+} & \xi_{--} \end{pmatrix}$$

so, for example

$$\langle m_2|X|m_1\rangle = \lambda \langle m_2|\sigma_x|m_1\rangle \begin{pmatrix} \xi_{++} & \xi_{+-} \\ \xi_{-+} & \xi_{--} \end{pmatrix}$$

Suppose we are calculating matrix elements relating to quadrapole moments. Then we want the matrix elements to transform when rotated such that they behave as tensors; i.e., the result of the rotation must behave like a tensor.

$\langle m_2|XP_x|m_1\rangle$

$\langle \quad |XP_y| \quad \rangle$

$\vdots$

} choose new matrix elements between vectors $|xP_x + yP_y + zP_z|$ vector

e.g. new matrix formed by taking linear combination -- get symmetric tensor of zero trace

$$xP_x - \tfrac{1}{3}(xP_x + yP_y + zP_z)$$

$$xP_y + yP_x$$

$$yP_y - \tfrac{1}{3}(xP_x + yP_y + zP_z)$$

$$yP_z + zP_y$$

$$xP_z + zP_x$$

} take 5 so they will be independent

So, when doing calculation of matrix elements like $\langle x p_y \rangle$, etc., follow 3 steps

i.) take matrix elements of a set of quantities which is a scalar

ii.) " " " " " vector

iii.) " " " " " tensor

Scalar component

$$\langle m_1 | x p_x + y p_y + z p_z | m_2 \rangle = \mu \langle m_1 | I | m_2 \rangle$$

Vector components

$$\langle m_1 | x p_y - y p_x | m_2 \rangle = \lambda \langle m_1 \left| \begin{matrix} \sigma_z \\ \sigma_x \\ \sigma_y \end{matrix} \right| m_2 \rangle$$

Tensor components

$$\langle m_1 | \text{tensor comp} | m_2 \rangle = \gamma \langle m_1 | \sigma_x \sigma_x - \tfrac{1}{3}(\sigma_x\sigma_x + \sigma_y\sigma_y + \sigma_z\sigma_z) | m_2 \rangle$$

Tensor components are zero ($\gamma = 0$) for spin $\frac{1}{2}$ problems since have in the end only 2 unknowns $\Rightarrow$ tensor components are not independent, i.e.

$$\langle \chi_J | \overset{\text{tensor}}{T_2} | \psi_I \rangle \qquad J = J+2, J+1 \cdots J-2$$

for $J = \frac{1}{2}$ $\quad J = \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \cdots -\frac{5}{2}$

We have been considering non-diagonal elements. Now let's try to get matrix elements for diagonal terms of angular momentum

$\langle m_2 | P_x | m_1 \rangle$; $\langle m_2 | \vec{P} | m_1 \rangle$
$\langle m_2 | P_y | m_1 \rangle$
$\langle m_2 | P_z | m_1 \rangle$

We have $\underbrace{I, J_x, J_y, J_z}_{4 \text{ numbers}}$

Matrix is

$2j+1 \left(\quad \overset{2j+1}{} \quad \right)$

Need $(2j+1)^2$ matrix elements -- numbers -- in operator we know we only have 4 numbers

But we also know $J_x J_x$, $J_x J_y$, $J_x J_z$, ... $J_y J_x J_x$ ...

Can't include $J_x J_y$ & $J_y J_x$ because of difference of J_z which we have, so must watch out for restrictions. Still have a # of combinations? However don't really know this many, e.g. for $j = 1$

$$(J_z+1) J_z (J_z-1) |m\rangle = 0 \quad \text{for all } m = \begin{matrix} 1 \\ 0 \\ -1 \end{matrix}$$

$\therefore J_z^3 - J_z = 0$ $\therefore$ we can't allow $J_z J_z J_z$ or $J_x J_y J_x$, so we are restricted.

Can make combination of 3, so we cannot make a vector from 2 J's

$$\langle m_2 | \vec{P} | m_1 \rangle = \lambda \langle m_2 | \vec{J} | m_1 \rangle$$

Generally, for arbitrary j,

$$\langle m_1 | \text{scalar} | m_2 \rangle = a \langle m_1 | I | m_2 \rangle$$

$$\text{vector} \qquad \vec{J}$$

$$\text{tensor} \qquad J_x^2 - \tfrac{1}{3}(J_x^2 + J_y^2 + J_z^2)$$

(tensor with zero trace)

For $j=1$, can get higher than terms like $J_x J_y + J_y J_x$
Terms like $J_x J_x J_x$ give 0 m.e. In general

$$\langle J=1 | T_{(3)} | 1 \rangle = 0$$

because ① + ③ = ④ so can have

$$J = 4, 3, 2$$

Putting m.e. together, e.g.

$$\langle m_2 | x P_x | m_1 \rangle = \langle m_2 | x P_x - \tfrac{1}{3}(P_x X + P_y Y + P_z Z) | m_1 \rangle + \tfrac{1}{3} \langle m_2 | P_x X + P_y Y + P_z Z | m_1 \rangle$$

Important point is a traceless tensor can be written as

$$\langle m_2 | x P_x | m_1 \rangle = c \langle m_2 | J_x^2 - \tfrac{1}{3}(J_x^2 + J_y^2 + J_z^2) | m_1 \rangle + \tfrac{1}{3} a \langle m_2 | I | m_1 \rangle$$

$$= c \langle m_2 | J_x J_x | m_1 \rangle + (\tfrac{1}{3}a - \tfrac{2}{3}c)\, \delta_{m_1, m_2}$$

$\sum (J+1)$

(traceless)

Can prove that a nucleus of spin ½ cannot have a quadrapole moment -- no magnetic moment if spin is 0, because need

$$\langle m_1 | \vec{\mu} | m_1 \rangle \propto \langle m_2 | I | m_1 \rangle$$

or vector ∝ scalar

$\Rightarrow$ scalar = 0, no mag. moment for $j = 0$ objects

SOLID STATE PHYSICS

1/6/67 LECTURE

To learn this field, one must read alot to gain experience of the various phenomenum. Return to us books idea to develop theory.

Types of crystals

molecular: sugar, odour, etc.

covalent: diamond

ionic: NaCl

metallic:

We will be concerned with 2 topics, phonon interactions and conduction in crystalline material.

From statistical mechanics, if a crystal is at temperature T at equilibrium, prob. of being in state i is

$$P_i \propto e^{-E_i/kT}$$

$$= Q e^{-E_i/kT}$$

where $Q = \sum_i e^{-E_i/kT}$ partition function

Can get all of thermo from this.

U = expected energy $= \sum_i E_i P_i = \dfrac{\sum_i E_i e^{-E_i/kT}}{Q}$

If we know $Q = Q(T)$

$$\frac{\partial Q}{\partial T} = \sum_i \frac{E_i}{kT^2} e^{-E_i/kT}$$

$$\Rightarrow U = \frac{kT^2}{Q} \frac{\partial Q}{\partial T}$$

Can write

$$Q = e^{-F/kT} \quad \text{where } F = -kT \ln Q$$

Helmholtz free energy

Then find

$$U = -T^2 \frac{\partial}{\partial T}\left(\frac{F}{T}\right) = F - T \underbrace{\frac{\partial F}{\partial T}}_{S \text{ entropy}}$$

$\therefore U + TS = F$

The energy of a molecule is a function of the position of the nuclei $U(R_1, R_2, \cdots)$. Thus

$$H\Psi = \sum_i \left(-\frac{\hbar^2}{2M_i}\nabla_i^2\right)\Psi(R_1, R_2, \cdots) + U(R_1, R_2 \cdots)\Psi = -\frac{\hbar}{i}\frac{\partial \Psi}{\partial t}$$

PROBLEM: Why is this equation right and how did we arrive at it. Assume that the correct S. equ is for Coulomb interactions and use mass differences of N. etc to try to separate electronic and nuclear motion.]

[First consider case of fixed nuclei

$$\sum_\alpha \frac{\hbar^2}{2m}\nabla_\alpha^2 \chi_{R\cdots}(r_\alpha) + V(R\cdots r\cdots)\chi_{R\cdots}(r_\alpha) = E\,\chi_{R\cdots}(r_\alpha)$$

↑ fixed constant

Note $E = E(R_1 \cdots)$ and idea is for $E = U$.
Want to show exact wave fcn

$$\Psi \simeq \Psi(R_1, R_2 \cdots)\,\chi_{R_1 R_2 \cdots}(r_\alpha)\ ]$$

PROBLEM: Find F and U for an harmonic oscillator of natural frequency ω, mass m, temperature T. 1/9/67 LECTURE

We were considering

$$\left\{\sum_i -\frac{\hbar^2}{2M_i}\nabla_i^2 + U(R_1, R_2 \cdots)\right\}\Psi(R) = -\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = \mathcal{E}\Psi(R_i \cdots) \qquad (1)$$

One of those laws of physics which seems to reproduce itself (like Newton's law $F = MA \Leftrightarrow f = ma$)

Since potential U rises very rapidly, molecular motion is quite small and nuclear wave functions are pretty localized for vibrations. Thus we can approx. solve (1) by expanding about equilibrium pt. Let $x_i \to R_1, R_2 \cdots$ from equilibrium

$$\sum_i -\frac{\hbar^2}{2M_i}\frac{\partial^2}{\partial x_i^2} + U(x_1, x_2 \cdots)$$

Expand $$U(0,0,\cdots) + x_i\left(\frac{\partial U}{\partial x_i}\right)_0 + \frac{1}{2}\sum_{ij} x_i x_j \underbrace{\left(\frac{\partial^2 U}{\partial x_i \partial x_j}\right)_0}_{V_{ij}} + \cdots \qquad (2)$$

Redefine energy at $U(0,0,\cdots)$. Note $\frac{\partial U}{\partial x_i}$ is zero.

Thus we use

$$\sum_i -\frac{\hbar^2}{2M_i}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\sum_{ij} x_i x_j V_{ij} = H$$

Redefine $q_i = \sqrt{M_i}x_i$, let $\hbar = 1$

$$\sum_i -\frac{1}{2}\frac{\partial^2}{\partial q_i^2} + \frac{1}{2}\sum_{ij} q_i q_j C_{ij} = H$$

where $$C_{ij} = \frac{1}{\sqrt{M_i M_j}}\left(\frac{\partial^2 U}{\partial x_i \partial x_j}\right)_0$$

This is just a set of coupled harmonic oscillators. First look at the classical analogue

$$\sum_i \frac{p_i^2}{2} + \frac{1}{2}\sum_{ij} q_i q_j C_{ij} = H$$

to find

$$\ddot{q}_i = -\frac{\partial}{\partial q_i}\left(\text{Pot. Energy}\right) = -\sum_j C_{ij} q_j$$

Use $q_{0i} = a_i e^{i\omega t}$

$$\omega^2 a_i = \sum_j C_{ij} a_j$$

$$\Rightarrow \det\left(C_{ij} - \omega^2 \delta_{ij}\right) = 0$$

Find $\omega^2_{(\alpha)}$ roots yielding then $a_i^{(\alpha)}$ eigenvectors

Also

$$\sum_i a_i^{(\alpha)} a_i^{(\beta)} = \delta_{\alpha\beta} \text{ since } C_{ij} \text{ is symmetric}$$

Apply to CO_2 molecule

9 modes:


$\omega = 0$


$\omega \neq 0$


$\omega = 0$


$\omega = 0$

$\omega = 0$


$\omega = 0$

} rotation


$\omega \neq 0$


$\omega \neq 0$


$\omega \neq 0$

Also $\sum_\alpha a_i^{(\alpha)} a_j^{(\alpha)} = \delta_{ij}$

We can reexpress $q_i = \sum_\alpha a_i^{(\alpha)} Q_\alpha$, i.e. q_i as a sum of the eigenmodes. Can show

$$Q_\alpha = \sum_i a_i^{(\alpha)} q_i$$

This separates the harmonic oscillators. Can also do this in q.m.

1/10/67 LECTURE

We were considering

$$H = \tfrac{1}{2}\sum_i p_i^2 + \frac{1}{2}\sum_{i,j} C_{ij} q_i q_j$$

$$p_j = \frac{1}{i}\frac{\partial}{\partial q_i}$$

and found

$$\omega_\alpha^2 a_i^{(\alpha)} = \sum_j C_{ij} a_j^{(\alpha)} \qquad \sum_i a_i^{(\alpha)} a_i^{(\beta)} = \delta_{\alpha\beta}$$

$$\sum_\alpha a_i^{(\alpha)} a_j^{(\alpha)} = \delta_{ij}$$

To simplify, we substitute the normal coordinates

$$Q_\alpha = \sum_i a_i^{(\alpha)} q_i$$

as new variables $q_i = \sum_\alpha a_i^{(\alpha)} Q_\alpha$ to find

$$H = \tfrac{1}{2}\sum_\alpha P_\alpha^2 + \tfrac{1}{2}\sum_\alpha \omega_\alpha^2 Q_\alpha^2$$

$$\frac{1}{i}\frac{\partial}{\partial Q_\alpha}$$

$$= \sum_\alpha h_\alpha \qquad \text{where } h_\alpha = \tfrac{1}{2} P_\alpha^2 + \tfrac{1}{2}\omega_\alpha^2 Q_\alpha^2$$

EXAMPLE:

i) $E_{\text{system}} = E_{\text{osc}_1} + E_{\text{osc}_2} + \cdots = \sum_\alpha E_\alpha$

$$= \hbar\omega_1(n_1 + \tfrac{1}{2}) + \hbar\omega_2(n_2 + \tfrac{1}{2}) + \cdots$$

$$= \sum_\alpha \hbar\omega_\alpha (n_\alpha + \tfrac{1}{2})$$

ii) Write wave functions as $\varphi_n(x)$ (Hermite polynomials)
then

$$\Psi = \varphi_{n_1}(Q_1)\,\varphi_{n_2}(Q_2)\cdots$$

$$= \prod_\alpha \varphi_{n_\alpha}(Q_\alpha)$$

iii) ground state of system: $n_\alpha = 0$, $E_g = \sum_\alpha \tfrac{1}{2}\hbar\omega_\alpha + U(0,0,0\cdots)$

" " wave function

$$\Psi_g = \prod_\alpha e^{-\frac{1}{2}\omega_\alpha Q_\alpha^2} = e^{-\frac{1}{2}\sum_\alpha \omega_\alpha Q_\alpha^2}$$

$$= e^{-\frac{1}{2}\sum_\alpha \omega_\alpha \sum_{ij} a_{\alpha i} a_{\alpha j} q_i q_j} = e^{-\frac{1}{2}\sum_{ij}\gamma_{ij} q_i q_j}$$

Might try to express $\gamma_{ij} = \sum_\alpha \omega_\alpha a_i^\alpha a_j^\alpha$ as a fcn of C

$$\gamma\gamma = C \qquad \left[\sum_k \gamma_{ik}\gamma_{kj} = C_{ij}\right]$$

iv) $\bar{n} = \dfrac{1}{e^{\hbar\omega/kT} - 1}$ very useful

Thus internal energy ↙ gives trouble later

$$U = \sum_\alpha \hbar\omega_\alpha(\bar{n}_\alpha + \tfrac{1}{2}) = \sum_\alpha \frac{\hbar\omega_\alpha}{2} + \sum_\alpha \frac{\hbar\omega_\alpha}{e^{\hbar\omega_\alpha/kT}-1}$$

To show $\bar{n}$, consider prob of occupation of n state by 1 osc.

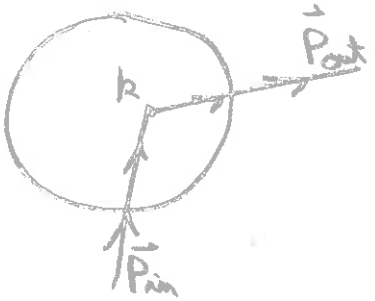
$$P_n = \frac{1}{Q} e^{-\frac{\hbar\omega(n+\frac{1}{2})}{kT}}$$

But $\sum_n P_n = 1 = \sum_n \frac{1}{Q} e^{-\frac{\hbar\omega(n+\frac{1}{2})}{kT}}$

$$\bar{n} = \sum_n n P_n \sim (1-x)\sum_n n x^n = \frac{x}{1-x}$$

EXAMPLE:

Neutron scattering off of a nucleus in a solid. What is chance that neutron loses no energy?



neutron-nucleon potential $V(R-q_k)$ is so space limited, use Born approx.

interaction $V(R-q_k) \approx a\delta(R-q_k)$

initial state $e^{i P_{in} \cdot R}\, \psi_i(q \ldots) = \psi(R, q)$

final state $e^{i P_{out} \cdot R}\, \psi_f(q \ldots)$

$$P_{rate\ of\ transition} = \ldots |M_{fi}|^2$$

$$M_{fi} = \int \psi_f^* e^{i P_{out} \cdot R}\, \delta(R-q_k)\, e^{i P_{in} \cdot R}\, \psi_i\, d^3R\, dq$$

Define $K = P_{in} - P_{out}$ = momentum transfer

$$\int \psi_f^*(q)\, e^{iKq_k}\, \psi_i(q)\, dq$$

[if sudden K given to part of ψ_i, $\psi_f = e^{iK \cdot R_{point}}\, \psi_i$]

or for us

$$\int \psi_0\, e^{iKq_k}\, \psi_0\, dq = \iiint e^{-\sum_\alpha \omega_\alpha Q_\alpha^2}\, e^{ik \sum_\alpha a_k^{(\alpha)} Q_\alpha}\, dQ_1 dQ_2 \ldots$$

$$= \prod_\alpha \left(\int e^{-\omega_\alpha Q_\alpha^2 + i\kappa a_k^\alpha Q_\alpha} dQ_\alpha \right) = \prod_\alpha e^{-(\kappa a_k^\alpha)^2/4\omega_\alpha}$$

Thus $\text{prob}_{\substack{\text{left in} \\ \text{ground} \\ \text{state}}} = e^{-\kappa^2 S}$ $\qquad S = \sum_\alpha \frac{(a_k^\alpha)^2}{2\omega_\alpha}$

PROBLEM: One can find $\langle q_k^2 \rangle = \int \psi_0 q_k^2 \psi_0 dq = S$

Thus

$$\text{prob} = e^{-\kappa^2 \langle q_k^2 \rangle / \hbar^2}$$

PROBLEM: Prove the same formula for the system at temperature T [i.e. that prob. that no energy is transferred to system is

$$\text{prob} = e^{-\kappa^2 \langle q_k^2 \rangle / \hbar^2}$$

where now $\langle q_k^2 \rangle$ is ave. at temp. T

1/13/67 LECTURE

We found

$$\text{Prob. to remain in ground state} = \text{Prob. of elastic scattering} = e^{-p^2\langle q_{0k}^2\rangle_0}$$

Debye-Waller Factor

Note we cannot elastically scatter from zero-ω modes (translations). Always define elastic scattering in center of mass system so as to throw out translational mode.

PROBLEM: Suppose system in ground state. Show

$$\langle \text{energy lost by neutron if } p \text{ final} \rangle = \frac{p^2}{2m_k}$$

mean energy gained by crystal
= matrix disturbance is e^{ipx} = $\frac{p^2}{2m_k}$ (classical result)

i.) prove for ground state
ii.) " " any state
iii.) " " " system

Can get a diffraction (only if we cannot distinguish which atom was hit). When is this true? When

$p_{neutron} > p_{zero\ point\ energy}$

PROBLEM: Show that elastic scattering gives a diffraction. Show that inelastic scattering does not give a diffraction pattern.

Nucleus inside a crystal emits a γ. Expect a recoil (classically)

$$E_\gamma = E_0 - \frac{p^2}{2m}$$

Then could absorb this γ in a similar nucleus (resonance absorption)

Mössbauer discovered recoilless emission and absorption. Analogue to elastic neutron scattering. Very precise effect.

Back to Harmonic Oscillator $m=1, \omega=1$

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\xi^2 \qquad p = \frac{1}{i}\frac{\partial}{\partial \xi}$$

Recall

$$H\phi_n = \epsilon_n \phi_n$$

$$\epsilon_n = (n+\tfrac{1}{2})$$

$$\phi_n(\xi) = \frac{1}{\pi^{1/4}\sqrt{2^n n!}} H_n(\xi) e^{-\frac{1}{2}\xi^2}$$

$n=0$ $\quad e^{-\frac{1}{2}\xi^2}$

$n=1$ $\quad \xi e^{-\frac{1}{2}\xi^2}$

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

Interesting that we can get a generating function

$$e^{-s^2+2s\xi} = \sum_n \frac{H_n(\xi) s^n}{n!}$$

Also have

$$\sum_n \frac{\phi_n(\xi) s^n}{\sqrt{n!\,2^n}} = \frac{1}{\pi^{1/4}} e^{-\frac{1}{2}(\xi-s)^2} e^{s^2/4}$$

EXAMPLE:

$$\lambda_{mn} = \int \phi_m^*(\xi)\, e^{i\rho\xi}\, \phi_n(\xi)\, d\xi$$

Calculate

$$\sum_{m,n} \frac{\lambda_{mn} s^m t^n}{\sqrt{2^m m!}\sqrt{2^n n!}} \equiv S(s,t)$$

$$= \sum_{m,n} \int \frac{s^m \phi_m(\xi)\, e^{i\rho\xi}\, \phi_n(\xi)\, t^n}{\sqrt{2^m m!}\sqrt{2^n n!}}\, d\xi$$

$$= \frac{1}{\sqrt{\pi}} \int e^{-\frac{1}{2}(\xi-s)^2} e^{s^2/4}\, e^{i\rho\xi}\, e^{-\frac{1}{2}(\xi-t)^2} e^{t^2/4}\, d\xi$$

$$= \frac{1}{\sqrt{\pi}} \int e^{-\xi^2 + \xi(s+t+i\rho)}\, e^{-s^2/4 - t^2/4}\, d\xi$$

$$= \frac{1}{\sqrt{\pi}} \int e^{-\left(\xi - \frac{s+t+i\rho}{2}\right)^2} e^{-\left(\frac{s^2}{4}+\frac{t^2}{4}\right)} e^{\left(\frac{s+t+i\rho}{2}\right)^2} d\xi$$

$$= e^{-\rho^2/4}\, e^{st/2}\, e^{i\rho s}\, e^{i\rho t}$$

Now just expand in $s^m t^n$

$$= e^{-\rho^2/4} \sum_{k,r,q} \frac{\left(\frac{st}{2}\right)^k}{k!} \frac{(i\rho s)^r}{r!} \frac{(i\rho t)^q}{q!}$$

$$= e^{-\rho^2/4} \sum_{k,r,q} (i\rho)^{r+q} 2^{-k}\, s^{k+r}\, t^{k+q} \qquad \therefore\ r = m-k,\ q = n-k$$

$$\therefore \frac{\lambda_{mn}}{\sqrt{2^m m!}\sqrt{2^n n!}} = e^{-\rho^2/4} \sum_{k=0}^{\min(m,n)} \frac{(i\rho)^{m+n-2k}\, 2^{-k}}{k!\,(m-k)!\,(n-k)!}$$

PROBLEM: a crystal at temp T. Find Prob for scattering neutron (for given p) elastically.

Hint: If simple oscillator, $P_{abs} = \langle n | e^{ip\cdot r} | n \rangle$

$$\therefore \frac{\sum_n e^{-\epsilon_n/kT} |\langle n | e^{ip\xi} | n \rangle|^2}{Q}$$

Then show

$$P_{scat} = e^{-p^2 \langle q_{av}^2 \rangle_T}$$

PROBLEM: Show

$$\sum_n \varphi_n(\xi) \varphi_n^*(\xi') e^{-it\epsilon_n}$$

$$= \left(\frac{m\omega}{2\pi i \sin\omega t}\right)^{1/2} e^{i\frac{m\omega}{2\sin\omega t}\left[(\cos\omega t)(\xi^2+\xi'^2) - 2\xi\xi'\right]}$$

PROBLEM: Consider

$$i\frac{\partial}{\partial t}\psi(\xi,t) = -\tfrac{1}{2}\frac{\partial^2}{\partial \xi^2}\psi(\xi,t) + \tfrac{1}{2}\xi^2\psi(\xi,t)$$

Suppose $\psi(\xi,0) = \delta(\xi-\xi_0)$. Try to solve the time-dependent eqn:

Hint: $\psi(\xi,t) = e^{a(t)\xi^2 t + b(t)\xi + c(t)}$

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$$H = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\xi^2 \qquad \varphi_0(\xi) = e^{-\xi^2/2}$$

$$p = \frac{1}{i}\frac{d}{d\xi} \qquad \varphi_n(\xi)$$

We can transform this to momentum space

$$H = \frac{1}{2}p^2 - \frac{1}{2}\frac{d^2}{dp^2}$$

and find we get exactly the same equations and

$$\psi_n(p) = i^n \varphi_n(p)$$

↖ phase from $\psi(p) = \int e^{ip\xi}\varphi(\xi)\,d\xi$

Recall we had given

$$\lambda_{mn} = \int \varphi_m^*(\xi)\, e^{iP\xi}\, \varphi_n(\xi)\,d\xi = \int \psi_m^*(p)\,\psi_n(p+P)\,dp$$

$$-\frac{d^2}{dr^2}\underset{f}{[r\psi]} + \frac{l}{r}\underset{f}{[r\psi]} = rE\underset{f}{[r\psi]}$$

$$-\frac{\hbar}{i}\frac{d}{dp}\left(\frac{p^2}{2}f(p)\right) + f(p) = -E\frac{\hbar}{i}\frac{df}{dp}$$ much easier

---

Now return to

$$H = \frac{1}{2}\frac{p^2}{m} + \frac{m\omega^2}{2}q^2$$

Now define

$$a = \sqrt{\frac{m}{2\omega}}\left(\omega q + i p/m\right) \qquad \left[\frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)\right]$$

$$a^\dagger = \sqrt{\frac{m}{2\omega}}\left(\omega q - i p/m\right) \qquad \left[\frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)\right]$$

Then

$$q = \frac{1}{\sqrt{2m\omega}}\left(a + a^\dagger\right)$$

$$p = (-i)\left(a - a^\dagger\right)$$

Note $pq - qp = -i$. To get this in a's

$$a^\dagger a = \frac{1}{\omega} H - \frac{1}{2}$$

$$a a^\dagger = \frac{1}{\omega} H + \frac{1}{2}$$

Thus $$a a^\dagger - a^\dagger a = 1$$

Also

$$H = \underbrace{\omega a^\dagger a}_{\text{excitation energy for harmonic oscillator}} + \frac{\omega}{2}$$

Can figure out eigenvalues and matrix elements

Sometimes define

$$N = a^\dagger a$$

If $N|n\rangle = n|n\rangle$, then

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

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

Thus $a^\dagger$ creation operator, a annihilation operator.

$$\langle m|a^\dagger|n\rangle = \delta_{m,n+1}\sqrt{n+1}$$

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

Can show

$$(a^\dagger)^n|0\rangle = \frac{1}{\sqrt{n!}}|n\rangle$$

where we define $|0\rangle$ by

$$a|0\rangle = 0$$

EXAMPLE: $q_{mn} = \langle m|(a+a^\dagger)|n\rangle$

$$= \langle 0|\frac{a^m}{\sqrt{m!}}(a+a^\dagger)\frac{a^{\dagger n}}{\sqrt{n!}}|0\rangle$$

Use $\langle 0|a^\dagger = 0$, $a|0\rangle = 0$ to work out.

$$\lambda_{mn} = \langle 0|\frac{a^m}{\sqrt{m!n!}}e^{i\frac{p(a+a^\dagger)}{\sqrt{2}}}(a^\dagger)^n|0\rangle$$

If we have α independent oscillators, define

$$a_\alpha^\dagger = \left(m_\alpha \omega_\alpha Q_\alpha + i \frac{P_\alpha}{m}\right)\sqrt{\frac{m_\alpha}{2\omega_\alpha}}$$

Can show

$$a_\alpha^\dagger a_\beta - a_\beta a_\alpha^\dagger = \delta_{\alpha\beta}$$

$$a_\beta a_\alpha = a_\alpha a_\beta$$

Thus

$$H = \underbrace{\sum_\alpha \frac{\hbar\omega_\alpha}{2}}_{\text{ground state energy}} + \sum_\alpha \omega_\alpha a_\alpha^\dagger a_\alpha$$

Can arbitrarily say when oscillator is in n^{th} state it has n "vibrations". Thus $a^\dagger$ & a create and annihilate vibrations.

This is very convenient for more complicated problems.

E & M cavity: photons

crystal phonons

"Calling a state of motion by a noun." Like "vortex". ["Can't step in same river twice". Eating & anti-process]
Humans as a pattern of motion.

Now return to our discussion of a polyatomic molecule

$$H = \sum_i \frac{p_i^2}{2} + \frac{1}{2} \sum_{ij} c_{ij} q_i q_j$$

and try to extend it to a crystal.

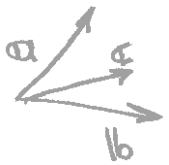
Label location in a crystal

$\mathbb{N}$ cell

r atom in cell

If p atoms/unit cell, r has $3p$ values

$\mathbf{a}, \mathbf{b}, \mathbf{c}$ are directions which reproduce the crystal



Then to find $\mathbb{N}$

$$\mathbb{N} = n_a \mathbf{a} + n_b \mathbf{b} + n_c \mathbf{c}$$

Now H for the crystal becomes

$$H = \sum_{\mathbb{N},r} \frac{P_{\mathbb{N},r}^2}{2} + \frac{1}{2} \sum_{\mathbb{N},r,\mathbb{M},s} c_{\mathbb{N},r,\mathbb{M},s} q_{\mathbb{N},r} q_{\mathbb{M},s}$$

Now $C_{N,r,M,s} = \Gamma_{r,s}(N-M)$

expressing fact that interaction doesn't depend on the absolute location of the cells, but only on relative distance between them.

We must solve for the frequencies using

$$\omega_\alpha^2 \phi_{N,r} = \sum_{M,s} \Gamma_{r,s}(M-N)\phi_{M,s}$$

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$$H = \sum_{N,r} \frac{P_{N,r}^2}{2} + \frac{1}{2}\sum_{N,r;M,s} \Gamma_{r,s}(N-M)\, q_{N,r}\, q_{M,s}$$

Now consider

$$\omega_\alpha^2 q_{N,r} = \sum_{M,s} \Gamma_{r,s}(N-M)\, q_{M,s}$$

EXAMPLE:

Choose as a potential $\sum_n \frac{A}{2}(q_n - q_{n+1})^2 + \sum_n \frac{B}{2}(q_n - q_{n+2})^2 + \cdots$

at first take B & longer range terms vanish. Then

$$H = \sum_n \frac{P_n^2}{2} + \frac{1}{2}\underbrace{\sum_n A(q_n - q_{n+1})^2}$$

$$\underbrace{\sum_n A q_n^2 - \sum_n A\, q_n\, q_{n+1}}$$

$$\sum_{n,m} \Gamma(n-m)\, q_n\, q_m \qquad \Gamma(0) = 2A,\ \Gamma(+1) = A,\ \Gamma(-1) = -A$$

Our e.v. problem becomes

$$\omega_\alpha^2 q_n = A(q_n - q_{n+1}) - A(q_{n-1} - q_n)$$

Set $\begin{pmatrix} 2A-\omega^2 & -A & & & -A \\ -A & 2A-\omega^2 & -A & & 0 \\ & -A & 2A-\omega^2 & -A & \\ & & \ddots & & \\ -A & & & & \end{pmatrix}$ a band matrix

and as b.c. use $q_{N+n} = q_n$

Rather than solve $\det| \; | = 0$, we merely solve eqn by letting

$$q_n = e^{in\delta}$$

to find

$$\omega_\alpha^2 e^{in\delta} = A\left[e^{in\delta} - e^{i(n+1)\delta}\right] - A\left[e^{in\delta} - e^{i(n-1)\delta}\right]$$

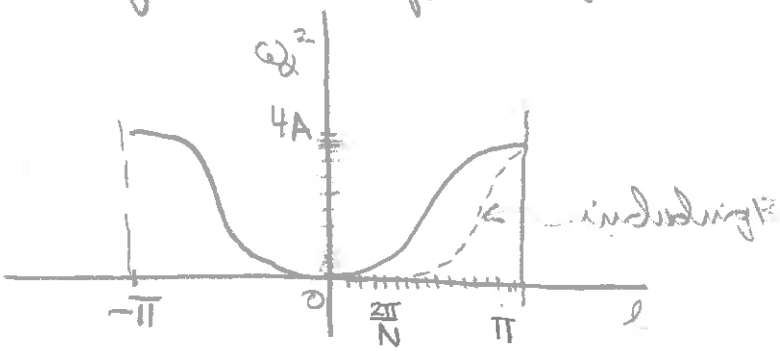
$$\omega_\alpha^2 = A\left[1 - e^{i\delta} - e^{-i\delta} + 1\right] = 2A(1-\cos\delta)$$

We also require $q_{N+n} = q_n$

$$\therefore \; e^{iN\delta} = 1 \quad \Rightarrow \quad \delta = \frac{2\pi}{N}\ell \qquad \ell = 0, \cdots N-1$$

$$\text{or} \quad \ell = \frac{N}{2} \text{ to } \frac{N}{2}$$

Then we find an ω_α for each ℓ



If we included B, $2A(1-\cos\delta) + 2(1-\cos 2\delta)$ which distorts the curve above

It is convenient to change α to δ to k, suggestive of a wave motion 

$$k = \frac{\delta}{a} \qquad \text{phase difference } \delta = ka.$$

Then

$$\omega_k^2 = 2A(1-\cos ka) \qquad k = -\frac{\pi}{a} \text{ to } \frac{\pi}{a}$$

$$\text{spacing of } k = \frac{2\pi}{Na} = \frac{2\pi}{L}$$

At long wavelength

$$\omega_k^2 \sim Aa^2k^2 \qquad \Rightarrow \omega \sim k \quad \text{like sound waves } \omega = ck$$

[which is what it is anyway]

$$\Rightarrow c_s = \sqrt{Aa^2}$$

Now for the normal modes

$$Q_k = \sum_i a_{ki} q_i = \sum_n \frac{e^{-ikan} q_n}{\sqrt{N}}$$

and H becomes

$$H = \sum_k \frac{p_k^2}{2} + \sum_k \frac{\omega^2(k)}{2} Q_k^2$$

Now have "phonons" of wavelength k. Thus sound has a maximum ω & min. wavelength [corresponding to a]

Now returning to our general problem

$$q_{lM,s} = q'_{ls}\, e^{i M\cdot K}$$

Thus we take into account the phase difference between cells, not between atoms. Find

$$\omega_\alpha^2 q'_{lr} e^{iN\cdot K} = \sum_{M,s} \Gamma_{r,s}(N-M) e^{iK\cdot M} q'_s$$

Now define

$$\sum_{N,} \Gamma_{r,s}(N) e^{-iK\cdot N} \equiv \gamma_{r,s}(K)$$

(kind of a Fourier transform)

Thus letting $\omega_\alpha \to \omega_\beta^2(K)$

$$\omega_\beta^2(K)\, q'_{lr} = \sum_s \gamma_{r,s}(K) q'_s$$

Now this problem is just for atoms in cell and we can revert to our analysis of polyatomic molecules [we handle the infinite periodic unit cells by the K]

β has $3p$ values for each K. Now spacing of K is $\frac{2\pi}{L_x}, \dots$ Thus

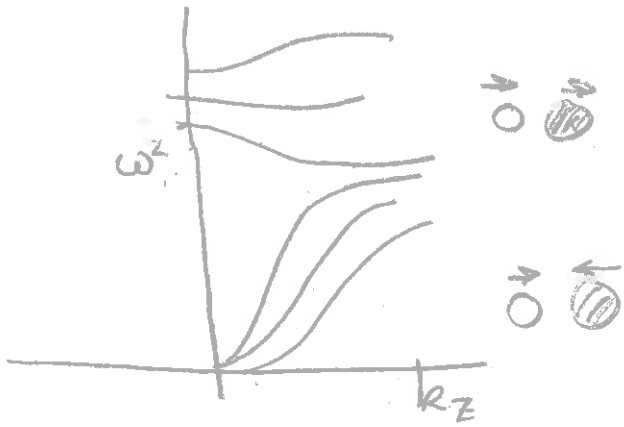
$$\sum_K \to \int \frac{d^3K}{(2\pi)^3} \text{Vol}$$

Where are repetition boundaries of K space? We'll return to this in a moment.

Consider a one dimensional k_z where each unit cell has
1 atom - 3 modes per k

Thus 3 types of sound waves - longitudinal & 2 transverse. [not actually either]

In other directions curves are different. Thus c_s are different in different directions.



2 atoms / unit cell (NaCl)

Acoustical & optical branches

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PROBLEMS:

1.) One-dimensional line of atoms, spacing a, limit case $ka \ll 1$. Try to develop the q.m. of a continuous material (long waves). $q_n \to q(x)$. This is quantum field theory.

2.) Find the frequency spectrum for some crystal. Specific heat. Like cubic crystal

Recall

$$C_{N,r;M,s} = \Gamma_{rs}(N-M)$$

$$\sum_N \Gamma_{rs}(N) e^{iK\cdot N} = \gamma_{rs}(K)$$

Then solved

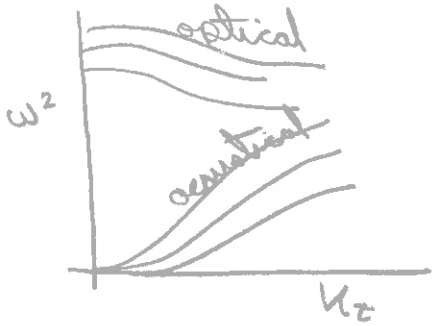
$$\omega_\beta^2(K)\, q_r' = \sum_s \gamma_{rs}(K)\, q_s'$$

and

$$Q_\beta'(K) = \sum_r a_r^\beta(K)\, q_r'$$

$$Q^\beta(K) = \sum_{r,N} a_r{}^\beta(K)\, e^{-iK\cdot N} q_{r,N}$$

Continues discussion polyatomic crystals

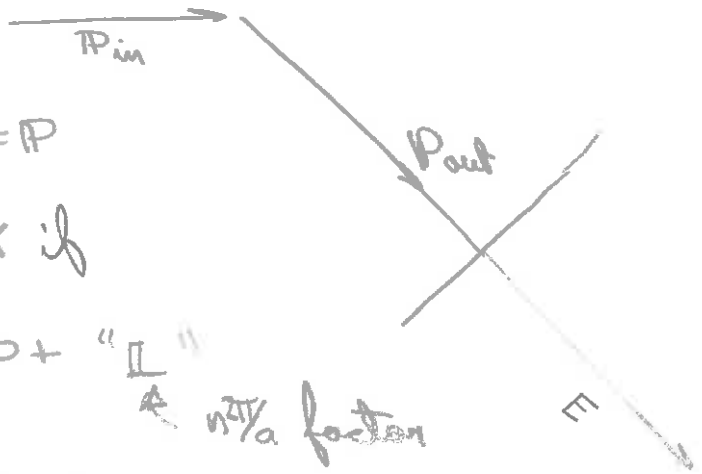


Because of dipole moment, one can excite modes in optical branch with infrared light. Thus NaCl has enormous absorption at these 3 frequencies as $k_z \to 0$. Reststrahl frequency. Thus reflects monochromatic beam. Would be an intense dye — if only not infrared. Greenish look — like green dye which absorbs red light.

Can use good guesses of coupling constants to determine physical properties -- or vice versa. Problem is essentially solved. Can also get elastic constants (21 for monoclinic crystal).

Determination of ω_j's:

For every K, $3p$ frequencies $\pm\omega_j(K)$
Not hard to show that if you bounce neutrons from crystals



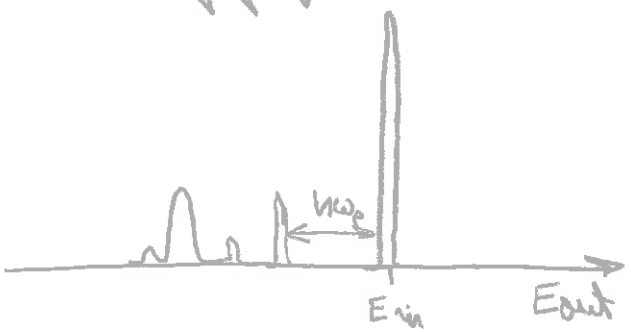
$$P_{in} - P_{out} = P$$

Excite a mode of K if

$$K = P + \text{"}L\text{"}$$

$\uparrow$ $n2\pi/a$ factor

Can plot energy of neutron



By looking at peaks, we can get ω_j directly.

Now in K space

$$\sum_K \rightarrow \int_R \frac{d^3K}{(2\pi)^3} \text{ vol}$$

Now $N = n_a a + n_b b + n_c c$

We can try to find L, such that
$K' = K + L$ gives same answer.

$$e^{i\mathbf{K}'\cdot\mathbf{N}} = e^{i\mathbf{K}\cdot\mathbf{N}}$$

$$\Rightarrow e^{i\mathbf{L}\cdot\mathbf{N}} = 1$$

Thus $(\mathbf{L}\cdot\mathbf{a}) = 2\pi$ (integer)

$(\mathbf{L}\cdot\mathbf{b}) = 2\pi$ (integer)

$(\mathbf{L}\cdot\mathbf{c}) = 2\pi$ (integer)

—o—

Say we know $(\mathbf{L}\cdot\mathbf{a}) = \mathcal{L}_a$ $(\mathbf{L}\cdot\mathbf{b}) = \mathcal{L}_b$ $(\mathbf{L}\cdot\mathbf{c}) = \mathcal{L}_c$

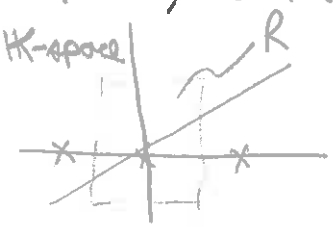
Then one can show we can invert the vector as

$$\mathbf{L} = \mathcal{L}_a \frac{\mathbf{b}\times\mathbf{c}}{|\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}|} + \mathcal{L}_b \frac{\mathbf{c}\times\mathbf{a}}{|\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}|} + \mathcal{L}_c \frac{\mathbf{a}\times\mathbf{b}}{|\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}|}$$

—o—

Here $\mathcal{L}_a, \mathcal{L}_b, \mathcal{L}_c = 2\pi$ integers. This forms a latticework of points in $\mathcal{L}$-space, analogous to the reciprocal of the original cubic crystal. Called the reciprocal lattice. Very important in diffraction work (which is elastic).

In K-space, can separate regions R which repeat using reciprocal lattice. This is first Brillouin zone of K-space.



Solid-state physicists (& liquid chemists) love cubic crystals. True physicists always work with cubic crystals.

Specific Heats:

These nuclear vibrations are main contribution to specific heat in most problems.

$$U(T) = \sum_{\beta,\mathbf{k}} \frac{\hbar\omega_\beta(\mathbf{k})}{e^{\hbar\omega_\beta(\mathbf{k})/kT} - 1}$$

$$= \sum_\beta \int_R \frac{\hbar\omega_\beta(\mathbf{k})}{e^{\hbar\omega_\beta(\mathbf{k})/kT} - 1} \frac{d^3\mathbf{k}}{(2\pi)^3} \cdot V$$

Can find

$$C_V = \frac{\partial U}{\partial T}, \text{ etc.}$$

$\omega_\alpha(\vec{k})$ = mode frequencies 1/23/67 LECTURE
↳ 3p values

U = Internal Energy (of vibration) $= \sum_\alpha \int_R \frac{d^3k}{(2\pi)^3} Vol \left[\frac{\hbar\omega_\alpha(\vec{k})}{e^{\hbar\omega_\alpha/kT}-1} + \frac{\hbar\omega_\alpha(\vec{k})}{2} \right]$

$\therefore C_V = \frac{\partial U}{\partial T} = kVol. \sum_\alpha \int_R \frac{d^3k}{(2\pi)^3} \frac{(\hbar\omega_\alpha/kT)^2 e^{\hbar\omega/kT}}{\left(e^{\hbar\omega_\alpha/kT}-1\right)^2}$

Phonon description is quite good for many crystals (not metals, magnets, etc. however). We can discuss C_V

High temperatures:

If $kT >$ highest frequency (usually at room temp.)

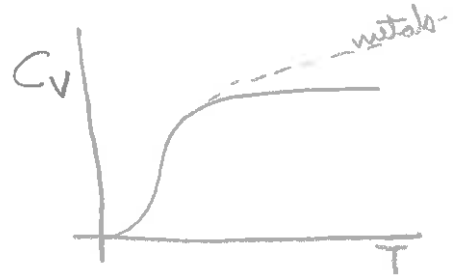
$$\frac{\hbar\omega_\alpha}{e^{\hbar\omega/kT}-1} \to kT$$

$$\therefore U = kT \cdot \underbrace{\sum_\alpha \int_R \frac{d^3k}{(2\pi)^3} 1 \; Vol}_{3 \text{ No. of } \vec{k}\text{'s in crystal}} = 3NkT$$

$C_V = 3Nk = 3R$ per °K, per mole

$\sim$ 6 cal per °K per mole

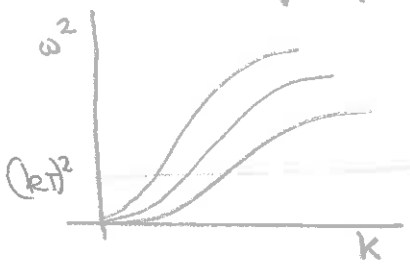
pretty good at high T



Low Temperatures:

$kT <$ any frequency ; get $e^{-\Delta/T}$ – essential singularity

But no lowest frequency



; only these modes contribute

Thus assume 3 values of αi survive and

$$\omega_{\alpha i}(k) = c_{\alpha i}|k|$$

$$U = kT \sum_{\alpha i} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar c_{\alpha i} k / kT}{e^{\hbar c_{\alpha i} k/kT} - 1} \quad \text{Vol}$$

($4\pi k^2 dk \left(\frac{d\Omega}{4\pi}\right)$)

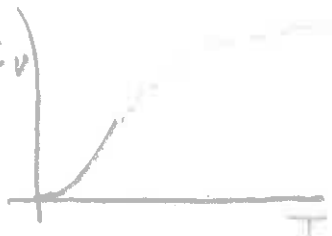
$$= kT \sum_{\alpha i} \int \frac{d\Omega}{4\pi} \left(\frac{kT}{\hbar c_{\alpha i}}\right)^3 \frac{1}{2\pi^2} \int_0^{\infty} \frac{x^3 dx}{e^x - 1} \sim \frac{\pi^4}{15} \quad \text{Vol}$$

$$= (kT)^4 \frac{\pi^2}{10} \int \frac{d\Omega}{4\pi} \frac{1}{3} \sum_{\alpha i} \frac{1}{(c_{\alpha i})^3} \quad \text{Vol}$$

$$= \frac{(kT)^4 \pi^2}{10 c_0^3} \quad \text{Vol}$$

c_0 ← one speed of sound $\quad \frac{1}{c_0^3} = \left\langle \frac{1}{c_{\alpha i}^3} \right\rangle$

$\therefore C_V \sim T^3$



# of modes at low T = # of acoustic modes $\sim K^3 \sim T^3$

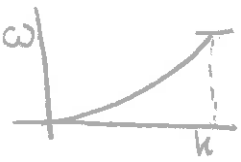
—o—

However as we approach 0° (10^{-6} degrees), we find $C_v \propto T^3$. Why? Because $\sum \to \int$ for very small crystals which are used at very low T. Then there is a lowest frequency. Then essential singularity

—o—

Mentions Debye theory

sphere of radius K_{max}



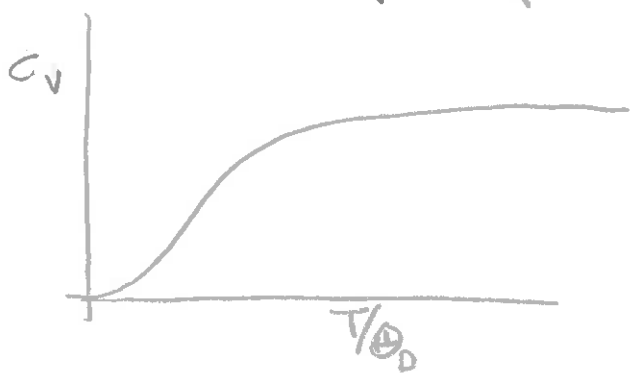
$$U = 3kT \int \frac{d^3K}{(2\pi)^3} \frac{\hbar C_0 K}{e^{\hbar C_0 K/kT} - 1}$$

$$= \frac{(kT)^4}{(\hbar C_0)^3} \frac{\pi^2}{10} \left(\frac{15}{\pi^4}\right) \int_0^{\Theta_D/T} \frac{x^3 dx}{e^x - 1}$$

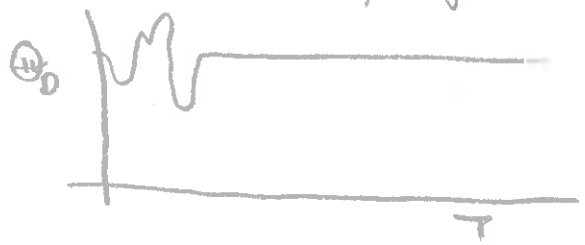
where $\Theta_D = \frac{K_{max} \hbar C_0}{k}$

Debye temperature

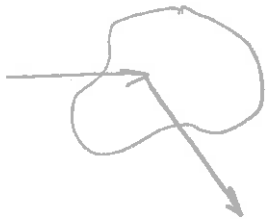
Debye temp. is a useful way to characterize a crystal.



But never plot C_v vs T, unfortunately. Always plot



Neutron Scattering



$$\langle f | \sum_i a_i e^{i\mathbf{p}\cdot\mathbf{R}_i} | i \rangle$$

Actually this is gotten from:

$$\left\langle e^{i\mathbf{k}_f\cdot\mathbf{r}_n} \middle| \sum_i V(\mathbf{r}_n - \mathbf{R}_i) \middle| e^{i\mathbf{k}_n\cdot\mathbf{r}_n} \right\rangle$$

where we assume Fermi pseudopotential $\Rightarrow a_i(p) = \text{const}$.

Now suppose elastic scattering $i=f$

$$\text{Prob}_{f=i} = |\langle i | \sum_i | i \rangle|^2$$

Put $\mathbf{R}_i = \mathbf{R}_{eq} + \mathbf{q}_i$

$$\text{Prob}_{f=i} = \left| \langle i | \sum_i e^{i\mathbf{p}\cdot\mathbf{R}_{oi}} e^{i\mathbf{p}\cdot\mathbf{q}_i} | i \rangle \right|^2$$

If we take $e^{i\mathbf{p}\cdot\mathbf{q}_i} \sim 1$, $\text{Prob}_{f\neq i} = \text{Prob}_{f=i}$

However carry $e^{i\mathbf{p}\cdot\mathbf{q}_i}$ along

$$\sum_i e^{i\mathbf{p}\cdot\mathbf{R}_{oi}} \underbrace{\langle i | e^{i\mathbf{p}\cdot\mathbf{q}_i} | i \rangle}_{e^{-\frac{p^2\langle q_i^2\rangle}{2}}}$$

Now for inelastic,

$$\sum a_i e^{iP\cdot R_i} \langle f | e^{iP\cdot q_i} | i \rangle$$

For some reason we don't get any interference from inelastic scattering [since we can always identify the excited atom

May be a tiny bit of interference due to coupling between nuclei in crystal.

Try to work it out for a linear chain.

Now $\psi_{after} = e^{iP\cdot x}\psi_{before}$ if given an impulse of momentum P

$$\langle \psi_a^* H \psi_a \rangle - \langle \psi_b^* H \psi_b \rangle$$

$$\left[\frac{P^2}{2m} + \text{other } p^2 + V(\ )\right]$$

$$\langle \psi_b^* | e^{-iP\cdot x} H e^{iP\cdot x} - H | \psi_b \rangle$$

Now use $\frac{\partial}{\partial x}(e^{ax} f) = e^{ax}\left(\frac{\partial}{\partial x} + a\right) f$

to find

$$\langle \psi_b^* | \left(\frac{p+P}{2m}\right)^2 + \quad - \left(\frac{p^2}{2m} + \cdots\right) | \psi_b \rangle$$

$$= \frac{P^2}{2m}\langle \psi_b^* | \psi_a \rangle + P \cdot \langle \psi_b^* \left(\frac{p}{m}\right) | \psi_a \rangle$$

when $\langle \psi_b^* \frac{p}{m} \psi_a \rangle = 0$, get classical result

The M.E. $\langle \psi_b^* | \frac{p}{m} | \psi_a \rangle$ is kind of a Doppler correction.

—o—

Prob: No excitation from e^{iPQ}. If initially state is n, Prob of no excitation is $|\langle n|e^{iPQ}|n\rangle|^2$. At thermal equilibrium

Prob of no excitation $= \sum_n e^{-E_n/kT} |\langle n|e^{iP\cdot Q}|n\rangle|^2$

$= \sum_n e^{-n\hbar\omega/kT}(1-e^{-\hbar\omega/kT}) |\langle n|e^{iP\cdot Q}|n\rangle|^2$

First find $\langle n|e^{iP\cdot Q}|n\rangle = \langle 0| \frac{a^n}{\sqrt{n!}} e^{iP\left(\frac{a+a^*}{\sqrt{2}}\right)} \frac{(a^*)^n}{n!}|0\rangle$

$= \sum_s \frac{(iP)^{2s}}{2^s} \frac{1}{n!} \langle 0|a^n(a+a^*)^{2s}(a^*)^n|0\rangle$

Use $a^n a^* = a^* a^n + n\cdot a^{n-1}$ — stuck

1/30/67 LECTURE

μ^- to stimulate $p+p \to d+e^+ + \nu$.

Great for nuclear physics. But μ only has $\lambda \sim 2.2\times10^{-6}$ sec, so can't be sustained too long. But maybe another longer-lived heavy neg. charged particle.

At high T, can get barrier penetration for
$p+p \to d+e^+ +\nu$.

—o—

PROBLEM: Changing line of atoms to a continuum

o o o o o q_n

$$H = \tfrac{1}{2}P_n^2 + \frac{\alpha}{2}(q_n - q_{n+1})^2 \qquad Q_k = \sum_n q_n \frac{e^{ikx_n}}{\sqrt{N}}$$

Set $x_n = an$. Thus $q(x)$ replaces q_n. Recall we found

$$\omega^2 = 2\alpha(1-\cos ka)$$

For ka small, $q(x)$ continuous

$$\omega^2 = \alpha a^2 k^2$$

$$Q_k = \int q(x)\, e^{ikx}\, \frac{dx}{a\sqrt{N}}$$

$$Q'_k = \int q(x)\, e^{ikx}\, dx \qquad Q' = \frac{Q}{a\sqrt{N}}$$

$$q(x) = \int Q_k \frac{dk}{2\pi}$$

$$\therefore H = \int \left\{ \underbrace{\frac{1}{2a}\left(\frac{\partial q}{\partial t}\right)^2}_{K.E.} + \underbrace{\frac{1}{2a}\alpha a^2 \left(\frac{\partial q}{\partial x}\right)^2}_{P.E.} \right\} dx$$

($\rho \sim \pi$, c^2)

$$\pi(x) = p_n a$$

$$q_n p_{n'} - p_{n'} q_n = -i\,\delta_{nn'}$$

$$q(x)\pi(x') - \pi(x') q(x) = i\,\delta(x-x')$$

$$\therefore H = \int \left[\frac{1}{2}\pi^2(x) + \frac{1}{2}c^2 \left(\frac{\partial q}{\partial x}\right)^2 \right] dx$$

Thus we have defined a field -- a q.m. field -- of two conjugate variables $q(x)$, $\pi(x)$. [Corresponds to vibrating string] Note we can "diagonalize" H using

$$q(x) = \int e^{ikx} Q(k) \frac{dk}{2\pi}$$

$$\pi(x) = \int e^{ikx} P(k) \frac{dk}{2\pi}$$

$$\Rightarrow P(k)Q(k') - Q(k')P(k) = -2\pi i\,\delta(k-k')$$

$$\therefore H = \frac{1}{2}\int \left\{ |P(k)|^2 + k^2c^2 |Q(k)|^2 \right\} \frac{dk}{2\pi}$$

$$\therefore \omega^2(x) = ck$$

We could have applied this to electrodynamics.
QED field theory in 3-d

$\vec{Q}(\vec{x})$: $Q_x(\vec{x})$, $Q_y(\vec{x})$, $Q_z(\vec{x})$

$$K.E. = \frac{1}{2}\int \frac{\partial \vec{Q}}{\partial t} \cdot \frac{\partial \vec{Q}}{\partial t}\, dVol$$

$$P.E. = \frac{1}{2}\int C_{ij,kl}\, C_{ij}\, C_{kl}\, d^3x$$

PROBLEM: Diffusion of phonons (finite mfp) 1/31/67 LECTURE

This is heat diffusion. Need higher order interactions $(q_i - q_{i+1})^3 + \cdots$. Could do a perturbation theory. (Use aaa^*) Phonon-phonon scattering

Umklapp processes: $\mathbb{K}' + \mathbb{K}'' = \mathbb{K}''' + \mathbb{L}$ because propagation vector goes into a new Brillouin zone. Thus we get thermal diffusion, not second sound (compression phonon waves as in He^4). At low T not much chance of leaving zone, thus small thermal resistance.

Impossible to define the momentum of phonon, since can be transferred to crystal as a whole.

$\mathbb{K}$, 0 (phonon, crystal)

$\mathbb{K} + \mathbb{L}$, $-\mathbb{L}$

etc.

PROBLEM: Low density of imperfections (atoms of different mass) so we can treat each flaw separately. Phonons will scatter off of these.

Effect on thermal conductivity

For small T, how does thermal conductivity depend on T? and n?

Continuum Approximation

2/4/67 Lecture

$q(x)$, $\pi(x)$ $\ni$ $\pi(x)q(x') - q(x')\pi(x) = -i\delta(x-x')$

$$K.E. = \tfrac{1}{2}\int \left(\frac{\partial q}{\partial t}\right)^2 dx = \tfrac{1}{2}\int [\pi(x)]^2 dx$$

$$P.E. = \frac{c^2}{2}\int \left(\frac{\partial q}{\partial x}\right)^2 dx$$

Thus

$$H = \tfrac{1}{2}\int [\pi(x)]^2 dx + \frac{c^2}{2}\int [\nabla q]^2 dx \qquad (1)$$

Can find

$$q(x) = \sum_k \frac{1}{\sqrt{2\omega_k}}\left[(a_k^* + a_{-k})e^{-ikx}\right] \qquad (2)$$

$$\pi(x) = \sum_k \frac{i\sqrt{\omega_k}}{\sqrt{2}}\left[(a_k^* - a_{-k})e^{ikx}\right]$$

we use $a_k a_L^* - a_L^* a_k = (2\pi)^3 \delta^3(k-L)$

$$\sum_k \to \int \frac{d^3k}{(2\pi)^3}$$

We demonstrates

$$[\pi(x), q(x')] = -i \sum_k e^{ik\cdot(x-x')} = -i\,\delta^3(x-x')$$

The representation (2) is very convenient for most physical problems. Can find

$$H = \int \frac{d^3k}{(2\pi)^3} \left[a_k^* a_k + \tfrac{1}{2}\right] \hbar\omega_k$$

We can return to play with (1). Note

$$\langle\psi|\dot{A}|\phi\rangle = \frac{d}{dt}\langle\psi|A|\phi\rangle$$

provided ψ, ϕ solve S-equ

$$= \langle\psi|\frac{\partial A}{\partial t}|\phi\rangle - i\langle\psi|AH|\phi\rangle + i\langle\psi|HA|\phi\rangle$$

$$\Rightarrow \quad \dot{A} = +\frac{\partial A}{\partial t} + i[H, A]$$

Thus

$$\dot{q}(y) = i[H, q(y)]$$

$$= i\left[\frac{1}{2}\int \underbrace{\{[\pi(x)]^2 q(y) - q(y)\pi(x)^2\}}_{\pi(x)[\pi(x)q(y) - q(y)\pi(x)] + [\pi(x)q(y) - q(y)\pi(x)]\pi(x)} d^3x\right.$$

$$\underbrace{\pi(x)[\pi(x)q(y) - q(y)\pi(x)]}_{-i\delta(x-y)} + \underbrace{[\pi(x)q(y) - q(y)\pi(x)]\pi(x)}_{-i\delta(x-y)}$$

$$= \int \pi(x)\,\delta(x-y)\,d^3x = \pi(y)$$

$$\therefore \quad \dot{q}(x) = \pi(x)$$

$$\dot{\pi}(y) = i[H, \pi] = i\int d^3x \left\{ (\nabla q(x))^2 \pi(y) - \pi(y) (\nabla q(x))^2 \right\}$$

$$\nabla q(x) \underbrace{\left\{ \nabla q(x)\, \pi(y) - \pi(y) \nabla q(x) \right\}}_{\nabla_x [i\delta(x-y)]} + \cdots$$

to find

$$\dot{\pi}(x) = + c^2 \nabla^2 q(x) \qquad (4)$$

Now can find from (3) & (4)

$$\frac{\partial^2 q}{\partial t^2} = c^2 \frac{\partial^2}{\partial x^2} q(x)$$

This is called quantum field theory. [variable at every point in space].

EXAMPLE:

In elastic theory we need a vector field

$$q_i(\vec{x}) \quad , \pi(\vec{x})$$

Now

$$\pi_i(x) q_j(y) - q_j(y) \pi_i(x) = -i\delta_{ij} \delta(x-y)$$

$$[q_i(x), q_j(y)] = 0 = [\pi_i(x), \pi_j(y)]$$

$$K.E. = \frac{1}{2}\int \left(\frac{\partial \vec{q}}{\partial t}\cdot\frac{\partial \vec{q}}{\partial t}\right) dV dt = \frac{1}{2}\int \Pi\Pi(x)\cdot\Pi\Pi(x)\, dV dt$$

$$P.E. = \frac{1}{2}\int \sum_{ij,kl} C_{ij,kl}\left(\frac{1}{2}\left(\frac{\partial q_i}{\partial x_j}+\frac{\partial q_j}{\partial x_i}\right)\right) dV dt$$

$$= \frac{1}{2}\int \sum_{ij,kl} C_{ij,kl}\left(\frac{\partial q_i(x')}{\partial x_j}\right)\left(\frac{\partial q_k}{\partial x_e}\right) dV dt \qquad \text{using symmetry}$$

One can find equation

$$\ddot{q}_i(\vec{x}) = \sum_{ijkl} C_{ij,kl}\frac{\partial}{\partial x_j}\frac{\partial}{\partial x_k} q_k(x)$$

[wave equation in anisotropic media]

Anisotropic media

$$\ddot{\vec{q}} = \lambda_1 \nabla^2 \vec{q} + \lambda_2 \nabla(\nabla\cdot\vec{q})$$

ELECTRODYNAMICS

For free fields

$$L = \frac{1}{2}\int \left[\mathbb{E}\cdot\mathbb{E} - \mathbb{B}\cdot\mathbb{B}\right] d\mathrm{Vol} + \int (\mathbb{J}\cdot\mathbb{A} + \rho\varphi)\, d^3\mathrm{Vol}$$

$$= \frac{1}{2}\int \left[\left(-\nabla\varphi - \frac{\partial \mathbb{A}}{\partial t}\right)^2 - (\nabla\times\mathbb{A})\cdot(\nabla\times\mathbb{A})\right] d^3x$$

$$\left(\frac{\partial \mathbb{A}}{\partial t}\right)^2 - 2\,\nabla\varphi\cdot\frac{\partial \mathbb{A}}{\partial t} + (\nabla\varphi\cdot\nabla\varphi)$$

$$\varphi\,\frac{\partial}{\partial t}(\nabla\cdot\mathbb{A}), \qquad \nabla\cdot\mathbb{A} = 0$$

Coulomb gauge $\nabla\cdot\mathbb{A}$

Can solve for φ statically from $\nabla^2\varphi = \rho$

Now identify $\mathbb{A}$ as an operator. Define a

$$\Pi(x) \sim \frac{\partial \mathbb{A}}{\partial t}$$

$$\Pi_i(x)\,\mathbb{A}_j(x') - \mathbb{A}_j(x')\,\Pi_i(x) = -i\,\delta^3(x-x')\,\delta_{ij}$$

$$H = \frac{1}{2}\int \Pi(x)\cdot\Pi(x)\, d^3x + \frac{1}{2}\int (\nabla\times\mathbb{A})^2 d^3x$$

2/6/67 LECTURE

In classical mechanics we use

$$\int L(q,\dot{q})\,dt = S$$

and Euler equations (principle of least action). For E&M we use

$$S = \frac{1}{2}\int\left[\underbrace{\left(-\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}\right)^2}_{E^2} - \underbrace{(\nabla \times \mathbf{A})^2}_{B^2}\right] d^3x\,dt$$

$$+ \int J_\mu(x,t)\,A_\mu(x,t)\,d^3x\,dt$$

Our variables corresponding to $q, \dot{q}$ are ϕ and $\mathbf{A}$. Using variation will produce Maxwell eqns.

We make our quantum theory in analogy, only take out the t. We use Coulomb-gauge $\nabla\cdot\mathbf{A} = 0$. Then no $\partial\phi/\partial t$ appears. Thus can determine ϕ from

$$\nabla^2\phi = \rho$$

via instantaneous Coulomb interaction. In q.m. just use " " in S-eqn.

Thus in q.m. we get variables

$$\mathbf{A}(x) \quad ; \quad \Pi(x)$$

and

$$H = \underbrace{\frac{1}{2}\int(\Pi\cdot\Pi)\,d^3x + \int(\nabla\times\mathbf{A})^2 d^3x}_{\text{free field}} + \int \mathbf{J}\cdot\mathbf{A}\,d^3x + \text{Matter}$$

Find

$$[\Pi_i(x), A_j(y)] = -i\,\delta^3(x-y)\,\delta_{ij}$$

PROBLEM: Derive Maxwell eqns as operator eqns.

$$\dot{\Pi} = i(H\Pi - \Pi H) \qquad \dot{A} = i(HA - AH)$$

PROBLEM: Find

$$[A_i(x,t), A_j(x',t)]$$

for free fields

One can write A as a superposition of plane waves (photons)

$$A(x) = \sum_{k,\alpha=1,2} \frac{1}{\sqrt{2\omega_k}}\left[\epsilon_\alpha a^*_{k,\alpha} e^{-ik\cdot x} + \epsilon^*_\alpha a^*_{-k,\alpha} e^{-ik\cdot x}\right]$$

$$\Pi(x) = \quad " \quad " \quad - \quad "$$

Comments: i.) Many more assumptions are needed in Q.E.D. than in our crystal theory (2nd quantization) assume the form of operators.

ii.) Very similar to elastic hamiltonian except for curl term (there an elastic solid which will reproduce E & M. No — more with proper $C_{ij,kl}$

This term is all the difference. In 19th century people didn't realize this, and since knew a lot about elastic waves, tried to study "ether" of EM wave propagation. Got into trouble. Mentions McCullagh who got right idea, but no one listened to him. We now listen to people like this (Dirac's ear). Learn from past mistakes. When we get stuck, it is only because we haven't tried all of what was done before. Need new ideas in strange particles. Every generation must invent its own methods.

PROBLEM: Surface interactions

Consider 2-dimensions "gas". Can get two dimensional condensation

In 3-dimensions, 3 phases. In 2-D, 2-phases are found: condensed or expanded phase. Why? Is the condensed phase a solid or liquid?

Might try scatter neutrons to see if we get a sharp diffraction pattern

Bragg says $q^2 = 0$ in $e^{-p^2/8\beta^2}$
$\Rightarrow$ no solid?

Try shear effects (by transmitting transverse waves). How do we define a solid.

ELECTRON THEORY OF METALS

Degenerate Electron Gas

Disregard ionic potential, Coulomb interaction [assume they are free] ‡

Consider a box of V with n elect/cc. What is behavior at 0 ° finite T? 0 means lowest temp.

0 Temp.

Plot K-space. Only discrete values for states. Fill up to a certain energy value of rad.

$K_{max} \equiv K_f$

Now No. of states filled is

$$2 \int_{sphere} \frac{d^3K}{(2\pi)^3} \text{ Vol} \qquad (2 \text{ spins})$$

$$= \text{Vol}\ 2\ \frac{4\pi}{3}\ \frac{K_f^3}{(2\pi)^3}$$

$$\therefore\ n = 2\ \frac{4\pi}{3}\ \frac{K_f^3}{(2\pi)^3}$$

$$\text{Energy of electrons} = 2 \int_0^{K_f} \frac{d^3K}{(2\pi)^3} (\text{Vol}) \frac{K^2}{2m} = \frac{3}{5} \frac{K_f^2}{2m} N$$

$$\text{Energy/particle} = \frac{3}{5} \epsilon_f \qquad \epsilon_f = \frac{K_f^2}{2m}$$

$$\text{Pressure} = \rho^{5/3} \qquad (\text{density} = \rho)$$

‡ Crazy, but it works.

PROBLEMS: Determine the size of stars from your armchair by balancing fermion repulsion against gravitational attraction. Find critical mass (gravitational collapse). Then find out what happens above critical mass (good luck). Take $T=0°$, $\rho \sim n$. Use electrons as fermions (forget about Coulomb potential. $P = \rho^{5/3}$ – modify relativistically ±

2/7/67 LECTURE

$$\frac{dP}{dr} = \frac{GM(r)}{r^2}\rho - f(\rho)$$

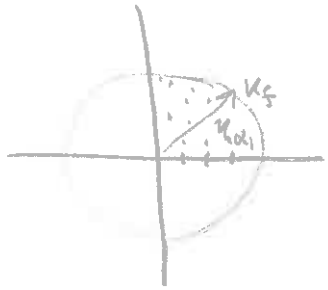
$$M(r) = \int_0^r \rho(r)\, r^2 dr\, 4\pi$$

PROBLEMS; Find magnetic effect of spin (Pauli's paramagnetism) Diamagnetic effect of spin in strong B. Consider Larmor precession – find energy levels using fermions and plot $\chi = \frac{\partial \mathcal{E}}{\partial B}$

± $U = \int \epsilon(k) \frac{d^3k}{(2\pi)^3} Vol \qquad \epsilon(k) = \sqrt{m^2 + k^2} - m$

From $P \sim \rho^{4/3}$ high density. Neglect mass of electrons (don't correct $M(\rho)$ due to U). Ignore general relativity.

What are characters of wave fcns.



What is

$\Psi(\mathbb{R}_1, \mathbb{R}_2 \cdots \mathbb{R}_i \cdots)$?

Use independent nature of electrons and consider only spin ↑. Use exclusion principle (antisymmetric Ψ)

$$\Psi(\mathbb{R}_1, \cdots) = e^{i\mathbb{K}_{\alpha_1}\cdot\mathbb{R}_1} e^{i\mathbb{K}_{\alpha_2}\cdot\mathbb{R}_2} \cdots$$

$$- e^{i\mathbb{K}_{\alpha_2}\cdot\mathbb{R}_1} e^{i\mathbb{K}_{\alpha_1}\cdot\mathbb{R}_2} \cdots$$

$$\vdots \qquad \text{etc.}$$

$$= \frac{1}{\sqrt{N!}} \sum_P (-1)^P \prod_i e^{i\mathbb{K}_{\alpha_{P(i)}}\cdot\mathbb{R}_i}$$

$$= \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \phi_{\alpha_1}(\mathbb{R}_1) & \phi_{\alpha_2}(\mathbb{R}_1) \cdots \\ \phi_{\alpha_1}(\mathbb{R}_2 & \phi_{\alpha_2}(\mathbb{R}_2) \\ \vdots & \end{pmatrix}$$

where $\phi_\alpha(\mathbb{R}) = e^{i\mathbb{K}_\alpha\cdot\mathbb{R}_i}$

Note this also means $\mathbb{K}_{\alpha_i} \neq \mathbb{K}_{\alpha_j}$ or $\Psi \equiv 0$.

Say we find electron at $\mathbb{R}_a$. What is prob. of finding one at $\mathbb{R}_b$.

Calculate instead prob of finding e at $\vec{R}_a$ & $\vec{R}_b$.
— indeed calculate average values

$$= \langle \Psi | \sum_i \delta(\vec{R}_a - \vec{R}_i) \sum_j \delta(\vec{R}_b - \vec{R}_j) | \Psi \rangle$$

$$= \langle \Psi | \delta(\vec{R}_a - \vec{R}_1)\, \delta(\vec{R}_b - \vec{R}_2) | \Psi \rangle$$

$$= \sum_{\substack{k_1 \text{ over all } \vec{k} \\ k_2 \text{ over all } \vec{k}}} 1 - \sum_{\substack{k_1' \text{ over all } \vec{k} \text{ occupied} \\ k_2' \text{ over all } \vec{k}}} e^{i(\vec{k}_{2'} - \vec{k}_{1'}) \cdot (\vec{R}_a - \vec{R}_b)}$$

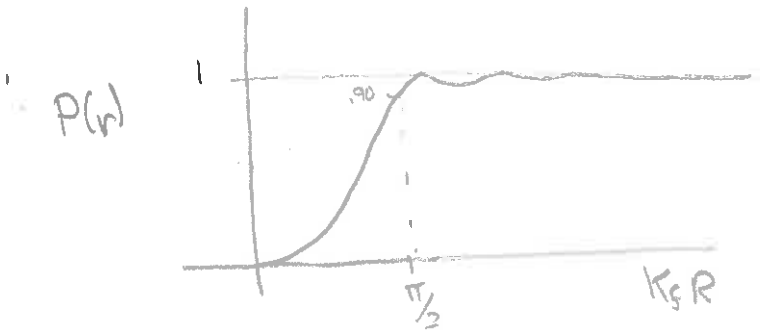
direct term exchange term

$$= \sum_{\substack{\vec{k}_1 \\ \vec{k}_2}} 1 - \left| \sum_{\vec{k}} e^{i \vec{k} \cdot \vec{R}} \right|^2$$

or pass from $\sum_{\vec{k}} \rightarrow \int_0^{k_f}$

$$= 1 - \left\{ \frac{3}{x^3} \left[\sin x - x \cos x \right] \right\}^2$$

$x = k_f R$



2/13/67 LECTURE

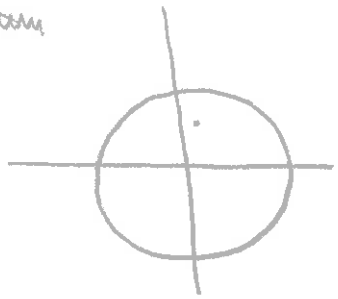
At high temp., the prob. of occupation of an electron state is

$$n_e \sim e^{-\epsilon/kT}$$

μ = Fermi energy or chemical potential.

Can find at low temp. $U \sim T^2$, $C \sim T$. At zero T we fill up the momentum sphere of radius μ.

Electrons are excited with energy kT. How many can be excited? Only ones on surface of sphere

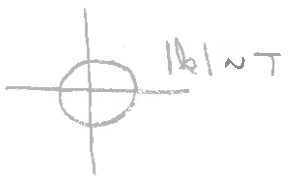


no. of electron ~ region within kT of surfaces of Fermispheres

$\sim kT$

Thus $U \sim (kT)(kT) \sim T^2$

For phonons, $\hbar\omega \sim kT$



$\therefore$ no. $\sim T^3$

$\therefore U \sim T^4$

since working with Bosons now and need entire volume of sphere.

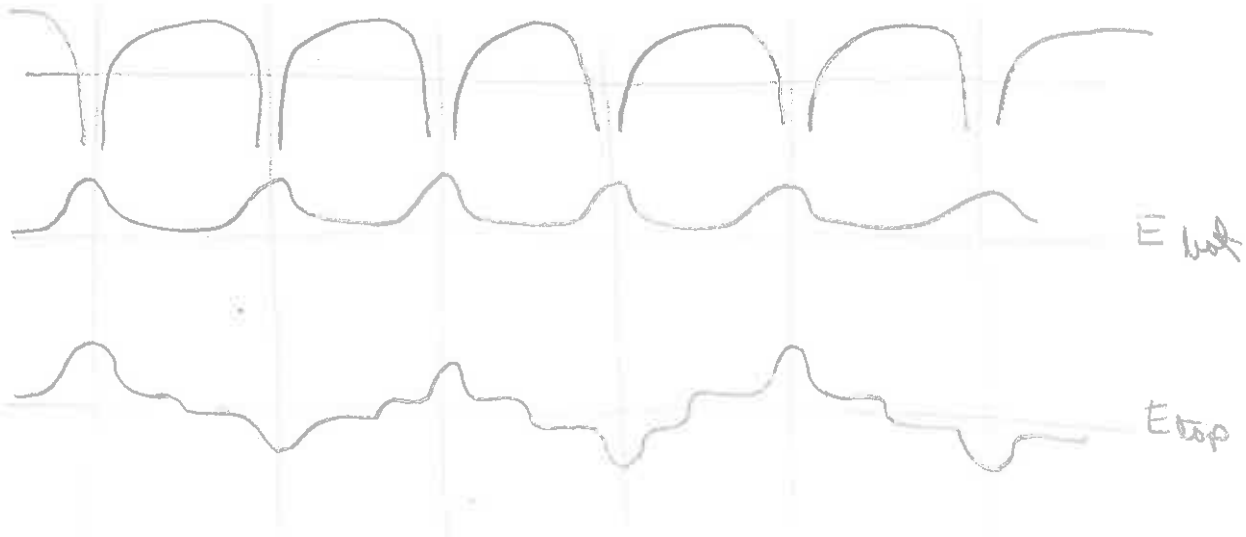
We can plot

Periodic Potentials

We now try to solve the S-eqn for this [need Hartree-Fock to get correct potential]

We consider bringing two potentials to get

Find degeneracy is destroyed. For many atoms



Now $-\frac{\hbar^2}{2m}\nabla^2\psi + V(R)\psi = E\psi$

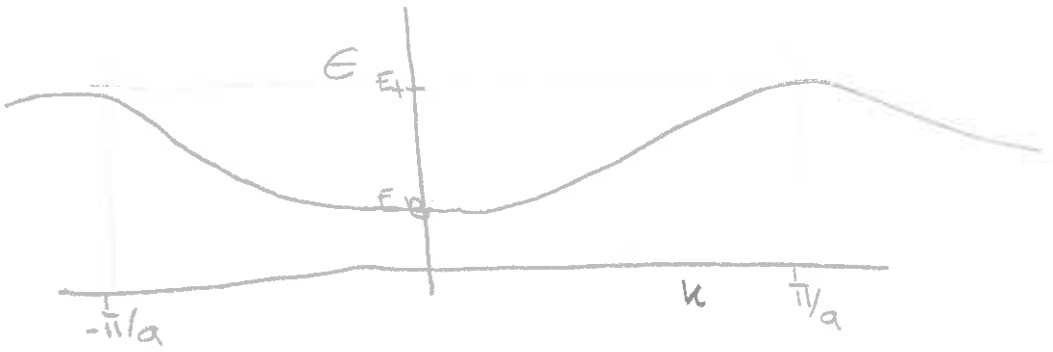
But

$$V(R) = V(R+a)$$

Using "phony-screwy" periodicity

$$\psi(R+na) = \psi(R)\, e^{ikna}$$

Can find



[Remember can only define k mod $\hat{1}$]

Frequently postulate $\psi(R) = e^{ikR}\, u_k(R)$

and

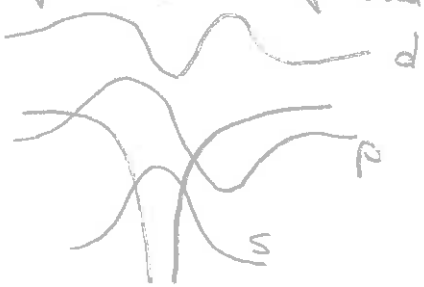
$$u_k(R+a) = u_k(R)$$

Mentions all of this as it applies to group theory

$$T[S\text{-eqn}] = [S\text{-eqn}]$$

$$\Rightarrow \quad T\psi(R) = \psi(R)$$

But this doesn't describe free propagation. We neglected higher states. Even as $V \to 0$, not free particle wavefunctions.



Weak Potentials

$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{R})\psi = \epsilon\psi$

2/14/67 Lecture

$$V(\mathbf{R}) = \sum_{\mathbf{L}} V_{\mathbf{L}} e^{i\mathbf{L}\cdot\mathbf{R}}$$

$$\psi(\mathbf{R}) = e^{i\mathbf{K}\cdot\mathbf{R}} u_{\mathbf{K}}(\mathbf{R})$$

$$= \sum_{\mathbf{L}} A_{\mathbf{L}} e^{i(\mathbf{K}+\mathbf{L})\cdot\mathbf{R}}$$

as wave-fun for one electron moving through a periodic potential

Hence

$$\left[\frac{\hbar^2}{2m}(\mathbf{K}+\mathbf{L})^2 - \epsilon\right] A_{\mathbf{L}} = -\sum_{\mathbf{L}'} V_{\mathbf{L}-\mathbf{L}'} A_{\mathbf{L}'} \qquad (1)$$

Choose $V_0 = 0$, all other V's small. Zeroth approximation $A_0 = 1$, other A_i very small. Then (1) for $\mathbf{L} = 0$ gives

$$\epsilon \sim \frac{\hbar^2}{2m}\mathbf{K}^2 \qquad \mathbf{L} = 0$$

$$A_{\mathbf{L}} = \frac{-V_{\mathbf{L}}}{\frac{1}{2m}(\mathbf{K}+\mathbf{L})^2 - \frac{1}{2m}\mathbf{K}^2} \qquad \mathbf{L} \neq 0$$

[Can solve for ϵ analytically for ⊓⊓⊓⊓ ··· or ∿∿∿. Otherwise use a computer or approximations as above]

For second order, use

$$\left(\frac{\hbar^2}{2m}K^2 - \epsilon\right) A_0 = -\sum V_{-\mathbf{L}'} A_{\mathbf{L}}' = \sum_{\mathbf{L}'} \frac{|V_{\mathbf{L}'}|^2}{\frac{1}{2m}\left[(\mathbf{K}+\mathbf{L}')^2 - \mathbf{K}^2\right]}$$

$$\therefore \quad \epsilon = \frac{1}{2m}K^2 - \sum_{\mathbf{L}} \frac{|V_{\mathbf{L}}|^2}{\frac{1}{2m}\left[(\mathbf{K}+\mathbf{L})^2 - \mathbf{K}^2\right]}$$

This is ok. except when $|K| = |K+L|$? Consider at L'

$$K^2 = (K+L_1)^2$$

get a gap now at edge of Brillouin zone.

If $|K| = |K+L_1|$, $(K+L_1)^2 - K^2 \sim V$, we can start even by considering A_0 and A_1 not small -- all other A_i small. Then (1) gives

$$L=0 \qquad \left(\frac{\hbar^2}{2m}K^2 - \epsilon\right)A_0 = -V_{-L_1}A_{L_1}$$

$$L=1 \qquad \left(\frac{\hbar^2}{2m}(K+L_1)^2 - \epsilon\right)A_1 = -V_{+L_1}A_0$$

$$\Rightarrow \underbrace{\left[\frac{1}{2m}(K+L_1)^2 - \epsilon\right]}_{\omega(K+L_1)}\underbrace{\left[\frac{1}{2m}K^2 - \epsilon\right]}_{\omega(K)} = |V_{L_1}|^2$$

using $V_{-L} = V_{+L}^*$

Can find

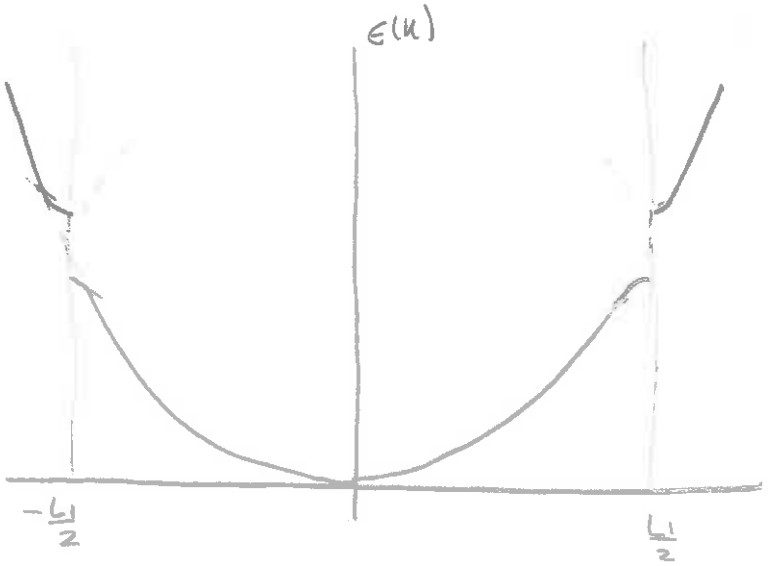
$$\epsilon = \frac{\omega(K+L_1)+\omega(K)}{2} \pm \sqrt{\left(\frac{\omega(K+L_1)-\omega(K)}{2}\right)^2 + |V_{L_1}|^2}$$

If $V_{L_1} << \frac{\omega(K+L_1)-\omega(K)}{2}$

$$= \omega(K) - \frac{|V_{L_1}|^2}{\omega(K+L_1)-\omega(K)}$$

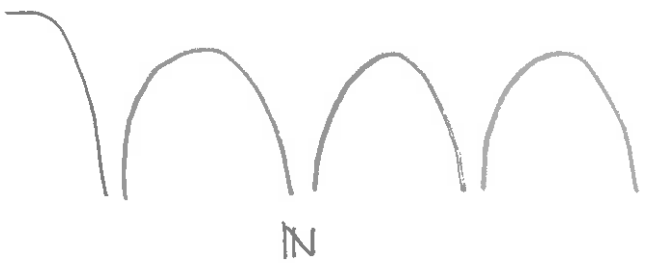
$$\omega(K+L_1) + \quad "$$

thus a discontinuity at gap



We now get an energy gap in which there is no solution.

Strong Potentials:



Try $\sum_{N} e^{ik\cdot lN} f(r-lN)$

where $f(|r|)$ is soln to S-eqn in one of these potentials

$-\frac{1}{2m}\nabla^2 f + v(|r|) f = E_0 f$ where $V = \sum_{lN} v(|R-lN|)$

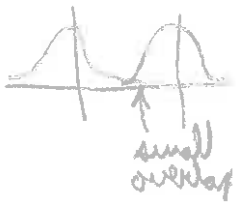
Can find

$$\epsilon = \frac{\int \psi^* H \psi \, dV}{\int \psi^* \psi \, dV} = \frac{N}{D}$$ where ψ is trial fun

Now

$$D = \sum_{\mathbf{N},\mathbf{N}'} e^{i\mathbf{k}\cdot(\mathbf{N}-\mathbf{N}')} \int f^*(\mathbf{r}-\mathbf{N}')\, f(\mathbf{r}-\mathbf{N})\, d^3\mathbf{r}$$

$$= 1 + \sum_{\mathbf{M}} e^{i\mathbf{K}\cdot\mathbf{M}}\, I(\mathbf{M})$$



$$I(\mathbf{M}) \equiv \int f^*(\mathbf{r}-\mathbf{M}) f(\mathbf{r})\, d^3\mathbf{r}$$

$$N = \sum_{\mathbf{N},\mathbf{N}'} e^{i\mathbf{k}\cdot(\mathbf{N}-\mathbf{N}')} \int f^*(\mathbf{r}-\mathbf{N}') \left\{ -\frac{\hbar^2}{2m}\nabla + \sum_{\mathbf{N}''} V(\mathbf{r}-\mathbf{N}'') \right\} f(\mathbf{r}-\mathbf{N})\, d^3\mathbf{r}$$

$E_0 - v(\mathbf{R}-\mathbf{N})$

Let

$$J(\mathbf{M}) = \int f(\mathbf{R}-\mathbf{M}) \left[V(\mathbf{R}) - v(\mathbf{R}) \right] f(\mathbf{R})\, d^3\mathbf{R}$$

$$\therefore \quad G = E_0 + \frac{J_0 + \sum_{\mathbf{M}\neq 0} J(\mathbf{M})\, e^{i\mathbf{K}\cdot\mathbf{M}}}{1 + \sum_{\mathbf{M}\neq 0} I(\mathbf{M})\, e^{i\mathbf{K}\cdot\mathbf{M}}}$$

Note if $\mathbf{M}=0$

$$J(0) = \int |f(\mathbf{r})|^2 \left[V(\mathbf{r}) - v(\mathbf{r}) \right] d^3\mathbf{r}$$

average of all potentials less $v(\mathbf{r})$

$J(\mathbf{M})$ falls off rapidly with $\mathbf{M}$.

Thus for say a cubic lattice

$$\epsilon = E_0 + \frac{J_0 + 2J_{100}(\cos k_x a + \cos k_y a + \cos k_z a)}{1 + 2I_{100}(\cos k_x a + \cos k_y a + \cos k_z a)}$$

2/17/67 LECTURE

We had found

$$\epsilon = E_0 + \frac{J_0 + 2J_{100}(\cos k_x a + \cos k_y a + \cos k_z a)}{1 + 2I_{100}(\cos k_x a + \cos k_y a + \cos k_z a)}$$

really don't use this, but books rarely mention this.

can get a "subband" using s-states of electron as base states

$$i\dot{a}_N = \eta_0 a_N + A[a_{N+1_y} + a_{N-1_x} + a_{N+1_y} + \cdots]$$

$$= \eta_0 a_N + \sum_{M1} A_M a_{N+M}$$

This model tells us all we need to know about bonds. Could also set it up for s & p states

$$i\dot{a}_n = \eta_{a0} a_N + \sum_{M1} A_M a_{N+M}$$

$$i\dot{b}_N = \eta_{b0} b_N + \sum_{M} B_M b_{N'}$$

He Li Be B C N O F
Ne Na Mg Al Si P S Cl

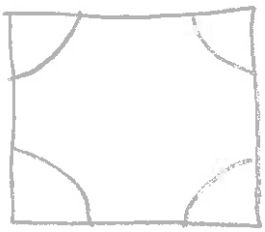
2/20/67 LECTURE

Comments again on naive view of band theory. Must consider electron interactions. Feynmann suggests that if we could expand Li lattice it would eventually become an insulator.

Any substance at all squeezed hard enough becomes a conductor.

Methods of analysis in solid state physics rely too heavily on experimental information. Try to analyze a non-laboratory situation (what is center of the earth). Life problem understand properties of materials at high pressures. Lots of experimental data.

PROBLEM: If we apply a const. field



$$\frac{d(\hbar k)}{dt} = e(E + V \times B)$$

$$V_x = \frac{\partial E(k)}{\hbar \partial k_x}$$

Prove these.

Band theory works quite well for semi-conductors however.

Coulomb interactions in a Fermi gas

$$\text{Energy per electron}/R_y = \frac{2.22}{r_s^2} - \frac{0.916}{r_s} + \epsilon_c$$

where $r_s = r_0/a_0$ ← Bohr radius

$\frac{4\pi r_0^3}{3}$ = Vol per electron

We use a uniform positive charge to neutralize electrons. The $\frac{0.916}{r_s}$ term is due to Coulomb interactions between electrons.

ϵ_c = "correlation energy" – all other junk
(Bad physics to call it this)

2/21/67 LECTURE

PROBLEM: Find the speed of sound in an ideal gas for long wavelengths. Now include effect of the Coulomb potential on $\omega(k)$

—o—

Conductivity of Metals:

Two origins of resistance due to collisions
i.) imperfections in crystal

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \sum_N V(r-N) + \underbrace{[U(r-M) - V(r-M)]}_{H_1 = \mu(r-M)}$$

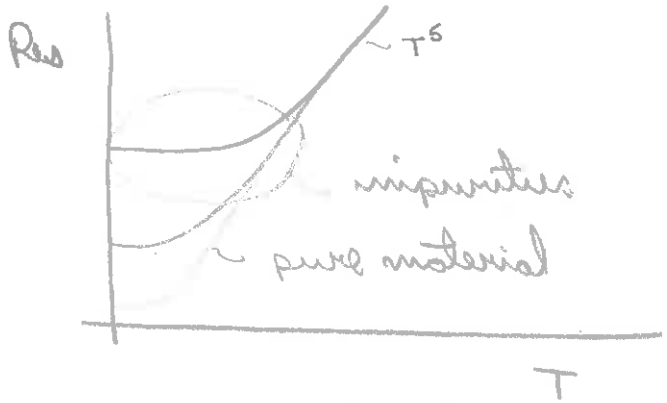
Idea is to find scattering cross-sections and then to solve Boltzmann equation.

$$\langle k'|H_1|k\rangle = \int u_{k'}(r)\,\mu(r-M)\,u_k(r)\,d^3r\,e^{i(k-k')\cdot r}$$

Must include charge shielding effects however. Very few have been able to do this correctly. The "nightmare of the inner shells" Van Vleck [Did not succeed.] Variational principle doesn't work to distinguish 2s from 1s in Li, for instance.

ii.) phonon scattering from atomic vibrations

find



Consider model with one atom / unit cell,

$$\sum_N V(r-N-q) = \underbrace{\sum_N V(r-N)}_{H_0} - \underbrace{\sum_N q_N \cdot (\nabla V(r-N))}_{H_1}$$

Need

$$\langle {}^{k'}_{\text{phonon}} | \sum_N q_N \cdot \nabla V(r-N) | {}^{k}_{\text{phon}} \rangle$$

$$= \sum_N \langle \text{phonon} | q_N | \text{phonon} \rangle \underbrace{\int u^*_{k',1}(r)\, e^{-ik'\cdot r}\, \nabla V(r-N)\, e^{ik\cdot r}\, u_{k,1}}$$

$$e^{-i(k'-k)\cdot N}\, \gamma_{1k,1k'}$$

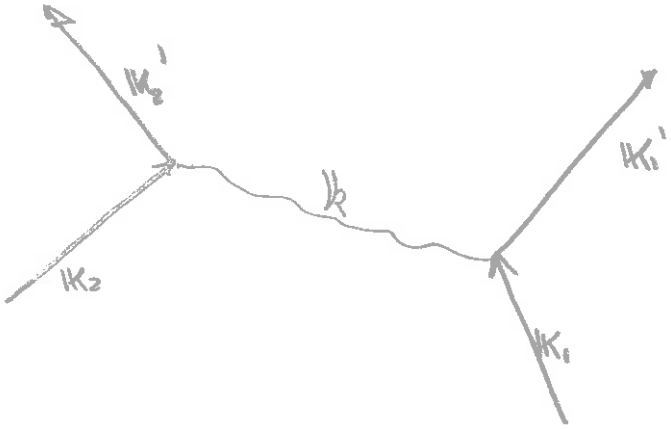
where $\gamma_{k,k'} = \int e^{-ik'\cdot r}\, u^*_{k',1}(r)\, \nabla V(r)\, u_{k,1}(r)\, e^{ik\cdot r}\, d^3r$

Use

$$\sum_N e^{ik\cdot N} e^{i(k'-k)\cdot N} \to \delta(k-k'+k+L)$$

Looks vaguely like conservation of momentum mod L

Can have electron-electron scattering using virtual phonons



This is very important in superconductivity since it tends to bind electrons in pairs (BCS)

CREATION OPERATORS FOR ELECTRONS 2/24/67 LECTURE

Recall we had defined for photons and phonons

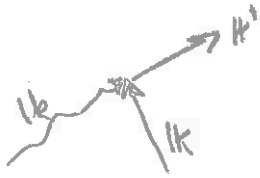
$a^*_{k,\beta}$ $a_{k,\beta}$

$$\rightarrow \quad a_i^* a_j - a_j a_i^* = \delta_{ij}$$

$$a_i^* a_j^* - a_j^* a_i^* = 0$$

$$a_i a_j - a_j a_i = 0$$

Similar operators are used for electrons. We denote these by $C_{k,\beta}$.
Last time we found the amplitude



Amp to absorb phonon wave k, and scatter electron k to k' $= \Gamma_{k,k,k'}$

Now define

C_k annihilate electron of wave k

C_k^* creates " " "

Then in H we include an interaction term to describe above

$$H_{int} = \sum_{k,k',k} \Gamma_{k,k,k'} a_k C_{k'}^* C_k$$

(annihilate phonon; create k'; annihilate k)

This is just formal mathematics for now

Actually to make H hermetian, use

$$H = \sum_{k,k',k} \Gamma_{k,k,k'} a_k C^*_{k'} C_k$$

$$+ \sum_{k,k',k} \Gamma^\dagger_{k,k',k} a^*_k C^*_k C_{k'}$$

Now consider the c's in general

c_i^* creates an electron in state i

Very useful since it is a way we can discuss things without knowing mechanism.

Exclusion principle allows only two states

| no electron in i > $\quad |0\rangle$

| one electron in i > $\quad |1\rangle$

Thus

$$C^*|0\rangle = |1\rangle$$

$$C^*|1\rangle = 0$$

$$C|1\rangle = |0\rangle$$

$$C|0\rangle = 0$$

= properties of operators

Now for correct adjoints

$$\langle n|c^*|n'\rangle^* = \langle n'|c|n\rangle$$

Applying this yields

$$\langle 1|c^*|0\rangle = 1$$

$$\langle 0|c|1\rangle = 1$$

so phase of states are properly fixed.

Now

$$c^*c^* = 0$$

since $c^*c^*|0\rangle = 0$, $c^*c^*|1\rangle = 0$

also

$$cc = 0$$

Now

$$cc^*|0\rangle = |0\rangle$$

$$cc^*|1\rangle = 0$$

$$c^*c|0\rangle = 0$$

$$c^*c|1\rangle = |1\rangle$$

Thus we see

$$c_i^*c_i = N_i$$ no. of electrons in state i

Now

$$(C^*C + CC^*)|0\rangle = |0\rangle$$

$$(C^*C + CC^*)|1\rangle = |1\rangle$$

Thus

$$\boxed{C^*C + CC^* = 1}$$

$$C^*C^* = 0$$

$$CC = 0$$

One could now work backwards and find the representation for these operators (eigenvalues and eigenstates) only from these equations.

Now consider different states

a	b
C_a^*	C_b^*
C_a	C_b

$$C_a^*C_a + C_aC_a^* = 1$$
$$C_b^*C_b + C_bC_b^* = 1$$
$$C_a^*C_a^* = 0 = C_aC_a$$
$$C_b^*C_b^* = 0 = C_bC_b$$

How do we combine these?

$$C_a^*C_b^* = -C_b^*C_a^*$$

since we are developing Fermi statistics.

Can also show

$$C_b^* C_a + C_a C_b^* = 0$$

Starting with

$$C_i^* C_i + C_i C_i^* = 1$$

can superimpose states to get new basis

$$|c\rangle = \alpha|a\rangle + \beta|b\rangle$$

$$|d\rangle = \beta^*|a\rangle - \alpha^*|b\rangle$$

Then

$$C_c^* C_c + C_c C_c^* = 0$$

$$C_d^* C_d + C_d C_d^* = 0$$

Can find $C_c^* = \frac{1}{\sqrt{2}}(C_a^* + C_b^*)$

Then use

$$1 = (\alpha \overset{C_a^*}{C_a^*} + \beta C_b^*)(\alpha^* \overset{C_c}{C_a} + \beta^* C_b) + (\alpha^* \overset{C_c}{C_a} + \beta^* C_b)(\alpha \overset{C_c^*}{C_a^*} + \beta C_b^*)$$

$$= \alpha\alpha^*(C_a^* C_a + C_a C_a^*) + \beta\beta^*(C_b^* C_b + C_b C_b^*)$$

$$+ \alpha\beta^*(C_a^* C_b + C_b C_a^*) + \beta\alpha^*(C_a C_b^* + C_b^* C_a)$$

Now normalized states $\Rightarrow |\alpha|^2 + |\beta|^2 = 1$

$$\Rightarrow \quad C_a^* C_b + C_b C_a^* = 0$$

$C_a^* C_b^* + C_b^* C_a^* = 0$ in same way.

2/27/67 LECTURE

For bosons

a_i^* creates particle in state i

$a_i a_j^* - a_j^* a_i = \delta_{ij}$ $\quad (= \langle i|j\rangle)$

$a_i^* a_j^* - a_j^* a_i^* = 0$

$a_i a_j - a_j a_i = 0$

For fermions

c_i^* creates particle in state i

$c_i c_j^* + c_j^* c_i = \delta_{ij}$

$c_i^* c_j^* + c_j^* c_i^* = 0$

$c_i c_j + c_j c_i = 0$

$c_i^* c_i = N_i =$ no. of electrons in i

EXAMPLE: Consider c_p^* creates electron with momentum p (no spin)

$c_p^* |\text{vacuum}\rangle =$ state for electron $e^{ip\cdot x}$

Now create one electron which has amplitude α_1 to have p_1 and α_2 to have p_2

$c_?^* |\text{vac}\rangle =$ state of one electron of $\alpha_1 e^{ip_1 x} + \alpha_2 e^{ip_2 x}$

$\Rightarrow \quad c_?^* = \alpha_1 c_{p_1}^* + \alpha_2 c_{p_2}^*$

C_ψ^* create one electron which has amplitude $\varphi(\mathbf{p})$ to be in momentum state $\mathbf{p}$, i.e.

$C_\psi^*|vac\rangle$ = state one electron which has wave fun

$$\sum_{\mathbf{p}} \varphi(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} = \psi(\mathbf{x})$$

where $\varphi(\mathbf{p}) = \int f(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}} d^3x$

Thus

$$C_\psi^* = \sum_{\mathbf{p}} C_{\mathbf{p}}^* \varphi(\mathbf{p})$$

$$= \langle *|\mathbf{p}\rangle \langle \mathbf{p}|\psi\rangle$$

$$= \langle *|\psi\rangle$$

where $C_{\mathbf{p}}^* = \langle *|\mathbf{p}\rangle$

$C_{\mathbf{p}} = \langle i|\mathbf{p}\rangle$

Now operator which creates electron at $\mathbf{x}_0 = \Psi^*(\mathbf{x}_0)$

$\Psi^*(\mathbf{x}_0)|vac\rangle$ = state of one electron with wave fun $\delta(\mathbf{x}-\mathbf{x}_0)$

$$= \sum_{\mathbf{p}} \underbrace{e^{-i\mathbf{p}\cdot\mathbf{x}_0}}_{\varphi(\mathbf{p})} e^{i\mathbf{p}\cdot\mathbf{x}_0}$$

Thus

$$\Psi^*(\mathbf{x}_0) = \sum_{\mathbf{p}} C_{\mathbf{p}}^* e^{-i\mathbf{p}\cdot\mathbf{x}_0}$$

Similarly

$$\Psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} C_{\mathbf{p}}$$

Note also

$$C_\psi^* = \int \Psi^*(\mathbf{x}) \psi(\mathbf{x}) d^3x$$

We expect then

$$\Psi^*(x)\,\Psi(y) + \Psi(y)\,\Psi^*(x) = \delta^3(x-y)$$

$$\Psi^*(x)\,\Psi^*(y) + \Psi^*(y)\,\Psi^*(x) = 0$$

$$\Psi(x)\,\Psi(y) + \Psi(y)\,\Psi(x) = 0$$

$\Psi^*(x)\,\Psi(x)$ = "no. of electrons at x" = density of electrons at x

EXAMPLE: We return to band theory. Recall we had for a single electron

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + U(\mathbf{R})\,\psi$$

We found solutions $\psi = e^{i\mathbf{k}\cdot\mathbf{r}}\,u_{\mathbf{k}}(\mathbf{r}) = f_{\mathbf{k}}(\mathbf{r})$

Then

$$H f_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}}\, f_{\mathbf{k}}(\mathbf{r})$$

Now to use our new notation, let

$C_{\mathbf{k}}^*$ create electron of propagation vector $\mathbf{k}$ with $f_{\mathbf{k}}(\mathbf{r})$

$$= \int f_{\mathbf{k}}(\mathbf{r})\,\Psi^*(\mathbf{r})\,d^3\mathbf{r}$$

Now for a system of independent electrons:

$$H_{\text{system}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} N_{\mathbf{k}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} C_{\mathbf{k}}^* C_{\mathbf{k}}$$

[note how similar this formulation is to phonon work]

Note

$$H_{\text{system}} = \sum_k \epsilon_k c_k^\dagger c_k = \int \Psi^*(x)\, h\, \Psi(x)\, dx \qquad (*)$$

To show this use

$$\Psi^\dagger(x) = \sum_k f_k^*(x)\, c_k^\dagger$$

$$\therefore h\Psi(x) = \sum_k h f_k(x)\, c_k = \sum_k \epsilon_k f_k(x)\, c_k$$

Now multiply by $\Psi^*(x)$ & integrate, and use orthogonality to find $(*)$

We had

$$\text{amp } \Gamma_{k_2 k'; k} = \text{amp electron } k \to k' \text{ absorbing phonon of mode } k_2$$

We can then write H for a system of electrons and phonons as

$$H = \underbrace{\sum_k \epsilon_k c_k^\dagger c_k}_{\text{electrons}} + \underbrace{\sum_{k_2} \omega_{k_2} a_{k_2}^\dagger a_{k_2}}_{\text{phonons}} + \underbrace{\sum_{k,k',k_2} \Gamma_{k_2 k'; k}\, c_{k'}^\dagger c_k a_{k_2}}_{\text{phonon-electron interaction}}$$

$$+ \sum_{k,k',k_2} \Gamma^*_{k_2 k; k'}\, c_k^\dagger c_{k'}\, a_{k_2}^\dagger$$

[remainder of H as before]

Note

$$\text{amp } \Gamma_{k_2 k'; k} = \text{amp electron } k' \to k \text{ emitting phonon of mode } k_2$$

This H is the basis of the theory of conductivity and superconductivity.

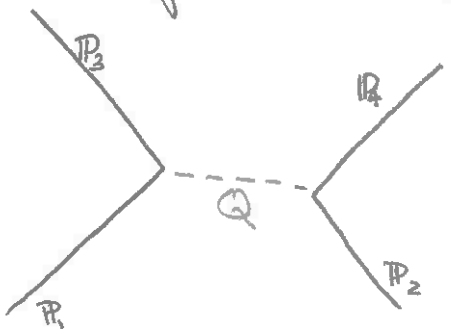
[Note the a's and b's commute.]

2/28/67 LECTURE

We now discuss electron electron interactions. Say by e^2/r_{12}. Ordinarily we would write

$$H = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_i U(x_i) + \frac{1}{2}\sum_{i,j} V(x_i - x_j)$$

Consider first order scattering of electrons for $P_1 + P_2 = P_3 + P_4$



aup. born scatt $v(Q)$

where $Q = P_3 - P_1$

$$v(Q) \equiv \int V(R)\, e^{-i(Q\cdot R)}\, d^3R$$

Then for $U = 0$,

$$H = \sum_P \left(\frac{p^2}{2m}\right) C_p^* C_p + \sum_{P_1 P_2 P_3 P_4} v(Q)\, C_{P_4}^* C_{P_3}^* C_{P_2} C_{P_1} \qquad (*)$$

($P_3 - P_1$)

Now H is quadratic in C. Thus we can represent interactions using the C_p operators.

We can try to represent this in terms of $\Psi(x)$'s where

$$C_P^* = \int e^{iP\cdot x}\, \Psi^*(x)\, d^3x$$

The first term in (*) yields

$$\int \Psi^*(x)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\Psi(x)\, d^3x$$

$$H_{int} = \iiint \frac{d^3P_1 d^3P_2 d^3P_3}{(2\pi)^{3\times 3}} \int\!\!\int V(Q)\, \delta^3(P_1+P_2-P_3-P_4)\, e^{i(P_3-P_1)\cdot X_1}\, e^{i(P_1+P_2-P_3)\cdot X_4}\, e^{i P_4 \cdot X_4}\, e^{i P_3 \cdot X_3}$$

$$e^{-i P_2 \cdot X_2}\, e^{-i P_1 \cdot X_1}\, \Psi^*(X_4)\Psi^*(X_3)\Psi(X_2)\Psi(X_1)\, d^3X_1 d^3X_2 d^3X_3 d^3X_4$$

$$= \iint d^3Q\, e^{iQ\cdot(X_3-X_4)}\, \Psi^*(X_4)\Psi^*(X_3)\Psi(X_4)\Psi(X_3)\, d^3X_3 d^3X_4$$

$$= \iint \Psi^*(X)\Psi^*(Y)\, V(X-Y)\, \Psi(X)\Psi(Y)\, d^3X d^3Y \qquad (2)$$

Suppose we invert the order using

$$\Psi^*(X)\Psi(Y) = -\Psi(Y)\Psi^*(X) + \delta^3(X-Y)$$

Then

$$H_{int} = -\iint \Psi^*(X)\Psi(X)\, V(X-Y)\, \Psi^*(Y)\Psi(Y)\, d^3X d^3Y \qquad (3)$$

$$+ \int \Psi^*(X)\Psi(X)\, V(0)\, d^3X$$

Classically we expect

$$\text{Energy} = \frac{1}{2}\iint \rho(X)\, V(X-Y)\, \rho(Y)\, d^3X d^3Y \qquad (4)$$

Three troubles

i) factor $\frac{1}{2}$

ii) sign

iii) extra term

The last term is a self-energy term (energy of particle acting on itself). This is true in classical too since (4) also includes self energy.

If we omit such self-energy, go back to (2)
[like with Coulomb interaction where $V(0) = \infty$]

$\frac{1}{2}$ comes from a mistake in original sum

$$\sum V(Q)\, C^*_{P_4} C^*_{P_3} C_{P_2} C_{P_1}$$

Then

$$H_{int} = -\frac{1}{2}\iint \Psi^*(x)\Psi^*(y)\, V(x-y)\Psi(x)\Psi(y)\, d^3x\, d^3y \qquad (5)$$

and

$$H_{int} = +\frac{1}{2}\int \Psi^*(x)\Psi(x)\, V(x-y)\, \Psi^*(y)\Psi(y)\, d^3x\, d^3y$$

$$-\frac{1}{2}\int \Psi^*(x)\Psi(x)\, V(0)\, d^3x \qquad (6)$$

The sign comes in also from initial ordering in Σ. Need

$$\frac{1}{2}\sum_{P_1 P_2 P_3 P_4} V(Q)\, C^*_{P_4} C^*_{P_3} C_{P_1} C_{P_2}$$

Gives a negative self energy term. Do you want it or not (of course not!)?

Thus neglecting self energy, our H for a system of electrons is

$$H = \int \Psi^*(x)\left[-\frac{\hbar}{2m}\left(\nabla_i - \frac{e}{c}A(x,t)\right)^2 + e\phi(x,t)\right]\Psi(x)\,d^3x \tag{7}$$

$$+ \frac{1}{2}\int\int \Psi^*(x)\Psi^*(y)\,\frac{e^2}{|x-y|}\,\Psi(y)\Psi(x)\,d^3x\,d^3y$$

Note because of the double annihilation, this contains no self energy term [consider H operating on a system of one electron]. Note also the number of electrons is not specified.

This is the H for say a quantum plasma, with fixed nuclei -- at least non-relativistically.

—o—

How do we use (7)? In the S-eqn

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi = H\Psi$$

Now $$N = \int \Psi^*(x)\Psi(x)\,d^3x$$

Can show $[H, N] = 0$. Thus can show

$N\Psi = n\Psi$ where n is an integer

How do we deal with "holes" in our formal theory? Again use

3/3/67 LECTURE

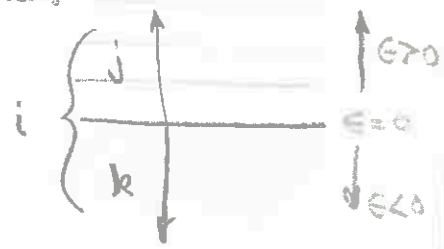
c_i^* creates electron in state i $\quad \varphi_i(\underline{x})$

Then $H = \sum_i \epsilon_i c_i^* c_i + \sum_{i,i'} \lambda_{i'i} c_{i'}^* c_i$

where $\lambda_{i'i} = \int \varphi_{i'}^*(\underline{x})\, \lambda(\underline{x})\, \varphi_i(\underline{x})\, d^3x$

is our perturbing potential

Suppose some empty levels above ground state. Try to imagine perturbation operating on hole-inground state. Define new indices as shown. Recall



$$c_i^* c_{i'} + c_{i'} c_i^* = \delta_{ii'}$$

If $i = j$ write $c_i = c_j$

$i = k$ write $c_i = b_k^* \Rightarrow b_k = c_i^*$

Ex: $c_i^* c_i + c_i c_i^* = 1 \rightarrow b_k b_k^* + b_k^* b_k = 1$ for $i \in S_k$.

$c_i c_i = 0 \rightarrow b_k^* b_k^* = 0$

$c_i^* c_i^* = 0 \rightarrow b_k b_k = 0$

We now regard b^* as "creating a hole"

c_j^* creates an electron in state j

b_j^* creates a hole in state k

Then if we neglect perturbation

$$H = \sum_j \epsilon_j \underbrace{c_j^* c_j}_{\text{no. of electrons}} + \sum_k \epsilon_k b_k b_k^*$$

$$\sum_k \epsilon_k - \sum_k \epsilon_k \underbrace{b_k^* b_k}_{\text{no. of holes}}$$

"0" if $\epsilon_0 = 0$

Our perturbation becomes

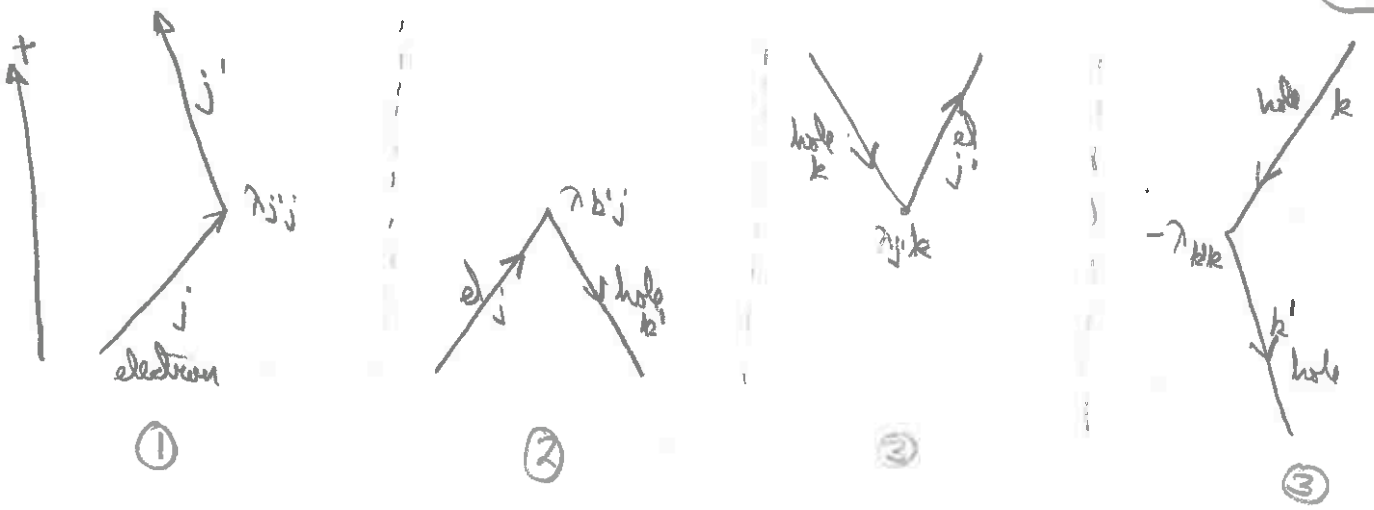
$$\sum_{j,j'} \lambda_{j'j} c_{j'}^* c_j + \sum_{k',j} \lambda_{k'j} b_{k'} c_j$$

① ②

$$+ \sum_{j',k} \lambda_{j'k} c_{j'}^* b_k^* + \sum_{k,k'} \lambda_{k'k} \underbrace{b_{k'} b_k^*}_{④ \; -b_k^* b_{k'} + \delta_{kk'}}$$

③

We must examine each term.



① ② ③

(like positron-electron annihilation) (pair production)

Use arrows to mark different types of particles.

$$\pi_{i'i} = \int \Phi_{i'}(\underline{x})\, \lambda(\underline{x})\, \Phi_i(\underline{x})\, d^3\underline{x}$$

exit state ↑ entrance state

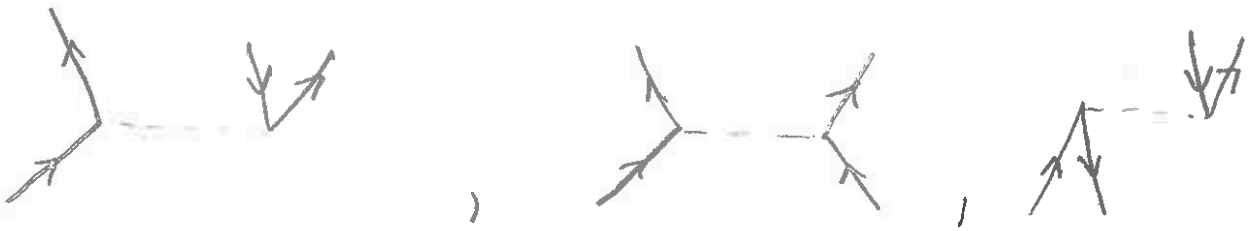
These arrows tell where to put states in matrix elements. Enter and leave types. Don't use initial and final states in time ordered concept or you'll get confused.

—o—

Can play now with more complicated interactions like

$$C_i^* C_{i'}^* C_{i''} C_{i'''}$$

Get things like



Can just picture this as bending the diagrams (arrows) around.

These schemes are used very frequently in perturbation theory -

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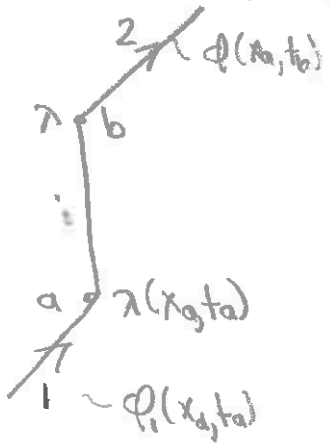
Consider now usual 2nd order perturbation theory in this formalism.



$$\text{amp} = \int \varphi^*(x_b,t_b)\,\lambda(x_b,t_b)\,K_0(x_b,t_b;x_a,t_a)$$

propagator

$$\lambda(x_a,t_a)\,\varphi(x_a,t_a)\,dx_a dt_a dx_b dt_b$$

where the propagator is

$$K_0(b,a) = \sum_i e^{-\epsilon_i(t_b-t_a)}\, u_i(x_b)\,u_i^*(x_a)\,H(t_b-t_a)$$

where $Hu_i = \epsilon_i u_i$

Now let $\varphi_{1_2} \to u_{1_2}(x_a)\,e^{-i\epsilon_{2_1}t_a}$ $\qquad \lambda_{1_2}(x_a,t_a) = e^{-i\omega_{2_1}t_a}$

We then find

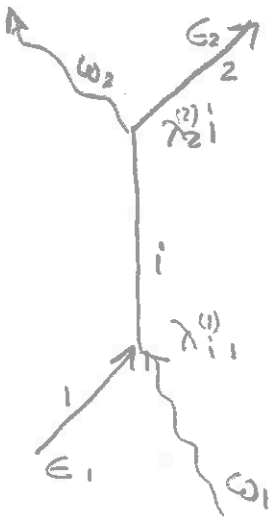
$$\text{amp} = \sum_i \int e^{+i\epsilon_2 t_b}\, e^{i\omega_2 t_b}\, e^{-i\epsilon_i(t_b-t_a)}\, e^{-i\omega_1 t_a}\, e^{-i\epsilon_1 t_a}\, dt_a\, dt_b \cdot \lambda^{(2)}_{2i}\,\lambda^{(1)}_{i1}$$

$= 0$ unless $\epsilon_2+\omega_2 = \epsilon_i+\omega_1$ as expected

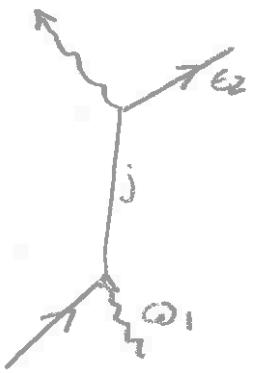
$$= \int_{t_a}^{\infty} e^{-i\epsilon_i(t_b-t_a)}\, e^{-i(\epsilon_1+\omega_1)(t_a-t_b)}\, dt_b\; \lambda^{(2)}_{2i}\,\lambda^{(1)}_{i1}$$

Then

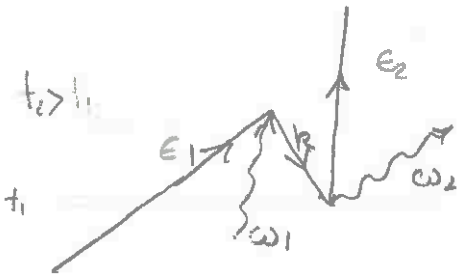
$$\text{Amp} = \sum_{\substack{i \\ \text{intermediate states}}} \lambda^{(2)}_{2i} \; \frac{-i}{\epsilon_i - (\epsilon_1 + \omega_1) - i\eta} \; \lambda^{(1)}_{i1}$$



Now can we write this allowing holes? We guess by drawing pictures.



$$\sum_j \lambda_{2j} \; \frac{-i}{\epsilon_j - (\epsilon_1 + \omega_1) - i\eta} \; \lambda_{j1}$$



"virtual pair production"

$$-\sum_k \lambda_{k1} \; \frac{-i}{|\epsilon_k| + \epsilon_2 + \omega_2 - i\eta} \; \lambda_{2k}$$

↑ from exchange symmetry of fermions

This is correct.

Can we combine these into (1) term and return to our general perturbation theory? Write second term as

$$+ \sum_k \lambda^{(2)}_{2k} \frac{-i}{\epsilon_k - (\epsilon_i + \omega) - i\eta} \lambda^{(1)}_{k,}$$

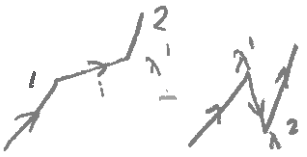
Thus just let i range over both i & k

$$H = \sum \epsilon_i C_i^* C_i + \sum |\epsilon_k| b_k^* b_k + H_{int}$$ 3/6/67 LECTURE

where $H_{int} = \sum_{i,i'} \lambda_{i'i} C_{i'}^* C_i + \sum_{ik'} \lambda_{k'i} b_{k'}^* C_i + \sum_{ik} \lambda_{ik} C_i^* b_k^*$

$$- \sum_{k'k} \lambda_{k'k} b_k^* b_{k'}$$

Perturbation gives



$$\lambda_{2i} \frac{\perp}{\epsilon_1 - \epsilon_i - \omega_1} \lambda_{i1} + \lambda'_{k_1} \frac{\perp}{|\epsilon_k| + \epsilon_i + \omega_1} \lambda^*_{ik}$$

This can also be written

$$\int \psi_2^*(x_2,t_2)\, \lambda(x_2,t_2)\, K_+(x_2,t_2;x_1,t_1)\, \lambda(x_1,t_1)\, \psi_1(x_1,t_1)\, dx_1\, dt_1\, dx_2\, dt_2$$

$$\text{if} \begin{cases} K_+(2,1) = \sum_{i\,(\text{electron})} e^{-i\epsilon_i(t_2-t_1)} \varphi_i(x_2)\, \varphi_i^*(x_1) & t_2 > t_1 \\ K_+(2,1) = -\sum_{k\,(\text{hole})} e^{-i\epsilon_k(t_2-t_1)} \varphi_k(x_2)\, \varphi_k^*(x_1) & t_1 > t_2 \end{cases}$$

k (hole) states the holes are missing electrons in (ϵ_k is neg)

[No violation of causality]

IV. RELATIVISTIC QUANTUM MECHANICS

A. INTRODUCTION

Some of the achievements of r.q.m. are
i.) prediction of antiparticles (CPT theorem)
ii.) can show particles with spin ½ obey Fermi statistics
iii.) fine structure of H-atom

There seem to be three ways to present this subject.

1.) One way is easiest to understand since it works from $-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi$ in form of Dirac eqn. However we lose the manifest covariance

2.) Relativistic invariance is obvious, but notation is heavier to understand [Feynman, Schwinger, etc.]

3.) Abstract formulation -- immediately implies positrons, spin statistics, etc [more recent formulation]

We will begin using Method 1, even though it is very dull.

EXAMPLE:

MAXWELL EQUATIONS (EXAMPLE OF METHOD 1)

$$\text{Action} = \int \left[\left(-\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t} \right)^2 - (\nabla \times \mathbf{A})^2 \right] dV\,dt + \int \left(\rho A|_x - \mathbf{j}\cdot\mathbf{A} \right) dV\,dt$$

Equivalent to (in gauge $\nabla \cdot \mathbf{A} = 0$ -- makes QED no longer manifestly covariant)

1.) Instantaneous Coulomb: $\sum_{i,j} \frac{q_i q_j}{r_{ij}}$

2.) $H = \sum_{\substack{k,i \\ \text{polarization } 1,2}} \omega_k a_k^* a_k + \text{coupling}$

where $\omega_k = kc$

coupling $\rightarrow \int \mathbf{j}(x) \cdot \mathbf{A}(x)\, d^3x$

and

$$\mathbf{A}(x) = \sum_{k,i} \frac{1}{\sqrt{2\omega_k}} \left[\varepsilon_{k,i} e^{i\mathbf{k}\cdot x} a_{k,i} + \varepsilon_{k,i}^* e^{-i\mathbf{k}\cdot x} a_k^* \right]$$

Recall in classical theory

$$E = \frac{m_0 c^2}{\sqrt{1 - v^2/c^2}} \quad ; \quad P = \frac{m_0 v}{\sqrt{1 - v^2/c^2}}$$

so that

$$E^2 - p^2 = m_0^2 \qquad c \equiv 1 \,, \; \hbar \equiv 1$$

or $$E^2 - \mathbf{P} \cdot \mathbf{P} = m_0^2$$

m always refers to m_0, rest mass in this notation

Hereafter we denote 4-vectors by

$$A_\mu = (A_1, A_x, A_y, A_z)$$

Also use summation convention

$$A_\mu B_\mu = A_1 B_1 - A_x B_x - A_y B_y - A_z B_z = \text{invariant}$$

We use also

$$\delta_{\mu\nu} = \begin{cases} 1 & \mu = \nu = t \\ -1 & \mu = \nu = x, y, z \\ 0 & \mu \neq \nu \end{cases}$$

and note $\delta_{\mu\nu} A_\nu = A_\mu$

Finally

$$\nabla_\mu = \left(\frac{\partial}{\partial t}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z} \right)$$

Then

$$p_\mu = (E, p_x, p_y, p_z)$$

$$k_\mu = (\omega, k_x, k_y, k_z)$$

De Broglie $p_\mu = \hbar k_\mu$ & wave goes as $e^{-i(k_\mu x_\mu)}$

Also $p_\mu p_\mu = m^2$

Note $\omega = \sqrt{k^2 + m^2}$

$$v_{gr} = \frac{\partial \omega}{\partial k} = \frac{\partial E}{\partial p} = v_{cl}$$

since

$$v_{gr} = \frac{\partial \omega}{\partial k} = \frac{k}{\sqrt{k^2+m^2}} = \frac{u}{\omega} = \frac{p}{E}$$

a free particle of momentum p has

$$\boxed{e^{-i(p_\mu x_\mu)}}$$

Also

$$\boxed{p_\mu p_\mu = m^2}$$

These contain all of classical special relativity (by De Broglie)

Now to formulate q.m, we need some eqn to generate

$$e^{-ip_\mu x_\mu} \quad \text{in r.q.m.}$$

Now $-\frac{\hbar}{i}\frac{\partial}{\partial t}\psi = \frac{\left(\frac{\hbar}{i}\nabla\right)\cdot\left(\frac{\hbar}{i}\nabla\right)}{2m}\psi$ held in n.r.q.m.

Thus we seek a linear eqn. The fool begins with

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\psi = \sqrt{m^2+\left(\frac{-\nabla^2}{2m}\right)}\,\psi$$

But trouble with $\sqrt{\ }$. If we include vector potential this gets fouled up.

Start over again "with soul"

$E^2 - p\cdot p = m^2$ leads to

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial t}\right)^2\psi - \left(\frac{\hbar}{i}\nabla\right)\cdot\left(\frac{\hbar}{i}\nabla\right)\psi = m^2\psi$$

or $$-\Box^2\psi = m^2\psi$$

or $$-\nabla_\mu\nabla_\mu\psi = m^2\psi$$

Now we must put in an interaction. Guess

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - A_4\right)^2\psi - \left(\frac{\hbar}{i}\nabla - A\right)\cdot\left(\frac{\hbar}{i}\nabla - A\right)\psi = m^2\psi$$

or $$(i\nabla_\mu - eA_\mu)(i\nabla_\mu - eA_\mu)\psi = m^2\psi$$

Is this eqn OK? Must test it

i.) cons. prob

ii.) reduce to S-eqn

iii.) H-atom

iv.) causality

PROBLEM: Try all of these to see if it works? iii.) is most serious.

[Doesn't include spin.]

3/7/67 LECTURE

$$(i\nabla_\mu - eA_\mu)(i\nabla_\mu - eA_\mu)\psi = m^2\psi$$

Klein-Gordon Equation

But it cannot represent spin. Maybe it is OK for spinless particles. Dirac thought it was wrong and thought only a first order time derivative should appear

$$H\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$

He then guessed only first-order derivatives in space appeared,

$$H = \left(\alpha_x \frac{\hbar}{i}\frac{\partial}{\partial x} + \alpha_y \frac{\hbar}{i}\frac{\partial}{\partial y} + \alpha_z \frac{\hbar}{i}\frac{\partial}{\partial z} + \beta m\right)$$

for a free particle

He also knew Pauli's results. Thus he proposed α's & β be matrices. If a potential

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right)\psi = \left[\alpha_x\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - eA_x\right) + \alpha_y\left(\frac{\hbar}{i}\frac{\partial}{\partial y} - eA_y\right)\right.$$

$$\left. + \alpha_z\left(\frac{\hbar}{i}\frac{\partial}{\partial z} - eA_z\right) + \beta m\right]\psi$$

Dirac Equation

In order that a free particle work we try

$$\psi = u\, e^{-i(Et - \mathbf{p}\cdot\mathbf{x})}$$

where α's and β's operate only on u.

If we substitute this in we find

$$Eu = \left[(\alpha \cdot \mathbf{p}) + \beta m\right] u$$

If we operate again

$$E^2 u = \left[(\alpha \cdot \mathbf{p}) + \beta m\right]^2 u$$

But we want $E^2 = p^2 + m^2$. Multiply out operator.

$$E^2 u = \alpha_x^2 p_x^2 + (\alpha_x \alpha_y + \alpha_y \alpha_x) p_x p_y +$$

$$+ (\alpha_x \beta + \beta \alpha_x) p_x u \quad + \beta^2 m$$

Thus we choose $\alpha, \beta \ni$

$$\left.\begin{aligned} \alpha_x^2 = 1 = \alpha_y^2 = \alpha_z^2 \\ \alpha_x \alpha_y + \alpha_y \alpha_x = 0 \\ \alpha_y \alpha_z + \alpha_z \alpha_y = 0 \\ \alpha_z \alpha_x + \alpha_x \alpha_z = 0 \\ \beta \alpha_x + \alpha_x \beta = 0 \\ \beta^2 = 1 \end{aligned}\right\}$$

Thus 4 operators $\alpha_x, \alpha_y, \alpha_z, \beta$ whose squares = 1 and which anticommute with each other. There are many different possible representations. Need 4×4 matrices. We set it up for a spin $\frac{1}{2}$ object (electrons, μ mesons, etc.)

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

$$\alpha_y = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Of course the u's are 4-component. For memory ease consider splitting up into spinors

$$u = \begin{pmatrix} u_1 \\ u_2 \\ \hline u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} u_a \\ u_b \end{pmatrix}$$

Then

$$\alpha = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Thus for a free particle

$$E^2 u = (\vec{\alpha}\cdot\vec{p} + m^2)\, u$$

We can rewrite the Dirac-eqn in various ways

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right)\psi = \alpha \cdot \left[-\frac{\hbar}{i}\nabla - A\right]\psi + \beta m \psi$$

Still another way is

$$\left\{\beta\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right) - \beta\alpha \cdot \left[-\frac{\hbar}{i}\nabla - A\right]\right\}\psi = m\psi$$

We can define other matrices

$$\gamma_t \equiv \beta$$

$$\gamma_x = \beta\alpha_x$$

$$\gamma_y = \beta\alpha_y$$

$$\gamma_z = \beta\alpha_z$$

Then Dirac eqn becomes

$$\gamma_\mu\left(i\nabla_\mu - eA_\mu\right)\psi = m\psi$$

where $\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu}$

$\gamma_t^2 = 1 \quad \gamma_x^2 = -1 \quad \gamma_y^2 = -1 \quad \gamma_z^2 = -1$

This eqn looks relativistically invariant. But support he makes a calculation with

$$\vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

But suppose someone unitary w.r.t. the two different ψs. Do we still have invariance? Yes! Commutation properties are invariant.

We can write the eqn in spinor form using

$$\psi = \begin{pmatrix} \psi_a(x,t) \\ \psi_b(x,t) \end{pmatrix}$$

and use

$$\alpha\psi = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = \begin{pmatrix} \sigma\psi_b \\ \sigma\psi_a \end{pmatrix}$$

we can find

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right)\psi_a = \sigma\cdot\left(-\frac{\hbar}{i}\nabla - eA\right)\psi_b + m\psi_a$$

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right)\psi_b = \sigma\cdot\left(-\frac{\hbar}{i}\nabla - eA\right)\psi_a - m\psi_b$$

The argument that relativity + qm $\Rightarrow$ spin is circular. Rests upon assumption that eqn takes the form

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi$$

Only for spin ½ particles. For neutrinos

$$-\frac{\hbar}{i}\frac{\partial\psi_a}{\partial t} = \sigma\cdot\left(-\frac{\hbar}{i}\nabla\right)\psi_b$$

$$-\frac{\hbar}{i}\frac{\partial\psi_b}{\partial t} = \sigma\cdot\left(-\frac{\hbar}{i}\nabla\right)\psi_a$$

(Not true for neutrons, protons, etc. May be just ok for leptons.

Suppose Klein-Gordon eqn was right. Write

$$\left(i\frac{\partial}{\partial t} - eV\right)\psi = \chi$$

$$\left(i\frac{\partial}{\partial t} - eV\right)\chi = \left(-i\nabla - eA\right)^2\psi - m^2\psi$$

We can then convert this into $\Psi = \begin{pmatrix}\chi\\ \psi\end{pmatrix}$

$$H = eV + \rho + \mu\left(-i\nabla - A\right)^2$$

which looks first order in time but obviously isn't. Indeed Dirac's eqn is actually 4-order in time. Thus Dirac's original logic was wrong.

Yes: Frequently bad logic leads to good answers.

Dirac Equation (Cont.) 3/10/67 LECTURE

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = H\psi$$

$$H = \beta m + eV + \alpha \cdot \left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)$$

$$\mathbf{p} \Rightarrow \frac{\hbar}{i}\nabla$$

α's, β 4x4 matrices which anticommute
squares = 1

Eg:

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \alpha = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix} \qquad \psi = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$$

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right)\psi_a = \sigma \cdot (\mathbf{p} - \mathbf{A})\psi_b + m\psi_a$$

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right)\psi_b = \sigma \cdot (\mathbf{p} - \mathbf{A})\psi_a - m\psi_b$$

To learn more about this equation we will play with things

Now H is hermitian. Thus we have

$$\frac{\partial}{\partial t}\int \psi^* \psi \, dVol = 0$$

Thus can normalize

$$\int \psi^* \psi \, dVol = 1$$

What does this mean? Write

$$\psi^* = \psi_1^* \; \psi_2^* \; \psi_3^* \; \psi_4^*$$

to find inner product. Can take matrix elements in usual manner

$$\int \psi^* \Pi \psi = \int \psi_i^* \left(\sum_k \frac{\partial}{\partial x_k} \psi_i \right) + \int ( ) \cdots$$

Now

$$\langle f | \alpha_k | i \rangle = \int \psi_f^* \alpha_k \psi_i \, d\text{vol}$$

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\therefore \alpha_x \psi_1 = \begin{pmatrix} \psi_4 \\ \psi_3 \\ \psi_2 \\ \psi_1 \end{pmatrix}$$

$$\langle f | \alpha_x | i \rangle = \int d\text{vol} \left[\psi_{f1}^* \psi_{i4} + \psi_{f2}^* \psi_{i3} + \psi_{f3}^* \psi_{i2} + \psi_{f4}^* \psi_{i1} \right]$$

Thus all of q.m. goes through in usual way.

We can set up a probability density ρ & current J s

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{j}$$

Find

$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$
$$= \psi_1^*\psi_1 + \psi_2^*\psi_2 + \psi_3^*\psi_3 + \psi_4^*\psi_4$$

$$j = \psi^*(x,t)\,\alpha\,\psi(x,t)$$

(unique since if α changes to $\alpha_x' = S^{-1}\alpha_x S$, then ψ also changes $\psi' = S\psi$)

---

4 components of Dirac wavefn. has nothing to do with a 4 vector.

EXAMPLE: for 3-d we get 2-component spinor. Again no connection.

However the matrices do form a 4-vector $[\alpha;\beta]$

If we use $\psi_S = \psi_a + \psi_b$, $\psi_A = \psi_a - \psi_b$ we find

$$[(E-eV)^2 - (p-eA)^2 + e\sigma\cdot(B+iE)]\,\psi_S = m^2\psi_S$$

Two-component wave eqn

Feynman used this to calculate effects of parity violation in β-decay.

What do 4 components mean? Can we get S-eqn?

First check S-eqn. Assume A, V time independent. Write

$$E = m + W \qquad W, V << m$$

$$\frac{p}{m} \sim V \qquad \left(\frac{V}{c}\right)^2 << 1$$

Writing out eqns

$$(m + W - eV)\psi_a = \sigma \cdot (p - eA)\psi_b + m\psi_a$$

$$(m + W - eV)\psi_b = \sigma \cdot (p - eA)\psi_a - m\psi_b$$

$$\therefore \quad \psi_b \sim \frac{1}{2m}\sigma \cdot (p - eA)\psi_a$$

"small amplitudes"

Subst in

$$(W - eV)\psi_a = \frac{[\sigma \cdot (p - eA)][\sigma \cdot (p - eA)]}{2m}\psi_a$$

Now $(\sigma \cdot a)(\sigma \cdot a) \neq a \cdot a$

But $(\sigma \cdot A)(\sigma \cdot B) = A \cdot B + i\sigma \cdot (A \times B)$

$$\therefore \quad \frac{[\sigma \cdot (p - eA)][\sigma \cdot (p - eA)]}{2m} = \frac{1}{2m}\left[(p - \tfrac{e}{c}A) \cdot (p - \tfrac{e}{c}A)\right]$$

$$+ \frac{e\hbar}{2mc}\sigma \cdot \underbrace{(\nabla \times A)}_{B}$$

Thus we find non-relativistic limit

$$H\psi_a = \left[eV + \frac{1}{2m}\left(p - \frac{e}{c}A\right)^2 + \frac{e\hbar}{2mc}(\sigma \cdot B)\right]\psi_a$$

$$\Rightarrow \mu = \frac{e\hbar}{2mc}$$

Thus we have deduced numerical value for magnetic moment of electron. One of great triumphs of Dirac equation!

Thus we get a spin correction to S-eqn.

—o—

Consider free particle at rest & assume

$$\psi = u e^{-i(Et - \underset{0}{p}\cdot x)} \quad \text{and put into Dirac eqn}$$

$$\therefore H = \beta m$$

$$\Rightarrow Eu = m\beta u$$

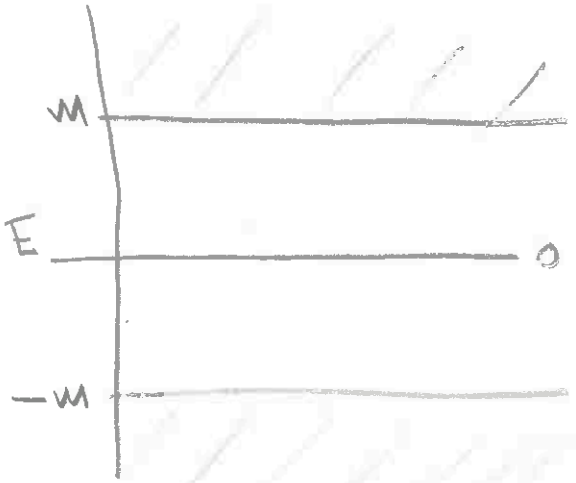
$$\text{or} \quad Eu_1 = mu_1 \quad Eu_2 = mu_2$$

$$Eu_3 = -mu_3 \quad Eu_4 = -mu_4$$

$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ spin up, $E = +m$

$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ spin down, $E = +m$

$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ spin up $E = -m$ $\qquad$ $\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ spin down $E = -m$



Both ± energy.

Dirac proposed our world has filled band of electrons with $E < 0$. Can get holes however $\Rightarrow$ positrons

3/28/67 LECTURE

Recall the Dirac equation in the form

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi \qquad (1)$$

where

$$H = \beta m + eV + \vec{\alpha}\cdot\left(\vec{p} - \frac{e}{c}\vec{A}\right)$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

If we multiply (1) by β, and note $\beta\cdot\beta = 1$

$$-\frac{\hbar}{i}\beta\frac{\partial\psi}{\partial t} = \left[m + e\beta V + \beta\vec{\alpha}\cdot\left(\vec{p} - \frac{e}{c}\vec{A}\right)\right]\psi$$

or regrouping

$$\left\{\underbrace{\beta\left[-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right]}_{B_0} - \underbrace{\beta\vec{\alpha}\cdot\left(\vec{p} - \frac{e}{c}\vec{A}\right)}_{B}\right\}\psi = m\psi$$

B_0: time-dependent part

B: time independent part

Define the γ matrices which are conventionally used to make non-relativistic part obvious:

$$\gamma_0 \equiv \beta \qquad \vec{\gamma} \equiv \beta\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}$$

Also define

$$\not{B} \equiv \gamma_0 B_0 - \vec{\gamma}\cdot\vec{B}$$

The Dirac equation then becomes

$$[\not{p} - \tfrac{e}{c}\not{A} - m]\psi = 0$$

Case I: $\vec{A} = 0$, $\vec{p} = 0$ (free particle at rest)

$$[p_0\gamma_0 - m]\psi = 0 \quad \text{where} \quad \psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix}$$

or

$$\left\{-\tfrac{\hbar}{i}\tfrac{\partial}{\partial t}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - m\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\right\}\begin{pmatrix}\phi\\ \chi\end{pmatrix} = 0$$

This yields

$$(E - m)\phi = 0$$

$$(-E - m)\chi = 0$$

Thus

$$\phi = \begin{pmatrix}a\\ b\end{pmatrix} e^{-i\hbar m t}$$

$$\chi = \begin{pmatrix}c\\ d\end{pmatrix} e^{+i\hbar m t}$$

Note the two 2 component spinors are decoupled.

Case II: $\vec{A}=0$, $\vec{p}\neq 0$ (moving free particle)

Then

$$[\not{p}-m]\psi=0$$

or

$$[E\gamma_0-\vec{p}\cdot\vec{\gamma}-m]\psi=0$$

or

$$\left\{E\begin{pmatrix}1&0\\0&-1\end{pmatrix}-\begin{pmatrix}0&\vec{p}\cdot\vec{\sigma}\\-\vec{p}\cdot\vec{\sigma}&0\end{pmatrix}-m\begin{pmatrix}1&0\\0&1\end{pmatrix}\right\}\psi=0$$

or

$$\begin{bmatrix}E-m & -\vec{p}\cdot\vec{\sigma}\\ \vec{p}\cdot\vec{\sigma} & -(E+m)\end{bmatrix}\begin{pmatrix}\phi\\ \chi\end{pmatrix}=0$$

or

$$(E-m)\phi-\vec{p}\cdot\vec{\sigma}\,\chi=0$$

$$\vec{p}\cdot\vec{\sigma}\,\phi-(E+m)\chi=0$$

Now ϕ & χ are coupled. Solve for

$$\chi=\left(\frac{\vec{p}\cdot\vec{\sigma}}{E+m}\right)\phi$$

and then

$$(E-m)\phi=\frac{(\vec{p}\cdot\vec{\sigma})(\vec{p}\cdot\vec{\sigma})}{E+m}\phi$$

Hence the energy must satisfy

$$E^2-m^2-p^2=0$$

Thus E can be + or −

$$E^2 = \sqrt{p^2+m^2}$$

To get Case I solution as $p \to 0$, we need the negative sign for the square root. Then

$$\psi_- = \begin{pmatrix} \frac{-\vec{\sigma}\cdot\vec{p}\ \chi}{m+\sqrt{p^2+m^2}} \\ \chi \end{pmatrix} e^{i\sqrt{p^2+m^2}t + i\vec{p}\cdot\vec{x}} \qquad (1)$$

The + sign gives

$$\psi_+ = \begin{pmatrix} \phi \\ \frac{\vec{p}\cdot\vec{\sigma}\ \phi}{E+m} \end{pmatrix} e^{-i\sqrt{p^2+m^2}t + i\vec{p}\cdot\vec{x}} \qquad (2)$$

Since (1) implies negative energies, we try to understand by rewriting soln to try & get it to look like (2). Define

$$\vec{p}' = -\vec{p} \qquad E' = +\sqrt{p^2+m^2}$$

Then

$$\psi_- = \begin{pmatrix} \frac{\vec{\sigma}\cdot\vec{p}'\ \chi}{E+m} \\ \chi \end{pmatrix} e^{-(-iE't + i\vec{p}'\cdot\vec{x})}$$

This now looks like ψ_+ except with momentum reversed.

Dirac Equation Including Electromagnetic Interactions

We first try to get the non-relativistic limit. Don't try to normalize ψ

$$\left[\not{p} - \tfrac{e}{c}\not{A} - m\right]\psi = 0$$

or writing it out

$$\begin{bmatrix} E - m - \frac{e}{c}V & (\vec{p} - \frac{e}{c}\vec{A})\cdot\vec{\sigma} \\ -\vec{\sigma}\cdot(\vec{p} - \frac{e}{c}\vec{A}) & -(E + m - \frac{e}{c}V) \end{bmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = 0$$

We can solve, taking χ as the smallest component, to find

$$\chi = \frac{-1}{(E + m - \frac{e}{c}V)}\,\vec{\sigma}\cdot(\vec{p} - \tfrac{e}{c}\vec{A})\,\phi$$

Then plugging back in

$$\underbrace{\left[E - m}_{w} - \tfrac{e}{c}V\right]\phi = \vec{\sigma}\cdot(\vec{p} - \tfrac{e}{c}\vec{A})\,\frac{1}{\underbrace{(E + m - \frac{e}{c}V)}_{2m+w}}\,\vec{\sigma}\cdot\underbrace{(\vec{p} - \tfrac{e}{c}\vec{A})}_{\pi}\,\phi$$

$$E = m + w \qquad \vec{\pi} = \vec{p} - \tfrac{e}{c}\vec{A}$$

To get the non-relativistic limit, assume potential energy small and expand

$$\frac{1}{2m + w - \frac{e}{c}V} \sim \frac{1}{2m} - \frac{(w - e/cV)}{(2m)^2}$$

Plug this in to get

$$(w - \tfrac{e}{c}V)\,\phi = \vec{\sigma}\cdot\vec{\pi}\;\frac{1}{2m}\;\vec{\sigma}\cdot\vec{\pi}\,\phi$$

alternatively: Let $V' = \frac{2}{c} V$

$$\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right](W-V')\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]\phi = \frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})\phi$$

$$+ \frac{1}{8m^2}\left[(\vec{\sigma}\cdot\vec{\pi})^2(W-V') - 2\vec{\sigma}\cdot\vec{\pi}(W-V')\vec{\sigma}\cdot\vec{\pi} + (W-V')(\vec{\sigma}\cdot\vec{\pi})^2\right]\phi \qquad (3)$$

Let

$$\boxed{\chi} = \left[1 - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]\phi$$

since to first order,

$$\psi^\dagger\psi = \phi^\dagger\phi + \chi^\dagger\chi \sim \phi^\dagger\phi\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]$$

and to first order

$$\phi \sim \boxed{\chi} - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\phi$$

$$\Rightarrow \quad \psi^\dagger\psi \sim \boxed{\chi}^\dagger\boxed{\chi}$$

Using this in (3) and using

$$\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]^{-1} \sim \left[1 - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]$$

we find

$$(W-V')\boxed{\chi} = \frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2\boxed{\chi} - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\boxed{\chi} \qquad (4)$$

$$+ \frac{1}{8m^2}\left\{(\vec{\sigma}\cdot\vec{\pi})^2(W-V') - 2\vec{\sigma}\cdot\vec{\pi}(W-V')\vec{\sigma}\cdot\vec{\pi} + (W-V')(\vec{\sigma}\cdot\vec{\pi})^2\right\}\boxed{\chi}$$

To rewrite the { } expression, use the commutation relation

$$A^2B - 2ABA + BA^2 = A[A,B] - [A,B]A$$

and let $A = \vec{\sigma}\cdot\vec{\pi}$ $\qquad B = W - V'$

Now since $E \to \mathcal{H}_+$, if $\vec{A}$ is time dependent it will commute with E. Assume

$$\frac{\partial \vec{A}}{\partial t} = 0$$

so that $\vec{A}$ commutes with E, m, V'. Now worry about $\vec{\sigma}\cdot\vec{p}$ which commutes with E. Thus

$$\left[\vec{\sigma}\cdot(\vec{p} - \tfrac{e}{c}\vec{A}),\ E - m - V'\right] \to \left[\vec{\sigma}\cdot\vec{p}, -V'\right] = -\lambda e\,\vec{\sigma}\cdot\vec{E}$$

Then in (4)

$$\{\quad\} = \kappa\left[\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}\right]$$

Now use

$$(\vec{\sigma}\cdot\vec{E})(\vec{\sigma}\cdot\vec{\pi}) = -(\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\vec{E})$$

and $(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = \vec{a}\cdot\vec{b} + i\,\vec{\sigma}\cdot(\vec{a}\times\vec{b})$

to find

$$\vec{E}\cdot\vec{\pi} + i\,\vec{\sigma}\cdot(\vec{E}\times\vec{\pi}) = \vec{\pi}\cdot\vec{E} - i\,\vec{\sigma}\cdot(\vec{\pi}\times\vec{E})$$

$$\vec{p}\times\vec{E} = -\vec{E}\times\vec{p}$$

Hence

$$\{\ \} = -e\left[\nabla\cdot\vec{E} - 2\vec{\sigma}\cdot(\vec{\pi}\times\vec{E})\right]$$

and (4) becomes

$$W\boxed{\chi} = V'\boxed{\chi} + \frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2\boxed{\chi} - \frac{(\vec{\sigma}\cdot\vec{\pi})^4}{8m^3}\boxed{\chi}$$

$$- \frac{e}{8m^2}\left[\nabla^2 E + 2\vec{\sigma}\cdot(\vec{\pi}\times\vec{E})\right]\boxed{\chi}$$

Use

$$(\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\vec{\pi}) = \vec{\pi}\cdot\vec{\pi} - e\,\vec{\sigma}\cdot\vec{B}$$

Then

$$W\boxed{\chi} = V\boxed{\chi} + \frac{1}{2m}\left[\vec{\pi}\cdot\vec{\pi} - e\vec{\sigma}\cdot\vec{B}\right]\boxed{\chi}$$

$W\boxed{\chi}$: total energy (non-rel); $V\boxed{\chi}$: P.E; $\vec{\pi}\cdot\vec{\pi}$: K.E.; $e\vec{\sigma}\cdot\vec{B}$: mag. moment coupling

$$-\frac{(\vec{p}\cdot\vec{p})^2}{8m^2}\boxed{\chi} - \frac{e}{8m^2}\left[\vec{\nabla}\cdot\vec{E} + 2\vec{\sigma}\cdot(\vec{\pi}\times\vec{E})\right]\boxed{\chi}$$

$-\frac{(\vec{p}\cdot\vec{p})^2}{8m^2}\boxed{\chi}$: 1st order relativistic correction to K.E.

$\vec{\nabla}\cdot\vec{E} + 2\vec{\sigma}\cdot(\vec{\pi}\times\vec{E})$: spin orbit coupling

3/31/67 LECTURE

$$W\chi = \left\{ V + \frac{1}{2m}\left(\mathbb{P} - \frac{e}{c}\mathbb{A}\right)^2 - \frac{1}{8m^3}\left(\mathbb{P} - \frac{e}{c}\mathbb{A}\right)^4 + \frac{e}{2m}\sigma\cdot\mathbb{B} + \frac{e}{2m}\left[\frac{1}{2}\sigma\cdot\left(\frac{\mathbb{P}-e\mathbb{A}}{m}\times\mathbb{E}\right) + \frac{1}{4m}\nabla\cdot\mathbb{E}\right]\right\}\chi$$

Significance of these terms:

$\frac{1}{8m^3}\left(\mathbb{P} - \frac{e}{c}\mathbb{A}\right)^4$

Consider

$$E = \sqrt{m^2 + p^2} = m + \frac{p^2}{2m} - \frac{p^4}{8m^3} \cdots$$

We can identify the terms directly ↑

$\frac{e}{2m}\left[\frac{1}{2}\sigma\cdot\left(\frac{(\mathbb{P}-e\mathbb{A})}{m}\times\mathbb{E}\right) + \frac{1}{4m}\nabla\cdot\mathbb{E}\right]$

Can understand $\sigma\cdot(\mathbb{V}\times\mathbb{E})$ as magnetic field seen by moving object. [But doesn't account for ½ term.]

Note $E = \frac{Ze^2}{4\pi}\frac{R}{r^3}$, Thus get a $\frac{L\cdot\sigma}{r^3}$ term — "spin orbit coupling." (Does example.)

In an H atom $\nabla\cdot\mathbb{E} \to 4\pi Ze\,\delta^3(R)$

Pauli's Correction for the Proton (Anomolous moment)

The electron has a moment $\frac{e}{2m}$. But the proton has $2.17\left(\frac{e}{2m}\right)$. Where does the extra 1.17 come from? ("anomalous magnetic moment"). Pauli suggested an alternate equation by adding terms to Dirac equation

$$\left[\gamma_\mu\left(i\nabla_\mu - eA\right) - m\right]\psi = \underbrace{\frac{\mu}{4}\gamma_\mu\gamma_\nu F_{\mu\nu}\psi}_{\text{anomalous moment term}} + \gamma_\nu \Box^2 A_\nu \psi \cdots$$

where $F_{\mu\nu}$ is field tensor

$$F_{\mu\nu} = \frac{\partial A_\mu}{\partial x_\nu} - \frac{\partial A_\nu}{\partial x_\mu}$$

Multiply by β to find

$$i\frac{\partial \psi}{\partial t} = \left[\beta m + V + \alpha\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\right]\psi + \mu\beta\left[\nabla_D \cdot \mathbf{B} - \alpha\cdot\mathbf{E}\right]\psi$$

In the non-relativistic limit this leads to

$$W\chi = \left\{V + \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 - \frac{1}{8m^3}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^4 + \left(\mu + \frac{e}{2m}\right)(\sigma\cdot\mathbf{B}) + \left(\mu + \frac{e}{4m}\right)\left[\sigma\cdot\frac{\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\times\mathbf{E}}{m} + \frac{\nabla\cdot\mathbf{E}}{2m}\right]\right\}\chi$$

where

$$\sigma_D = \begin{pmatrix}\sigma & 0\\ 0 & \sigma\end{pmatrix}$$ spin operator for Dirac equn

$$\sigma_z = i\alpha_x\alpha_y$$

Note the $\left(\mu + \frac{e}{tm}\right) = \left(\mu + \frac{e}{2m} - \frac{e}{2m}\right)$ term.

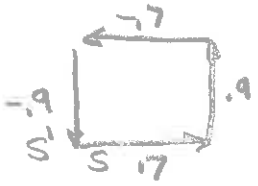
The extra $-\frac{1}{2}$ term comes from Thomas precession.

Thomas Precession

⊗

Must account for fact that electron rest system is accelerating. Thus need system of electron processes slowly.

$\vec{v}$



$S' \neq S$

since Lorentz transformation don't commute. Their commutator involves a rotation operator.

At present we don't know what makes the μ_e comes from guts of proton (maybe mesons & such). Maybe "ideal proton" satisfies Dirac eqn, while mesons about it satisfy Klein-Gordon eqn. (Yukawa's idea).

Recoil appear electron has guts, although if Dirac eqn predicts 1.000, measurements give 1.001147. But we can handle this if we consider e.g.m. interaction potential (use Q.E.D.). Same thing works for muons.

Thus electrons and muons seem to satisfy the Dirac eqn -- at least to within experimental evidence.

4/3/67 LECTURE

We also have an "ideal" electron which satisfies

$$\gamma_\mu \left(i\nabla_\mu - \frac{e}{c} A_\mu\right) \psi = m\psi$$

and an ideal photon which satisfies Maxwell eqns. However there is an interaction which gives rise to anomalous electron moment. (Like radiation resistance term in classical E&M

$$m \frac{d^2 x_\mu}{ds^2} = \gamma_\mu F_{\mu\nu} = \gamma_\mu \left(F_{\mu\nu}^{self} + F_{\mu\nu}^{ext}\right)$$

No experiment to date predicts any failure in these eqns. Any disagreement can be attributed to lack of knowledge about strong interaction.

Law of motion of electron	Dirac eqns
" " " photon	Maxwell eqns
" " " strongly interacting particles	(Gell-Mann eqn 1970)

PROBLEM: Explain physical interpretation of $\frac{1}{4\pi} \nabla \cdot E$ term.

PROBLEM: Can write Dirac H as

$$H_D = \alpha_0 \left(iP - \frac{e}{c} A\right) + \beta m$$

But from q.m.

$$\dot{Q} = i\left(H_D Q - Q H_D\right)$$

In S. eqn we found $\dot{\vec{x}} = \left(\vec{p} - \frac{e}{c}\vec{A}\right)/m$ $\quad \dot{\vec{p}} = -\nabla V + \cdots$

Try this game with Dirac eqn.

PROBLEM: Isiven ① 1; ② $\alpha_x, \alpha_y, \alpha_z, \beta$; ③ $\alpha_x\alpha_y, \beta\alpha_x$; ④ $\alpha_x\alpha_y\alpha_z$
Find how many are really different (to get used to commutation laws).

Now want to study free particle Dirac solutions to try to interpret components of Dirac spinor.

$\psi = \begin{pmatrix}\psi_a \\ \psi_b\end{pmatrix}$ and $\psi = e^{-i(Et - \vec{p}\cdot\vec{x})}\psi_{a,b}$

$$(E+m)\psi_b = (\vec{\sigma}\cdot\vec{p})\psi_a$$

$$(E-m)\psi_a = (\vec{\sigma}\cdot\vec{p})\psi_b \qquad \vec{p}, E \text{ are numbers}$$

Combined $(E^2 - m^2)\psi_a = (\vec{\sigma}\cdot\vec{p})(E+m)\psi_b = (\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\vec{p})\psi_a = (\vec{p}\cdot\vec{p})\psi_a$

$$\Rightarrow \quad E^2 - m^2 = \vec{p}\cdot\vec{p}$$

$$E = E_p = \left|\sqrt{m^2 + p\cdot p}\right|$$

$$= -E_p$$

Suppose $E = E_p$ and solve

$$\psi_b = \frac{1}{E_p + m} (\sigma \cdot p) \psi_a$$

Consider case where p is in z direction.
Also

$$\sigma_z \psi_a = +\psi_a \qquad \left(\psi_a = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right)$$

Then

$$\psi_b = \frac{1}{m + E_p} \sigma_z p \psi_a = \frac{p}{E+m} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\therefore \quad \sigma_z \psi_b = +1 \, \psi_b$$

spin is in up direction

But usually want to normalize $\psi_b^* \psi_b + \psi_a^* \psi_a = 1$
then find ψ

$$\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} \sqrt{E_p + m} \\ 0 \\ \sqrt{E_p - m} \\ 0 \end{pmatrix}$$

particle in z direction,
up spin since
$\sigma_z \psi = +1 \, \psi$

Now for spin down

$$\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} 0 \\ \sqrt{E_p + m} \\ 0 \\ -\sqrt{E_p - m} \end{pmatrix}$$

particle in z direction
down spin

Now for spin in x-direction, recall in n.r. q.m.,

if $\chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ $\quad \sigma_x \chi = \chi$

Thus we expect

$$\psi = \frac{1}{\sqrt{2E_p}} \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{E_p+m} \\ \sqrt{E_p+m} \\ \sqrt{E_p-m} \\ -\sqrt{E_p-m} \end{pmatrix}$$

p in z-direction
spin in x-direction (?)

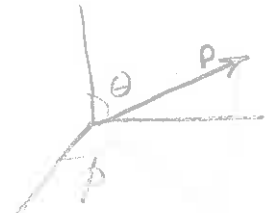
But $\sigma_x \psi_a = +\psi_a$ $\quad \sigma_x \psi_b = -\psi_b$?

What's the matter? ψ is certainly a soln of the eqn.
But σ_x does not commute with H. Mentions helicity?
left helicity concept.

4/4/67 LECTURE

We have seen that $[\sigma_x, H_D] \neq 0$. Thus no definite ang. mom in x-direction.

Now say
$\vec{p}$ not in z-direction



For case of positive helicity, we require

$$\underbrace{\left(\frac{\vec{\sigma}\cdot\vec{p}}{p}\right)}_{\sigma_p}\psi = +\psi$$

Now

$$\sigma_p \psi_a = +\psi_a \qquad \text{where} \quad \psi_a = \begin{pmatrix} \cos\theta/2\, e^{i\phi/2} \\ \sin\theta/2\, e^{-i\phi/2} \end{pmatrix}$$

from n.r.q.m.

Thus in r.q.m.

$$\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} \sqrt{E_p+m}\cos\theta/2\, e^{i\phi/2} \\ \sqrt{E_p+m}\sin\theta/2\, e^{-i\phi/2} \\ \sqrt{E_p-m}\cos\theta/2\, e^{i\phi/2} \\ \sqrt{E_p-m}\sin\theta/2\, e^{-i\phi/2} \end{pmatrix}$$

for positive helicity $\sigma_p = +1$

Now consider $E = -E_p$

p in z-direction, $\sigma_z = +1$

$$\frac{1}{\sqrt{2E_p}} \begin{pmatrix} -\sqrt{E_p - m} \\ 0 \\ +\sqrt{E_p + m} \\ 0 \end{pmatrix}$$

$\sigma_z = -1$

$$\frac{1}{\sqrt{2E_p}} \begin{pmatrix} 0 \\ +\sqrt{E_p - m} \\ 0 \\ +\sqrt{E_p + m} \end{pmatrix}$$

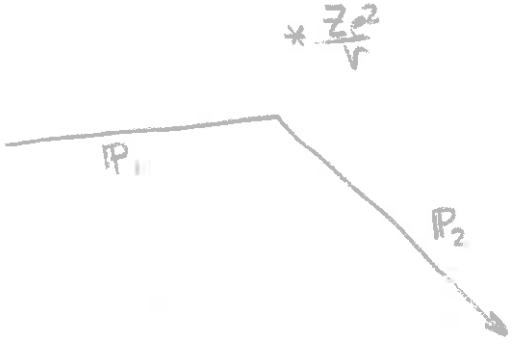
Note 4 orthog. spinors for free particle (4 basis states).

These components cannot be easily interpreted.

Eg. $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ has no simple meaning.

Dirac proposed all negative states in a vacuum are full. A "hole" is a positron.

EXAMPLE: Scattering cross-section of an electron from a nucleus of Ze. Use Born approx.



$$H_D = \underbrace{\alpha_0 \mathbb{P} + \beta m}_{H_0} + \underbrace{V \underline{\underline{1}}}_{H_{int}}$$

$$\text{Rate} = \sigma v_{in} = 2\pi \delta(E_f - E_i) \frac{d^3\mathbb{P}_2}{(2\pi)^3} |M_{fi}|^2$$

[Note relativity only enters into H_D, note into state density]

$$M_{fi} = \int \psi_f^\dagger(x) H_{int} \psi_i(x) d^3x$$

Now we use free wave-fcns

$$\psi(x) = e^{i\mathbb{P}\cdot x} u \qquad \text{where } u \text{ is } \begin{pmatrix} \\ \\ \\ \\ \end{pmatrix} \text{ 4 numbers (spinor)}$$

$$M_{fi} = \int u_2^\dagger e^{-i\mathbb{P}_2\cdot x} \frac{Ze^2}{r} e^{i\mathbb{P}_1\cdot x} u_1 d^3x$$

$$= (u_2^\dagger \underline{\underline{1}} u_1) \underbrace{\int e^{i(\mathbb{P}_1 - \mathbb{P}_2)\cdot x} \frac{Ze^2}{r} d^3x}_{\frac{4\pi Ze^2}{Q^2}}$$

Note that except for $(u_2^+ | u_1)$ everything is the same as in n.r.q.m. However actually we have differences in δ-fcn

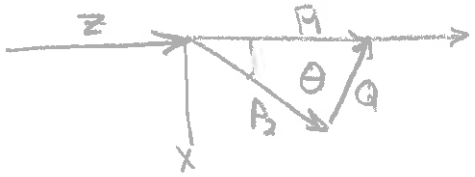
$$\sigma v_1 = 2\pi\, \delta\left(\sqrt{m^2+p_2^2} - \sqrt{m^2+p_1^2}\right) \frac{p_2^2\, dp_2\, d\Omega_2}{(2\pi)^3} \left(\frac{4\pi Z e^2}{Q^2}\right)^2 |(u_2^+ | u_1)|^2$$

$$= \frac{1}{(2\pi)^2} \frac{\sqrt{m^2+p_2^2}}{p_2}\, p_2^2\, d\Omega_2 \left(\cdots\right)^2 |\;|^2$$

$\frac{E_2}{p_2}$ $\qquad$ $E_2 dp_2 = dp_2^2$

[Note $\quad \delta(E_2 - E_1)\, p_2^2 dp_2 = \delta(E_2 - E_1)\, p_2 \cdot p_2 \cdot dp_2$]

Now $\underbrace{E_2 = E_1}_{E} \quad \therefore \underbrace{|p_2|^2 = |p_1|^2}_{p}$



$Q = 2p \sin\theta/2$

Now to calculate $(u_2^+ | u_1)$. We need more information about initial and final spins

in state 1 $\quad$ + helicity $\quad u_1 = \frac{1}{\sqrt{2E_1}} \begin{pmatrix} \sqrt{E_1+m} \\ 0 \\ \sqrt{E_1-m} \\ 0 \end{pmatrix}$

$\quad$ − helicity $\quad u_1 = \frac{1}{\sqrt{2E_1}} \begin{pmatrix} 0 \\ \sqrt{E_1+m} \\ 0 \\ -\sqrt{E_1-m} \end{pmatrix}$

out state 2 $\quad$ + helicity $\quad u_2 = \frac{1}{\sqrt{2E_2}} \begin{pmatrix} \sqrt{E_2+m}\cos\theta/2 \\ \sqrt{E_2+m}\sin\theta/2 \\ \sqrt{E_2-m}\cos\theta/2 \\ \sqrt{E_2-m}\sin\theta/2 \end{pmatrix}$

$\quad$ − helicity $\quad u_2 = \frac{1}{\sqrt{2E_2}} \begin{pmatrix} -\sqrt{E_2+m}\sin\theta/2 \\ \sqrt{E_2+m}\cos\theta/2 \\ \sqrt{E_2-m}\sin\theta/2 \\ -\sqrt{E_2-m}\cos\theta/2 \end{pmatrix}$

$$(+ \to +) = \frac{1}{\sqrt{2E\,2E}} \left[\sqrt{E+m}\sqrt{E+m}\cos\theta/2 + 0 + \sqrt{E-m}\sqrt{E-m}\cos\theta/2 + 0 \right]$$

$$= \cos\theta/2 \qquad \text{(no spin flip)}$$

$$(+ \to -) = \frac{1}{\sqrt{2E\,2E}} \left[\sqrt{E+m}\sqrt{E+m}\sin\theta/2 + \sqrt{E-m}\left(-\sqrt{E-m}\sin\theta/2\right) \right]$$

$$= -\frac{m}{E}\sin\theta/2 \qquad \text{(spin flip)}$$

If (+ → unknown helicity)

$$\sigma v = \frac{4Z^2e^4}{Q^4} E_p \, d\Omega \left(\cos^2\theta/2 + \frac{m^2}{E^2}\sin^2\theta/2 \right)$$

relativistic modification

Note as $m/E \to 1$ we get usual Coulomb scattering, i.e.

$$\cos^2\theta/2 + \frac{m^2}{E^2}\sin^2\theta/2 = 1 - \frac{v^2}{c^2}\sin^2\theta/2$$

To get ($- \to$ anything) just use parity invariance of EM interactions to get [illegible] thing.

4/6/67 LECTURE

"Quantum Mechanics + Relativity + Causality"

R.P. Feynman

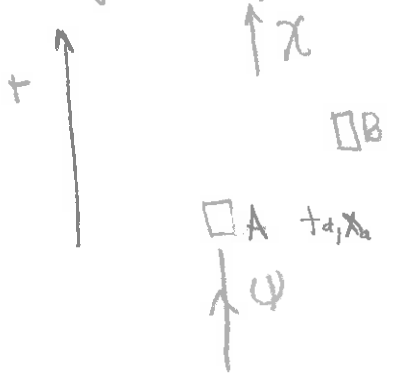
Consequences
1.) Antiparticles
2.) Spin & Statistics related
3.) CPT invariance (in definite way)
4.) No arbitrary functions
5.) Divergence problems

THEOREM: In general we can expand $f(t)$ in $\omega > 0$

$$f(t) = \int_0^\infty \varphi(\omega) e^{-i\omega t} d\omega$$

impossible for $f(t) \equiv 0$ over a finite t.
(identity theorem)

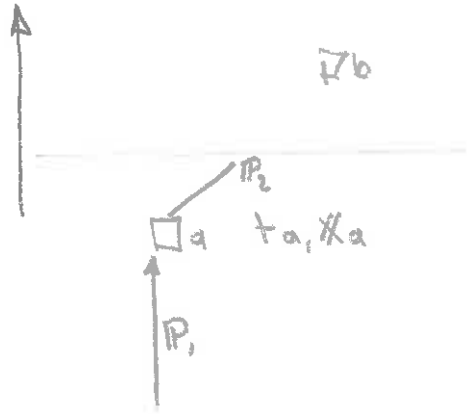
We want to include causality in q.m. What one does in future cannot affect the past. We imagine the state of system at a certain time $|\psi\rangle$. Consider second order scattering in a potential.



$$\langle \chi|\psi\rangle = \sum_{\varphi} \langle \chi|B|\varphi\rangle\langle\varphi|A|\psi\rangle$$

future past

If ψ is a particle only, and scattering is local



$$\text{Scatt. amp } \vec{P}_1 \to \vec{P}_2 \propto e^{i[(E_3 - E_1)t_a - (\vec{P}_3 - \vec{P}_1)\cdot\vec{x}_a]}$$

$$E_3 = \sqrt{\mu^2 + \vec{P}_3 \cdot \vec{P}_3}$$

$$\therefore \text{Scat} = \sum_{\vec{P}_3}{}' \beta\alpha\, e^{i[E_2 t_b - \vec{P}_2\cdot\vec{x}_b]}\, e^{-i[E_3(t_b - t_a) - \vec{P}_3(\vec{x}_b - \vec{x}_a)]}\, e^{i[E_1 t_a - \vec{P}_1\cdot\vec{x}_a]}$$

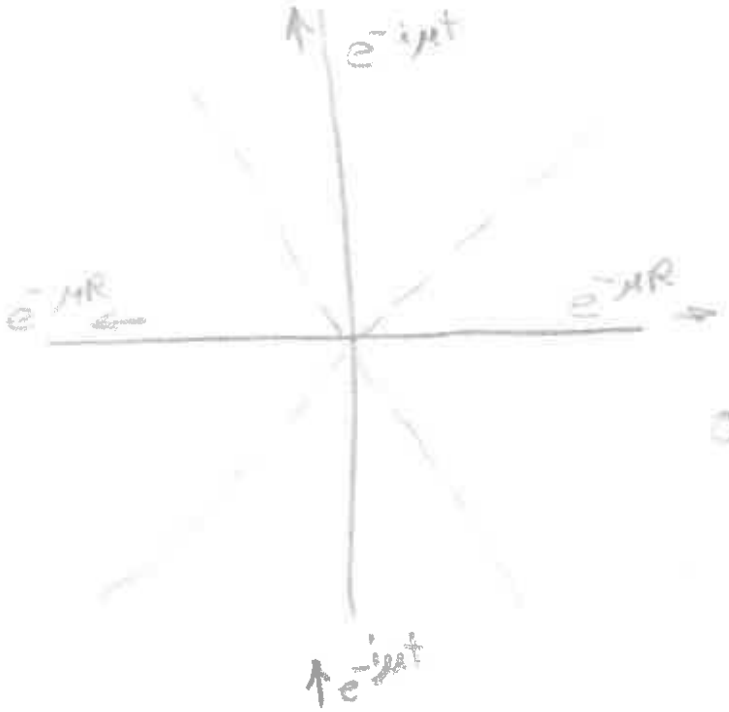
$t_b > t_a$

e.g. for muoniums, $\alpha, \beta = \text{const.}$

$$\sum_{\vec{P}_3}{}' \to \int \frac{d^3\vec{P}_3}{(2\pi)^3 \cdot 2E_3}$$

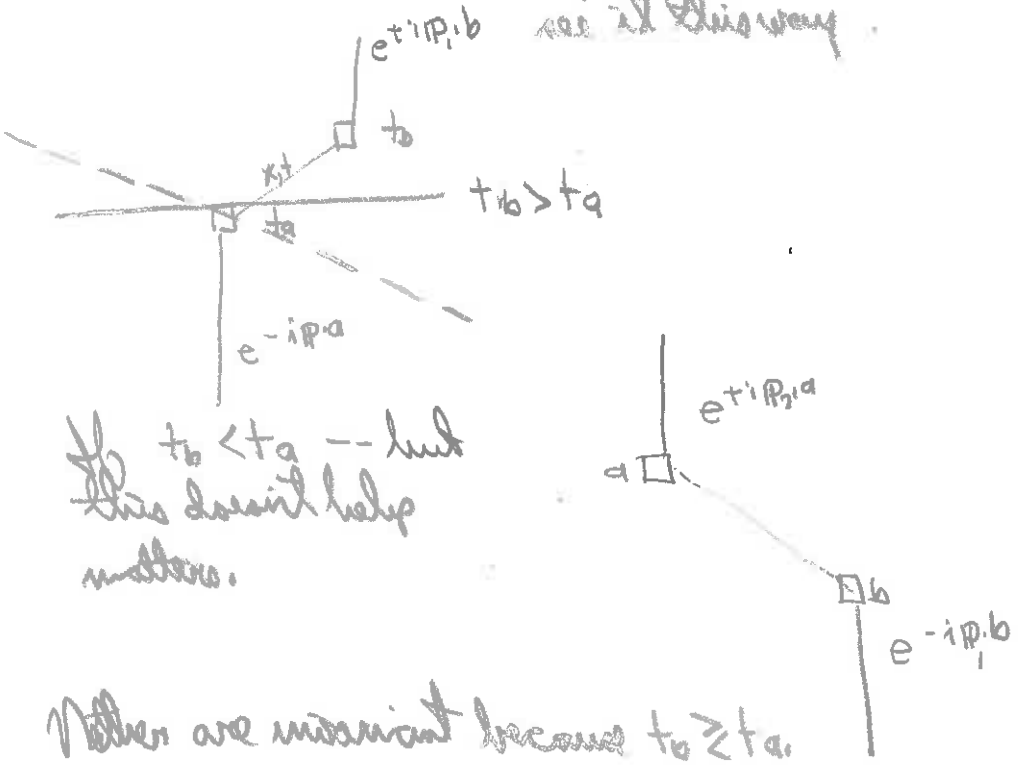
$$\therefore \text{Scat} = \beta\alpha\, e^{i\vec{P}_2\cdot\vec{b}}\, e^{-i\vec{P}_1\cdot\vec{a}}\, N(\vec{b}-\vec{a}) \quad \text{for } t_b > t_a$$

$$N(\vec{x}, t) = \int \frac{d^3\vec{P}}{(2\pi)^3\sqrt{\mu^2+\vec{P}^2}}\, e^{-i[\sqrt{\mu^2+\vec{P}^2}\, t - \vec{P}\cdot\vec{x}]}$$



Outside light cone $N(x,t) \neq 0$, But $\tilde{N}$ real there [$N = N^*$]

Causality can't mean $N \to 0$ across time like line because a ray in another coord system would hit it this way.



Neither are invariant because $t_b \gtrless t_a$.

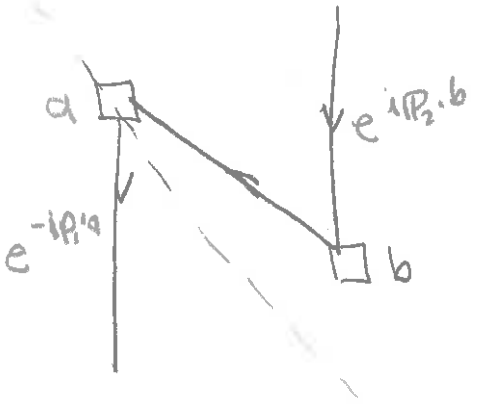
Consider emission from a pt. We expect velocity of particle $< c$ i.e. no influence outside light cone. But if we try to superimpose

$$\sum_p C_p e^{+ip\cdot x} e^{-i\sqrt{\mu^2+p^2}t}$$

$$\delta(x) = \int e^{ip\cdot x} d^3p\, e^{-i\sqrt{\mu^2+p^2}t}$$

But by our theorem, $\alpha \neq 0$, can't be zero over a finite range, and locality is not compatible with relativity (invariance).

Only one way out, and that is to take $t_b \leq t_a$



$$\sum_{p_3} \beta\alpha\, e^{ip_2\cdot b}\, e^{-i\left[E_3(t_b-t_a) - p_3\cdot(x_b-x_a)\right]}\, e^{-ip_1\cdot a}$$

$$= \sum_{p_3} \beta\alpha\, e^{ip_2 b}\, e^{-i\left[E_3(t_a-t_b) - p_3\cdot(x_a-x_b)\right]}\, e^{-ip_1\cdot a}$$

if b is outside light cone of a.

∴ use first form for $t_a > t_b$
" second form for $t_b < t_a$

to get invariant result & causality.

In vacuum, amp for pair prod. in vacuum:

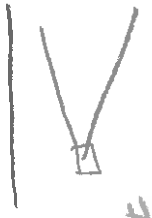
amp for pair a
prob of pair $\chi|a|^2$

nothing
amp 1

pair produced + passes unscathed
amp $-\frac{1}{2}(\chi+i\chi')|a|^2$
prob $= 1 - \chi|a|^2$

1 particle present

scatt amp a
prob scatt $c|a|^2$



no scatt + pair
$\chi|a|^2$

nothing

$1 - \frac{1}{2}(c+ic)|a|^2 - \frac{1}{2}(d+id')|a|^2 - \frac{1}{2}(\chi+i\chi')|a|^2$

Prob something happens $= c|a|^2 + \chi|a|^2$

Prob nothing happens $= 1 - c|a|^2 - d|a|^2 - \chi|a|^2$

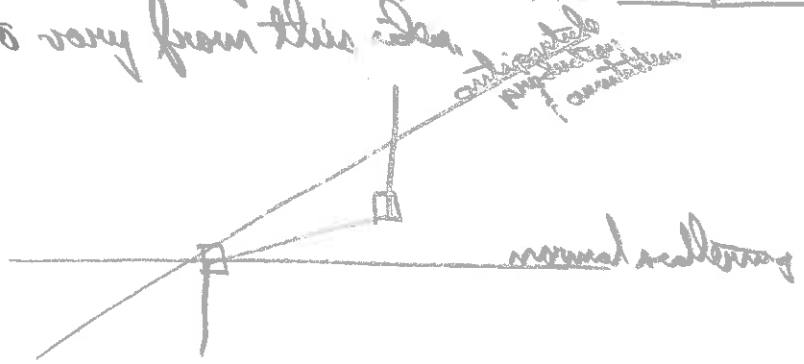
Note it doesn't add up. -- unless we suppose amp for pair prod in vacuum is less than in presence of new particle

$\Rightarrow$ prob something happens $c|a|^2 + \chi|a|^2 + d|a|^2$

$\Rightarrow$ Bose statistics (since we assumed no spin)

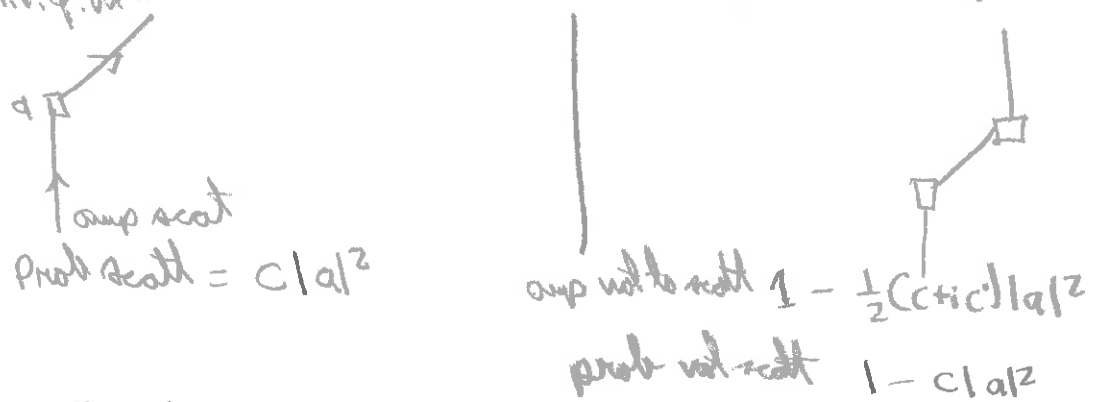
"One manic particle is another manic antiparticle."

Outside light cone we have antiparticle. No freedom to vary from this idea.



This leads to C=PT invariance.

Not quite as direct to get spin ½ statistics. Basic idea is unitarity ($\Sigma (\text{amp})^2 = 1$). Consider first n.r.q.m.



$\therefore \Sigma(\text{prob}) = 1$ if $C = C'$.

Spin ½: For particle standing still $|+,0\rangle$
$|-,0\rangle$

For particle moving he uses Lorentz transformations.
(lost me here) Shows spin ½ ⇒ pseudoscalar.

Now

prob something
$c|a|^2 + \chi|a|^2 - \delta|a|^2$

prob nothing happens
$1 - c|a|^2 + \delta|a|^2 - \chi|a|^2$

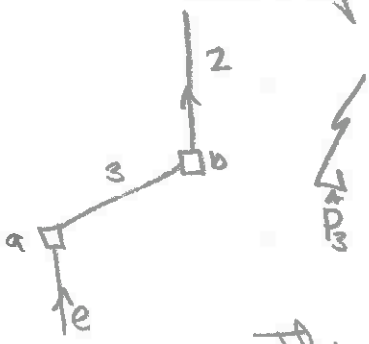
He has tried to invent a non-local theory (doesn't assume causality). Difficult.

If locality fails, it will fail for all theories.

But CPT, causality look OK so far.

4/7/67 LECTURE

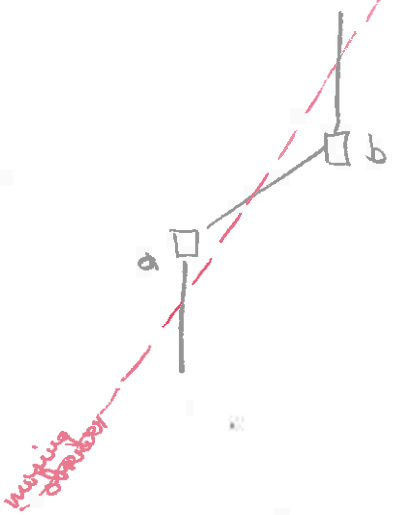
In order to get rid of negative energy states, we must introduce antiparticles. Consider again 2-nd order scattering and sum over intermediate states.

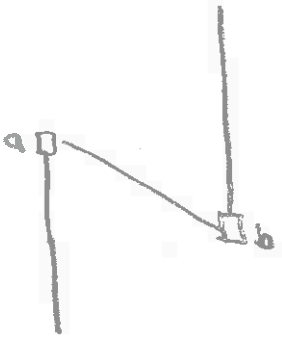


$$e^{i\vec{p}_2\cdot b}\,\beta\, e^{-i\vec{p}_3\cdot b}\quad e^{+i\vec{p}_3\cdot a}\,\alpha\, e^{-i\vec{p}_1\cdot a} \qquad (*)$$

valid only for $\rightarrow t_b > t_a$

This amplitude should invariant, but the condition $t_b > t_a$ is not invariant. One way to avoid this is to remove the restriction $t_b > t_a$. Then we can use the diagram below





But if we use it as we did the earlier diagram we find $\mathcal{E} = E_1 - E_3 + E_2$ may be negative. But we can't have $\mathcal{E} < 0$ since then vacuum would be unstable. Thus we must try something else.

Thus can't just extend the formula (*) for negative times directly.

The correct way out is to notice in the sum (*) that

$$N(\vec{x},t) = \int \frac{d^3p}{(2\pi)^3\sqrt{\mu^2+p^2}}\, e^{-i\left(\sqrt{\mu^2+p^2}\,t - \vec{p}\cdot\vec{x}\right)}$$

& $R = \sqrt{\vec{x}\cdot\vec{x}} > t$, N real

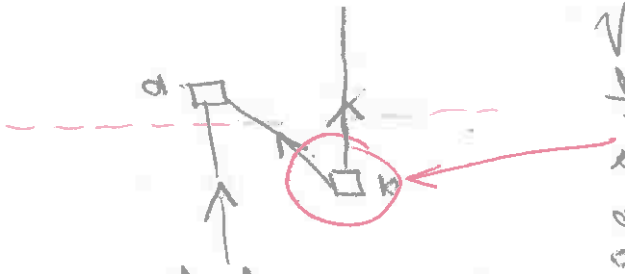
Thus we can propose for $t_b < t_a$ to use the same formula as for $t_b > t_a$

$$(*) = \cdots e^{-i(E_3 t_b - \vec{p}_3\cdot\vec{x}_b)} e^{+i(E_3 t_a - \vec{p}_3\cdot\vec{x}_a)} \cdots \qquad t_b > t_a$$

except

$$(*) = \alpha'\beta \cdots e^{+i(E_3 t_b - \vec{p}_3\cdot\vec{x}_b)} e^{-i(E_3 t_a - \vec{p}_3\cdot\vec{x}_a)} \cdots \qquad t_b < t_a$$

Then the diagram is



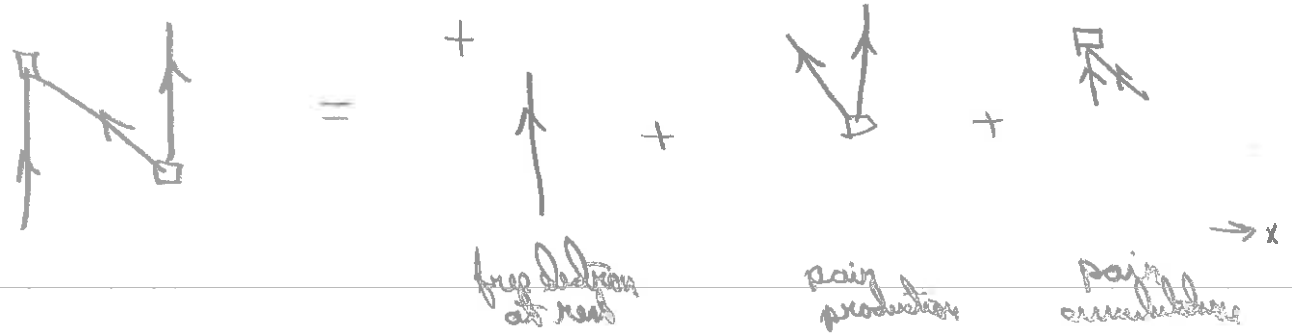
Now causality requires us to continue to allow "backward scatt" -- pair production -- for all situations (doesn't know about quantization when pair is produced)

Now the formula (*) is relativistically invariant for $t_b \geq t_a$, because $N(\vec{x},t)$ is real in space-like region

The new diagram gives us new physics -- antiparticles.

PROBLEM: Do Compton effect

Note we can think of



Actually we must integrate

$$\int dt_a d^3x_a\, dt_b d^3x_b \left[\sum_{p_3} e^{+i(p_2 \cdot x_b)} e^{-i \vec{p}_2 \cdot (x_b - x_a)} e^{-i \vec{p}_1 \cdot x_a} \right] \chi(x_b, t_b) \chi(x_a, t_a) \qquad t_b > t_a$$

$$\text{"} \qquad \left[\sum_{p} e^{i(\vec{p}_1 \cdot x_b)} e^{+i \vec{p}_2 \cdot (x_b - x_a)} e^{-i \vec{p}_1 \cdot x_a} \right] \text{"} \qquad t_b < t_a$$

SPIN-½ 4/10/67 LECTURE

Tried to describe spin-½ particles without hypothesizing the Dirac equation (which presupposes antiparticles). We found

$$[J_x, J_y] = i J_z$$

Also Lorentz generators $1 + i \in N_z$. Found

$$[J_x, N_x] = 0$$

$$[N_x, N_y] = -i J_z$$

$$[N_x, J_y] = i N_z$$

Also a momentum operator P

$$[J_z, P_x] = i P_y$$

$$[J_x, P_x] = 0 = [J_z, P_z]$$

$$[N_z, P_z] = i P_z$$

$$[N_z, P_+] = i P_z \quad \text{etc.}$$

Can try to find representation for these groups.

However consider a particle at rest. Let i be rotation index. State $|0, i\rangle$

Consider uniform motion

$$e^{i v N_z} |0, i\rangle \equiv |p_z, i\rangle$$

center state of uniform motion

or $$\tanh v = \frac{p}{E}$$

$$\sinh v = \frac{p}{\mu}$$

$$\cosh v = \frac{E}{\mu}$$

Can prove

$$P_z |p_x p_y p_z, i\rangle = p_z |p_x p_y p_z, i\rangle$$

and

$$P_z e^{i N_z v} = e^{i N_z v} \left[P_z \cosh v + P_z \sinh v \right]$$

The indices i give the spin in the rest system only.
A rotation

$$J_z = i\left[p_x \frac{\partial}{\partial p_y} - p_y \frac{\partial}{\partial p_x}\right] + j_z$$

and

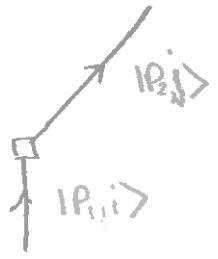
$$N_z = i\left[\underbrace{p_z \frac{\partial}{\partial p_t}}_{0} - p_t \frac{\partial}{\partial p_z}\right] + \left(\frac{\vec{j} \times \vec{p}}{E + \mu}\right)_z \qquad p_t = \sqrt{\mu^2 + p^2} = E$$

He then used these to set up a system of states for spin ½ particle.

Now we wanted to apply this to scattering problems using

$$|\psi\rangle = \sum_p \{a_{p,+}|p,+\rangle + a_p|p,-\rangle\}$$

For elastic scattering



Use interaction $f(p_1,p_2) + \sigma \circ F(p_1,p_2)$
which includes σ matrices.

We now consider scattering from a scalar potential (invariant under N & J. E.g. $f(p_1-p_2)$. Turns out this is enough to determine 2 solutions.

$$\frac{(E_1+M)(E_2+M) - p_1\cdot p_2 - i\sigma\circ(p_1\times p_2)}{\sqrt{2M(E_1+M)}\,\sqrt{2M(E_2+M)}} \qquad \text{scalar}$$

and

$$\frac{(E_1+M)(\sigma\circ p_2) - (E_2+M)(\sigma\circ p_1)}{\sqrt{2M(E_1+M)}\,\sqrt{2M(E_2+M)}} \qquad \text{pseudoscalar} \;]$$

Now considered 2nd order scattering

Turns out amp. for creation is

$$\frac{(E_2+M)(\mathbb{P}\cdot\mathbb{P}_3)-(E_3+M)(\mathbb{P}\cdot\mathbb{P}_2)}{\sqrt{2M(E_3+M)}\;\sqrt{2M(E_2+M)}}$$

annihilation

$$\frac{(E_1+M)(\mathbb{P}\cdot\mathbb{P}_3)-(E_3+M)(\mathbb{P}\cdot\mathbb{P}_1)}{\sqrt{2M(E_3+M)}\;\sqrt{2M(E_1+M)}}$$

But turns out these are not "Hermitian". Then this causes Fermi statistics. Note also these formulas look pseudoscalar even though potential was scalar. Means positron has negative parity from electron.

He did it for general i. If i even, all p's, E's are even & mx. el. are hermitian. If i odd, all powers of p's, E's are odd & non-hermitian $\Rightarrow$ Fermi statistics.

A simpler but incomplete argument assumes time reversal. For every state $\exists$ a time reversed state, but phase not defined. E.g.

$|+\rangle$ $\qquad T|+\rangle = \epsilon|-\rangle$

(phase $\epsilon = e^{i\delta}$)

However T is strange because it causes

$$T\{\alpha|a\rangle + \beta|b\rangle\} = \alpha^* T|a\rangle + \beta^* T|b\rangle$$

Also

$$T|-\rangle = \eta|+\rangle$$

Actually can fix either ϵ or η. Fix?

$$T|+\rangle = |-\rangle$$

$$T|-\rangle = \epsilon|+\rangle$$

Now

$$T|+ \text{in x-dir}\rangle = e^{i\theta}\{|- \text{in x dir}\rangle\}$$

$$\frac{1}{\sqrt{2}} T\{|+\rangle + |-\rangle\} = \frac{e^{i\theta}}{\sqrt{2}}\{|+\rangle - |-\rangle\}$$

or

$$|-\rangle + \epsilon|+\rangle = e^{i\theta}\{|+\rangle - |-\rangle\}$$

$\Rightarrow$

$$T|+\rangle = |-\rangle$$

$$T|-\rangle = -|+\rangle$$

for spin $\frac{1}{2}$

(2 time reversals changes sign)

∴ Double time reversal throws in a − phase for spin ½

$T(T|+\rangle) = T|-\rangle = -|+\rangle$

$T(T|-\rangle) = T(-|+\rangle) = -|-\rangle$

For 0 spin

$T|0\rangle = e^{i\delta}|0\rangle$

$T(T|0\rangle) = T(e^{i\delta}|0\rangle) = e^{-i\delta} T|0\rangle = |0\rangle$

$\Rightarrow$ + phase for integral spin

COMPTON SCATTERING 4/11/67 LECTURE

This first calculation will be rather clumsy. As we learn more we will streamline our calculations.

Photon scattering off of a free-electron

$$\gamma + e^- \rightarrow \gamma + e^-$$

First make a picture } define a coord. system. We take lab system

Now

$$p_1 = (m, 0, 0, 0) \qquad [p = (E, p_x, p_y, p_z)]$$

$$k_1 = \omega_1(1, 0, 0, 1)$$

$$k_2 = \omega_2(1, \sin\theta, 0, \cos\theta)$$

$$p_2 = (E_2, -p_2 \sin\varphi, 0, p_2 \cos\varphi)$$

Note

$$p_2 = p_1 + k_1 - k_2$$

Squaring

$$m^2 = m^2 + 0 + 0 + 2p_1 \cdot p_1 - 2p_1 \cdot k_2 - 2k_1 \cdot k_2$$

or using our 4-vectors

$$0 = m\omega_1 - m\omega_2 - \omega_1\omega_2(1-\cos\theta)$$

or

$$\frac{1}{\omega_2} - \frac{1}{\omega_1} = \frac{1}{m}(1-\cos\theta)$$

This was all just kinematics and is always done first. (Compton result)

Now add in polarizations

$$e_1 = (0,0,1,0) \quad \perp \text{ plane}$$
$$\text{or} \quad = (0,1,0,0) \quad \text{in plane}$$

$$e_2 = (0,\cos\theta,0,-\sin\theta) \quad \text{in plane}$$
$$= (0,0,1,0) \quad \perp \text{ plane}$$

[To get recoil electron, square

$$p_2 = p_1 + k_1 - k_2$$

to get $0 = \cdots$ etc.]

Now we develop Klein-Nishina formula for σ:

$$\text{Prob/sec} = 2\pi\,\delta(E_{out} - E_{in})\,\frac{d^3K_2}{(2\pi)^3}\,|m|^2$$

Now recall

$$H = \beta m + \alpha\cdot\left(p - \frac{e}{c}A\right) = H_0 + H_{int}$$

where

$$H_0 = \beta m + \alpha\cdot p$$

$$H_{int} = \frac{e}{c}\alpha\cdot A$$

Now recall $A = \frac{1}{\sqrt{2\omega}}\sum_{k}\left(a_k^{*}\, e^{ik\cdot x} + a_k e^{-ik\cdot x}\right)$

Then

$$m = \sum_{i} \frac{\langle 2|H'_{int}|i\rangle\langle i|H_{int}|1\rangle}{E - E_{i}}$$

Now write

$$\text{Prob/sec} = 2\pi\,\delta\left(\underbrace{\sqrt{\mu^2 + (K_1 - K_2)^2}}_{\text{energy of electron}} + \underbrace{\omega_2}_{\text{energy of photon}} - \underbrace{m - \omega_1}_{E_{in}}\right)\frac{K_2^2\,dK_2\,d\Omega}{(2\pi)^2}\,|m|^2$$

E_{out}

$$\left(\sqrt{\mu^2 + K_1^2 + K_2^2 - 2K_1K_2\cos\theta} + K_2 - m - \omega_1\right)$$

We use $\int \delta[f(x)]\,dx = \frac{1}{|f'(x_0)|}$

$$\frac{\partial}{\partial k_2}(\quad) = \frac{k_2 - k_1\cos\theta}{\sqrt{\quad}} + 1 = \frac{k_2 - k_1\cos\theta + E_2}{E_2}$$

or using conservation of energy $= \dfrac{E_1 + \omega_1 - \omega_1\cos\theta}{E_2}$

or " Compton formula $= \dfrac{\overset{m}{E_1} + \omega_1 m\left(\frac{1}{\omega_2} - \frac{1}{\omega_1}\right)}{E_2}$

$$= \frac{m\omega_1}{E_2\omega_2}$$

Thus integrating over k_2

$$\text{Prob/sec} = \sigma v = \sigma c = \omega_2^2 \frac{\omega_2 E_2}{m\omega_1} \frac{d\Omega_2}{(2\pi)^2} |M|^2$$

Now for matrix element, we consider possible intermediate states

$$\sum(\text{photon 2 emitted})(\text{photon 1 emitted}) \qquad A$$

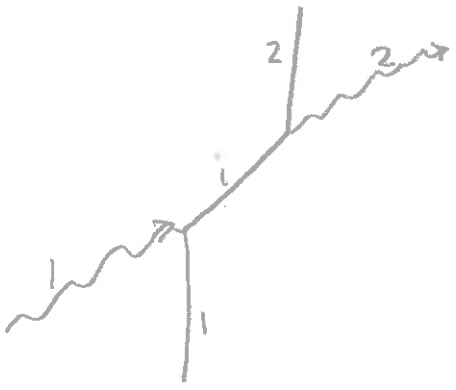
$$+ \sum(\text{photon 1 emitted})(\text{photon 2 emitted}) \qquad B$$

Then

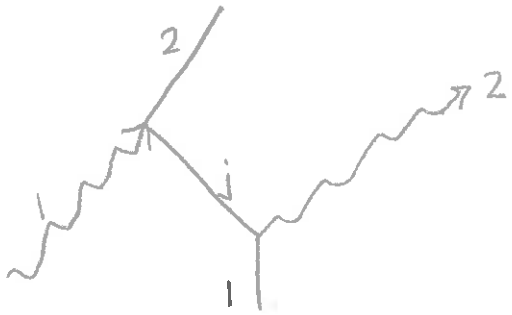
$$A = \sum_i \frac{\langle 2 | \alpha \cdot \epsilon_2^* e^{-i k_2 \cdot x} | i \rangle \langle i | \alpha \cdot \epsilon_1 e^{i k_1 \cdot x} | 1 \rangle}{E_1 + \omega_1 - E_i}$$

$$B = \sum_j \frac{\langle 2 | \alpha \cdot \epsilon_1 e^{i k_1 \cdot x} | j \rangle \langle j | \alpha \cdot \epsilon_2 e^{-i k_2 \cdot x} | 1 \rangle}{E_1 - \omega_2 - E_j}$$

Can associated pictures with these



A



B

[Have already calculated

$$M \sqrt{2\omega_1 2\omega_2} \left(\frac{e}{c}\right)^2 = A + B \ ]$$

In more elaborate problems we need ie for resonances.

Note we have made these calculations in conventional non-relativistic way -- but they contain that relativistically plane wave states

Can write using Dirac plane waves

$$\underline{A} = \sum_{\vec{P}_i = \vec{P}_1 + \vec{K}_1} \frac{\langle u_2^* | \alpha_2 | u_i \rangle \langle u_i^* | \alpha_1 | u_1 \rangle}{E_1 + \omega_1 - E_i} \qquad \vec{P}_i = \vec{P}_1 + \vec{K}_1$$

$$= \sum_{\substack{\text{2 spins} \\ \text{pos } E}} \frac{\langle u_2^* | \alpha_2 | u_i \rangle \langle u_i^* | \alpha_1 | u_1 \rangle}{E_1 + \omega_1 - |E_i|} \qquad |E_i| = \sqrt{\mu^2 + |\vec{P}_j|^2}$$

$$+ \sum_{\substack{\text{2 spins} \\ \text{neg } E_i}} \frac{\langle u_2^* | \alpha_2 | u_i \rangle \langle u_i^* | \alpha_1 | u_1 \rangle}{E_1 + \omega_1 + |E_i|}$$

Also

$$\underline{B} = \sum_{\text{pos } E} \frac{\langle u_2^* | \alpha_1 | u_j \rangle \langle u_1^* | \alpha_2 | u_1 \rangle}{E_1 - \omega_2 - |E_j|} \qquad \vec{P}_j = \vec{P}_1 - \vec{K}_2$$

$$+ \sum_{\text{neg } E} \frac{\langle u_2^* | \alpha_1 | u_j \rangle \langle u_j^* | \alpha_2 | u_1 \rangle}{E_1 - \omega_2 + |E_j|}$$

But all negative E states are full. Need 2 new possibilities — "pair theory". (Full sea)

Pair theory

C { 1st: photon ① knocks electron in sea (neg. k) to a positive energy state ②, leaving a hole at k
  { 2nd: photon ② makes electron ① go into negative hole k.

$$C = -\sum_{\substack{k \\ \text{neg. } E}} \frac{\langle 2 | \alpha_1 e^{-iK_1 \cdot X} | k \rangle \langle k | \alpha_2 e^{-iK_2 \cdot X} | 1 \rangle}{E_1 + \omega_1 - (E_1 + E_2 + |E_k|)}$$

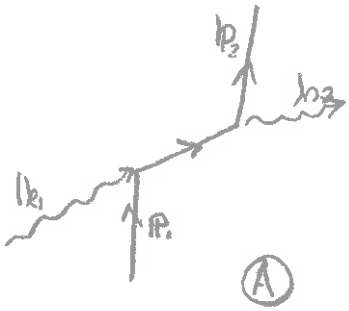
Find $P_k = P_2 - K_1 = P_1 - K_2 \equiv P_i$ before

Can also show denom $= \omega_2 - E_1 - |E_k|$

4/14/67 LECTURE

$$\text{Rate} = \sigma v = 2\pi \delta(E_{out} - E_{in}) \frac{d^3 k_2}{(2\pi)^3} \cdot |M|^2$$

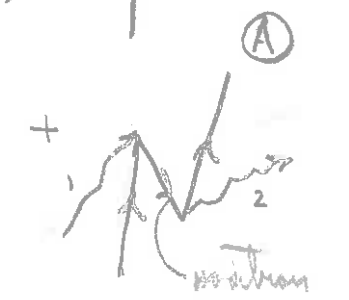
$$\sqrt{2\omega_1 2\omega_2}\, \frac{1}{e^2} M = A + B$$



$$A = \sum_{\substack{\text{spins } i \\ (\text{pos } E)}} \frac{(u_2^* \alpha_2 u_i)(u_i^* \alpha_1 u_1)}{E_1 + \omega_1 - |E_i| + i\epsilon} \qquad P_2 = P_1 + k_1$$

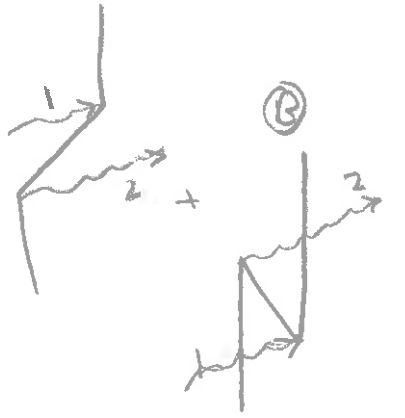
$$|E_i| = +\sqrt{\mu^2 + (P_1 + k_1)^2}$$

$$+ \sum_{\substack{\text{spin } i \\ (\text{neg } E)}} \frac{(u_2^* \alpha_2 u_i)(u_i^* \alpha_1 u_1)}{E_1 + \omega_1 + |E_i| - i\epsilon}$$



$$B = 2 \leftrightarrow 1$$

$$k_1, \omega_1 \leftrightarrow -k_2, -\omega_2$$



Technically the main difference in the last theory is in the $\pm i\epsilon$. Only important for resonances. But since denominators can't vanish in Compton scattering, we disregard this.

Now can pick polarization of electron & photons and calculate σ after some algebra. We will go on to the short cuts however.

Consider

$\overbrace{(u_2^* \alpha_2 u_1)}^{v} \overbrace{(u_1^* \alpha_1 u_1)}^{w}$

spin 1
E, p⃗

or

$$(v^* u_1)(u_1^* w)$$

$$\sum_{\text{spins}} \sum_b \sum_a v_a^* u_a u_b^* w_b$$

or

$$\sum_b \sum_a v_a^* \lambda_{ab} w_b \qquad \lambda_{ab} = \sum_{\text{spin } u} u_a u_b^*$$

$$\sum (u_2^* \alpha_2 u_1)(u_1^* \alpha_1 u_1) \rightarrow (u_2^* \alpha_2 \lambda' \alpha_1 u_1)$$

This if we can find λ we don't have to sum. We will work it out -- p⃗ in pure z $\quad E = \sqrt{u^2 + p^2} = E_p$

$$u = \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{E+\mu} \\ 0 \\ \sqrt{E-\mu} \\ 0 \end{pmatrix} \qquad u_a u_b^* = \frac{1}{2E} \begin{pmatrix} \quad \end{pmatrix} = \frac{1}{2E} \begin{pmatrix} E+\mu & 0 & p & 0 \\ 0 & 0 & 0 & 0 \\ p & 0 & E-\mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$u = \frac{1}{\sqrt{2E}} \begin{pmatrix} 0 \\ \sqrt{E+\mu} \\ 0 \\ -\sqrt{E-\mu} \end{pmatrix}$$

some idea $= \frac{1}{2E} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & E+\mu & 0 & -p \\ 0 & 0 & 0 & 0 \\ 0 & -p & 0 & E-\mu \end{pmatrix}$

$$\lambda = \frac{1}{2E}\begin{pmatrix} E+\mu & 0 & p & 0 \\ 0 & E+\mu & 0 & -p \\ p & 0 & E-\mu & 0 \\ 0 & -p & 0 & E-\mu \end{pmatrix}$$

$$= \frac{1}{2E}\left(E1 + \mu\beta + \alpha_z p\right)$$

In general

$$\lambda = \frac{1}{2E}\left(E1 + \mu\beta + \alpha \cdot \mathbb{P}\right)$$

Then

$$A = \frac{u_2^* \alpha_2 \left(|E_i| + \mu\beta + \alpha \cdot \mathbb{P}_i\right) \alpha_1 u_1}{2|E_i|\left(E_1 + \omega_1 - |E_i|\right)}$$

$$+ \frac{u_2^* \alpha_2 \left(E_i - \mu\beta - \alpha \cdot \mathbb{P}_i\right) \alpha_1 u_1}{2|E_i|\left(E_1 + \omega_1 + |E_i|\right)}$$

$$E_i = \sqrt{\mu^2 + (|\mathbb{P}_1| + |\mathbb{K}_1|)^2}$$

Note we might have deduced this by using

$$\sum_i \langle 2|A|i\rangle\langle i|B|1\rangle = \langle 2|AB|1\rangle$$

But note also

$$\sum_i (u_2^* N)\frac{(H_{HP;i} + |E;i|)}{2E;i}(u_i M u_1)$$

$$= \sum_{\text{pos } E} (u_2^* N u_i)(u_i^* M u_i)$$

$$= \frac{u_2^* N(|E|+H) M u_1}{2E_1}$$

This is what we could have done to get π. Used concept of projection operator $|E,|+H$. (Kramers)

Now add terms to find

$$A = \frac{u_2^* \alpha_2 (E_1 + \omega_1 - \mu\beta - \alpha\cdot P_i)\alpha_1 u_1}{(E_1+\omega_1)^2 - |E_i|^2}$$

We now find a way to write this directly.

$$A = \frac{u_2^* \alpha_2 (E_1 + \omega_1 + \alpha \cdot (\mathbf{P}_1 + \mathbf{K}_1) + \mu\beta) \alpha_1 u_1}{\underbrace{(E_1 + \omega_1)^2 - (\mathbf{P}_1 + \mathbf{K}_1)^2 - \mu^2}_{\Delta \text{ vector}}}$$

Note how this appears rel. invariant. How can we make the invariance obvious by cleaning up Dirac notation.

Recall we had

$$\gamma_4 \equiv \beta$$

$$\gamma_{x_i} = \beta \alpha_x \quad \gamma_4 = \beta \alpha_4 \quad \gamma_z = \beta \alpha_z$$

so we can rewrite Dirac eqn as

$$\underbrace{(E p\beta - \beta \alpha \cdot \mathbf{P})}_{P_\mu \gamma_\mu} u = mu$$

or

$$P_\mu \gamma_\mu u = mu$$

Thus put A in terms of γ's.

$$A = \frac{(u_2^* \beta [\gamma \cdot e_2] [(p_{1\mu} + k_{1\mu})\gamma_\mu + \mu](\gamma \cdot e_1) u_1)}{(p_{1\mu} + k_{1\mu})(p_{1\mu} + k_{1\mu}) - \mu^2}$$

Can imagine $\gamma \cdot e_1 = \gamma_\mu e_\mu$ where $e_\mu = (0, \cdots 0)$

Define $u^* \beta = \bar{u}$ relativistic conjugate

If $u^* = u_1^* u_2^* u_3^* u_4^*$

$$\bar{u} = u_1^* u_2^* - u_3^* - u_4^*$$

and

$$\gamma_\mu a_\mu \equiv \not{a}$$

Then

$$A = \frac{\bar{u}_2 \not{e}_2 (\not{p}_1 + \not{k}_1 + \mu) \not{e}_1 u_1}{(\not{p}_1 + \not{k}_1)^2 - \mu^2}$$

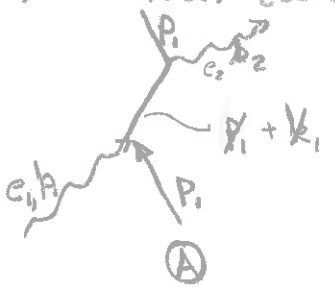
note "strength" of intermediate state depends on

$$\frac{1}{(p_1 + k_1)^2 - \mu^2}$$

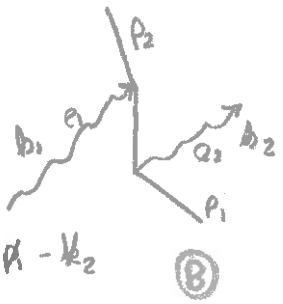
4/17/67 Lecture

Problem:
Positron annihilation $e^+ + e^- \to 2\gamma$ (disregard e^- motion)
Estimate lifetime of positronium
Discuss polarization character of photons

Compton Effect (continued)



Ⓐ



Ⓑ

Note Ⓑ is topologically different from Ⓐ. Now write amplitudes in new notation

$$Ⓐ = \frac{(\bar{u}_2 \not{e}_2 (\not{p}_1 + \not{k}_1 + m) \not{e}_1 u_1)}{(p_1 + k_1)^2 - m^2}$$

$$Ⓑ = \frac{(\bar{u}_2 \not{e}_1 (\not{p}_1 - \not{k}_2 + m) \not{e}_2 u_1)}{(p_1 - k_2)^2 - m^2}$$

Can we figure out a way to write these directly? Recall notation

$$a_\mu b_\mu = a \cdot b = a_4 b_4 - a_x b_x - a_y b_y - a_z b_z$$

$$\nabla_\mu = \left(\frac{\partial}{\partial t_1}, -\frac{\partial}{\partial x_1}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}\right)$$

$$\gamma_\mu = (\beta, \beta\alpha_x, \beta\alpha_y, \beta\alpha_z)$$

$$a_\mu \gamma_\mu \equiv \not{a} = a_4 \gamma_4 - a_x \gamma_x - a_y \gamma_y - a_z \gamma_z$$

$$= \beta(a_4 - \vec{\alpha} \cdot \vec{a})$$

$$\not{\nabla} = \nabla_\mu \gamma_\mu = \gamma_4 \frac{\partial}{\partial t} + \gamma_1 \frac{\partial}{\partial x} + \gamma_4 \frac{\partial}{\partial y} + \gamma_2 \frac{\partial}{\partial z}$$

$$= \beta \left[\frac{\partial}{\partial t} + \vec{\sigma} \cdot \vec{\nabla} \right]$$

Now

$$\not{a}^2 = a_\mu \cdot a_\mu$$

$$\not{a} = \not{b} \Longrightarrow a_\mu = b_\mu$$

Sometimes he uses / for 4-vectors also $(\not{p}, \vec{p})$

$$\not{a}\not{b} = 2(a \cdot b) - \not{b}\not{a} \qquad \text{[expresses commutation laws of } \gamma\text{'s]}$$

$$\not{a}\gamma_\nu + \gamma_\nu \not{a} = 2a_\nu$$

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\delta_{\mu\nu}$$

The Dirac equation now becomes

$$\left(i\not{\nabla} - \frac{e}{c}\not{A} - m \right) \psi = 0$$

—o—

Ex: $\not{e}_1 = -\gamma_x \qquad \not{p} = m\gamma_4$, etc.

—o—

Current density

$$j_\mu = \bar{\psi} \gamma_\mu \psi$$

$$\left[\begin{array}{l} \psi^* \psi \text{ density} \\ \psi^* \alpha \psi \text{ current} \end{array} \right]$$

$$\bar{\psi} = \underline{\psi_1^* \psi_2^* - \psi_3^* - \psi_4^*}$$

Now our matrix element looks relativistic invariant.

1.) But u_1 & u_2 are not strictly invariant because of normalization

2.) Formula for prob/sec & phase space density etc

3.) Rel. inv. of e

1.) Normalization: we have been taking

$$u^* u = 1 = \bar{u} \beta u = a \gamma_4 u$$

This rep. 1 particle/unit vol. But not invariant.

Our new normalization will be

$$\bar{u} u = 2m$$

[2m instead of 1 to get rid of $\sqrt{2E}$ factor in front of spinor]

$$\bar{u} \gamma_4 u = 2E = u^* u$$

Also change M as

$$M = M \underbrace{\sqrt{2E_1}\ \sqrt{2E_2} \sqrt{2\omega_1} \sqrt{2\omega_2}}$$

$\sqrt{2}$ energy of every free particle

2.) Our dd formula was

$$\text{Rate} = 2\pi\,\delta(E_f - E_i)\,\frac{d^3|K_2}{(2\pi)^3}\,\frac{1}{2E_1 2E_2 2\omega_1 2\omega_2}\,|\mathcal{M}|^2$$

$$= \frac{(2\pi)^4}{2E_1 2\omega_1}\,\delta(E_f - E_i)\,\delta^3(\mathbb{P}_f - \mathbb{P}_i)\,\frac{d^3|K_2}{(2\pi)^3 \cdot 2\omega_2}\,\frac{d^3\mathbb{P}_2}{(2\pi)^3 \cdot 2E_2}\,|\mathcal{M}|^2$$

4-vector 6-fun

$dP_z \neq dP_z'$ but $\frac{dP_z}{E} = \frac{dP_z'}{E'}$ for invariance

Actually rate isn't invariant due to $\frac{1}{E_1 \omega_1}$

Sometimes people use

$$2\pi\,\delta(p^2 - m^2)\,\frac{d^4p}{(2\pi)^4}$$ as invariant differential.

This in general

$$\text{Rate} = (2\pi)^4\,\delta^4(\text{4mom in} - \text{4mom out})$$

$$\prod_{in}\frac{1}{2E_{in}}\prod_{out}\frac{d^3|P_{out}}{(2\pi)^3 2E_{out}}\,|\mathcal{M}_{fi}|^2$$

Inv. matrixelement

4/18/67 LECTURE

$$\text{Rate} = \left(\prod_{in} \frac{1}{2E_{in}}\right)\left(\prod_{out} \frac{1}{2E_{out}}\right) \cdot \text{Density of final states/unit energy range} \; 2\pi |M|^2$$

$$= \left(\prod_{in} \frac{1}{2E_{in}}\right)(2\pi)^4 \delta^4\left(\textstyle\sum p_{in} - \sum p_{out}\right) \prod_{out} 2\pi\, \delta(p_i^2 - m_i^2) \frac{d^4p_i}{(2\pi)^4} |M|^2$$

where $$2\pi\, \delta(p_i^2 - m^2) \frac{d^4p_i}{(2\pi)^4} = \frac{d^3p_i}{(2E_i)(2\pi)^3}$$

Compton scattering yields

$$M = \bar{u}_2 \not{\epsilon}_2 \frac{(\not{p}_1 + \not{k}_1 + m)\not{\epsilon}_1 u_1}{(p_1 + k_1)^2 - m^2} + \bar{u}_2 \not{\epsilon}_1 \frac{(\not{p}_1 - \not{k}_2 + m)\not{\epsilon}_2 u_1}{(p_1 - k_2)^2 - m^2}$$

The main idea was to write the Rate in a manner in which the relativistic invariance is obvious. Note for 2 particles in

$$\text{Rate} = \sigma v_{rel} \qquad v_{rel} = |V_1 - V_2|$$

The cross-section should be invariant. Note from earlier this means $v_{rel} E_1 E_2$ is invariant since the rate transforms as $Y_{E_1 E_2}$. Continue to demonstrate this.

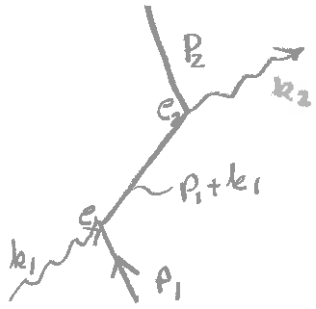
For only one particle in,

$$\text{Rate} = \frac{1}{\tau} \quad , \; \tau = \text{lifetime}$$

In our expression for M, $\frac{\not p_1 + \not k_1 + m}{(p_1+k_1)^2 - m^2}$ is called the propagator of a virtual proton

In general for an electron propagator

$$\frac{\not p + m}{p^2 - m^2 + i\epsilon}$$



For interaction with a photon of pol. vector e_μ,

$$\text{amp} = \sqrt{4\pi}\, e \not e$$

The amplitude for a free electron to enter is u
" " " " " " leave " $\bar{u}$

Thus we can synthesize the matrix element directly

(amp for electron to leave ②)	(amp. to interact with photon ②)	(propagation from ① to ②)	(amp to absorb photon at ①)	(amp. for electron to enter at ①)
$\bar{u}_2$	$\not e_2$	$\frac{\not p_1 + \not k_1 + m}{(p_1+k_1)^2 - m^2}$	$\not e_1$	u_1

Note the propagator is usually written as

$$\frac{1}{\not{p}-m}$$

or the reciprocal of a matrix

Must solve $(\not{p}-m)\chi = 1$

$$\frac{(\not{p}-m)(\not{p}+m)}{p^2-m^2} = \frac{p^2-m^2}{p^2-m^2} = 1$$

$$\Rightarrow \quad \frac{1}{\not{p}-m} = \frac{\not{p}+m}{p^2-m^2+i\epsilon}$$

Thus the propagator is in general the reciprocal of a Dirac operator. Consider

$(i\not{\partial}-m)\psi = S$ as Dirac eqn for free particle

Take F.T.

$$(\not{p}-m)\psi = S$$

$$\text{or} \quad \psi = \frac{1}{\not{p}-m+i\epsilon} S$$

Thus a mnemonic is to regard each interaction as a source of mass

$$\bar{u}_2 \not{\epsilon}_2 \frac{1}{\not{p}+\not{k}_1-m} \not{\epsilon}_1 u_1$$

Consider

$$(i\not\partial - \not K - m)\psi = 0$$

or

$$(i\not\partial - m)\psi = \not K \psi$$

Solve by Neumann series

$\psi_0 = \phi_1$ zeroth approx $\Rightarrow (i\not\partial - m)\phi = 0$

Next solve

$$(i\not\partial - m)\psi_1 = \not K \phi_1$$

$$\psi_1 = \phi_1 + \frac{1}{i\not\partial - m}\not K \phi_1$$

and so on until

$$\psi = \phi + \frac{1}{i\not\partial - m}\not K \phi + \frac{1}{i\not\partial - m}\not K \frac{1}{i\not\partial - m}\not K \phi + \cdots$$

(~ propagate ~ any # of interactions potential ~ free waves)

This is just a perturbation expansion.

Thus it is important to learn these tricks because they make the calculations so much simpler.

Also idea of representing a scattering as a 2-nd order process

In general for $\nabla \cdot A = 0 \quad \varphi = 0$

$$A_\mu = e_\mu e^{-ik\cdot x} = e_\mu e^{-i(\omega t - k\cdot x)}$$

$\therefore \quad \nabla \cdot A = 0 \Rightarrow e \cdot k = 0 \qquad \varphi = 0 \Rightarrow e_t = 0 \qquad e \cdot e = 1$

But note

$$e_\mu k_\mu = e_t \omega - e \cdot k = 0$$

$$e_\mu e_\mu = -1$$

But expect that we could Lorentz transform to system where $e_t \neq 0$. How do we get right answer? This has to do with an additional property of electrodynamics and concerns gauge invariance

$$A''_\mu = A_\mu + \nabla_\mu \chi$$

Has nothing to do with Lorentz invariance. It is true for Dirac eqn

$$(i\not{\nabla} - \not{k} - m)\psi = 0$$

$$(i\not{\nabla} - \underbrace{\not{A} - \not{\nabla}\chi}_{\not{A}''} - m)\psi'' = 0$$

If we use $\psi'' = e^{i\chi}\psi$, we get same physics. Thus gauge invariance introduces a phase.

Substituting in

$$\gamma_\mu (i\nabla_\mu - A'_\mu) e^{i\chi}\psi - m e^{-i\chi}\psi = 0$$

$$e^{-i\chi}\left[\gamma_\mu(+\nabla_\mu\chi + i\nabla_\mu - A''_\mu)\psi\right] = m e^{-i\chi}\psi$$

or

$$\gamma_\mu\left[i\nabla_\mu - \underbrace{(A'_\mu - \nabla_\mu\chi)}_{A_\mu}\right]\psi = m\psi \qquad \text{Q.E.D.}$$

Thus rule is to use

$$A''_\mu = A_\mu + \nabla_\mu\chi$$

$$\psi'' = e^{i\chi}\psi$$

Thus suppose we have plane wave

k_1 $\qquad A_\mu = e_\mu e^{-ik_1\cdot x}$

$$A''_\mu = e''_\mu e^{-ik_1\cdot x} = A_\mu + \nabla_\mu\chi$$

$$= e_\mu e^{-ik_1\cdot x} + k_\mu\alpha e^{-ik_1\cdot x}$$

Thus $e_\mu'' = e_\mu + \alpha k_\mu$ without changing physics.

Can always use the gauge invariance to get rid of the time component e_t. Thus can always wipe out ϕ, the scalar potential.

We then demonstrate this on Compton matrix element.

$$M^{new} = M^{old} + \underbrace{\alpha \bar{u}_2 \not{k}_2 \frac{1}{\not{p}_1 + \not{k}_1 - m} \not{k}_1 u_1}_{\bar{u}_2 \not{p}_2 \frac{1}{\not{p}_1 + \not{k}_1 - m} (\not{p}_1 + \not{k}_1 - m) u_1 \; - \; \bar{u}_2 (\not{p}_2 - \not{k}_1 - m) \frac{1}{\not{p}_2 - \not{k}_1 - m} \not{\epsilon} u_1} + \bar{u}_2 \not{k}_1 \frac{1}{\not{p}_1 - \not{k}_2 - m} \not{\epsilon}_2 u_1$$

$$\bar{u}_2 \not{\epsilon}_2 u_1 - \bar{u}_2 \not{\epsilon}_2 u_1 = 0$$

$\Rightarrow M^{new} = M^{old}$ $\Rightarrow$ formula is gauge invariant

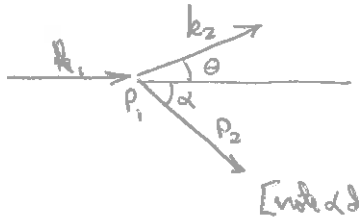
Note both terms in the matrix element are of equal significance in determining gauge invariance. Thus arguments that one diagram is "larger" than another are misleading

In general, a simple diagram is relativistic invariant but not gauge invariant

Need all diagram for gauge invariance

4/21/67 LECTURE

We now do the arithmetic of the Compton formula



[note α defined <0]

$p_1 = m(1,0,0,0)$

$p_2 =$

$k_1 = \omega_1(1,0,0,1)$

$k_2 = \omega_2(1,\sin\theta,0,\cos\theta)$

Recall $\quad \frac{1}{\omega_2} - \frac{1}{\omega_1} = \frac{1}{m}(1-\cos\theta)$

Also need $\cos\alpha$:

$$p_2 + k_2 = p_1 + k_1 \quad \text{yields} \quad m\omega_2 = \omega_1(E_2 - p_2\cos\alpha)$$

Now recall

$$M = \frac{\bar{u}_2 \not{e}_2 (\not{p}_1 + \not{k}_1 + m)\not{e}_1 u_1}{(p_1+k_1)^2 - m^2} + \frac{\bar{u}_1 \not{e}_1 (\not{p}_1 - \not{k}_2 + m)\not{e}_2 u_1}{(p_1 - k_2)^2 - m^2}$$

$$\text{Rm}\,M = \frac{\bar{u}_2 \not{e}_2 (\not{p}_1 + \not{k}_1 + m)\not{e}_1 u_1}{\omega_1} - \frac{\bar{u}_1 \not{e}_1 (\not{p}_1 - \not{k}_2 + m)\not{e}_2 u_1}{\omega_2}$$

Possible cases: $\quad u_{1+} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}\sqrt{m}$ pos z spin ; $u_{1-} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}\sqrt{m}$ neg z spin

$$u_{2+} = \begin{pmatrix}\sqrt{E_2+m}\cos\alpha/2\\ -\sqrt{E_2+m}\sin\alpha/2\\ \sqrt{E_2-m}\cos\alpha/2\\ -\sqrt{E_2-m}\sin\alpha/2\end{pmatrix} \text{pos helicity}; \quad u_{2-} = \begin{pmatrix}\sqrt{E_2+m}\sin\alpha/2\\ \sqrt{E_2+m}\cos\alpha/2\\ -\sqrt{E_2-m}\sin\alpha/2\\ -\sqrt{E_2-m}\cos\alpha/2\end{pmatrix} \text{neg helicity}$$

- $\not{e}_{1a} = \gamma_x$ or $\not{e}_{1b} = \gamma_y$

- $\not{e}_{2a} = \gamma_x\cos\alpha + \gamma_z\sin\alpha$ or $\not{e}_{2b} = \gamma_y$

($\perp$ plane pol) ($\parallel$ plane pol)

$$\not{p}_1 = m\gamma_+ \qquad \not{k}_1 = \omega_1(\gamma_+ - \gamma_z) \qquad \not{k}_2 = \omega_2(\gamma_+ - \gamma_z\cos\theta - \gamma_x\sin\theta)$$

Thus must workout M for 16 different cases. We do 1 case

$u_{1+}, u_{2+}, e_{1a}, e_{2a}$

$$\textcircled{A} = \frac{\bar{u}_{2+}}{\omega_1}(\gamma_x\cos\theta - \gamma_z\sin\theta)(m\gamma_+ + m + \omega_1\gamma_+ - \omega_1\gamma_z)\gamma_x u_{1+}$$

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

$\gamma_+ = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $\gamma_x = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}$

$\gamma_+\gamma_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$ $\gamma_x\gamma_y = -i\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$ $i\gamma_x\gamma_y = \sigma_z$

$\gamma_x\gamma_y\gamma_z = \gamma_5\gamma_+ = -i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$\gamma_x\gamma_y\gamma_+ = \gamma_5\gamma_+ = -i\begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}$

where $\gamma_5 \equiv \gamma_x\gamma_y\gamma_z\gamma_+ = i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\textcircled{A} = \frac{\bar{u}_{2+}}{\omega_1}(\gamma_x\cos\theta - \gamma_z\sin\theta)\gamma_x(-\cancel{m}\gamma_+ + m - \cancel{\omega_1}\gamma_+ + \cancel{\omega_1}\gamma_z)u_{1+}$$

note $\gamma_+ u_1 = u_1$

$$= \bar{u}_{2+}(-\cos\theta - \gamma_z\gamma_x\sin\theta)(-1 + \gamma_z)u_{1+}$$

$$= \begin{pmatrix} \sqrt{E_2+\mu}\cos\frac{\alpha}{2}, & -\sqrt{E_2+\mu}\sin\frac{\alpha}{2}, & -\sqrt{E_2-\mu}\cos\frac{\alpha}{2}, & \sqrt{E_2-\mu}\sin\frac{\alpha}{2} \end{pmatrix} \begin{pmatrix} \cos\theta \\ \sin\theta \\ \cos\theta \\ \sin\theta \end{pmatrix}$$

$$= \sqrt{E_2+\mu}\left(\cos\tfrac{\alpha}{2}\cos\theta - \sin\theta\sin\tfrac{\alpha}{2}\right) - \sqrt{E_2-\mu}\left(\cos\theta\cos\tfrac{\alpha}{2} - \sin\theta\sin\tfrac{\alpha}{2}\right)$$

$$= \left(\sqrt{E_2+\mu} + \sqrt{E_2-\mu}\right)\cos\left(\theta + \tfrac{\alpha}{2}\right)\sqrt{2m}$$

UNRELATIVISTIC FORM OF Q.E.D. (many electron systems) 4/23/67 LECTURE

$$H = \underbrace{\frac{1}{8\pi}\int (E^2+B^2)\,dV\lambda}_{\text{E \& M field}} + \underbrace{\int \Psi^*(x)\left[\beta m + e\phi(x) + \alpha\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}A\right)\right]\Psi(x)\,d^3x}_{\text{energy of electron}}$$

$$= \underbrace{\frac{1}{8\pi}\int (E^2+B^2)\,dV\lambda}_{\text{H field}} + \underbrace{\int \Psi^*(x)\left[\beta m + \alpha\cdot\left(\frac{\hbar}{i}\nabla\right)\right]\Psi(x)\,d^3x}_{\text{H electron-positron}}$$

$$+ \underbrace{e\int \Psi^*(x)\left[\phi(x) - \alpha\cdot A\right]\Psi(x)\,d^3x}_{\text{H int of electron-field with matter}}$$

Now choose $\nabla\cdot A = 0$ $\left[\nabla^2\phi = \rho,\ \phi = \frac{\rho}{r}\right]$

Then write

$$A(x) = \sum_{i,k} \sqrt{\frac{4\pi}{2\omega_k}}\left(e_i a_{k,i} e^{ik\cdot x} + e_i^* a_{k,i}^* e^{-ik\cdot x}\right)$$

$e_{k,i}$ = polarization vector of photon of momentum k

i = index of photon pol. (2 values)

$a_{k,i}$ = annihilation op. for photons

Then

$$H = \underbrace{\sum_{k,i} \hbar\omega_{ik}\, a^*_{k,i}\, a_{k,i}}_{H_{field}} + \underbrace{\int \Psi^* \left[\beta m + \alpha \cdot p\right] \Psi \, d^3x}_{H_{el,pos}}$$

$$+ \underbrace{\frac{e^2}{2} \iint \frac{\Psi^*(x)\Psi(x)\,\Psi^*(y)\Psi(y)}{r_{xy}} \, d^3x\, d^3y}_{H_{coulomb}} \qquad \underbrace{- e \int \Psi^* \alpha \Psi \cdot A \, d^3x}_{H_{int}}$$

Now write

$$\Psi(x) = \sum_{p,l} c_{p,l}\, u_{p,l}\, e^{i p \cdot x}$$

$$\Psi^*(x) = \sum_{p,l} c^*_{p,l}\, u^*_{p,l}\, e^{-i p \cdot x}$$

where $(\beta m + \alpha \cdot p)\, u_{p,l} = \varepsilon\, u_{p,l}$

where $\varepsilon = +E_p$ or $-E_p$

Use index

$u_{p,k}$ = spinor for (+energy soln) k spin index 2 values

$u_{-p,j}$ = " " (− energy soln) j

Then

$$H_{el,pos} = \sum_{p,l} \varepsilon\, c^{*}_{p,Q}\, c_{p,l}$$

$$= \sum_{p,k} E_p\, c^{*}_{p,k}\, c_{p,k} - \sum_{p,j} E_p\, c^{*}_{p,j}\, c_{p,j}$$

Define

$c_{p,k}$ = means annih. electron of mom p, spin k

$c_{p,j} = d^{*}_{-p,j}$ creates positron of mom $-p$

$d_{p,j}$ annih. positron of mom p, spin j

$$H_{el,pos} = \sum_{p,k} E_p\, c^{*}_{p,k} c_{p,k} + \sum_{p,j} E_p\, d^{*}_{p,j} d_{p,j} - \sum_{p,j} E_p$$

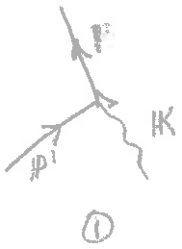
subtract out p energy of Fermi sea

Now

$$H_{int\ el.pos.-photons} = -e \sum_{p,k,p',k',K,i} \sqrt{\frac{4\pi e^2}{2\omega_K}} \left[u^{*}_{p,k}(\alpha \cdot \varepsilon_{K,i})\, u_{p',k'}\right] c^{*}_{p,k} c_{p',k'} a_{K,i} \cdot \delta(p-p'-K) \quad (1)$$

$$\sqrt{\frac{4\pi e^2}{2\omega_K}} \left[u^{*}_{p,k}(\alpha \cdot \varepsilon^{*}_{K,i})\, u_{p',k'}\right] c^{\dagger}_{p,k} c_{p',k'} a^{\dagger}_{K,i}\, \delta(p-p'+K) \quad (2)$$

3 more terms like these. Easy to see. Diagrammatically



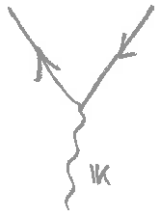
(1)

(2)

Another term is

$$-\sum_{\vec{p},k,\vec{p}',j,\vec{k},i} \sqrt{\frac{4\pi e^2}{2\omega_{\vec{k}}}} \left[u^*_{\vec{p},k} (\alpha \cdot e_{\vec{k},i}) v_{\vec{p}',j} \right] c^*_{\vec{p},k} d^*_{\vec{p}',j} a_{\vec{k},i} \delta(\vec{p}+\vec{p}'-\vec{k}) \quad (3)$$

$$\left[u^*_{\vec{p},k} (\alpha \cdot e^*_{\vec{k},i}) v_{\vec{p}',j} \right] c^*_{\vec{p},k} d^*_{\vec{p}',j} a^*_{\vec{k},i} \delta(\vec{p}+\vec{p}'+\vec{k}) \quad (4)$$



(3)

(4)

$$-\sum_{\vec{p},j,\vec{p}',k,\vec{k},i} \sqrt{\frac{4\pi e^2}{2\omega_{\vec{k}}}} \left[v^*_{\vec{p},j} (\alpha \cdot e_{\vec{k},i}) u_{\vec{p}',k} \right] d_{\vec{p},j} c_{\vec{p}',k} a_{\vec{k},i} \delta(\vec{p}+\vec{p}'+\vec{k}) \quad (5)$$

" e^* " $a^*_{\vec{k},i} \delta(\vec{p}+\vec{p}'-\vec{k})$ (6)

(5)

(6)

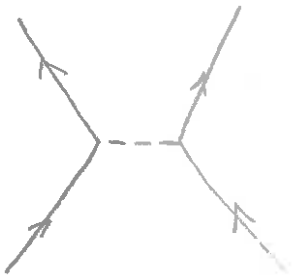
$$-\sum_{\vec{p},j,\vec{p}',j',\vec{k},i} \sqrt{\frac{4\pi e^2}{2\omega_{\vec{k}}}} \left[v^*_{\vec{p},j} (\alpha \cdot e_{\vec{k},i}) v_{\vec{p}',j} \right] d_{\vec{p},j} d^*_{\vec{p}',j} a_{\vec{k},i} \delta(\vec{p}+\vec{k}-\vec{p}') \quad (7)$$

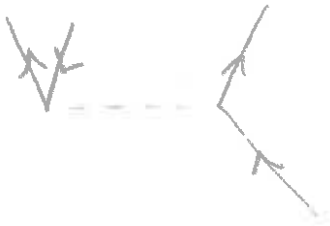
" e^* " " a^* $\delta(\vec{p}-\vec{k}-\vec{p}')$ (8)

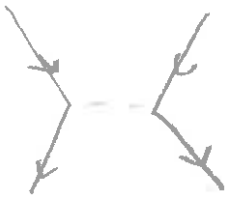
(7)

(8)

Now have 16 terms from H_int. int with diagrams like



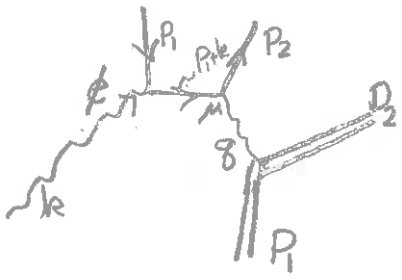




Pair Production

5/1/67 LECTURE 6

Our diagrams are



$\not{q} = \not{p}_2 - \not{p}_1$

$$\sqrt{4\pi e^2}^3 \left(\bar{u}_2 \gamma_\mu u_1\right) \frac{1}{q^2} \left(u_2 \gamma_\mu \frac{1}{p_1 + k - m} \not{\epsilon}\, u_1\right)$$

(propagator; propagator)

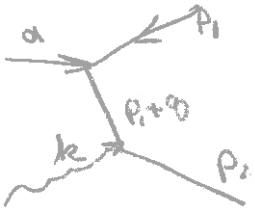
For considering girls of proton, replace $(\bar{u}_2 \gamma_\mu u_1)$ by

$\bar{\psi}_2 \left(\gamma_\mu F_1(q) + \frac{\kappa}{4m} (\gamma_\mu \not{q} - \not{q}\gamma_\mu) F_2(q)\right) \psi_1$ where is current operator

Bremsstrahlung

Assume fixed potential $V(R) = \frac{Ze^2}{R}$ usually
since most amp. comes from small $q^2 \Rightarrow$ nucleus not affected

Also a diagram

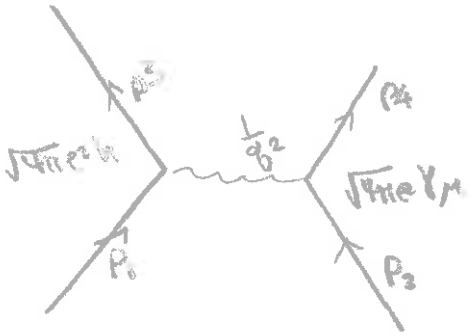


Other diagrams

$$\left(\bar{u}_2 \gamma_\mu \frac{\not{p}_1 + \not{k} + M}{(p_1+k)^2 - M^2} e \not{\epsilon}_1\right) \frac{1}{(p_1 + k - p_2)^2} (\bar{u}_2 \gamma_\mu u_1) \quad (4\pi e^2)^{3/2}$$

Note pair prod. formula is same as bremsstrahlung

Mentions shower or cascade problems



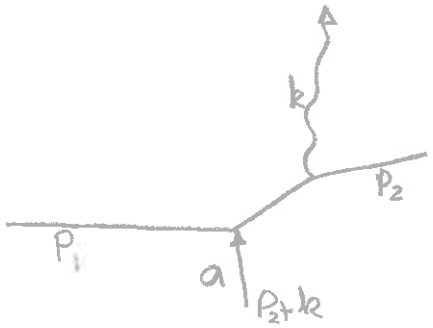
$$\frac{4\pi e^2 \,(\bar{u}_3 \gamma_\mu u_1)_\mu \,(\bar{u}_4 \gamma_\mu u_2)_\rho}{(p_3 - p_1)^2}$$

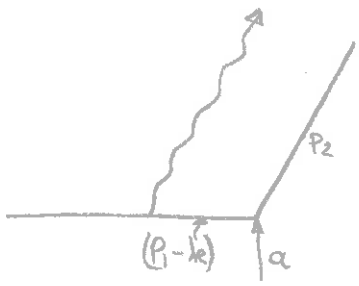
and so on.

If positive muon, expect same in first order. If potential acts [illegible] Lamb shift difference.

Pair prod

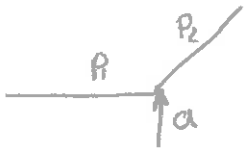
Bremsstrahlung (from potential scattering $a_\mu(q)$) 5/2/67 Lecture





$q = P_2 + k_2 - P_1$

[Scattering with no emission



$$\text{Rate} = 2\pi\delta(E_2-E_1)\frac{d^3P_2}{(2\pi)^3 2E_1 2E_2}\left|(\bar{u}_2 a_\mu u_1)\right|^2 \quad]$$

For both processes above

$$\text{Rate} = 2\pi\,\delta(E_2+\omega-E_1)\frac{d^3P_2}{(2\pi)^3\,2E_2\cdot 2E_1}\,\frac{d^3k}{2\omega\,(2\pi)^3}\,|M|^2$$

$$M = \bar{u}_2 \not{\epsilon}\,\frac{1}{\not{P}_2+\not{k}-m}\not{A}u_1 + \bar{u}_2\not{A}\,\frac{1}{\not{P}_1-\not{k}-m}\not{\epsilon}\,u_1 \quad \sqrt{4\pi e^2}$$

$$= \bar{u}_2\not{\epsilon}\,\frac{(\not{P}_2+\not{k}+m)}{2P_2\cdot k}\not{A}u_1 + \frac{\bar{u}_2\not{A}(\not{P}_1-\not{k}+m)\not{\epsilon}\,u_1}{-2P_1\cdot k}$$

We want to consider low ω behavior (neglect $k \ll P_2+m$)

Using commutation law $\not{a}\not{b} = -\not{b}\not{a} - 2(a\cdot b)$

$$M = \frac{\bar{u}_2 \left(-\not{p}_2^{m} \not{\epsilon} + 2p_2\cdot\epsilon + \not{\epsilon}\, m\right) \not{k}\, u_1}{2p_2\cdot k} + \frac{(\bar{u}_2 \not{\epsilon}\, u_1)\, 2p_1\cdot\epsilon}{-2p_1\cdot k}$$

$$= (\bar{u}_2 \not{\epsilon}\, u_1) \left\{ \frac{p_2\cdot\epsilon}{p_2\cdot k} - \frac{p_1\cdot\epsilon}{p_1\cdot k} \right\} \sqrt{4\pi e^2}$$

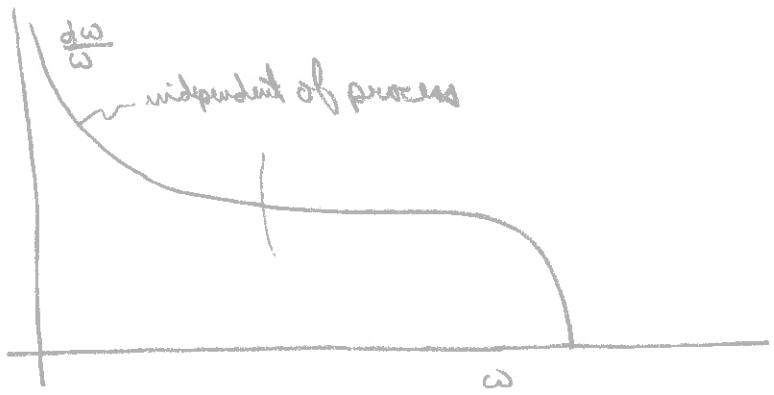
↳ matrix element for scattering without emission of photons

amp. that if scattering results in photon

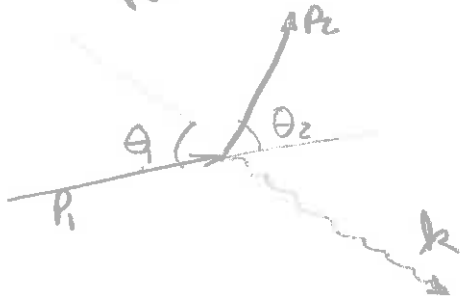
Thus

$$\text{Rate} = \underbrace{2\pi\, \delta(E_2 - E_1)\, \frac{d^3 p_2}{(2\pi)^3 2E_2 2E_1}\, (\bar{u}_2\, a(q)\, u_1)^2}_{\text{Prob with no photon emitted}} \underbrace{\left\{ \omega \left(\frac{p_2\cdot\epsilon}{p_2\cdot k} - \frac{p_1\cdot\epsilon}{p_1\cdot k} \right) \right\}^2 4\pi e^2 \frac{d\omega}{\omega} \frac{d\Omega_2}{4(2\pi)^3}}_{\text{prob that if electron scattering it emits a soft photon}}$$

Prob.



To analyze in more detail, consider coordinates



$$p_1 \cdot k = E_1\omega - p_1\omega\cos\theta_1 = \omega E_1(1 - v_1\cos\theta_1)$$

where $v_1 = \frac{p}{E}$

$$p_1 \cdot \epsilon = -\mathbf{p}_1 \cdot \boldsymbol{\epsilon} = -E v_1 \cdot \boldsymbol{\epsilon}$$

Then

$$\{\ \} = \frac{\mathbf{v}_1 \cdot \boldsymbol{\epsilon}}{1 - v_1\cos\theta_1} - \frac{\mathbf{v}_2 \cdot \boldsymbol{\epsilon}}{1 - v_2\cos\theta_2}$$

$$= \frac{v_1 \sin\theta_1}{1 - v_1\cos\theta_1} - \frac{v_2 \sin\theta_2}{1 - v_2\cos\theta_2}$$ part. in plane of collision

Can get same result from classical physics

PROBLEM: Emission of two independent photons.

Classical Bremsstrahlung:

Instead of using Lienard-Wiechert potentials, do a different way. Consider a path in 4-d space. Now to write current density

$$j_\mu(x) = e\int \dot{z}_\mu(\alpha)\,\delta^4(x - z(\alpha))\,d\alpha$$

Now must solve $\Box^2 A_\mu = j_\mu$. Also Fourier FT.

$$a_\mu(k) \equiv \int A_k(x)\, e^{-ik\cdot x}\, d^4x$$

Now take F.T. of eqn,

$$k^2 a_\mu(k) = \int e^{-ikx}\, j_\mu(x)\, d^4x$$

$$= \int e^{-ikx} \int \dot{z}_\mu(\alpha)\,\delta^4(x - z(\alpha))\,d\alpha\, d^4x$$

$$= \int \dot{z}_\mu(\alpha)\, e^{-ik\cdot z(\alpha)}\, d\alpha = j_\mu(k)$$

For $\alpha < 0$, $z_\mu(\alpha) = p_{1\mu}\,\alpha$

$\alpha > 0$, $z_\mu(\alpha) = p_{2\mu}\,\alpha$

Thus

$$j_\mu(k) = \int_{-\infty}^{0} p_{1\mu}\, e^{-ik\cdot p_1 \alpha}\, d\alpha + \int_{0}^{\infty} p_{2\mu}\, e^{-ik\cdot p_2 \alpha}\, d\alpha$$

or $$J_\mu(k) = i\left(\frac{p_{1\mu}}{p_1\cdot k} - \frac{p_{2\mu}}{p_2\cdot k}\right)$$

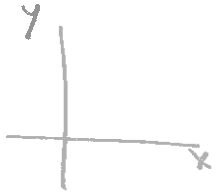
which agrees with what we found from QED.

Classical expected energy in $d\omega = \hbar e^2 C(\omega)\,d\omega$. In q.m., mean energy liberated is $\hbar e^2 C(\omega)\,d\omega$. But mean no. of photons is $e^2 C(\omega)\,d\omega$. Like Poisson distribution

$$\frac{(\bar{n})^n}{n!} e^{-\bar{n}}$$

5/3/67 LECTURE

Group



$$Uf(x,y) = \xi(x,y)\frac{\partial f}{\partial x} + \eta(x,y)\frac{\partial f}{\partial y}$$

Once-extended group

$$U'f(x,y,y') = \xi(x,y)\frac{\partial f}{\partial x} + \eta(x,y)\frac{\partial f}{\partial y} + \eta'(x,y,y')\frac{\partial f}{\partial y'}$$

where

$$\eta'(x,y,y') = \frac{D}{Dx}\eta(x,y) - y'\frac{D}{Dx}\xi(x,y)$$

$$= \frac{\partial \eta}{\partial x} + \left(\frac{\partial \eta}{\partial y} - \frac{\partial \xi}{\partial x}\right)y' - \frac{\partial \xi}{\partial y}y'^2$$

The general form of the ODE is

$$\Omega(x,y,y') = 0 \qquad \text{-- a surface}$$

We want $U'\Omega = 0$ for invariance

$$= \xi\frac{\partial \Omega}{\partial x} + \eta\frac{\partial \Omega}{\partial y} + \eta'\frac{\partial \Omega}{\partial y'} = 0 \qquad (*)$$

We know there can be two independent integrals of (*) $u(x,y,y')$, $v(x,y,y')$. The general solution is some

$$W(u,v) = 0$$

More explicitly $W(u,v) = v - w(u) = 0$

We are free to choose

$$u(x,y,y') = u(x,y) \quad \Rightarrow \quad \xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} = 0$$

or $\dfrac{dx}{\xi(x,y)} = \dfrac{dy}{\eta(x,y)} \Rightarrow u(x,y) = \text{const} = c$

$\Rightarrow y = y(x,c)$

Suppose pathcurves $u(x,y) = \text{const}$ are known. Then can solve

$$\frac{dx}{\xi(x,\, y(x,c))} = \frac{dy'}{\eta_x + (\eta_y - \xi_x) y' - \xi_y y'^2} \Rightarrow v(x,y';c) = c_1$$

or

$$\frac{d(y')}{dx} = \frac{1}{\xi}\frac{\partial \eta}{\partial x} + \frac{1}{\xi}\left(\frac{\partial \eta}{\partial y} - \frac{\partial \xi}{\partial x}\right) y' - \frac{\partial \xi}{\partial y} y'^2$$

$$= F(x;c) + F_1(x;c)\, y' + F_2(x;c)\, y'^2 \qquad (*)$$

General form of Riccati equation

Then can write $\quad y'(x) = y'_p(x) + \dfrac{1}{g(x)} \qquad (**)$

where $y'_p(x) = \dfrac{\eta}{\xi}$ is particular solution

[$\xi y' - \eta = 0$

or $(\xi_x + y'\xi_y)\, y' + \xi \dfrac{dy'}{dx} - (\eta_x + y'\eta_y) = 0$]

Now if we stick (*) into (**) we get a linear equation for $g(x)$

$$\frac{dg}{dx} = -F_1(x,c)\,g(x) - 2y_p' F_2(x,c)\,g(x) - F_2(x,c)$$

This can be integrated by quadratures to find $g(x)$.

An alternative method is to introduce canonical coordinates: $r(x,y)$, $s(x,y)$ $\Rightarrow$ $Uf \equiv \frac{\partial f}{\partial r} \equiv U^1 f$

Now ODE is $W(r, s, \frac{ds}{dr}) = 0$. To admit translation group we require

$$\frac{ds}{dr} - F(r) = 0$$

Now to get back to (x,y), use

$$\frac{s_x + s_y y'}{r_x + r_y y'} - F(r(x,y)) = 0$$

EXAMPLE: Similarity Transformation $Uf = x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y}$

Then

$$Uf = x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} + 0\frac{\partial f}{\partial y'} \quad \text{as extended group}$$

$$= Uf$$

Now to find $u(x,y)$, $v(x,y,y')$ which satisfy

$$x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} + 0\frac{\partial f}{\partial y'} = 0$$

$$\frac{dx}{x} = \frac{dy}{y} \quad \Rightarrow \quad u = \frac{y}{x} = \text{const}$$

By inspection take $v = f(y) = y'$, for instance.

$$\Rightarrow \quad y' = \frac{dy}{dx} = F\left(\frac{y}{x}\right)$$

$\Rightarrow$ general form of ODE admitting U.

EXAMPLE: Rotation Group $Uf = -y\frac{\partial f}{\partial x} + x\frac{\partial f}{\partial y}$

$$Uf = -y\frac{\partial f}{\partial x} + x\frac{\partial f}{\partial y} + (1+y'^2)\frac{\partial f}{\partial y'}$$

To find invariants

$$\frac{dx}{-y} = \frac{dy}{x} = \frac{dy'}{1+y'^2}$$

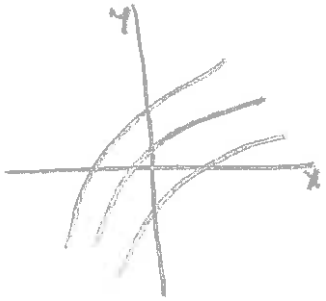
find $u(x,y) = x^2+y^2$

take $\tan^{-1} y' - \sin^{-1}\frac{y}{\sqrt{u}} = \text{const} = \tan^{-1} v$

$$\therefore V = \tan\left(\tan^{-1} y' - \tan^{-1}\frac{y}{x}\right) = \frac{y' - y/x}{1 + y'\,y/x} = \frac{xy' - y}{x + yy'} = f(x^2+y^2)$$

In this way you can use different groups to generate a table of 1st order ODE which admit those groups.

Second Order ODE's



Now two parameter family of curves
(2 initial conditions or b.c.)

∞^2 family of curves

$$\omega(x, y; a, b) = 0$$

where a, b are essentially independent

Invariance under point transformations

$$X_1 = \varphi(x, y)$$

$$Y_1 = \psi(x, y)$$

$$\Rightarrow \quad T[\omega] = \omega(x_1, y_1; a_1, b_1) = 0$$

Example: all st. lines in plane

$$\omega(x, y; a, b) = y - ax - b = 0$$

Should be invariant under rotation:

$$X = x_1 \cos\theta + y_1 \sin\theta$$
$$Y = y_1 \cos\theta - x_1 \sin\theta$$

Can verify this by direct calculation

Now consider $\omega(x, y; a, b) = 0$

$$D_x \omega = \omega_x + \omega_y y' = 0$$

$$\frac{d^2\omega}{dx^2} = \omega_{xx} + \omega_{xy} y' + \omega_y y'' = 0$$

Can eliminate a & b from these to obtain some 2nd order ODE

$$\Omega(x, y, y', y'') = 0 \qquad (***)$$

Can now talk about invariance of this ODE $\Rightarrow$

$$\Omega(x_1, y_1, y_1', y_1'') = 0 \qquad [\Omega \text{ is same fn as in } (***)]$$

Now use extended group concept.

$$x_1 = \phi(x, y)$$

$$y_1 = \psi(x, y)$$

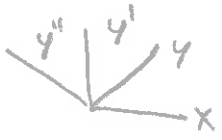
$$y_1' = \frac{\psi_x + \psi_y y'}{\phi_x + \phi_y y'} = \chi(x, y, y')$$

Need also

$$y_1'' = \frac{dy_1'}{dx} = \frac{d\chi}{d\phi} = \frac{\chi_x + \chi_y y' + \chi_{y'} y''}{\phi_x + \phi_y y'}$$

Need to construct twice extended infinitesimal transformation

$$U''f(x, y, y', y'')$$



or

$$U''f = \xi(x,y)\frac{\partial f}{\partial x} + \eta(x,y)\frac{\partial f}{\partial y} + \eta'(x,y,y')\frac{\partial f}{\partial y'} + \eta''(x,y,y',y'')\frac{\partial f}{\partial y''}$$

Now

$$\eta' = \frac{D}{Dx}\eta - y'\frac{D\xi}{Dx}$$

Can show

$$\eta'' = \frac{D}{Dx}\eta' - y''\frac{D\xi}{Dx}$$

4/28/67 LECTURE

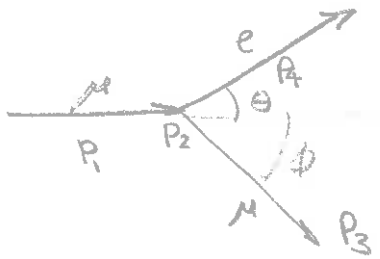
Directions

QED → (lowest order) Compt, Brems, Pair Prod. → go round results

→ High order corrections

→ β-decay, meson theory

EXAMPLE – μ-e scattering



$P_2 = (m_e, 0, 0, 0)$

$P_1 = (E, p, 0, 0)$

$P_4 + P_3 = P_1 + P_2$

$P_1^2 = \mu^2$ $\quad P_3^2 = \mu^2$

$P_2^2 = m_e^2$ $\quad P_4^2 = m_e^2$

$P_4 (W, \pi \cos\theta, \pi \sin\theta, 0)$ → all kinematic formulas.

Then

$$\text{Rate} = \sigma v_m = (2\pi)^4 \delta^4(\Sigma P_{in} - \Sigma P_{out})\, \delta(P_3^2 - \mu^2)\, \delta(P_4^2 - m_e^2)\, (2\pi)^2 \frac{d^4 P_3}{(2\pi)^4} \frac{d^4 P_4}{(2\pi)^4}$$

$$\frac{1}{2E_1 2m_e} \qquad |m|^2$$

The rate for emission of one soft photon   5/5/67 LECTURE

$$\text{Rate} = \underbrace{\frac{d^3p_2}{(2\pi)^3 2E_2 2E_1} |\bar{u}_2 \mathcal{M} u_1|^2}_{\substack{\text{Rate disregarding} \\ \text{radiation coupling}}} \frac{d\Omega\, d\omega}{(2\pi)^3 \omega} 4\pi e^2 \left\{ \omega \frac{p_1 \cdot e}{p_1 \cdot k} - \omega \frac{p_2 \cdot e}{p_2 \cdot k} \right\}^2$$

A more elaborate calculation gives

$$\sigma_{\text{no photons}} = \sigma_{\text{dis. rad}}\ C$$

$$\sigma_{1\ \text{photon}\ \omega_1} = \sigma_{\text{dis. rad}} \left(\frac{d\omega_1}{\omega_1} f(\theta_1) d\Omega_1 \right) C$$

$$\sigma_{2\ \text{photons}\ \omega_1, \theta_1, \omega_2, \theta_2} = \sigma_{\text{dis. rad}} \frac{1}{2} \left(\frac{d\omega_1}{\omega_1} f(\theta_1) d\Omega_1 \right) \left(\frac{d\omega_2}{\omega_2} f(\theta_2) d\Omega_2 \right) C$$

$$\vdots$$

$$\sigma_{\text{scatt \& don't care how many photons}} = \sigma_{\text{dis. rad}}\ C\, e^{\int \frac{d\omega}{\omega} f(\theta) d\Omega}$$

Now will find $\quad C = e^{-\int \frac{d\omega}{\omega} f(\theta) d\Omega}$ for soft photons

If $\omega \to 0$, integral diverges

However for an experiment with finite precision Δ, find

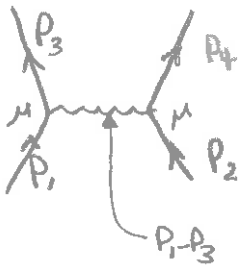
$$\sigma_{\substack{\text{NO PHOTON} \\ E > \Delta}} = \sigma_{\text{DIS RAD}}\ e^{-\alpha \ln \frac{E}{\Delta}} \qquad \alpha \sim \frac{1}{137}$$

This was originally called the "infrared catastrophe."

c is merely the result of a unit question.

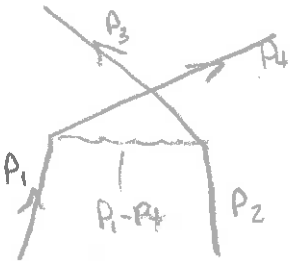
BACK TO DIAGRAMS

Consider e-e scattering



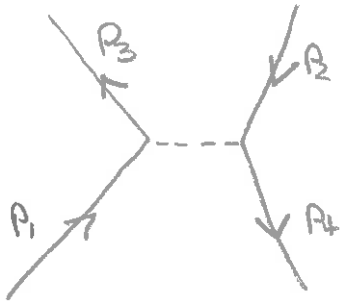
$$M = \sqrt{4\pi e^2}\,\frac{(\bar{u}_4 \gamma_\mu u_2)\,(\bar{u}_3 \gamma_\mu u_1)}{(P_1-P_3)^2}$$

But there is an exchange possibility. Must also consider



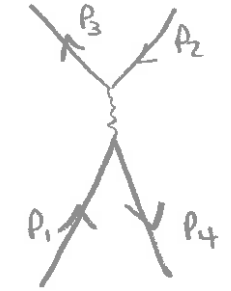
$$-\sqrt{4\pi e^2}\,\frac{(\bar{u}_3 \gamma_\mu u_2)\,(\bar{u}_4 \gamma_\mu u_1)}{(P_1-P_4)^2}$$

Now consider annihilation into, $e^+ - e^-$ scattering



$$M = \sqrt{4\pi e^2}\,\frac{(\bar{u}_4 \gamma_\mu u_2)\,(\bar{u}_3 \gamma_\mu u_1)}{(P_1-P_3)^2}$$

But also can have annihilation + pair production



$$\mathcal{M} = -\sqrt{4\pi e^2}\ \frac{(\bar{u}_3 \gamma_\mu u_2)(\bar{u}_4 \gamma_\mu u_1)}{(p_1 - p_4)^2}$$

Thus matrix elements are the same for e-e^+ as for e-e scattering.

Kind of suggests a generalization of the exclusion principle.

Technical Trick:

p_2

p_1

$$\text{Rate} = \cdots |(\bar{u}_2 N u_1)|^2$$

Suppose we don't want to measure exit spin. Then need

$$\sum_{\text{2 spins}} |\bar{u}_2 N u_1|^2 = \sum (\bar{u}_2 N u_1)^* (\bar{u}_2 N u_1)$$

Now define $\bar{N} \ni (\bar{g} N f)^* = (\bar{f} \bar{N} g)^*$ (relativistic adjoint)

Then

$$= \sum_{\substack{\text{2 spins} \\ \text{of } u_2}} (\bar{u}_1 \bar{N} u_2)(\bar{u}_2 N u_1)$$

$\uparrow$ insert $(\not{p}_2 + m)$

$$\sum_{\substack{\text{spins} \\ \text{of } u_2}} |\bar{u}_2 N u_1|^2 = \left(\bar{u}_1 \bar{N} (\not{p}_2 + m) N u_1\right)$$

Con due fermioni

$$\sum_{\substack{\text{spins of} \\ u_2 \, ; \, u_2}} |(\bar{u} N u_1|^2 = \mathrm{Tr}\left[(\not{p} + m) \bar{N} (\not{p}_2 + m) N\right]$$

Fermione $\bar{N}$ dove $N = \not{a} \not{b} \not{c}$

$$\bar{N} = \overset{+}{\not{c}} \not{b}^* \not{a}^*$$

3/8/67 LECTURE

Recall

$$H_D = \beta m + \alpha \cdot (p - A) + V$$

Now calculate velocity operator

$$\dot{x} = i(H_D x - x H_D) = \alpha_x$$

But $\alpha_x \alpha_x = 1$. $\Rightarrow$ e.v. are ± 1. Thus if you measure velocity in x-direction, you get $\pm c$? Swiss Dirac's explanation using simultaneous measurements -- and was wrong. If you make measurements over long times

$$\left\langle \frac{x_{t+T} - x_t}{T} \right\rangle^2 \sim \frac{p}{\sqrt{p^2 + m^2}} \quad \text{if} \quad T > \frac{\hbar}{mc^2}$$

Whole idea is that Dirac eqn does not describe motion of a single electron, but rather a combination of electron & positron motion.

No one has been able to interpret $\alpha_x \alpha_x = 1$ directly. Other interpretations trouble with

$$\frac{\partial}{\partial t}(\alpha_x \alpha_y \alpha_z), \text{ etc.}$$

Only one interpretation is $\dot{p} = E + \alpha \times B$

No one has ever made a detailed study of how to interpret the Dirac eqn. Not just a one electron eqn.

How do we know Dirac eqn is relativistically invariant.

: $\gamma_\mu (\nabla_\mu - A_\mu - m)\psi = 0$

If Joe uses $\xrightarrow{u_z}$ and his Moe uses

γ_x	$\gamma_x' = \gamma_x$
γ_y	$\gamma_y' = \gamma_y$
γ_z	$\gamma_z' = (\gamma_z - u\gamma_t)/\sqrt{1-u^2}$
γ_t	$\gamma_t' = (\gamma_t - u\gamma_z)/\sqrt{1-u^2}$

then all measurements will be OK.

Suppose Moe's professor uses

$\gamma_x' = \gamma_x$
$\gamma_y' = \gamma_y$
$\gamma_z' = \gamma_z$
$\gamma_t' = \gamma_t$

Must show Moe's prof. gets same answer as Moe. This is challenge. How unique are matrices γ.

Let $\gamma_x \to \gamma_x''$
$\gamma_y \to \gamma_y''$
$\gamma_z \to \gamma_z''$
$\gamma_t \to \gamma_t''$

and ask questions as to whether physics can be maintained.

Note have some problem in relativity

5/9/67 LECTURE

PROBLEM: mass corrections to electron in fourth order self-interaction

$$2m\,\Delta m = \left(\frac{e^2}{2\pi}\right) \int \frac{(\bar{u}\gamma_\mu(\not{p}-\not{k}+m)\gamma_\mu u)}{(p-k)^2-m^2} \; \frac{d^4k}{k^2(2\pi)^4}$$

Try to derive this from non-relativistic thinking

$$\Delta E = \sum_n \frac{H_{in} H_{ni}}{E_n - E_i}$$

[Easy to do in relativistic notation]

Back to our examination of γ matrices. Consider

$$[\gamma_\mu(i\nabla_\mu - A_\mu) + m]\psi = 0$$

Consider $\psi'' = S\psi$ $\qquad S = S(\gamma's)$

Then

$$[\gamma_\mu''(i\nabla_\mu - A_\mu) + m]\psi'' = 0 = [\gamma_\mu''(i\nabla_\mu - A_\mu) + m]S\psi = 0$$

or

$$[S^{-1}\gamma_\mu'' S(i\nabla_\mu - A_\mu) + m]\psi = 0$$

$\Rightarrow$ physics are same if

$$\gamma_\mu'' = S\gamma_\mu S^{-1}$$

That is, all ψ's related by equivalent transformations will give same physics. All commutation relations hold if

$$\bar{S} = S^{-1} \qquad \text{"relativistically unitary"}$$

where $\bar{S}$ defined by

$$(\bar{f} M g)^* = (\bar{g} \bar{M} f) \qquad \text{relativistic adjoint}$$

$$\Rightarrow \quad \bar{M} = \beta M^\dagger \beta^\dagger$$

In the standard representation of Dirac and

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad , \quad \bar{M} = \begin{pmatrix} a^\dagger & -c^\dagger \\ -b^\dagger & d^\dagger \end{pmatrix}$$

Note this means

$$\overline{\gamma_\mu} = \gamma_\mu \qquad \gamma \text{ matrices are self-adjoint relativistically.}$$

Demonstrates with

$$\gamma_t' = (\cosh w)\gamma_t - (\sinh w)\gamma_z$$

$$\gamma_x = \gamma_x$$

$$\gamma_y = \gamma_y$$

$$\gamma_z = (\cosh w)\gamma_z - (\sinh w)\gamma_t$$

where $\frac{v}{c} = \tanh w$

$$\cosh w = \frac{1}{\sqrt{1-v^2}} \qquad \sinh w = \frac{v}{\sqrt{1-v^2}}$$

Find $S = e^{\frac{\theta}{2}\gamma_+\gamma_z}$

Recall in rotations

$\gamma_+' = \gamma_+$

$\gamma_x' = \gamma_x \cos\theta + \gamma_y \sin\theta$

$\gamma_y' = -\gamma_x \sin\theta + \gamma_y \cos\theta$

$\gamma_z = \gamma_z$

$S = e^{\frac{\theta}{2}\gamma_x\gamma_y}$

Can find

$$J_z = \underbrace{(p \times r)_z}_{L_z} + \underbrace{\tfrac{1}{2}\gamma_x\gamma_y}_{\frac{1}{2}\sigma_z} = L_z + \tfrac{1}{2}\sigma_z$$

If we have to sum

$$\sum_{\substack{\text{spins} \\ \text{of } 1}} (\bar{u}_3 A u_1)(\bar{u}_1 B u_2)$$

Note: if we had to sum over

$$\sum_{\substack{\text{spins of} \\ \text{all } u\text{'s}}} (\bar{u}_3 A u_1)(\bar{u}_1 B u_2) = (\bar{u}_3 AB\, u_2)$$

So

$$\sum_{\substack{\text{spins} \\ \text{of } u_1}} (\bar{u}_3 A u_1)(\bar{u}_1 B u_2) = \bar{u}_3 (A(\not{p}_1 + m) B)\, u_2$$

$$\sum_{\substack{\text{spins} \\ \text{of } u_1, u_2}} |(\bar{u}_2 M u_1)|^2 = \sum_{\substack{\text{spins} \\ \text{over all}}} (\bar{u}_2 M(\not{p}_1 + m) \bar{M}(\not{p}_2 + m) u_2$$

$$= \mathrm{Sp}\left[M(\not{p}_1 + m)\bar{M}(\not{p}_2 + m)\right]$$

Now

$\bar{M}$: reverse order of all γ_n
change explicit i to $-i$

Useful information: $\mathrm{Sp}\, 1 = 4$ $\mathrm{Sp}\,\gamma_n = 0$ $\mathrm{Sp}\,\gamma_x\gamma_y = 0$

$$Sp[AB] = Sp[BA]$$

$$Sp[ABC] = Sp[CAB] = Sp[CBA] \quad [\text{must maintain cyclic order}]$$

$$Sp[\not{a}] = 0 \qquad [\not{a} = a_\mu \gamma_\mu \leftarrow \text{matrix}, \ a_\mu \leftarrow \text{number}]$$

$$Sp[\not{a}\not{b}] = 4(a \cdot b)$$

$$Sp[\not{a}\not{b}\not{c}] = 0$$

$$Sp[\not{a}\not{b}\not{c}\not{d}] = 4\{(a \cdot b)(c \cdot d) + (b \cdot c)(a \cdot d) - (a \cdot c)(b \cdot d)\}$$

Summing over photon polarizations ϵ_i

$$\sum_{\text{pol}} Sp[\cdots \not{\epsilon}_i \cdots \not{\epsilon}_i \cdots] \qquad (\not{\epsilon}_i \to -\gamma_\mu, \ \not{\epsilon}_i \to \gamma_\mu)$$

from gauge invariance

SUMMARY OF RULES FOR PERTURBATION CALCULATIONS

$$\frac{\text{Prob. transition}}{\text{sec}} = 2\pi \rho(E) \prod_{in}\left(\frac{1}{2E}\right) \prod_{out}\left(\frac{1}{2E}\right) |M|^2$$

$$= (2\pi)^4 \delta^4\left(\sum_{in} p - \sum_{out} p\right) \prod_{i\,out} 2\pi\, \delta(p_i^2 - m_i^2) \frac{d^4p}{(2\pi)^4} \times$$

$$\times \prod_{in}\left(\frac{1}{2E_{in}}\right) |M|^2$$

Now for calculation of matrix element M

$e_\mu e_\mu = -1$

$\bar{u} u = 2m$

Sum on states because for one electron in and out

$$\mathrm{Sp}\left[(\not{p}_2 + m)\,\bar{M}\,(\not{p}_1 + m M\right]$$

Electron propagator: $\dfrac{1}{\not{p} - m + i\epsilon}$

Photon propagator: $\dfrac{1}{p^2 + i\epsilon}$

Meson propagator (scalar or pseudoscalar): $\dfrac{1}{p^2 - m^2 + i\epsilon}$

Couplings

Real photon $\not{\epsilon}$

Potential $\not{A}(q) \equiv \int e^{-iqx} \not{A}(x) d^4x$

Closed loop (fermion) $-\not{p}$

Virtual photon: $\gamma_\mu \cdots \gamma_\mu$

$\sqrt{4\pi e^2}$ for each photon coupling

$\sqrt{4\pi g^2}$ for each meson coupling

Pseudoscalar meson $\gamma_5 \cdots \gamma_5$

Scalar meson $1 \cdots 1$

Sum each indeterminant momentum by $\int \frac{d^4p}{(2\pi)^4}$

To get phases right,

i each electron propagator

$-i$ each photon "

$+i$ " spin zero meson "

$-i$ " photon coupling

Energy $\cdot 2E$ = expectation value of $i\mathcal{M}$

In second. per. th.

$$M_{fi} = \sum_n \frac{H_{fn} H_{ni}}{E_i - E_n}$$

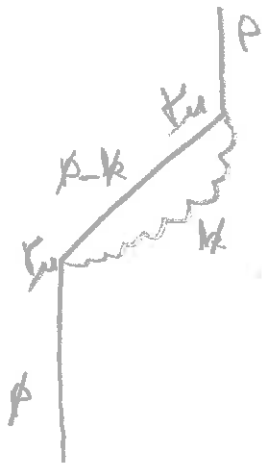
also

$$\Delta E_i = M_{ii} = \sum_n \frac{H_{in} H_{ni}}{E_i - E_n}$$

Thus if we adopt rule formulas to calculate diagonal elements, first

Δ Energy $\cdot \Delta E =$ sum value of $i M$

Self-Energy of Electron



Corresponding energy of electron due to interaction with E/M field.

Note momentum k is not determinable.

$$2E \cdot \Delta E = \int \frac{d^4k}{(2\pi)^4} \left(\bar{u} \gamma_\mu \frac{1}{\not p - \not k - m + i\epsilon} \gamma_\mu u \right) \frac{1}{k^2 + i\epsilon} 4\pi e^2$$

$$(+i)(-i)(-i)^2(i)$$

5/16/67 LECTURE

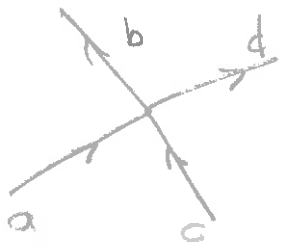
PROBLEM: β-decay Ref. Phys Rev 109, 193 (1958) Feynman & Gell-Mann

Example: $\mu \to e + \bar{\nu}_e + \nu_\mu$

ν satisfies Dirac eqn with $m = 0$

Suppose amplitude M for such decay.

Suppose a 4 pt. interaction



$$M = \frac{(\bar{u}_a \gamma_\mu a u_c)(\bar{u}_b \gamma_\mu a u_a)}{(\bar{a}c)(\bar{b}a)} \; G\sqrt{8}$$

G ← strength factor

where $a = \frac{1+i\gamma_5}{2}$

From experiment

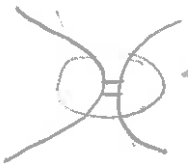
$$\frac{GM_p^2}{\hbar c} = 1.01 \times 10^{-5}$$

For our example $(\bar{e}\nu_e)(\bar{\nu}_\mu \mu) = (\bar{u}_e \gamma_\mu a u_{\nu_e})(\bar{u}_{\nu_\mu} \gamma_\mu a u_\mu)$

But this looks like $\mu + \nu_e \to e + \nu_\mu$. However using antiparticle we get right result

Find spectrum & lifetime of μ-decay, and also demonstrate non conservation of parity.

[Notice that this is lowest order perturbation theory process -- no propagators, etc. Actually if we do not assume a contact interaction, get a intermediate interaction.



Suppose we can represent this by current operators

$$M = G\sqrt{8}\, J_\mu^* J_\mu$$

where

$$J_\mu = (\bar{\nu}_{\nu_\mu} \gamma_\mu a \nu_\mu) + (\bar{\nu}_{\nu_e} \gamma_\mu a \nu_e) + J_\mu^{\text{strong interactions}}$$

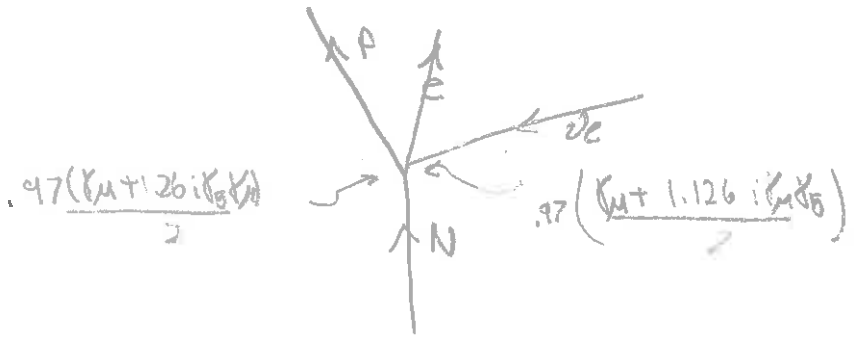
$$J_\mu^* = (\bar{\nu}_\mu \gamma_\mu a \nu_{\nu_\mu}) + (\bar{\nu}_e \gamma_\mu a \nu_{\nu_e}) + J_\mu^{*\,\text{strong}}$$

Note these introduce a number of other processes like

$$e + \nu_e \to e + \nu_e \,, \quad e + \bar{\nu}_e \to e + \bar{\nu}_e \,, \quad e + \bar{e} \to \nu_e + \bar{\nu}_e$$

We need J_μ^{strong} for $N \to p + e + \bar{\nu}_e$. Use things like

$$\langle \text{proton} | J_\mu | \text{neutron} \rangle = (\bar{u}_p \left[\frac{\gamma_\mu + 1.26 i \gamma_\mu \gamma_5}{2} \right] u_n)(.97)$$



Also E-M corrections of $O(1\%)$.

5/15/67 LECTURE

$$\Delta(m^2) = -4\pi e^2 i \int \left(\bar{u} \gamma_\mu \frac{1}{\not p - \not k - m + i\epsilon} \gamma_\mu u \right) \frac{d^4k}{(2\pi)^4 k^2 + i\epsilon}$$

$$= -\frac{4\pi e^2 i}{m} \int \frac{2m^2 + 2p\cdot k}{k^2 - 2p\cdot k} \frac{d^4k}{k^2 (2\pi)^4}$$

$$\sim \frac{2m^2}{k^4} d^4k + \frac{4(p\cdot k)^2}{k^2 k^4} d^4k$$

$$\sim \int 3m^2 \frac{d^4k}{k^4}$$ log. divergent integral

If we could cut this integration off @ Λ

$$\sim \frac{3e^2}{\pi} \ln \frac{\Lambda}{m}$$

Infinite correction to QED. End of theory.

How can we keep theory for calculations? Any problem with regard to indeterminate momentum gives ∞'s. Invent ways to stop integration.

Multiply integrand by $C(k^2)$ $\Rightarrow$ $C \sim 0$ for $k > \Lambda$.

Eg.

$$C(k^2) = \frac{-\Lambda^2}{k^2 - \Lambda^2}$$

Find that all physically measurable processes do not depend on Λ, then can take $\Lambda \to \infty$ and get invariant predictions of QED.

Idea is to use

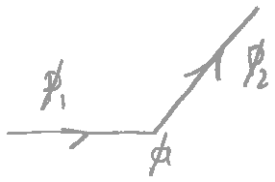
$$m_{eff}^2 = m_0^2 + \frac{3e^2 m^2}{\pi} \ln \frac{\Lambda}{m} + \dots$$

to cancel out logs before taking $\lim_{\Lambda \to \infty}$.

[Mass renormalization]. Current state of research.

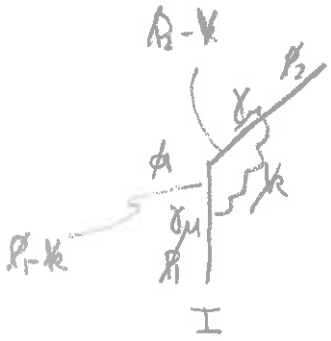
SCATTERING IN A POTENTIAL TO $O(e^2)$

5/19/67 LECTURE



$(\bar{u}_2 \not{\phi} u_1)$

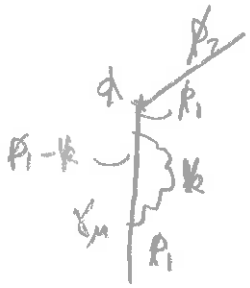
$\phi(q) \qquad q = p_2 - p_1$



I

$$I = (4\pi e^2) \int \left(\bar{u}_2 \gamma_\mu \frac{1}{p_2 - k - m} \not{\phi} \frac{1}{p_1 - k - m} \gamma_\mu u_1 \right) \frac{1}{k^2} \frac{d^4k}{(2\pi)^4}$$

Complication arising for any free particle problem

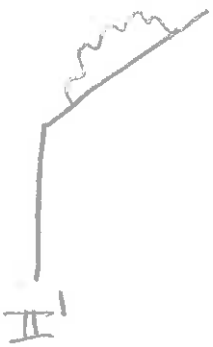


II

$$II = \bar{u}_2 \left(\not{\phi} \frac{(4\pi e^2)}{p_1 - m} \int \gamma_\mu \frac{1}{p_1 - k - m} \gamma_\mu \frac{d^4k}{k^2} \frac{C(k^2)}{(2\pi)^4} \right) u_1$$

mass correction

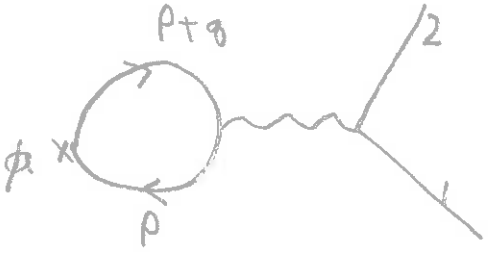
$$\frac{p_1 + m}{(m_{ap}^2 - m_{th}^2)} (m_{ap}^2 - m_{th}^2)$$



II'

$$= \bar{u}_2 \not{\phi} u_1 \, r/2$$

5/26/67 LECTURE

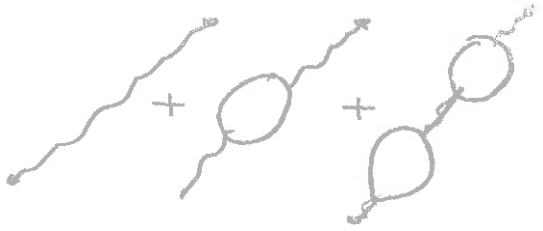


$$4\pi e^2 (\bar{u}_2 \gamma_\mu u_1) \frac{1}{q^2} \int \mathrm{Sp}\left[\frac{1}{\not p - m} \gamma_\mu \frac{1}{\not p + \not q - m} \not A\right] \frac{d^4p}{(2\pi)^4}$$

Need a new type of cutoff (Invariant regularization)
Subtract 3 terms

$$\mathrm{Sp}\left[\frac{1}{\not p - M} \gamma_\mu \frac{1}{\not p + \not q - M} \not A\right] - \mathrm{Sp}\left[M_2\right] - \mathrm{Sp}\left[M_3\right]$$

As before, this is



Use

$$e^2_{exp} = \frac{e_{+\Lambda}^2}{1 - (\ln \frac{\Lambda}{m}) e^2_{+\Lambda}}$$

as charge renormalization

See my book.

We were calculating 5/22/67 LECTURE

$$r = \frac{4\pi e^2}{(2\pi)^4}\int \gamma_\mu \frac{1}{p_1 - k - m}\frac{\not p}{m}\frac{1}{p_1 - k - m}\frac{d^4k}{k^2}\, C(k^2)\Big|_{p_1 = m}$$

Consider the probability of the the virtual process for long time propagation

$$\frac{1}{\not p - m_0} + \frac{1}{\not p - m_0}(a\not p + b)\frac{1}{\not p - m_0} + \cdots = \frac{1}{\not p - m_0 - (a\not p + b)}$$

Want to examine this near pole

$$= (1+r)\frac{1}{\not p - M} \quad \text{near } p^2 = M^2$$

Examine

$$\frac{1}{[1 - a(p^2)]}\quad \frac{1}{[\not p - f(p^2)]} \quad \text{where } f = \frac{m_0 + b(p^2)}{1 - a(p^2)}$$

$$= \frac{1}{1-a}\left[\frac{\not p + f(p^2)}{p^2 - [f(p^2)]^2}\right]$$

Suppose M satisfies $M = f(M^2)$. For a, b small

$$M = m_0 + b(\overset{\sim m_0}{m^2}) + m_0\, a(\overset{\sim m_0}{m^2}) = m_0 + [m_0 a(m_0^2) + b(m_0^2)]$$

just old formula for mass correction

Use $f(p^2) = M^2 + 2M(p^2 - M^2) f'(M^2) + \cdots$

$$= \frac{1}{1-a} \frac{\not{p} + f(M^2)}{(p^2 - M^2)\left[1 - 2M f'(M^2)\right]} = (1+r) \frac{1}{\not{p} - M}$$

where

$$1 + r = \frac{1}{\left[1 - a\right]\left[1 - 2M \frac{df(M^2)}{dM^2}\right]} \sim \frac{1}{1-r}$$

$$\therefore r \sim a + 2M(b' + Ma')$$

$$= p_\mu \frac{d}{dp_\mu} \left[a(p^2)\not{p} + b(p^2)\right] \Big|_{\not{p}=M}$$

To differentiate $1/A$, use

$$\frac{1}{A + \Delta A} = \frac{1}{A} - \frac{1}{A} \Delta A \frac{1}{A} + \cdots$$

Rather than using a new propagator, easier to include $(1+r)$ in coupling as

$$\sqrt{4\pi e^2}\, \not{\epsilon}_\mu \underbrace{(1+r)}_{Z_1}$$

Thus shift in pole $\Rightarrow$ shift in mass
Change in strength of pole $\Rightarrow$ change in coupling

r, unfortunately is divergent

Now returning to

$$4\pi e^2 \int \gamma_\mu \frac{1}{\not p_2 - \not k - m} \not A \frac{1}{\not p_1 - \not k - m} \gamma_\mu \frac{d^4k}{k^2} C(k^2)$$

$$= 4\pi e^2 \int \frac{\gamma_\mu (\not p_2 - \not k + m) \not A (\not p_1 - \not k + m) \gamma_\mu}{(k^2 - 2p_2\cdot k)(k^2 - 2p_1\cdot k)} \frac{d^4k}{k^2} C(k^2)$$

Setan infrared divergence as well as an ultraviolet divergence. Best technique to handle former is to set photon mass (the usual $\lambda \Rightarrow k^2 \to k^2 - \lambda^2$. Or better, use $\frac{\lambda - \Lambda^2}{k^2 - \Lambda^2}$

Returning to Pauli correction of Dirac eqn

$$\left[i\partial_\mu \gamma_\mu - e A_\mu \gamma_\mu - \frac{\mu}{4} (\gamma_\mu \gamma_\nu \tilde{F}_{\mu\nu}) \right] \psi = m\psi$$

$$i\gamma_\mu \gamma_\nu (q_\nu a_\mu - q_\mu a_\nu) = i(\not q \not a - \not a \not q)$$

After adding all above diagrams we get an expansion in powers of q

$$\bar{u}_2 \left[X \not a + Y (\not a \not b - \not b \not a) + Z (\not b^2 \not a) + \dots \right] u_1$$

Charge renormalization — Correction to μ_e — Anomalous moment

Thus to find μ_e, we need only calculate integral to first order. Thus we examine a technique for doing integrals.

$$\int \frac{1}{(k^2-L)^3}\frac{d^4k}{(2\pi)^4} = \frac{i}{32\pi^2 L}$$

$$\int \frac{1}{(k^2-2p\cdot k+\Delta)^3}\frac{d^4k}{(2\pi)^4} = \int \frac{1}{[(k-p)^2-(\Delta+p^2)]^3}\frac{d^4k}{(2\pi)^4}$$

$$= \frac{1}{32\pi^2(p^2+\Delta)}$$

$$\int \frac{k_\mu}{(k^2-L^2)^3}\frac{d^4k}{(2\pi)^4} = 0$$

$$\int \frac{k_\mu}{(k^2-2p\cdot k-\Delta)^3}\frac{d^4k}{(2\pi)^4} = \frac{i}{32\pi^2}\frac{p_\mu}{p^2+\Delta}$$

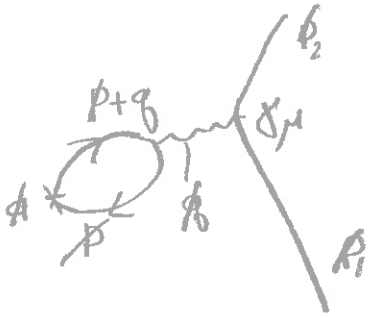
$$\int \frac{1}{(k^2-2p_1\cdot k+\Delta_1)(k^2-2p_2\cdot k+\Delta_2)}\frac{d^4k}{(2\pi)^4}$$

$$= \int_0^1 \frac{dx}{(k^2-2p_x\cdot k-\Delta_x)^2}$$

$$p_x = xp_1+(1-x)p_2$$

$$\Delta_x = x\Delta_1+(1-x)\Delta_2$$

using $\frac{1}{a\cdot b} = \int_0^1 \frac{dx}{[ax+b(1-x)]^2}$ very useful



closed loop

$$\text{III} = (\bar{u}_2 \gamma_\mu u_1) \frac{4\pi e^2}{q^2} \int Sp \left[\frac{1}{\not p - m} \gamma_\mu \frac{1}{\not p + \not q - m} \not A \right] (-1) \frac{d^4p}{(2\pi)^4}$$

vacuum polarization term

$$\Gamma = 4\pi e^2 \int \gamma_\mu \frac{1}{\not p - \not k - m} \left(\frac{\not p}{m}\right) \frac{1}{\not p - \not k - m} \gamma_\mu \frac{d^4k}{k^2} C(k^2)$$

roughly

$p_1 = p_0 + \Delta p$

$$\gamma_\mu \frac{1}{\not p_0 + \Delta\not p - \not k - m} \gamma_\mu = \gamma_\mu \frac{1}{\not p_0 - \not k - m} \gamma_\mu + \gamma_\mu \frac{1}{\not p - \not k - m} \Delta\not p \frac{1}{\not p - \not k - m} \gamma_\mu + \cdots$$

$$\left[\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A} B \frac{1}{A} + \frac{1}{A} B \frac{1}{A} B \frac{1}{A} + \cdots \right]$$

add virtual photons e^2

write

PHYSICS 205a

Week of November 7

Problem: Neutral K decay

Background: a K meson is a boson with mass more than three times the mass of the more common pi meson. There are four K mesons - two neutral ones, one each with positive and negative charge. These particles are produced in strong interactions of the form $\pi^- p \rightarrow \Lambda^0 K^0$

It was found experimentally that if the initial state contained only pions and nucleons, measurements of reactions with two particle final states showed only K^+ particles, never K^-. Gell-Mann came up with the idea of assigning to particles an additional quantum number called strangeness to predict this pattern.

$$S(\Lambda^0) = S(\Sigma^{+0-}) = S(\Xi^{-0}) = -1$$

$$S(K^+) = S(K^0) = +1 \qquad S(K^-) = S(\bar{K}^0) = -1$$

$$S(P) = S(n) = 0$$

If we postulate that strangeness be conserved in strong (i.e. fast) reactions, we predict

$$\pi^- p \not\rightarrow \Sigma^+ K^-$$

$$\pi^- p \rightarrow \Sigma^- K^+$$

To date predictions of this sort have always worked. However, the theory is rather peculiar in that it predicts <u>two</u> neutral K particles with opposite values of strangeness. If there were no way of distinguishing between this case and the case of only one neutral K, there would be questions raised about the theory. One way of distinguishing the two cases is to compare the rates of reactions between different members of the same multiplet. The ratios depend only on the isospins of the different constitutents - thus they will be different if the K forms two isospin doublets or one isospin triplet.

Another way of distinguishing the cases is in the K^0 decay. If only one K^0 were present, it would decay exponentially with time in the usual fashion. Your problem is to figure out what happens when two K^0's exist.

STATEMENT OF PROBLEM:

$$K^0 \rightarrow \pi^+ \pi^- \qquad \bar{K}^0 \rightarrow \pi^+ \pi^-$$

Assume that the two neutral K's have the same mass and the same matrix element for this

decay. Assume that this is by far the most important reaction in the decays.

Given a K^0 all alone in a box at t=0, what is the probability as a function of time of finding a K^0 in the box for $t > 0$?

For people who worry about infinities:

There are some reactions which distinguish between K^0 & $\bar{K}^0$ although they have small Probability.

$K^0 \to \pi^- + \begin{pmatrix} \mu^+ \\ e^+ \end{pmatrix} + \nu$ $\qquad$ $K^0 \not\to \pi^+ + \begin{pmatrix} \mu^- \\ e^- \end{pmatrix} + \bar{\nu}$

$\bar{K}^0 \to \pi^+ + \begin{pmatrix} \mu^- \\ e^- \end{pmatrix} + \bar{\nu}$ $\qquad$ $\bar{K}^0 \not\to \pi^- + \begin{pmatrix} \mu^+ \\ e^+ \end{pmatrix} + \nu$

MORE ON THE THEORY OF LINE WIDTHS

Suppose $H = H_0 + H_I$

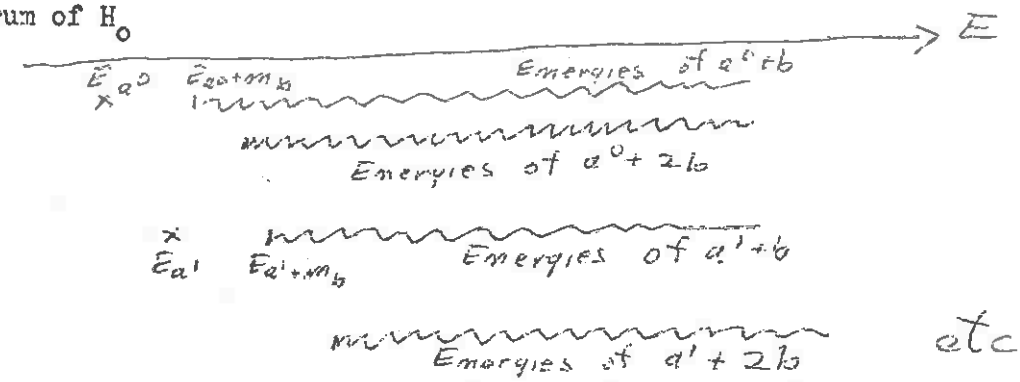
Consider the following model:

H_0 has as its eigenstates both

1) a collection of discrete states $a^0, a^1, a^2 \cdots$ with energies E^i

2) a continuum. Each state in the continuum consists of one a^i state, and n particles of a different type called b. Each b particle has an energy E_{b_i}. The a^i state or particle is assumed to always have energy E^i (i.e. it never gets kinetic energy in this model).

Spectrum of H_0



H_I, as usual, induces transitions between the states of H_0

Because the states of the discrete spectrum are usually simpler to analyze, it is desirable to eliminate the other states from our equations.

Label the coefficients of the discrete spectrum by a_m ; those of the continuum states by b_k

$$i\dot{a}_m(t) = \sum_m v_{mm}(t)\, a_m(t) + \sum_k v_{mk}(t)\, b_k(t)$$

Assume for ease of computation that the perturbation connecting continuum and discrete states is roughly independent of time (in practice this is almost always true - most of the "leakage" to continuum states is not connected with the turning on and off of laboratory apparatus)

Further, assume that at t=0 you have no continuum states populated. Then the b_k are small compared to the a_m ; the feeding of continuum states may be assumed to comm mostly from the discrete ones. Hence we arrive at

$$i\dot{a}_n(t) = \sum_m V_{nm}(t)\, a_m(t) + \sum_k M_{nk}\, b_k(t)\, e^{-i(E_n - E_k)t}$$

$$i\dot{b}_k(t) = \sum_m M_{km}\, e^{i(E_m - E_k)t}\, a_m(t)$$

integration gives

$$\dot{a}_m = -i \sum_m V_{nm}(t)\, a_m(t) - \int^t \sum_k |M_{km}|^2 e^{-i(E_m - E_k)(t-t')}\, a_m(t')\, dt'$$

$$- \int^t \sum_{\substack{k,m \\ m \neq n}} M_{nk} M^*_{km}\, e^{-i(E_n - E_k)t}\, e^{i(E_m - E_k)t'}\, a_m(t')\, dt'$$

The last piece has no average effect over large periods of time. Hence we may neglect it.

(General edification: a small perturbation which produces a large effect after a long time is called a secular disturbance)

As shown in last week's notes we may then define quantities $\Delta + \Gamma$ such that

$$\dot{a}_m = -i \sum_m [V_{nm}(t) + \Delta_n \delta_{nm}]\, a_m(t) - \Gamma_m/2\, a_m(t)$$

$$\Gamma = 2\pi \sum_k \delta(E_k - E_n) |M_{km}|^2$$

Define $V_{nm}(t) + \Delta\delta_{nm} = V'_{nm}(t) = V'_{mn}(t)\, e^{-i(E_m - E_n)t}$

Last week we computed the probability for light emission by an atomic transition between states with widths. If it began in state n with the atom in a

and went to state m with atom in b, and photon of energy w

then

$$P_m = |a_m(t)|^2 = \frac{|V'_{nm}|^2 \left[e^{-\Gamma_n t} + e^{-\Gamma_m t} - 2e^{-(\Gamma_n + \Gamma_m)t/2} \cos(E_n - E_m)t \right]}{\left[(E_n - E_m)^2 + \left(\frac{\Gamma_n - \Gamma_m}{2} \right)^2 \right]}$$

is the probability to be in state m at time t; this goes to 0 as t goes to infinity.

Suppose you just want the total probability at time t to find a photon of frequency ν which came from this transition. This is

P_m + probability that this took place and then the atom in state b decayed

As t goes to infinity, this total probability approaches $P_{decayed}$

Rate of decay = $\frac{d}{dt}$ [Probability that the state has decayed]

$* = \Gamma_b P_m(t)$ {From rate formula}

$P_{decayed} = \Gamma_b \int_0^\infty P_m(t)\,dt$

Assuming $V'_{mm}(t) = V'(0)$, we find ($V'_{mm} = V_{mm}$, $m \neq m$)

$$P_\nu(\infty) = |V_{mm}|^2 \frac{\Gamma_b}{\left[\nu^2 + \left(\frac{\Gamma_a - \Gamma_b}{2}\right)^2\right]}\left[\frac{1}{\Gamma_a} + \frac{1}{\Gamma_b} - \frac{2\left(\frac{\Gamma_a+\Gamma_b}{2}\right)}{\left[\nu^2 + \left(\frac{\Gamma_a+\Gamma_b}{2}\right)^2\right]}\right]$$

$$= |V_{mm}|^2 \left[\Gamma_b + \Gamma_a\right] \frac{1}{\Gamma_a} \frac{1}{\left[\nu^2 + \left(\frac{\Gamma_a+\Gamma_b}{2}\right)^2\right]}$$

Notice that the line shape as $t \to \infty$ is a "Lorentzian curve" with a width $\Gamma_a + \Gamma_b$.

If the resolution of our apparatus is crude, the line looks sharp enough that we may make the replacement

$$\frac{\Gamma_a+\Gamma_b}{\nu^2 + \left(\frac{\Gamma_a+\Gamma_b}{2}\right)^2} \longrightarrow 2\pi\delta(\nu)$$

thus

$$P_\nu(\infty) = |V_{mm}|^2 2\pi\delta(\nu)/\Gamma_a$$

and the total probability of emitting some photon is

$$\int P_\nu(\infty) \frac{d^3k}{(2\pi)^3} = \frac{2\pi}{\Gamma_a} |V_{mm}|^2 \rho(E_a - E_b)$$

This looks different from what we had before, because of the $1/\Gamma_a$

However, it is easily explained:

Rate = $2\pi |V|^2 \delta(\Delta E) \times$ Probability to be in upper state

$= 2\pi |V|^2 \delta(\Delta E)\, e^{-\Gamma_a t}$

Total probability of emission = $\int \text{Rate}\, dt = \dfrac{2\pi |V_{mm}|^2 \rho(E_a - E_b)}{\Gamma_a}$

= Rate × mean lifetime

Notice that the line shape changes as a function of time. In fact, if you look at only part of the line, the intensity is expected to change with t. This has been experimentally detected using the Mossbauer effect. Hence one must be careful in making arguments about probabilities and rates.

To see how the inclusion of widths removes certain infinities in the scattering problems.

Previously in the second order terms we had factors like $\frac{1}{E_c - E_a + \omega}$

Clearly difficulties might arise for $\omega = \Delta E$

Example of Present Formalism:

Work out the case of light scattering by an atom with stable ground state but unstable excited states.

$$\dot{a}_g = -i \sum_k V_{gk} a_k(t) e^{-i(E_k - E_g)t}$$

$$\dot{a}_e = -\Gamma_e a_e/2 - i \sum_m V'_{em} a_m(t) e^{-i(E_m - E_e)t}$$

$$a_g = a_g(0) - i \int_0^t \sum V_{gk} a_k(t') e^{-i(E_k - E_g)t'} dt'$$

Assume we start with $a_g = 1$, all other states unpopulated.

a_e the amplitude to reach some excited state is, to a first approximation

$$\dot{a}_e = -\Gamma_e a_e/2 - i V_{eg} e^{-i(E_g - E_e)t}$$

$$a_e = e^{-\Gamma_e t/2} f \quad ; \quad f = -i \int_0^t e^{\Gamma_e t'/2} V_{eg} e^{-i(E_g - E_e)t'} dt'$$

$$a_e \approx \frac{V_{eg}}{E_g - E_e + i\Gamma_e/2} \left[e^{-i(E_g - E_e)t} - e^{-\Gamma_e t/2} \right]$$

Then the transitions to another stable state are given by

$$a_j' = -i \int_0^t \sum V_{jk} a_k(t') e^{-i(E_k - E_j)t'} dt'$$

$$= -i \int_0^t \sum_{k \neq j, k \neq g} \frac{V_{jk} V_{kg} e^{-i(E_k - E_j)t'}}{E_g - E_k + i\Gamma_k/2} \left[e^{-i(E_g - E_k)t'} - e^{-\Gamma_e t'/2} \right] dt'$$

$$-i \int_0^t V_{jj} a_j(t) e^{-i(E_j - E_j)t'} dt' - i \int_0^t V_{jg} a_g(t') e^{-i(E_g - E_j)t'} dt'$$

For light scattering V_{jj}, V_{jg} are second order. a_j is first order; $a_g = 1 + f$

f is first order.

Hence keeping only second order terms gives

$$a_j \to -i \left[V_{jg} + \sum_{k \neq j, k \neq g} \frac{V_{jk} V_{kg}}{E_g - E_k + i\Gamma_k/2} \right] \int_0^t e^{-i(E_g - E_j)t'} dt'$$

$$+ i \int_0^t \sum_{k \neq i, k \neq g} \frac{V_{jk} V_{kg}}{E_g - E_k + i\Gamma_k/2} e^{-\Gamma_k t'/2 - i t'(E_k - E_j)} dt'$$

Explicit calculation shows that the last terms can be neglected compared to the other terms at long t.

Hence if $M_{ji} = V_{ji} + \sum_k \frac{V_{jk} V_{ki}}{E_i - E_k + i\Gamma_k/2}$ we find

$$\text{Probability} = |M_{ji}|^2 \frac{\sin^2 (E_j - E_i) T/2}{(E_j - E_i)^2}$$

$$\text{Rate} = 2\pi \delta (E_i - E_j) |M_{ji}|^2$$

Near the resonance the scattering amplitude looks like

$\frac{1}{E_i - E_R + i\Gamma_R/2}$ = a Breit-Wigner form

(this method of treating widths is sometimes called the Wigner-Weisskopf method)

Ph 205a

Thanksgiving Week

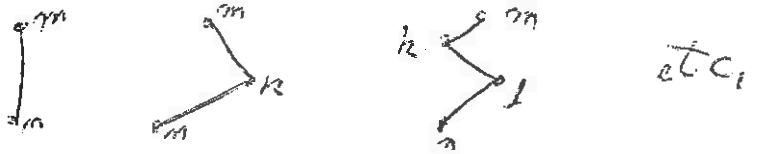
Last week we obtained GOLDEN RULE # 2

$$R_{m\to m} = 2\pi \delta(E_m - E_n)\,|T_{mm}|^2$$

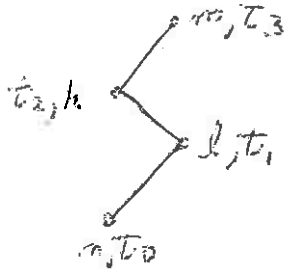
where $T_{m,n} = V_{mm} + \sum_k V_{mk}\frac{1}{E_m - E_k + i\varepsilon} V_{km} + \sum_{k,l} V_{mk}\frac{1}{E_m - E_k + i\varepsilon} V_{kl}\frac{1}{E_m - E_l + i\varepsilon} V_{lm} + \cdots$

Rehash of derivation:

Draw all graphs possible for the path between n and m, with this perturbation



Remember that the energies involved are those of the unperturbed Hamiltonian. Then think what a graph actually means



System moves from n to l in eigenstate $|m\rangle$ of the unperturbed system. At l it gets bumped into state $|l\rangle$ by the perturbation. It moves from l to k in state $|k\rangle$, then it is bumped into state $|m\rangle$, etc.

Associate a time with each corner. Along a given straight line,

state $|n\rangle$ at t_0, n becomes state $|n\rangle$ at t_1, l. $\quad |m, t_1\rangle = e^{-iE_m(t_1 - t_0)}|m, t_0\rangle$

Hence the graph, which might be written

$$(-i)^2 \langle m, t_2 | V | l, t_2\rangle \langle l, t_1 | V | n, t_1\rangle$$

takes on the form

$$(-i)^2 e^{iE_m(t_2 - t_0)} \langle m, t_0 | V | l, t_0\rangle e^{-iE_l(t_2 - t_0)} e^{iE_l(t_1 - t_0)} \langle l, t_0 | V | n, t_0\rangle e^{-iE_n(t_1 - t_0)}$$

$$(-i)^2 V_{ml} V_{ln} e^{-iE_l(t_2 - t_1)} e^{iE_m t_2} e^{-iE_n t_1} e^{-it_0(E_m - E_n)}$$

Since t_0 is just a constant, set it equal to 0 (this won't influence the rate)

$$(-i)^2 V_{ml} V_{ln} e^{-i(E_l - E_m)(t_2 - t_1)} e^{-it_1(E_n - E_m)}$$

The perturbation could act at any points $t_1, t_2 \Rightarrow t_3 > t_2 > t_1 > t_0$

To sum the contributions, integrate over t_1 & t_2

Change of variables gives

$$(-i)^2 \int_{t_1=0}^{t_3} \int_{x=0}^{t_3 - t_1} V_{ml}(x + t_1) V_{ln}(t_1) e^{-i(E_l - E_m)x} e^{-it_1(E_n - E_m)}\, dx\, dt_1$$

Consider first

$$\int_0^{t_3 - t_1} V_{ml}(x + t_1) e^{-i(E_l - E_m)x}\, dx$$

In most cases V varies very slowly with time compared to the exponential.

Thus we have $V_{mn}(t_1)\int_0^{t_3-t_1} e^{-i(E_l-E_m-i\varepsilon)x}\,dx$

$$V_{mn}(t_1)\left[\frac{e^{-i(E_l-E_m-i\varepsilon)(t_3-t_1)}-1}{-i(E_l-E_m-i\varepsilon)}\right]$$

It is reasonable to replace t_3 by ∞ in most situations. Then the final result is

$$\frac{(-i)^2 V_{ml}V_{lm}(i)}{E_m-E_l+i\varepsilon}\int_0^\infty e^{-it_1(E_m-E_m)}\,dt_1$$

Notice that all terms in the expansion of T have the same number of i's

$$(-i)^m \quad i^{m-1} = -i\times 1^{m-1} = -i$$

($(-i)^m$: from V; i^{m-1}: from propagators)

The factor $\frac{i}{E_m-E_l+i\varepsilon}$ is just the propagator in energy space (E_m is the energy variable) obtained by Fourier transforming e^{-iE_lt} (t is a time difference). In the representation where H_0 is diagonal, $e^{-iE_lt}=e^{-iH_0t}$

Thus we may write $\int_0^\infty e^{iEt}e^{-iH_0t}\,dt = \frac{i}{E-H_0+i\varepsilon}$

Pursuing this leads to the formal expression

$$T(E)= V+V\frac{1}{E-H_0+i\varepsilon}V+\cdots$$

In interpreting operator inverses like the above, keep in mind that

$$\frac{1}{A+B}=\text{GloTch} \iff (A+B)(\text{GloTch})=(\text{GloTch})(A+B)=1$$

where $A, B, 1$ & Gloтch are all operators.

$$\text{Gloтch}=\frac{1}{A}-\frac{1}{A}B\frac{1}{A}+\frac{1}{A}B\frac{1}{A}B\frac{1}{A}-\cdots$$

works here. Thus we set it equal to $\frac{1}{A+B}$

By use of this trick, $T=V+V\cdot W(E)\cdot V$

with $W(E)=\frac{1}{E-H_0+i\varepsilon}+\frac{1}{E-H_0+i\varepsilon}V\frac{1}{E-H_0+i\varepsilon}+\cdots$

may be written

$$W(E)=\frac{1}{E-H_0-V+i\varepsilon}=\frac{1}{E-H+i\varepsilon}$$

$$\boxed{T(E)=V+V\frac{1}{E-H+i\varepsilon}V}$$

This expression as it stands is absolutely exact. However, it is also almost absolutely useless. For suppose you tried to find $T_{m,n}$ for m,n eigenstates of H_0.

The evaluation of $\langle\psi_p|\frac{1}{E-H+i\varepsilon}|\psi_k\rangle$ is non-trivial.

Hence one is forced to try approximation schemes.

Example # 1

$$\langle \phi_m | T | \phi_m \rangle = \langle \phi_m | V | \phi_m \rangle + \sum_k \langle \phi_m | V | \psi_k \rangle \left(\frac{1}{E - E_k' + i\varepsilon} \right) \langle \psi_k | V | \phi_m \rangle$$

Here $|\psi_k\rangle$ is an eigenstate of H_{Total} . Of course you don't know what it is, but you can try to get close to it by different methods:

a) perturbation theory and the unperturbed eigenstates

b) sometimes the wave functions can be approximated more accurately by some physical guesswork than by blind series summing. For example, it might be convenient to use the variational method to get $|\psi_k\rangle$ and E_k'.

Example # 2

In certain contexts it is useful to replace V by $H-H_0$.

Consider a two body process $A + B \rightarrow C + D$

like $He^+ + H \rightarrow p + He$

It is only reasonable to split up the Hamiltonian in a different way in the initial state than in the final one

$$H_{tot} = K_1(A_{nuc}) + K_2(A_{elec}) + K_3(B_{nuc}) + K_4(B_{elec})$$
$$+ C_1(A_{nuc} - B_{nuc}) + C_2(A_{elec} - B_{nuc}) + C_3(A_{nuc} - A_{elec})$$
$$+ C_4(B_{nuc} - B_{elec}) + C_5(B_{elec} - A_{elec}) + C_6(B_{elec} - A_{nuc})$$

where K is kinetic energy; C is Coulomb energy

$$V^I = C_1 + C_2 + C_5 + C_6$$

$$V^{II} = C_1 + C_2 + C_4$$

The V's contain those pieces not in the individual Hamiltonians of the ions and atoms.

Then the formula for T becomes

$$(H - E_I) + (H - E_{II}) \left(\frac{1}{E - H + i\varepsilon} \right) (H - E_I)$$

$$V_I + V_{II} \left(\frac{1}{E_I - H + i\varepsilon} \right) V_I$$

To apply this, one must still approximate H.

Notice that $\langle M_I | V_I | N_I \rangle = \langle M_{II} | H - E_1 | N_I \rangle$

$$\langle M_{II} | V_{II} | N_I \rangle = \langle M_{II} | H - E_2 | N_I \rangle$$

These matrix elements are the same because the T matrix is multiplied by

$$\delta(E_1 - E_2)$$

K^0 decay problem

$$i\dot{a}_{K^0} = E_1 a_{K^0} + \sum_\pi M_{K^0,\pi\pi} b_{\pi\pi}$$

$$i\dot{a}_{\bar{K}^0} = E_2 a_{\bar{K}^0} + \sum_\pi M_{\bar{K}^0,\pi\pi} b_{\pi\pi} = E_1 a_{\bar{K}^0} + \sum_\pi M_{K^0,\pi\pi} b_{\pi\pi}$$

$$i\dot{b}_{\pi\pi} = \mathcal{E}_{\pi\pi} b_{\pi\pi}(t) + M^*_{K^0,\pi\pi} a_{K^0}(t) + M^*_{\bar{K}^0,\pi\pi} a_{\bar{K}^0}(t)$$

set the energy scale such that $E_1 = 0$

$$b_{\pi\pi} = e^{-i(\mathcal{E}_{\pi\pi} - E_1)t} \int_0^t e^{i(\mathcal{E}_{\pi\pi} - E_1)t'} M^*_{K^0,\pi\pi} [a_{K^0}(t') + a_{\bar{K}^0}(t')]\, dt'$$

$$i\dot{a}_{K^0} = \sum_\pi M_{K^0,\pi\pi} e^{-i(\mathcal{E}_{\pi\pi} - E_1)t} \int_0^t e^{i(\mathcal{E}_{\pi\pi} - E_1)t'} M^*_{K^0,\pi\pi} [a_{K^0}(t') + a_{\bar{K}^0}(t')]\, dt'$$

and

$$= [\Delta - i\Gamma/2][a_{K^0}(t) + a_{\bar{K}^0}(t)]$$

$$i\dot{a}_{\bar{K}^0} = (\Delta - i\Gamma/2)[a_{K^0} + a_{\bar{K}^0}]$$

Solving gives

$$a_{K^0} + a_{\bar{K}^0} = e^{-2i\Delta t - \Gamma t}$$

$$a_{K^0} - a_{\bar{K}^0} = 1$$

$$|a_{K^0}|^2 = \tfrac{1}{4}[1 + e^{-2\Gamma t} + 2\cos(2\Delta)t\, e^{-\Gamma t}]$$

$$|a_{\bar{K}^0}|^2 = \tfrac{1}{4}[1 + e^{-2\Gamma t} - 2\cos(2\Delta)t\, e^{-\Gamma t}]$$

It is clear that 2Δ represents a mass difference between the states a_{K^0} and $a_{\bar{K}^0}$ and $a_{K^0} - a_{\bar{K}^0}$. The relatives size of Δ : Γ determines whether it is possible to detect the wiggles. The wiggles can be seen and Δ comes out to be $\sim .45\,\Gamma$

For $\tau \sim 10^{-10}$ sec, this gives an energy difference of $5\,\mu$ ev !

This mass split is of interest because:

i) it is really there. Hence there can be no question that a perturbation changes the mass in the way indicated by the formula. (in certain other applications of perturbation theory only the final (perturbed) mass is physical - hence the formal manipulations required seem much less meaningful)

ii)it is small. If the $\bar{K}^0$ had a negative mass compared to K^0 this mass difference, as measured by the wiggles, would be enormous ($\sim 2 \times 494$ MeV)

Thus we can dispose of speculations that antiparticles have negative masses.

$a_{K^0} + a_{\bar{K}^0}$ & $a_{K^0} - a_{\bar{K}^0}$ are eigenstates of the operator CP (which takes an antiparticle into its particle and vice versa). Our result showed that one CP eigenstate decays into two π's (also an eigenstate of CP), whereas the other doesn't.

For some time after its discovery, the long lived eigenstate K_2^0 was observed to go only into 3 π's and lepton pairs (lepton pairs aren't CP eigenstates, so the K_1^0's go into them as well). Hence it was believed that CP was conserved in all interactions.

It is now known that K_2^0 does go into two π's, but with a very low rate. So far, no theory has managed to a)explain all observed phenomena and b) maintain CP conservation. Thus CP appears to be broken, although with very small probability.

Furthermore, it appears that this CP nonconservation cannot be studied very well in any presently observed reactions other than K^0 decay. Hence it will be difficult to fit it into the total picture of things until there are new developments (either in theory of experiment).

Now we have been alluding to the ionized state as a plasma wave. This is not quite correct however. Due to the ∞-range of the Coulomb potential we must actually use the Coulomb wave form [coulomb-yukawa-potential form]

PROBLEM: Consider excitations in He and find the energy as a function of momentum to

$$\epsilon(p) = \Delta + \frac{1}{2m}(p-p_0)^2 \tag{1}$$

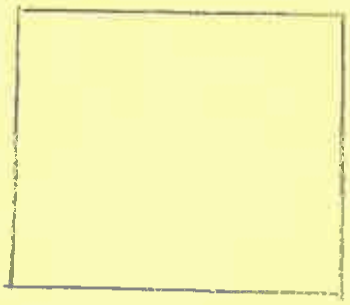
where Δ and p_0 are constants. Suppose also

$$\Delta(\rho) = \Delta_0 + (\rho-\rho_0)d + O(\rho-\rho_0)^2 \tag{2}$$

What is the probability of emitting a phonon of momentum $\hbar k$ in terms of p_0, Δ_0, d, and c_s?

Consider the He contained in a box of volume Vol. Now the density in the box obeys the wave eqn

$$\nabla^2\rho - \frac{1}{c_s^2}\frac{\partial^2\rho}{\partial t^2} = 0 \quad \text{classically.} \tag{3}$$



We want to quantize this fluid field. First if we imagine harmonic b.c., we can represent ρ as the sum of plane wave modes

$$\rho(\vec{r},t) = \sum_{\vec{k}} Q_{\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{r}} \tag{4}$$

If we plug this into (3) we find

$$-k^2 c_s^2 Q_{\vec{k}} - \ddot{Q}_{\vec{k}} = 0$$

just SHO. of $\omega = kc_s$

Now to apply p.m., we find the energy

$$\mathcal{E} = \int \rho \, \mathcal{E}_0 \, dV_0$$

Now we can write the interaction by writing

$$\mathcal{E}(\rho) = \frac{1}{2m}(\rho - \rho_0)^2 + \Delta_0 + \underbrace{(\rho - \rho_0)d}_{\text{interaction term}}$$

Thus

$$H_{\text{int}} = \frac{1}{2m}(\hat{p} - \hat{p}_0)^2 + \Delta_0 - \rho_0 d + \sum_k H_{k\,\text{osc}} + \sum_k d\, Q_k$$

where $H_{\text{osc}} = \frac{p_k^2}{2m} + \mu \frac{(kc)^2}{2} Q_k^2$

$$\mu = \frac{\rho_0 V}{2}$$

Now our unperturbed system H_0 is

$$H_{\text{system}} = \frac{1}{2m}(\hat{p} - \hat{p}_0)^2 + \Delta_0 - \rho_0 d$$

Note these will give system states corresponding to that of a free particle since $\Delta_0 - \rho_0 d = \text{const}$, e.g. $V = \text{const}$ in the S-eqn. Which have as

$$\langle r | \vec{p}' \rangle = \frac{e^{i \vec{k} \cdot \vec{r}}}{\text{vol}}$$

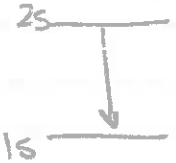
Thus we find

$$\underset{\vec{p} \to \vec{p}'}{\text{Rate}} = 2\pi\,\delta\!\left(\frac{p^2}{2m} - \frac{p'^2}{2m} - \hbar k c_s\right) \left|\langle p' | V_k | p \rangle\right|^2 \frac{1}{2\rho_0 V \hbar \frac{kc}{2}}$$

roton → 1 phonon of k

The remainder of the analysis should be obvious. Note the p_0 means that the roton will eventual decay to a ground state energy of $\frac{p_0^2}{2m} + \Delta_0$. One should be able to say something about the behavior of He II from this.

3.) Our problem is now to consider



2 photon emission

This immediately suggests the use of 2nd order perturbation theory, since a 2 photon process is 2nd order.

Thus we try to generalize our result on p. 31. This corresponds to the

$$\frac{qe^2}{2\mu}\,\vec{A}(\vec{r}_e)\cdot\vec{A}(\vec{r}_e)$$

term for the field interaction. The field, of course, is

$$H = \tfrac{1}{2}\sum_{\vec{k},\vec{\epsilon}}\left[\frac{p^2_{\vec{k},\vec{\epsilon}}}{2\mu} + \mu\frac{(kc)^2}{2}Q^2_{\vec{k},\vec{\epsilon}}\right]$$

$$H_{\text{interaction}} = \sum_{\vec{k},\vec{\epsilon}}\gamma_{\vec{k},\vec{\epsilon}}\,Q_{\vec{k},\vec{\epsilon}} + \sum_{\vec{k}',\vec{\epsilon}'}\sum_{\vec{k},\vec{\epsilon}}\frac{qe^2}{2\mu}\,e^{i(\vec{k}'+\vec{k})\cdot\vec{r}}\,Q_{\vec{k}',\vec{\epsilon}'}\,Q_{\vec{k},\vec{\epsilon}}$$

where $\gamma_{\vec{k},\vec{\epsilon}}$ is the first order operator on p. (34).

Now since the first order transitions is forbidden, we can conclude

$$\langle 1s|\gamma|2s\rangle = 0 \qquad \left[\begin{array}{c}\text{parity violated}\\ \text{in } \epsilon\end{array}\right]$$

What we now need is a nice handy dandy formula like

$$R_{a\to b} = 2\pi\,\delta(\epsilon_a - \epsilon_b - \hbar kc)\,|\langle b|\gamma_{\vec{k},\vec{\epsilon}}(a)\rangle|^2\,\frac{N_j+1}{2\epsilon_0\hbar\omega^{\frac{1}{2}}\omega}$$

for 2nd order theory. I'll wait for F to derive it -- if he doesn't, then I'll do it myself.

COMMENTS ON TIME-DEPENDENT PERTURBATION THEORY

We want to solve

$$-\frac{1}{i}\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \tag{1}$$

Write

$$H(t) = H_0 + V(t)$$

and expand

$$|\psi(t)\rangle = \sum_n c_n(t)\,|\phi_n\rangle$$

$$\Rightarrow H_0|\phi_n\rangle = E_n|\phi_n\rangle$$

Plug into (1)

$$\sum_n -\frac{1}{i}\dot{c}_n(t)\,|\phi_n\rangle = \sum_n c_n(t) E_n|\phi_n\rangle + \sum_n c_n(t) V(t)|\phi_n\rangle$$

Take a scalar product with $\langle\phi_m|$

$$-\frac{1}{i}\dot{c}_m(t) = E_m c_m(t) + \sum_n c_n(t)\langle\phi_m|V(t)|\phi_n\rangle \tag{2}$$

This suggests we try

$$c_m(t) = e^{-iE_m t}\,\gamma_m(t)$$

Then (2) becomes

$$\dot{\gamma}_m(t) = -i\sum_n \gamma_n(t)\underbrace{e^{-iE_m t}\langle\phi_m|V(t)|\phi_n\rangle\, e^{iE_n t}}_{v_{mn}(t)}$$

$$= i\sum_n v_{mn}\,\gamma_n(t) \tag{3}$$

(What relation does v_{mn} have to λ_{mn}?) Now we want

$$\gamma_m(t_f) = \sum_n \lambda_{mn}(t_f, t_i)\,\gamma_n(t_i).$$ Thus

λ_{mn} is some integral of $v_{mn}(t)$.

To evaluate the λ_{mn} (amplitude that if a state is in $\gamma_n(t_i)$ it will be in $\gamma_m(t_f)$), we take a specific case of $\gamma_n(t_i)$ and compute $\gamma_m(t)$ by integrating (3) and iterating

$$\gamma_m(t) = \delta_{mn} + (-i)\int_{t_i}^{t} V_{mn}(t_1)\,dt_1 + (-i)^2 \int_{t_i}^{t} dt_1 \int_{t_i}^{t_1} dt_2 \sum_k V_{mk}(t_1)\,V_{kn}(t_2) \qquad (4)$$

$$+ \cdots$$

and then identify $\gamma_m(t_f) = \lambda_{mn}(t_i, t_f)$ such that

$$\lambda_{mn}(t_i,t_f) = \delta_{mn} + (-i)\int_{t_i}^{t_f} V_{mn}(t_1)\,dt_1 + (-i)^2 \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 \sum_k V_{mk}(t_1)\,V_{kn}(t_2) \qquad (5)$$

If we consider a CONSTANT perturbation V applied at time t_i, we find

$$\lambda_{mn}(t_i,t_f) = \lambda_{mn}(t_i - t_f) = \delta_{mn} + (-i)\int_{t_i}^{t_f} V_{mn}\, e^{i(E_m - E_n)t}\,dt + \cdots$$

$$= \delta_{mn} + \frac{e^{i(E_m-E_n)T} - 1}{(E_m - E_n)} + \cdots \qquad (6)$$

Idea here is that if we can represent the state at t_i as a pure state $|\phi_n\rangle$ of the unperturbed Hamiltonian H_0, then the probability the state will be in an unperturbed state $|\phi_m\rangle$ at t_f is $|\lambda_{mn}|^2$. Note that since $|\lambda_{mn}|^2 \neq 0$ in general, the perturbation V mixes the pure state $|\phi_n\rangle$ and requires we represent $|\psi(t)\rangle$ as a superposition of the $|\phi_m\rangle$'s. Of course this merely expresses the fact that $|\phi_n\rangle$ is not a C.O.M. for the perturbed system.

Now we can define the S-matrix as

$$S_{mn} = \lambda_{mn}(-\infty, +\infty) \tag{7}$$

Then

$$S_{mn} = \delta_{mn} + (-i)\int_{-\infty}^{\infty} e^{i(E_m - E_n)t_1} V_{mn}(t_1)\,dt_1 + (-i)^2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \sum_l e^{i(E_m - E_l)t_1} V_{ml}(t_1)$$

$$e^{i(E_l - E_n)t_2} V_{ln}(t_2)$$

$$+ \cdots$$

$$= \delta_{mn} + (-i)\, V_{mn}^{F.T.}(E_m - E_n) + (-i)^2 \sum_l V_{ml}^{F.T.}(E_m - E_l)\, V_{ln}^{F.T.}(E_l - E_n) \tag{8}$$

$$+ \cdots$$

Thus we can express the Born expansion of S_{mn} as the Fourier transforms of the matrix elements of the perturbation.

Now suppose again at $t = t_i$, $|\psi(t)\rangle = |\varphi_n\rangle e^{-iE_n t_i}$. Then we require by conservation of probability,

$$\sum_m |c_{mf}(t)|^2 = 1 \qquad \sum_m |\gamma_{mf}(t)|^2 = 1 \tag{9}$$

or since $c_n = e^{-iE_n t}\gamma_n$,

Thus $\sum_m |\lambda_{mf}(t_i, t_f)|^2 =$ or

$$\sum_m \left| \delta_{mn} + (-i)\int_{t_i}^{t_f} v_{mn}(t_1)\,dt_1 + (-i)^2 \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 \sum_l v_{ml}(t_1)\, v_{ln}(t_2) + \cdots \right|^2 = 1$$

This seems pretty messy.

Instead try a different tact. Consider the first term of (9) as an integral equation

$$\gamma_m(t) = \gamma_m(t_i) + (-i)\int_{t_i}^{t} \sum_n v_{mn}(t_1)\,\gamma_n(t_1)\,dt_1 \tag{10}$$

Define the integral operation

$$\mathcal{L}(t,t_i) = (-i)\int_{t_i}^{t} \sum_n v_{mn}(t_1)\,[\;]\,dt_1 \tag{11}$$

so that (10) becomes

$$\gamma_m(t) = \gamma_m(t_i) + \mathcal{L}\{\gamma_m(t)\}$$

or

$$\gamma_m(t) = [1-\mathcal{L}(t,t_i)]^{-1}\gamma_m(t_i) \tag{12}$$

Thus we can identify an "evolution operator" $U_m(t,t_i)$

$$U_m(t,t_i) \equiv [1-\mathcal{L}(t,t_i)]^{-1} \tag{13}$$

such that

$$\gamma_m(t) = U_m(t,t_i)\,\gamma_m(t_i)$$

It would even be better to define a $U(t_s,t_i)$ such that

$$|\psi(t_f)\rangle = U(t_s,t_i)\,|\psi(t_i)\rangle \tag{14}$$

CENTRAL POTENTIAL SCATTERING:

(space limited potential)

Let $H = \underbrace{\frac{p^2}{2m}}_{H_0} + V(r)$

If we use plane wave fcns

$$H_0|\varphi_n\rangle = H_0|\vec{k}\rangle = \frac{k^2}{2m}|\vec{k}\rangle$$

Thus $|\varphi_n\rangle = |\vec{k}\rangle$, $|\varphi_m\rangle = |\vec{k}'\rangle$

Thus we expand

$$|\psi(t)\rangle = \sum_{\vec{k}} c_{\vec{k}}(t)\,|\vec{k}\rangle \qquad \langle\vec{r}|\vec{k}\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\text{vol}}}$$

Actually we usually consider scattering from one continuum $\vec{k}$ to another continuum $\vec{k}'$. Using our work on first Born approx

$$\text{Rate}_{\vec{k}\to\vec{k}'} = 2\pi\,\delta(E_k - E_{k'})\,|V_{\vec{k}\vec{k}'}|$$

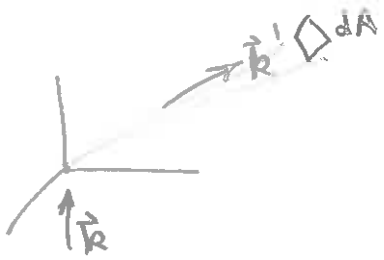
note the $\delta(k^2 - k'^2)$ merely ensures conservation of energy

where $V_{\vec{k}\vec{k}'} = \langle\vec{k}'|V(r)|\vec{k}\rangle$

$$= \iiint e^{i\vec{q}\cdot\vec{r}}\,V(\vec{r})\,\frac{d^3r}{\text{vol}} = V(\vec{q})$$

$$= 2\pi\int_{-1}^{+1} d\mu \int_0^{\infty} r^2 dr\, e^{iqr\mu}\,\frac{V(r)}{\text{vol}}$$

where $\vec{q} = \vec{k} - \vec{k}'$


$\vec{k}'$
Δp
$\vec{k}$

Physics 205a

Week of December 5

Problem: Due first class of second term

Choose one of the following:

a) Something you thought of yourself

b) It is commonly claimed in classes like Ph 205 that one can prove from the commutation relations for the rotation group that only half integer spins will appear.

Is this true?

The following has been suggested as a counterexample:

Take operators $J_z = \frac{1}{i}\left[V_x \frac{\partial}{\partial V_y} - V_y \frac{\partial}{\partial x}\right] + \lambda V_z$

$J_x = \frac{1}{i}\left[V_y \frac{\partial}{\partial V_z} - V_z \frac{\partial}{\partial V_y}\right] - \lambda V_y \phi$

$J_y = \frac{1}{i}\left[V_z \frac{\partial}{\partial V_x} - V_x \frac{\partial}{\partial V_z}\right] + \lambda V_x \phi$

$\phi = \arctan V_x / V_y$

It is claimed that: these commute like rotation group generators, but the J associated with them is not half integral.

Where does the inconsistency lie?

c) Suppose a system in which two spins ~~were~~ are combined, with a Hamiltonian of the form

$$H = A \vec{J}_a \cdot \vec{J}_b + B_z \left[\frac{\mu_a}{j_a} (J_a)_z + \frac{\mu_b}{j_b} (J_b)_z\right]$$

where B is a fixed field.

i) For small B, general spins, what are the energy levels of the combined system?

ii) Find the energy as a function of B for arbitrary B, in some special cases

e.g. $j_a = j \quad j_b = 1/2$

or something similar

(of course, if you can solve the problem in complete generality....)

Combination of angular momentum states

Suppose there are two particles of spins j_1 & j_2 together in a system. The spin of each individual particle tells how it transforms when a rotation of the coordinates is made. Now we must determine how the entire system transforms.

$$|\psi\rangle = |\psi_1\rangle |\psi_2\rangle$$

Symbolize the rotation operation by R $\quad R|\psi\rangle = R|\psi_1\rangle\, R|\psi_2\rangle$

$$R|\psi_1\rangle = \mathcal{D}_{j_1}(R)|\psi_1\rangle$$

$$R|\psi_2\rangle = \mathcal{D}_{j_2}(R)|\psi_2\rangle$$

where $\mathcal{D}_j$ is a matrix which acts on the spin indices of the wave functions

Thus we presumably have some matrix $\mathcal{D}$ such that $\quad R|\psi\rangle = \mathcal{D}(R)|\psi\rangle$

$$\mathcal{D}(R) = \mathcal{D}_{j_1}(R) \otimes \mathcal{D}_{j_2}(R)$$

To see what size $\mathcal{D}$ should have:

$|\psi_1\rangle$ has $(2j_1+1)$ components

$|\psi_2\rangle$ has $(2j_2+1)$ components

$|\psi\rangle$ has $(2j_1+1)(2j_2+1)$ components

However, $\mathcal{D}$ is not necessarily one of the fundamental ("irreducible") representations of rotations - i.e. it does not necessarily correspond to one particluar spin. Because it <u>is</u> a representation, it can be broken up into a direct sum of these irreducible representations.

This means that $|\psi\rangle$ can be written as $\sum a_i|\psi_i\rangle$ where the $|\psi_i\rangle$ correspond to each to a particular spin, and the a_i are completely determined by $|\psi_1\rangle$ and $|\psi_2\rangle$

$$|\psi_1^{j_1}\rangle\,|\psi_2^{j_2}\rangle = \sum_i a_i\,|\psi_i^{j_i}\rangle$$

The problem is to determine:

a) Which j_i will appear

b) What are the a_i

Both of these questions are answered by mechanically applying rotation operators and seeing how the state transforms. It may seem dull to go through this machinery, because in practice the a_i (Clebsch-Gordon coefficients) are usually found by looking in a table.

However, other continuous groups are sometimes relevent, and not all the coupling coefficients have been calculated. Thus it is worthwhile knowing what to do.

ONWARD!

I) Apply an infinitesimal rotation about the z axis $\quad (1+i\varepsilon J_z')|\psi_1^{j_1}\rangle\,(1+i\varepsilon J_z^2)|\psi_2^{j_2}\rangle$

$$= (1+i\varepsilon m_1)(1+i\varepsilon m_2)|\psi_1^{j_1}\rangle|\psi_2^{j_2}\rangle = (1+i\varepsilon J_z)|\psi\rangle$$

Here J_z is just the appropriate operator in $\mathcal{D}$

$$\Rightarrow \quad J_z|\psi\rangle = m|\psi\rangle \qquad m = m_1 + m_2$$

Rule 1) The magnetic quantum numbers always add

II) To find which j appear

As m_1 ranges over its $2j_1+1$ values

m_2 " " " $2j_2+1$ "

$\text{Max}(m_1+m_2) = j_1+j_2$

Hence this is the maximum value of J allowed in the decomposition

$|\psi\rangle - a_{J_{max}M} |\psi_{J_{max}M}\rangle$ is then a new thing whose possible maxJ is j_1+j_2-1 etc.

This goes on until $|\psi\rangle$ is exhausted.

to see how many steps are allowed, do a little calculation:

$$(2j_1+1)(2j_2+1) = \sum_{m=0}^{M} [2(j_1+j_2-m)+1]$$

$$= 2(j_1+j_2)(M+1) - M^2 + 1$$

$$\Rightarrow M = 2j_1 \text{ or } 2j_2$$

$$j_1+j_2-2j_1 = j_2-j_1$$

$$j_1+j_2-2j_2 = j_1-j_2$$

Then the minimum J is j_2-j_1 or j_1-j_2 whichever is physical

Rule 2) The J's allowed vary in steps of 1 from J_1+J_2 to $|J_1-J_2|$

(the steps are 1 because m steps necessarily come in ones)

III) To determine the a_j

Clearly it makes no difference whether we begin with a basis $|JM\rangle$

and expand it as $\sum b_{m_1 m_2} |j_1 m_1\rangle |j_2 m_2\rangle$

or start with $|j_1 m_1\rangle |j_2 m_2\rangle = \sum a_J |JM\rangle$

It is most convenient to find the $b_{j_1 j_2}$

$$|JM\rangle = \sum b_{m_1 m_2} |j_1 m_1\rangle |j_2 m_2\rangle$$

Clearly $|J_M J_M\rangle = |j_1 j_1\rangle |j_2 j_2\rangle$ if $J_M = j_1+j_2$

We then just apply J_- to both sides. Use of the relations derived last week $J_- |J_M M\rangle = C_M |J_M M-1\rangle$ will then completely specify the $b_{m_1 m_2}$

A word of caution is in order here:

In the most general case it is quite possible that beginning at $|J_M - J_M\rangle$ and applying Λ might lead to different phases for the $b_{j_1 j_2}$ than beginning at the top and working down. For the rotation group it happens that the states can be chosen

such that the phases for the two cases come out the same. However, not all Clebsch-Gordon tables use the same phase convention. Thus, unless you generate all your own Clebsch-Gordon coefficients it is absolutely essential never to use more than one table of C-G coeffs. at a time (i.e. within a given problem).

Assume all the states $|J_M M\rangle$ have been determined by this method. We next must find $|J_{M-1} M\rangle$. To do this, notice that $|J_M J_{M-1}\rangle$ is orthogonal to $|J_{M-1} J_{M-1}\rangle$ and that there are only two possible states with $m = J_{M-1}$ made up of $|j_1 m_1\rangle |j_2 m_2\rangle$

Then just ladder down from this new state. etc.

Suppose you just want some state which would be in the middle of one of the above series and can't bear the thought of constructing all the others.

Then the following trick may help:

$$|JM\rangle = \sum_{m_1+m_2=M} b_{m_1 m_2} |j_1 m_1\rangle |j_2 m_2\rangle$$

$$\vec{J}\cdot\vec{J}\,|JM\rangle = J(J+1)\,|JM\rangle = (\vec{J}_a+\vec{J}_b)\cdot(\vec{J}_a+\vec{J}_b)\sum b_{m_1 m_2}|j_1 m_1\rangle|\rangle$$

$$= (J_a^2 + J_b^2 + 2\vec{J}_b\cdot\vec{J}_a)\sum b_{m_1 m_2}|j_1 m_1\rangle|j_2 m_2\rangle$$

$$J_a^2 \to j_1(j_1+1) \qquad J_b^2 \to j_2(j_2+1)$$

Comparison of the equations

$$|JM\rangle = \sum b_{m_1 m_2}|j_1 m_1\rangle|j_2 m_2\rangle$$

$$|JM\rangle = \frac{1}{J(J+1)} \sum \text{mess}$$

will often allow you to determine the b's

Suppose you start out with n objects of spin $\frac{1}{2}$, all spinning up ↑↑↑↑ ...

and then ladder down.

The state is initially symmetric under permutations of the spinning objects. The ladder operator is also symmetric. Hence all the states of this J, the highest one possible for combinations of these spinors, are symmetric (This is one of those things its useful to have filed away somewhere)

It happens that all the representations of the rotation group can be found by appropriately combining spinors in this way.

i.e. the representation with $J = n/2$ is obtained from a symmetric combination of n spinors

OTHER CONTINUOUS GROUPS COMMON IN MODERN PHYSICS

Isotopic Spin

One of the symmetries first noticed in nuclear physics is that the nuclear forces between neutron and proton appear to be the same as those between neutron and neutron, and proton and proton.

Further, one can even apply a transformation of the sort

$$|p\rangle \rightarrow \alpha|p\rangle + \beta|n\rangle$$
$$|n\rangle \rightarrow -\beta^*|p\rangle + \alpha^*|n\rangle \qquad \ni \ |\alpha|^2 + |\beta|^2 = 1$$

without changing any of the forces.

The pair α, β determines an element of this group of transformations

The matrix $\begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$ acts on the pair $\begin{pmatrix} p \\ n \end{pmatrix}$ in exactly the same way as an element of the rotation group acts on an object of spin $\frac{1}{2}$. Hence the set (p, n) is called an isotopic spinor; and all the Clebsch-Gordonry involved with isotopic spin is identical to that for rotations

If the only representation of isotopic spin present in nature were the neutron-proton pair, this analogy would not be particularly useful. However, many isotopic families have now been identified:

spin 0 representation Λ

spin $\frac{1}{2}$ representations $n \quad p$
$\Xi^- \quad \Xi^0$

spin 1 representations: $K^+ \quad K^0$
$\pi^- \pi^0 \pi^+$
$\Sigma^+ \Sigma^0 \Sigma^-$

spin 3/2 representation $\Delta^- \Delta^0 \Delta^+ \Delta^{++}$

are a few examples

Notice that the rules derived above for coupling angular momentum already tell us something about strong interaction forces:

if we wish to make a Λ particle as a bound state of 2 particles, we must use a $\Sigma\pi$ combination - a $\Lambda\pi$ one will not work ($T=0 \otimes T=1$ cannot couple to $T=0$)

The fact that Δ has $T=3/2$ makes its decay into $\pi \quad N$ easily classified
$T=1 \quad T=1/2$

SU(3)

Both isotppic spin and rotations can be built up from a group of transformations on spinors, where the matrices acting on the spinors have the form

$$\begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} \qquad |\alpha|^2 + |\beta|^2 = 1$$

This is the group of special (i.e.determinant = 1) unitary transformations on two dimensions SU(2)

Suppose that instead of two "fundamental" objects there were three. Then we would have SU(3) as the matrix group.

We could go ahead and combine the fundamental 3 dimensional representation with itself to make more representations, as we did with the two dimensional spinors for SU(2). Unfortunately it is not possible to get all the representations of SU(3) this way. One other three dimensional representation must be introduced. Then products of $\underset{\sim}{3} \times \underset{\sim}{3}$ (the two 3 dimensional reps.) will generate all the representations.

It is easy to classify particles into isotopic spin multiplets because the masses of particles within a multiplet are very close together (they would be the same if there were no electromagnetic perturbations acting)

Classifying particles into SU(3) representations is more difficult because the symmetry is not exact (see discussion of Wigner-Eckart Theorem below). This means that the particles which belong to a given multiplet may have masses which differ by several hundreds of Mev. Nevertheless several representations have been identified:

Baryons

Octet Spin $\frac{1}{2}$ Parity +

$$n \quad p$$
$$\Sigma^+ \quad \Sigma^0, \Lambda \quad \Sigma^-$$
$$\Xi^0 \quad \Xi^-$$

Decuplet Spin 3/2 Parity +

$$\Omega^-$$
$$\Xi^{*-} \quad \Xi^0$$
$$\Sigma^{*-} \quad \Sigma^{*0} \quad \Sigma^{*+}$$
$$\Delta^- \quad \Delta^0 \quad \Delta^+ \quad \Delta^{++}$$

Mesons Octet Spin 0 Parity -

$$K^- \quad \bar{K}^0$$
$$\pi^- \quad \pi^0, \eta \quad \pi^+$$
$$\bar{K}^0 \quad K^+$$

Octet Spin 1 Parity -

$$K^{*-} \quad \bar{K}^{*0}$$
$$\rho^- \quad \rho^0, \omega' \quad \rho^+$$
$$K^{*0} \quad \bar{K}^{*+}$$

No one has yet found members of the $\underset{\sim}{3}$ or $\underset{\sim}{\bar{3}}$ representations. In most theories these are expected to have the following properties

particle a) strangeness-1 isospin 0 charge 0

particle b) strangeness 0 $T=\frac{1}{2}$ charge 1/3

particle c) strangeness 0 $T=\frac{1}{2}$ charge -2/3

lists the particles in one rep. The ones in the others are charge conjugates of these. b) and c) would be easily spotted (we hope) due to their fractional charge. People have looked for these in quite a number of experiments and have not yet found anything that is statistically believable.

All of the physics involved with the above groups has to do with calculating matrix elements of operators between states which belong to various representations of the group. The most powerful tool for doing this uses the transformation properties of the operators under generators of the group. In many books this method can be found masquerading behind the name WIGNER ECKART THEOREM

1) Given any operator, decompose it into pieces according to its transformation properties under spatial rotations

scalars: $\vec{x}, \vec{p}$ and other dot products

vectors: $\vec{x}, \vec{p}, \vec{x} \times \vec{p}$ etc

tensors $\vec{x}\,\vec{p}$

2) Re-express these so that they are separated into things with exact spin transformation properties:

$\vec{x} \cdot \vec{p}$ is an exact scalar which transforms like spin 0

$\vec{p}$ is an exact vector with transforms like spin 1

What do we mean "transforms like spin i?"

The spherical harmonics Y_J^M are eigenfunctions of total angular momentum with z projection M. Under a rotation of the coordinates, the Y_J^M for a given J transform among themselves according to the appropriate D^J

$$Y_J^{M'}(\theta_2) = \sum_M D^J_{M M'}(\theta_2 - \theta_1)\, Y_J^M(\theta_1)$$

Any wave function with these properties transforms like Spin J.

Now look at operators of the type shown above.

The components γ_1^m can be made to correspond to certain combination of a_i for a vector $V = \sum a_i \hat{e}_i$

$$\gamma_1^1 \leftrightarrow -1/\sqrt{2}(\hat{e}_x + i\hat{e}_y) \qquad \gamma_1^{-1} \leftrightarrow 1/\sqrt{2}(\hat{e}_x - i\hat{e}_y)$$

$$\gamma_1^0 \leftrightarrow \hat{e}_z$$

But γ_2^m has only 5 components, whereas the spatial tensor $\hat{e}_i \hat{e}_j$ has 9. Hence $\vec{x}\vec{p}$ cannot transform exactly like spin 2.

To figure out the proper spin decomposition of something like $\vec{x}\vec{p}$, notice the following:

a) a generalization of the arguments for spinor representations made above shows that every integral spin n representation can be formed from a <u>symmetric</u> combination of n spin 1 objects.

Hence if we have two spin 1 objects ($\vec{x}\vec{p}$), the spin two piece (highest spin formed) must not contain any antisymmetric combinations.

symmetric piece

$\hat{e}_x\hat{e}_x$ | $\hat{e}_y\hat{e}_x + \hat{e}_x\hat{e}_y$ | $\hat{e}_z\hat{e}_x + \hat{e}_x\hat{e}_z$

$\hat{e}_x\hat{e}_y + \hat{e}_y\hat{e}_x$ | $\hat{e}_y\hat{e}_y$ | $\hat{e}_z\hat{e}_y + \hat{e}_y\hat{e}_z$

$\hat{e}_x\hat{e}_z + \hat{e}_z\hat{e}_x$ | $\hat{e}_y\hat{e}_z + \hat{e}_z\hat{e}_y$ | $\hat{e}_z\hat{e}_z$

There are 6 independent symmetric pieces. We still can't hope to put this in one-to-one correspondence with a spin 2 object

antisymmetric piece

0 | $\hat{e}_y\hat{e}_x - \hat{e}_x\hat{e}_y$ | $\hat{e}_z\hat{e}_x - \hat{e}_x\hat{e}_z$

$\hat{e}_x\hat{e}_y - \hat{e}_y\hat{e}_x$ | 0 | $\hat{e}_z\hat{e}_y - \hat{e}_y\hat{e}_z$

$\hat{e}_x\hat{e}_z - \hat{e}_z\hat{e}_x$ | $\hat{e}_y\hat{e}_z - \hat{e}_z\hat{e}_y$ | 0

There are three independent elements here.

We recognize this as $\vec{x}\times\vec{p}$, a vector and thus a spin 1 object.

$\vec{x}\vec{p}$ can contain only spins 2,1,0 because $\vec{x}$ and $\vec{p}$ are spin 1. The only remaining problem is to separate the spin 0 from the spin 2.

spin 0 looks like $\vec{x}\cdot\vec{p}$ and thus corresponds to $\hat{e}_x\hat{e}_x + \hat{e}_y\hat{e}_y + \hat{e}_z\hat{e}_z$

Therefore any piece of our tensor of the form $a\hat{e}_x\hat{e}_x + b\hat{e}_y\hat{e}_y + c\hat{e}_z\hat{e}_z$ is a linear combination of spin 2 and spin 0.

It is clear that there are many ways to separate out the two, but to preserve the

symmetry under interchange of x,y and z one writes

$$\hat{e}_x\hat{e}_x\left[a-\tfrac{1}{3}(a+b+c)\right]+\hat{e}_y\hat{e}_y\left[b-\tfrac{1}{3}(a+b+c)\right]+\hat{e}_z\hat{e}_z\left[c-\tfrac{1}{3}(a+b+c)\right]+\frac{(a+b+c)}{3}\left[\hat{e}_x\hat{e}_x+\hat{e}_y\hat{e}_y+\hat{e}_z\hat{e}_z\right]$$

Spin decomposition of

spin 0 $\tfrac{1}{3}\vec{x}\cdot\vec{p}$

spin 1 $\vec{x}\times\vec{p}$

spin 2

$xp_x-\tfrac{1}{3}\vec{x}\cdot\vec{p}$	yp_x+xp_y	zp_x+xp_z
xp_y+yp_x	$yp_y-\tfrac{1}{3}\vec{x}\cdot\vec{p}$	zp_y+yp_z
xp_z+zp_x	yp_z+zp_y	$zp_z-\tfrac{1}{3}\vec{x}\cdot\vec{p}$

Having explicitly constructed all 5 independent elements of the spin 2 tensor, we put them in one-to-one correspondence with the Y_2^m's

Define $X_1^{\,1}=-1/\sqrt{2}\,(x+iy)$ $\qquad P_1^{\,1}=-1/\sqrt{2}\,(p_x+ip_y)$

$X_1^{-1}=1/\sqrt{2}\,(x-iy)$ $\qquad P_1^{-1}=1/\sqrt{2}\,(p_x-ip_y)$

$X_1^{\,0}=z$ $\qquad P_1^{\,0}=p_z$

Solving backwards gives

$$X_1^{\,1}P_1^{\,1}=\tfrac{1}{2}\{i(yp_x+xp_y)+xp_x-yp_y\}$$

$$X_1^{-1}P_1^{-1}=\tfrac{1}{2}\{-i(yp_x+xp_y)+xp_x-yp_y\}$$

$$X_1^{-1}P_1^{\,1}+X_1^{\,1}P_1^{-1}+2X_1^{\,0}P_1^{\,0}=-3(xp_x+yp_y)+2\vec{x}\cdot\vec{p}$$

$$X_1^{\,0}P_1^{-1}+P_1^{\,0}X_1^{-1}=-i/\sqrt{2}\{i(zp_x+xp_z)+zp_y+yp_z\}$$

$$X_1^{\,0}P_1^{\,1}+P_1^{\,0}X_1^{\,1}=-i/\sqrt{2}\{-i(zp_x+xp_z)+zp_y+yp_z\}$$

Now refer to a table of Clebsch-Gordon coefficients and construct spin 2 from two spin 1 objects

$(1\,1\,1\,1|2\,2)=1$ $\qquad (1\,1\,-1\,-1|2\,-2)=1$

$(1\,1\,1\,-1|2\,0)=1/\sqrt{6}$ $\qquad (1\,1\,-1\,1|2\,0)=1/\sqrt{6}$ $\qquad (1\,1\,0\,0|2\,0)=2/\sqrt{6}$

$(1\,1\,0\,-1|2\,-1)=1/\sqrt{2}$ $\qquad (1\,1\,-1\,0|2\,-1)=1/\sqrt{2}$

$(1\,1\,1\,0|2\,1)=1/\sqrt{2}$ $\qquad (1\,1\,0\,1|2\,1)=1/\sqrt{2}$

Hence $Y_2^{\,2}=X_1^{\,1}P_1^{\,1}$ $\qquad Y_2^{-2}=X_1^{-1}P_1^{-1}$

$$Y_2^{\,1}=1/\sqrt{2}\,(X_1^{\,0}P_1^{\,1}+P_1^{\,0}X_1^{\,1}) \qquad Y_2^{-1}=1/\sqrt{2}\,(X_1^{\,0}P_1^{-1}+P_1^{\,0}X_1^{-1})$$

$$Y_2^{\,0}=1/\sqrt{6}\,(X_1^{-1}P_1^{\,1}+X_1^{\,1}P_1^{-1}+2X_1^{\,0}P_1^{\,0})$$

Thus certain linear combinations of the $X_i P_j$ correspond exactly to spherical harmonics

In general the rule is:

Take the operator in question and break it up into pieces which transform under rotation like the spherical harmonics. Call these pieces $\boxed{Y_J^M}$

$$\Theta = \sum a_J^M \boxed{Y_J^M}$$

Then the rule for matrix elements is simple.

$$\langle \alpha j_1 m_1 | \boxed{Y_J^M} | \alpha j_2 m_2 \rangle = C_\alpha (j_2 J m_2 M | j_1 m_1)$$

where α specifies additional quantum numbers of the system.

Here C_α is a number that cannot be obtained by angular momentum arguments

To prove this:

$\boxed{Y_J^M} | \alpha j_2 m_2 \rangle$ transforms under rotation like $\sum a_i | \psi_{J_i}^{\nu} \rangle$

$|j_2 - J| \leq J_i \leq j_2 + J \qquad \nu = M + m_2$

where the a_i are the Clebsch-Gordon coefficients $(J\ j_2\ M\ m_2 | J_i\ \nu)$

A matrix element is just a number; hence it must be a rotational scalar. We can form this only if $\langle j_1 m_1 | = \langle J_i\ \nu |$ same J_i, ν

As far as the rotational character of the states and operators is concerned, a_i completely specifies the matrix element.

Notice that it is not necessary to think of operators in terms of spherical harmonics - you can do exactly the same thing by considering only the $\vec{J}$ operator, as follows:

$$[\vec{x}\cdot\vec{p}, \vec{J}] = 0$$

an operator's angular momentum properties are determined completely by its commutation relations with $\vec{J}$. Because $\vec{x}\cdot\vec{p}$ commutes with $\vec{J}$ in the same way as the unit operator, we know

$$\langle m_1 j_1 | \vec{x}\cdot\vec{p} | m_2 j_2 \rangle = a \langle m_1 j_1 | 1 | m_2 j_2 \rangle = a \delta_{m_1 m_2} \delta_{j_1 j_2}$$

where a has no dependence

$$[J_i, p_j] = a_{ij}^{\ k} p_k$$

where the $a_{ij}^{\ k}$ are the same as in $[J_i, J_j] = a_{ij}^{\ k} J_k$

Hence $\langle m_1 j_1 \alpha | \vec{p} | m_2 j_2 \alpha' \rangle = C \langle m_1 j_1 \alpha | \vec{J} | m_2 j_2 \alpha' \rangle$

The operator $\vec{x}\vec{p}$, as one would expect from the above discussion, does not have exactly the same commutation relations as the most simple tensor of the form $\vec{J}\vec{J}$

Exercise(for fun)do the operator decomposition of $\vec{x}\vec{p}$ that corresponds to our spherical harmonic decomposition

It is often helpful in computation to realize that algebraic simplifications exist for a system of given spin.

Example

$$(J_z+1)\,J_z\,(J_z-1)\,|1\,m\rangle = 0$$

allows you to reexpress products J_z^3 in terms of $J_z^2 + J_z$

Similar things can be done for $J_x + J_y$

APPLICATIONS OF WIGNER-ECKART THEOREM

Directly:

a nucleus of spin 0 has no magnetic moment

a nucleus of spin $\frac{1}{2}$ has no quadrupole moment

Suppose the Hamiltonian is invariant under rotation. It is thus a scalar ($\propto Y_0^0$)

Hence it cannot alter the J of M of a system $\langle j_1 m_1 | H | j_2 m_2 \rangle \propto \delta_{j_1 j_2}\,\delta_{m_1 m_2}$

Angular momentum is thus conserved in interactions governed by this Hamiltonian.

When viewed in the light of isotopic spin, this argument is repeated as follows:

If H is invariant under rotations in isotopic spin space, then it cannot connect states of different isotopic spin and z component of isospin. T & T_z must then be conserved.

The energy of a particle at rest is its mass; this is just the expectation value of the Hamiltonian in that state.

H a scalar in isospin space implies

$$\langle \alpha\, T\, T_z | H | \alpha'\, T\, T_z \rangle = C_\alpha \langle T\, 0\, T_z\, 0 | T\, T_z \rangle$$

which is independent of T_z. Thus states which differ only in T_z should have the same mass.

The strong interaction Hamiltonian is believed to be invariant under rotations in isospin space. It follows that if this were the only force acting, one would expect that all particles in a given isospin multiplet (which differ only by T_z) should have the same mass.

Neutron and proton have masses differing by about 1.3 Mev. They differ only in T_z. However there is another piece in our total Hamiltonian, formed by the

electromagnetic interaction.

The electromagnetic energy must have a piece proportional to the charge. In the neutron-proton system this would be written $K(1+\sigma_z)$. But $T_z \propto \sigma_z$

Thus the Hamiltonian contains an isospin vector. It is this piece which (in a general sense) accounts for the mass difference

Suppose that the Strong Interaction Hamiltonian were invariant under rotations in SU(3) space. Then all the elements of an SU(3) multiplet would be expected to have the same masses (The Wigner-Eckart Theorem generalizes easily to a group like SU(3))

However it is observed that the particles assigned to a multiplet do not all have the same mass. Hence the first conclusion to draw is that SU(3) is only an "approximate" symmetry of the Hamiltonian.

In fact, the "broken" symmetry is much more interesting in one sense than a complete symmetry would be. This is because we can expand the Hamiltonian in the SU(3) equivalent of

$$H = \sum \alpha \left[S_\alpha \right]$$

Study of the mass differences and coupling constants indicates that most of the non-symmetric piece belongs to one representation of SU(3) (the octet representation)

This is analogous to the $+\sigma_z$ electromagnetic term; but so far the explanations of "octet dominance" are not as simple to understand as is the presence of electric charge

An elegant and reasonably complete discussion of the properties of operators under rotation (and decomposition into irreducible tensor operators) can be found in Messiah Vol.II (first chapter and appendix)

In practice one usually ends up constructing things explicitly out of vectors by use of Clebsch-Gordon coefficients, as shown above.

Lectures 1–3 Physics 205b

Solid State Physics

There is a rich variety of phenomena associated with materials in the solid state. A very general approach is likely to lose this variety, so it is wise to think in terms of specific examples.

There are many places to read about the phenomena (eg., the Scientific American). The best way to understand how a phenomenon works is to figure it out for yourselves. The second-best way is to read a book. I suggest

C. Kittel, Introduction to Solid State Physics, 3rd ed. (Wiley).

In books and courses, there is an (unhealthy?) emphasis on methods. Examples, however, are essential, because very different approximations are used for different solids.

Types of Solids

1) Groups of atoms form molecules, and periodic arrangements of molecules form a molecular crystal. The molecules have no permanent electric dipole moment and are held together by Van der Waals forces.

Ex. Octane.

2) Another type of solid is known as a covalent crystal. The molecules are held together by covalent bonds (electron sharing) between molecules

Ex. Diamond

3) Ionic Crystal. Ex. NaCl

Each atom in the crystal has a net charge and is held in place by electrostatic attraction.

4) Metals. Certain electrons are no longer even approximately localized at definite atomic sites.

Ex. Liquid Mercury is a metal.

Metals are relatively soft. That is because the atoms can be moved with respect to each other (as in bending) without serious modification of the electron wavefunctions. Distortion of the perfect lattice generally results in increased hardness.

We will develop two topics in our excursion into solid state and molecular physics:

1) Vibrational motions of atoms about equilibrium positions.
2) Phenomena associated with the movement of electrons through the metallic lattice.

First, we will consider briefly the effect of temperature.

Consider an arbitrary crystal (or molecule). There exist energy levels E_i for the crystal, and the relative occupation probability p_i at temperature T is given by the Boltzmann law:

$$p_i \propto e^{-E_i/kT}$$

Normalization: $p_i = \frac{1}{Q} e^{-E_i/kT}$

$$\sum_i p_i = 1 \Rightarrow Q = \sum_i e^{-E_i/kT}$$

Then the average energy of the crystal is

$$U = \sum_i p_i E_i = \frac{1}{Q} \sum_i E_i e^{-E_i/kT}$$

There are common mathematical tricks that are useful in calculations at temperature T:

1) If you've found $Q = \sum_i e^{-E_i/kT}$

Then $\frac{\partial Q}{\partial T} = \frac{1}{kT^2} \sum_i E_i e^{-E_i/kT} = \frac{UQ}{kT^2}$

so that $U = \frac{kT^2}{Q} \frac{\partial Q}{\partial T}$.

Q is called the Partition Function

2) Let $Q = e^{-F/kT}$

then $F = -kT \log Q$

F is called the Free Energy.
(A note of caution: there are several different kinds of "free energy" in use.)

$$U = -T^2 \frac{\partial}{\partial T}\left(\frac{F}{T}\right)$$

$$= F - T\frac{\partial F}{\partial T}$$ ← entropy

I) Vibrations of Nuclei in a Crystal (or Polyatomic Molecule)

Problem: The Schrödinger Equation for the whole system (nuclei + electrons) is

$$\left[\sum_{j=i,\alpha} -\frac{\hbar^2}{2M_j}\nabla_j^2 + V(\underset{\sim}{R}_1, \underset{\sim}{R}_2, \ldots, \underset{\sim}{r}_\alpha, \underset{\sim}{r}_\beta, \ldots)\right]\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$$

where $\underset{\sim}{R}_k$ is the position vector of the k^{th} nucleus
$\underset{\sim}{r}_\alpha$ " " " " " " α^{th} electron

and $V = \sum_{i,j=k,\alpha} \frac{Z_i Z_j e^2}{r_{ij}}$ $\qquad r_{ij} = \begin{cases} |\underset{\sim}{R}_i - \underset{\sim}{R}_j| \\ \text{or } |\vec{r}_i - \vec{r}_j|, \text{ etc.} \end{cases}$

The problem is to show that the following equation is a good approximation for the state of lowest energy:

$$\sum_{\alpha\ (\text{electrons only})} -\frac{\hbar^2}{2m_e}\nabla_\alpha^2 \chi(\underset{\sim}{r}_\alpha) + V(\underset{\sim}{R}_i, \underset{\sim}{r}_\alpha)\,\chi(\underset{\sim}{r}_\alpha) = -\frac{\hbar}{i}\frac{\partial \chi}{\partial t} = E\chi$$

where the $\underset{\sim}{R}_i$ are fixed in such a way that

$$E = E(\underset{\sim}{R}_i) \text{ is a minimum.}$$

Show that to an excellect approximation

$$\Psi = \psi(\underset{\sim}{R}_k)\,\chi_{\underset{\sim}{R}_1 \cdots \underset{\sim}{R}_k \cdots}(\underset{\sim}{r}_\alpha, \underset{\sim}{r}_\beta \cdots)$$

Discuss the terms that make the equation an approximation and estimate the size of the errors involved.

Exercise: (Don't hand in)

Find F and U for a harmonic oscillator with natural frequency ω and mass m at temperature T.

The problem says that a Schrödinger Equation is approximately valid for the electron motion with fixed nuclei. Consider now the motion of the nuclei as small vibrations about the equilibrium configuration. Suppose the nuclei alone approximately obey a Schrödinger Equation with hamiltonian H,

$$H = \sum_i -\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial x_i^2} + U(x_i)$$

where (x_1, x_2, x_3) = displacement vector 1st nucleus

(x_4, x_5, x_6) = disp. vector of 2nd nucleus etc.

Then $U(x_i) = U(0) + \sum_i x_i \left.\frac{\partial U}{\partial x_i}\right|_0 + \frac{1}{2}\sum_{ij} x_i x_j \left.\frac{\partial^2 U}{\partial x_i \partial x_j}\right|_0 + \cdots$

Choose the zero of energy so that $U(0) = 0$ for convenience.

At the equilibrium configuration, $\left.\frac{\partial U}{\partial x_i}\right|_0 = 0$

Consider the displacements to be small (valid for many applications)

then $$H = \sum_i \frac{-\hbar^2}{2m_i}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\sum_{ij} x_i x_j V_{ij}$$

where $V_{ij} = \left.\frac{\partial^2 U}{\partial x_i \partial x_j}\right|_0$

Let $q_i = \sqrt{m_i}\, x_i$ and $c_{ij} = \frac{1}{\sqrt{m_i m_j}}\left(\frac{\partial^2 U}{\partial x_i \partial x_j}\right)_0$

Then

$$H = \sum_j \frac{1}{2} p_j^2 + \frac{1}{2}\sum_{ij} q_i q_j c_{ij},$$

where $p_j = \frac{1}{i}\frac{\partial}{\partial q_j}$

This problem can be analyzed classically and this is worthwhile because the results are rather similar to the quantum-mechanical case.

Classically, $$\ddot{q}_i = -\frac{\partial V}{\partial q_i} = -\sum_j c_{ij} q_j$$

A possible solution (periodic motion, really $\cos \omega t$) is

$$q_i = a_i e^{i\omega t}$$

Then we obtain the equation

$$\omega^2 a_i = \sum_j c_{ij} a_j .$$

This is an eigenvalue equation and has solutions in ω^2 where

$$\det |C - \omega^2 I| = 0.$$

This equation is of the n^{th} degree in ω^2, and has n real solutions (real because c_{ij} real and $c_{ij} = c_{ji}$).

Label these solutions $\omega_\alpha^2 \qquad \alpha = 1, \ldots n$

(n = number of coordinates $= 3N$, N = no. of nuclei)

Let the corresponding eigenvectors be designated $a_i^{(\alpha)}$.

i.e., $$\omega_\alpha^2 a_i^{(\alpha)} = \sum_j c_{ij} a_j^{(\alpha)}$$

α is known as the <u>mode number</u>.

We can choose normalization of the a's so that

$$\sum_{ij} a_i^{(\alpha)} a_j^{(\beta)} = \delta_{\alpha\beta}$$

Then it is also true that $\sum_\alpha a_i^{(\alpha)} a_j^{(\alpha)} = \delta_{ij}$

(That the a's, corresponding to different eigenvalues, are orthogonal is a well known property of the eigenvectors of hermitean matrices).

<u>Example:</u> CO_2 molecule

If you push one of the atoms, the other two atoms will respond and a complex motion will ensue.

Guess at the normal modes:

(Arrows indicate initial displacement)

$x_{(1)} = x_{(2)} = x_{(3)} = \frac{1}{\sqrt{3}}$

3 Modes of frequency 0 (no restoring force)
(same in y, z directions for other 2 modes)

(2) 

$$x^{(1)} = -x^{(3)} = \frac{-1}{\sqrt{2}} \quad , \quad x^{(2)} = 0$$

other displacements 0.

The same in the other 2 directions yields 3 modes of this type. All three frequencies are the same.

(3) 

$$\frac{1}{\sqrt{6}} \qquad \frac{-2}{\sqrt{6}} \qquad \frac{1}{\sqrt{6}}$$

+ same in other directions
3 modes of same frequency.

(The numbers were chosen so as to ensure orthogonality and normalization to unity).

Quantum-mechanically, instead of talking about displacements, we write the motion as a superposition of the different modes, giving the amplitude to be in each mode.

Let us make a linear transformation of coordinates, using the $a_i^{(\alpha)}$ we found classically,

viz., $$q_i = \sum_\alpha a_i^{(\alpha)} Q_\alpha$$

Then $$Q_\alpha = \sum_i a_i^{(\alpha)} q_i$$

The modes separate when we use these coordinates.

Let $$P_\alpha = \frac{1}{i} \frac{\partial}{\partial Q_\alpha}$$

Then $\frac{\partial}{\partial q_i} = \sum_\alpha \frac{\partial Q_\alpha}{\partial q_i}\frac{\partial}{\partial Q_\alpha} = \sum_\alpha a_i^{(\alpha)} \frac{\partial}{\partial Q_\alpha}$

$\therefore \quad p_i = \sum_\alpha a_i^{(\alpha)} P_\alpha$ (and, incidentally, $P_\alpha = \sum_i a_i^{(\alpha)} p_i$)

$$\therefore \frac{1}{2}\sum_i p_i^2 = \frac{1}{2}\sum_i \sum_\alpha a_i^\alpha P_\alpha \sum_\beta a_i^\beta P_\beta$$
$$= \frac{1}{2}\sum_{\alpha\beta} \delta_{\alpha\beta} P_\alpha P_\beta = \frac{1}{2}\sum_\alpha P_\alpha^2$$

$$\text{And } \frac{1}{2}\sum_{ij} c_{ij} q_i q_j = \frac{1}{2}\sum_{ij}\sum_{\alpha\beta} c_{ij} a_i^{(\alpha)} a_j^{(\beta)} Q_\alpha Q_\beta$$
$$= \frac{1}{2}\sum_i \sum_{\alpha\beta} \omega_\beta^2 a_i^{(\beta)} a_i^{(\omega)} Q_\alpha Q_\beta$$
$$= \frac{1}{2}\sum_\alpha \omega_\alpha^2 Q_\alpha^2$$

So that $H = \sum_\alpha (H_\alpha)_{osc.}$, where $(H_\alpha)_{osc.} = \frac{P_\alpha^2}{2} + \frac{1}{2}\omega_\alpha^2 Q_\alpha^2$

First, what does a particular energy level look like?

$$E = \sum_\alpha (n_\alpha + \tfrac{1}{2})\hbar\omega_\alpha$$ n_α are nonnegative integers.

Each choice of the set of n_α corresponds to a possible state of the system.

Wavefunctions $\psi = \prod_\alpha \phi_{n_\alpha}(Q_\alpha)$

where $\phi_{n_\alpha}(Q_\alpha)$ is the wavefunction for the n_α^{th}-excited state of a harmonic oscillator.

$\phi_0(x) \propto e^{-\frac{1}{2}\omega x^2}$ ($= e^{-\text{P.E.}/\hbar\omega}$ is a mnemonic for remembering this)

Ground state: All $n_\alpha = 0$

$$E_{\text{gnd-state}} = \sum_\alpha \frac{1}{2}\hbar\omega_\alpha + U(0)$$

$U(0)$: 0 (zero of energy)

And wavefunction $\propto \prod_\alpha e^{-\frac{1}{2}\omega_\alpha Q_\alpha^2} = e^{-\frac{1}{2}\sum_\alpha \omega_\alpha Q_\alpha^2}$

$$= e^{-\frac{1}{2}\sum_{ij}\gamma_{ij}q_i q_j}$$

where $\gamma_{ij} = \sum_\alpha \omega_\alpha a_i^\alpha a_j^\alpha$ = function of matrix C

Exercise: Show $\gamma^2 = C$.

At temperature T, the average excitation of a harmonic oscillator is

$$\bar{n} = \frac{1}{1 - e^{-\hbar\omega/kT}}$$

∴ at temperature T, internal energy of vibration

$$= U = \sum_\alpha \hbar\omega_\alpha (\bar{n}_\alpha + 1/2)$$

$$= \sum_\alpha \frac{\hbar\omega_\alpha}{2} + \sum_\alpha \frac{\hbar\omega_\alpha}{1 - e^{-\hbar\omega_\alpha/kT}}$$

$\frac{\hbar\omega_\alpha}{2}$: zero-pt. energy

And to obtain the specific heat, merely calculate $\frac{\partial U}{\partial T}$

Theorem: Average degree of excitation of an oscillator at temp. T is $\bar{n} = \frac{1}{1 - e^{-\hbar\omega/kT}}$

Proof: $p_n = e^{-n\frac{\hbar\omega}{kT}} \frac{e^{-\frac{1}{2}\hbar\omega/kT}}{Q}$, But $\sum_n p_n = 1 \Rightarrow Q = \frac{e^{-\frac{1}{2}\hbar\omega/kT}}{1 - e^{-\hbar\omega/kT}}$

So that $\bar{n} = \sum_n n p_n$

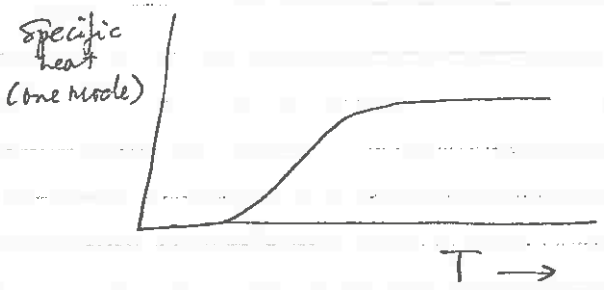
$$= (1 - e^{-\hbar\omega/kT}) \sum_n n x^n \qquad x = e^{-\hbar\omega/kT}$$

$$= (1-x) \frac{d}{dx}\left(\frac{1}{1-x}\right)$$

$$= \frac{1}{1 - e^{-\hbar\omega/kT}}$$

Comment on $U = \dfrac{\hbar\omega e^{\hbar\omega/kT}}{e^{\hbar\omega/kT} - 1}$

This gives a specific heat curve as a function of temperature like



This freezing-out of the contribution of the modes as $T \to 0$ was the first indication of the failure of classical mechanics, since this was discovered experimentally but not predicted theoretically. This discovery was made in the 19th century by Maxwell.

Application: Scattering of a neutron by a molecule.

Question: Suppose the molecule is in its groundstate before the collision. What is the probability that after the collision the molecule remains the ground state?

As an interaction, take $V(\underset{\sim}{R}) = a \sum_k \delta(\underset{\sim}{R} - \underset{\sim}{q}_k)$

initial state $\psi_i(R, q) = e^{i p_{in} \cdot R} \psi_i(q_1, q_2 \ldots)$

final state $\psi_f(R, q) = e^{i p_{out} R} \psi_f(q)$

Probability $\propto |M_{fi}|^2$

Make Born approximation for M:

$$M \propto \int \psi_f^* e^{i(p_{in}-p_{out})\cdot R} \delta(R - q_k) \psi_i \, d^3R \, dq$$

$$\propto \int\int\int \cdots e^{-\sum_\alpha \omega_\alpha^2 Q_\alpha^2} e^{i \sum_\alpha \kappa a_k^\alpha Q_\alpha} dQ_1 dQ_2 \cdots \quad \text{let } K = p_{in} - p_{out}$$

$$\propto \prod_\alpha \frac{1}{\sqrt{\omega_\alpha}} e^{-\frac{K^2 a_k^{\alpha\,2}}{4\omega_\alpha}} \propto e^{-K^2 S} \quad \text{where } S = \langle q_k^2 \rangle .$$

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Physics 205b

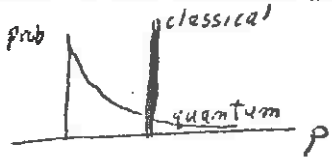
January 13,16, 17

MORE ON INTERACTIONS OF MULTI-ATOMIC SYSTEMS

Last week we found that the probability for a polyatomic system in the ground state to gain momentum p in some elastic collision (i.e. neither system changes energy state) is $e^{-p^2\langle q_K^2\rangle}$

where $\langle q_K^2\rangle$ is the average square displacement of the oscillator.

P is here measured in the center of gravity system. Hence this is quite different from what one would expect classically, for a classical elastic collision between an incident neutron and an atom in the lattice would impart just one definite momentum to the lattice.



Some things, however, are similar to the classical case:

(DO ANY ONE OF THE EXERCISES LISTED HERE OR IN THE JAN 20 LECTURE)

EXERCISE A:

Show that if the system is initially in the ground state, the mean value of the energy lost by a neutron is $p^2/2m_{osc}$, for a disturbance with matrix element

$$\langle \varphi_f | e^{ipx} | \varphi_i \rangle$$

It is only because the momentum transferred does not have a definite value that one can obtain a diffraction pattern from the crystal. Diffraction patterns are possible only if it is impossible after the scattering to tell which atom the neutron hit. Hence the scattering must be elastic as inelasticity would lead to changes in the crystal which could be detected. (See the sophomore physics text if you don't really understand this).

The oscillator has, along with its position q_K, a momentum p_K. To ensure elastic scattering we would expect $p < |p_K| \approx \hbar/|q_K|$ which agrees with $e^{-|p|^2/|p_K|^2}$

If the momentum transfer is too big the probability of elastic scattering is small and hence one cannot achieve a good diffraction pattern.

EXERCISE B: Show that elastic scattering from a crystal gives a diffraction pattern related to the structure of the crystal and that inelastic scattering does not. Disregard the fact that the momentum of the neutron is changed in the scattering

$B\frac{1}{4}$:Construct a theory of inelastic scattering from a crystal or a polyatomic molecule

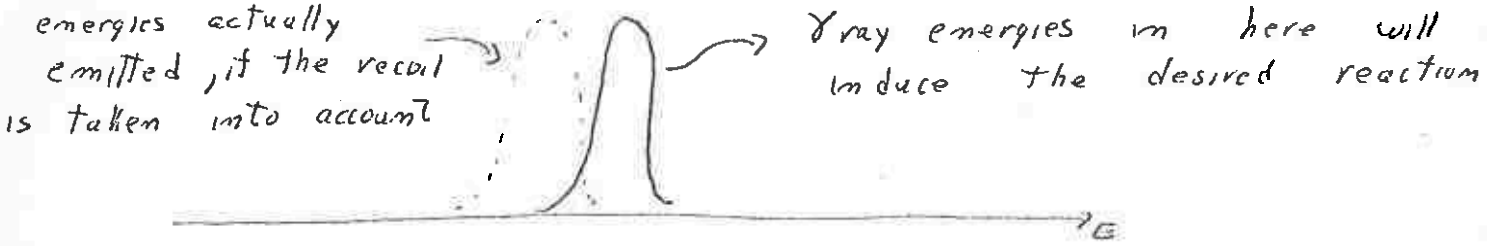
$B\frac{1}{2}$: The probability $e^{-\rho^2\langle q_x^2\rangle}$ derived above is called the Debye-Waller factor. We calculated it only for the simple case where the scattering is off only one particular kind of atom in the crystal. Figure out how to take into account the fact that there are different types of atoms in each unit cell.

Consider further implications of the fact that the lattice system can emit or gain momentum $\vec{p}$ and still remain in the ground state of energy.

Suppose a nucelus in a crystal undergoes some transition and emits a gamma ray of momentum $\vec{p}$. Classically you would expect that

E_γ = change of nuclear energy = $(\Delta E)_{Transition} - p^2/2M_{atom}$

This is, in fact, true in a gas where the atoms are not bound. To detect the emitted gamma ray, one would like to have it induce the inverse process in some other nucleus. However, the recoil energy is so big that the energy expected of the gamma ray is shifted far from the transition energy, even considering its width



Thus if one wants to do the experiment

one is forced to shift the effective ΔE_{II} in order that the lines overlap. This is accomplished by moving the second system. Then the Doppler effect shifts the gamma ray frequency seen by the system to the proper level.

This method of detecting resonance absorption has actually been carried out by putting one system on a spinning wheel.

However, if you think of the nucleus involved as simply one of the masses in a system of coupled harmonic oscillators, you see that there is a finite probability that the energy of this system will not change when the gamma ray is emitted. Hence the energy of the gamma ray will be exactly that of the nuclear transition. To detect this recoilless emission (Mossbauer effect), one slowly moves the receiver back and forth

and notices that the peak absorption is at zero relative velocity (i.e. no shift). The lines are so closely matched that a relative velocity of $1 mm/sec$ is sufficient to put you off resonance.

PROPERTIES OF THE HARMONIC OSCILLATOR

"Why do we spend so much time on the harmonic oscillator, Daddy?"

1) because it is one of the few problems in quantum mechanics which can be solved exactly by practically every method

2) because of the great similarities between quantum mechanicsland classical mechanics here

3) because whenever you expand a system about equilibrium you get a harmonic oscillator

4) because it is used all the time in talking about solid state, light, particles... etc.

For convenience set $m = 1 \quad \omega = 1$

$$H = \tfrac{1}{2} p^2 + \tfrac{1}{2} \xi^2 \qquad p = \tfrac{1}{i} \frac{\partial}{\partial \xi}$$

$$H \phi_n = \epsilon_n \phi_n$$

$\epsilon_n = n + \tfrac{1}{2}$ are the eigenvalues

$$\phi_n = \frac{1}{\pi^{1/4}} \frac{H_n(\xi)}{\sqrt{2^n n!}} e^{-\frac{1}{2}\xi^2}$$

Examples:

$H_0 = 1 \qquad H_1 = 2\xi$

$H_2 = 4\xi^2 - 2$

They can all he written compactly in terms of a generating function

$$e^{-s^2 + 2s\xi} = \sum_n \frac{H_n(\xi)\, s^n}{n!}$$

Hence

$$\sum \frac{\phi_n(\xi)\, s^n}{\sqrt{n!}\sqrt{2^n}} = \frac{e^{-\frac{1}{2}\xi^2}}{\pi^{1/4}} \sum \frac{H_n(\xi)}{n!} \left(\frac{s}{2}\right)^n = \frac{e^{-\frac{1}{2}(\xi - s)^2 + s^2/4}}{\pi^{1/4}}$$

Sometimes you can make up other generating functions, for fun and profit.

Example: to compute the general matrix element

$$\lambda_{mn} = \int \phi_m^*(\xi)\, e^{ip\xi}\, \phi_n(\xi)\, d\xi$$

Define $$f(s,t) = \sum_{mn} \frac{\partial_{mn}\, s^m t^n}{\sqrt{2^n 2^m\, m!\, n!}}$$

It happens to be simpler to compute f and expand in s and t to get ∂_{mn} than to do the explicit integral every time

$$f = \sum_{mn} \int_{-\infty}^{\infty} \frac{s^m t^m\, e^{i\rho\xi}\, \phi_m(\xi)\, \phi_n(\xi)\, d\xi}{\sqrt{2^m 2^n\, m!\, m!}}$$

$$= \int \frac{e^{i\rho\xi}}{\pi^{1/2}}\, e^{-\frac{1}{2}(\xi-s)^2 + s^2/4 - \frac{1}{2}(\xi-t)^2 + t^2/4}\, d\xi$$

$$= e^{-\rho^2/4} \iint e^{i\rho s/2}\, e^{i\rho t/2}\, e^{st/2} = e^{-\rho^2/4} \sum \frac{(i\rho s)^n}{2^n n!} \frac{(i\rho t)^k}{2^k k!} \frac{(st)^m}{m!\, 2^m}$$

Thus

$$\frac{\partial_{ij}}{\sqrt{2^i 2^j (i!)(j!)}} = e^{-\rho^2/4} \sum_m \frac{(i\rho/2)^{i+j-2m}\, 2^m}{(i-m)!\,(j-m)!\, m!}$$

EXERCISE C: For a crystal at temperature T, find the probability for elastic scattering with a given p.

Hint: if we had just a single oscillator, the answer would look like

$$(\text{normalization}) \sum_n |\langle n|e^{i\rho\xi}|n\rangle|^2\, e^{-E_n/kT}$$

because $e^{-E_n/kT}$ is the probability to be in the n'th state

One should find that the probability distribution for the energy lost again looks like

$$e^{-\rho^2 \langle q^2\rangle_T}$$

EXERCISE D:

Prove

$$\sum_n \phi_n(\xi)\, \phi_n^*(\xi')\, e^{it\epsilon_n} = \sqrt{\frac{m\omega}{2\pi i \sin\omega t}}\, e^{\frac{im\omega}{2\sin\omega t}\left[(\cos\omega t)(\xi^2+\xi'^2) - 2\xi\xi'\right]}$$

EXERCISE E: Unlike any other problem in quantum mechanics (with the exception of the free particle), the time dependent equation can be solved exactly.

Solve:

$$i\frac{\partial}{\partial t}\psi(\xi,t) = -\frac{1}{2}\frac{d^2}{d\xi^2}\psi(\xi,t) + \frac{1}{2}\xi^2\psi(\xi,t)$$

for some set of initial conditions - e.g. $t=0 \qquad \psi = \delta(\xi-\xi_0)$

Hint: Try $\psi(\xi,t) = e^{a(t)\xi^2 + b(t)\xi + c(t)}$

Another nice property of the harmonic oscillator equation is that it looks exactly the same in momentum space as in configuration space. Hence the normalized eigenfunctions must be the same up to phase. The phase is defined by Fourier transform from the configuration space functions. $\psi(p) = \int e^{ip\xi} \phi(\xi) d\xi$

(Feynman's guess is that $\psi_n(p) = i^n \phi_n(p)$. What do you get?)

It may on occasion be more convenient to use the momentum space wave functions

$$\lambda_{mn} = \int \phi_m^*(\xi) e^{iP\xi} \phi_n(\xi) d\xi$$

$$= i^{m-n} \int \psi_m^*(p) \psi_n(p+P) dp$$

shows explicitly that momentum P has been transferred to one of the oscillators

ASIDE:

Notice that a lot of these techniques which suggest themselves naturally in the harmoni oscillator problem can be used to advantage elsewhere. Consider the hydrogen atom:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{l(l+1)}{r^2} R + \frac{2m}{\hbar^2}\left[E - e^2/r\right] R = 0$$

For simplicity take $l = 0 \qquad 2me^2 = 1$

$$rR = f$$

$$-r\frac{d^2}{dr^2} f + f = Erf$$

This can be easily transformed to momentum space

$$-\frac{\hbar}{i}\frac{d}{dp}\left(\frac{p^2}{2}\phi(p)\right) + f(p) = -E\frac{\hbar}{i}\frac{df}{dp}$$

Now it is a first order differential equation, which is presumably easier to solve than the previous second order differential equation.

This equation (with $\hbar$ left in) can also be factorized into "creation" and "annihilation" operators in a manner not too unlike the one used below for the harmonic osciallator. These can then be used to find the eigenvalues. Interested persons should consult Morse and Feshbach pp. 270,729

CREATION AND ANNIHILATION OPERATORS FOR THE HARMONIC OSCILLATOR

$$H = \frac{1}{2} p^2/m + \frac{m\omega^2 q^2}{2}$$

$$a = \sqrt{\frac{m}{2\omega}}\left(\omega q + \frac{ip}{m}\right) = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$$

$$a^+ = \sqrt{\frac{m}{2\omega}}\left(\omega q - \frac{ip}{m}\right) = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)$$

a^* is called a creation operator and a an annihilation operator

$[p,q] = -i \Rightarrow \quad a a^+ - a^+ a = 1$

$a a^+ = 1/\omega H + 1/2$

$a^+ a = 1/\omega H - 1/2$

The most useful form is $H = \omega a^* a + \frac{\omega}{2}$, following a general rule of thumb wherein all the annihilation operators are written to the right of all the creation operators (normal ordering)

$a|0\rangle = 0 \Rightarrow \quad H|0\rangle = \omega/2 |0\rangle$

and $\omega/2$ can thus be interpreted as the energy of the ground state; $\omega a^* a$ as the energy above the ground state

$N = a^* a$ has integer eigenvalues $\quad N|n\rangle = n|n\rangle$

on which the creation and annihilation operators act like

$a^*|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad a|n\rangle = \sqrt{n}\,|n-1\rangle$

Hence $\quad \frac{(a^*)^n |0\rangle}{\sqrt{n!}} = |n\rangle$

All matrix elements written in terms of p's and q's can be reexpressed in terms of creation and annihilation operators (although this is not necessarily worthwhile)

$$q_{mn} = \langle m | \frac{q+q^*}{\sqrt{2}} | n \rangle = \langle 0 | \frac{a^m}{\sqrt{m!}} \frac{(a+a^*)}{\sqrt{2}} \frac{a^{*n}}{\sqrt{n!}} | 0 \rangle$$

This can then be calculated explicitly by commuting until all operator products are in normal order form $\quad q_{01} = \langle 0 | \left(\frac{a+a^*}{\sqrt{2}}\right) a^+ |0\rangle =$

$$\langle 0 | \frac{a^+ a^*}{\sqrt{2}} + \frac{1}{\sqrt{2}} (1 + a^+ a) |0\rangle = 1/\sqrt{2} \qquad e^+ c$$

Thus $\quad \lambda_{mn} = \langle 0 | \frac{a^m}{\sqrt{m!}} e^{ip(a+a^+)/\sqrt{2}} \frac{(a^+)^n}{\sqrt{n!}} |0\rangle$

If several independent oscillators are involved

$$a^*_\alpha = \sqrt{\frac{m_\alpha}{2\omega_\alpha}} \left(\omega_\alpha Q_\alpha + i \frac{P_\alpha}{m_\alpha}\right)$$

$$a_\beta a_\alpha^* - a_\alpha^* a_\beta = \delta_{\alpha\beta}$$

$$[a_\beta, a_\alpha] = 0 \qquad [a_\beta^+, a_\alpha^*] = 0$$

$H =$ (Ground state energy) $+ \sum_\alpha \omega_\alpha a^*_\alpha a_\alpha$

↳ notice the embarrassing fact that if there are an infinity of osciallators the ground state energy is infinite

In usage the harmonic oscillator formalism drags along some terminology. This can be

put in general form as follows:

when the oscillator is in the n th state it contains n vibratons

$a^\dagger$ creates a vibraton

a takes one away

The word vibraton is then replaced by phonon, roton, photon, meson, nucleon, etc. depending on your audience.

HOW TO APPLY ALL THIS TO CRYSTALS

Last week we discussed the Hamiltonian $H = p_i^2/2 + \frac{1}{2} C_{ij} q_i q_j$ for a small set of coupled oscillators (e.g. in a polyatomic molecule).

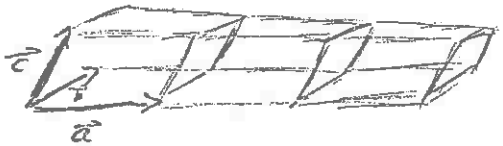
The point is to change coordinates by an orthogonal transformation which diagonalizes the C_{ij} ; the new coordinates are called normal modes of vibration and in terms of them $H = P_i^2/2 + 1/2\, Q_i^2$

Diagonalizing C_{ij} can be done by brute force for the case of molecules which contain only a few atoms; however in the case of a crystal with 10^{23} or so atoms some other approach must clearly be used.

The most obvious distinguishing characteristic of crystals is their periodic structure. By exploiting this symmetry we are able to reduce the potentially complicated problem of crystal vibrations to one with as few independent factors as the polyatomic molecule case Most of the definitions which follow are simply bookkeeping procedures to this end.

BASIC CRYSTAL STRUCTURE

The lattice is a neatly stacked array of unit cells



Each cell is identified by a vector $\vec{N} = n_a \vec{a} + n_b \vec{b} + n_c \vec{c}$ where $\vec{a}, \vec{b}, \vec{c}$ are fundamental vectors characteristic of the crystal lattice and (n_a, n_b, n_c) is a triplet of integers characterizing the cell.

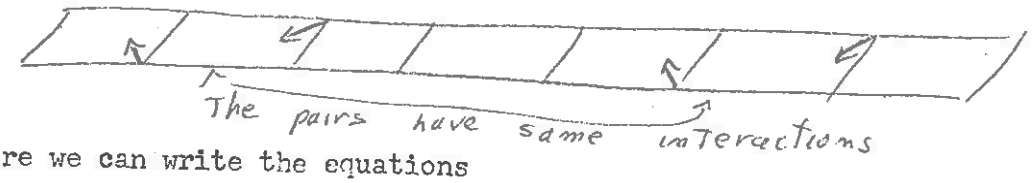
Within each cell there is the same (usually complicated) arrangement of atoms and molecules. Label the units within a cell by $\vec{r}$

Then the total Hamiltonian for the system takes the form

$$\sum_{N,r} \frac{P_{N,r}^2}{2} + \frac{1}{2} \sum C_{N,r,M,s}\, q_{N,r}\, q_{M,s}$$

where $C_{N,r;M,s} = \Gamma_{n,s}(\vec{N}-\vec{M})$

i.e. the forces between atoms depend only on the differences between the cell positions, not on the individual cell position



As before we can write the equations

$$\omega_a^2 q_{N,n} = \sum_{M,s} \Gamma_{n,s}(\vec{M}-\vec{N})\, q_{N,s}$$

but the method of solution used before is no good.

To see how we will use the periodicity of the lattice, consider a one dimensional crystal

Let q_N be the displacement of the n th atom from equilibrium

Then the potential energy takes the form $\sum_n \frac{A}{2}(q_n - q_{n+1})^2$

Differentiate with respect to q_N to get the force

$$\omega_a^2 q^n = A(q_n - q_{n+1}) - A(q_{n-1} - q_n) = A(2q_n - q_{n+1} - q_{n-1})$$

To patch up the end points we define the conditions $\Gamma(-1) = A \quad \Gamma(0) = 2A$

Then our previous techniques would be to find the determinant of

$2A-\omega^2$	$-A$							$-A$
$-A$	$2A-\omega^2$	$-A$						
	$-A$	$2A-\omega^2$	$-A$					
				etc				

If we wished to consider interactions not only of nearest neighbors, but also of next nearest neighbors, the Hamiltonian would have an additional term of the form $\sum_n \beta/2 (q_n - q_{n+2})^2$ and the matrix would become correspondingly more complicated.

There is a theorem which tells you that it is possible to find the determinant of a matrix with the above form, regardless of its size. But all this says is that it is possible to find the solution of a linear homogeneous differential equation which involves only differences between the displacements (note that the differential equation involved has time as the variable - this has already been factored out).

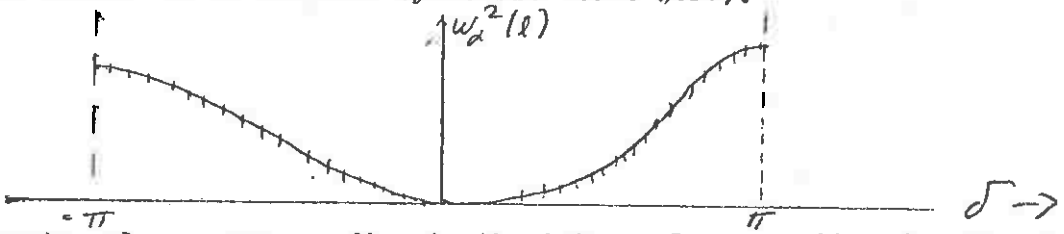
We know this already (by intuition). Therefore, try $q_n = e^{ina\delta}$

$$\omega_a^2 e^{ina\delta} = A\left[2e^{ina\delta} - e^{i(n+1)a\delta} - e^{i(n-1)a\delta}\right] \Rightarrow \omega_a^2 = 2A\left[1-\cos\delta\right]$$

At first sight one feels that δ may be arbitrary and hence that there is a continuum of solutions for ω_a. However, this is not the case because of the periodic boundary conditions imposed (from the matrix above we see that we have in effect hooked the first atom in the chain onto the last one). The imposition of periddic boundary conditions is one quite standard technique in these crystal problems. It means that if m is the number of atoms in the crystal, then $q_{m+s} = q_s$

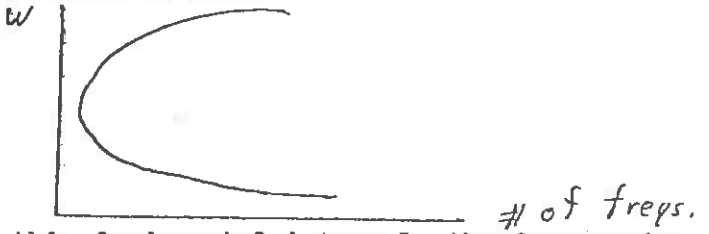
For our example this means $e^{ima\delta} = 1$

Hence $\delta = \frac{2\pi l}{ma}$ where l is an integer from 0 to $m-1$ (or it may assume an equal number of values in an interval symmetric about zero).

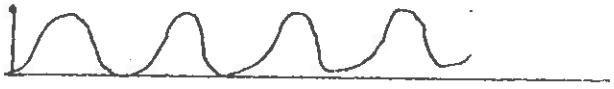


Only discrete values corresponding to the integer l's are allowed. This treatment is really valid only if a large number of cells is involved, however, so no harm is done in drawing the curve as a continuum. (if there were not large numbers of cells involved, the surface effects would become important and our imposition of periodic boundary conditions would be dubious).

Another interesting property is the number of vibrational frequencies at a given frequency (i.e. the density of points along the curve.) For fun, figure out how to calculate this and check the curve drawn in class



If δ continued outside this fundamental interval, the frequencies would simply repeat



Hence we always limit ourselves to the first zone constructed in the way.

If β should be non zero, it is easy to see that the answer will have the form

$$\omega = 2A(1-\cos\delta) + 2\beta(1-\cos 2\delta)$$

and so forth for more distant interactions

Solid state physicists do not in general talk about δ, however. The quantity normally used is $k = \delta/a$ = phase difference/cm. For a three dimensional crystal, k becomes a vector $\vec{k} = (\delta_1/a, \delta_2/b, \delta_3/c)$ in a space called reciprocal lattice space (since $1/a, 1/b, 1/c$ are the units of length along the respective crystal directions)

Because the spacing of δ is $\frac{2\pi}{m}$, the spacing of k is $\frac{2\pi}{ma} = \frac{2\pi}{\text{Length}}$ For very small k (i.e. very long waves) we get from above that $\omega^2 \simeq Aa^2k^2$; $\omega = ck$ where c may be thought of as the spped of sound. Hence at long wavelengths the spped of sound is very nearly independent of the wavelength.

Given an allowed k, define a mode of vibration by $Q_k = \sum_{\text{atoms}} e^{-ikam} \frac{q_m}{(\text{norm})}$ Then the Hamiltonian assumes the form $H = \sum \left(\frac{P_k^2}{2} + \frac{\omega(k)^2}{2} Q_k^2 \right)$ where $\omega^2(k) = 2A(1 - \cos ka)$

Notice again that just as there is only a region of δ which is significant, there is only a region of k which is significant. For k too large, the wavelengths get smaller than the spacing between the atoms  and these can't have any extra significance for the vibrations of the atoms. Thus there is only a fundamental zone of k which is important (a region in reciprocal lattice space called the first Brillouin zone). After this point things just repeat.

Thus sound has a maximum frequency of importante (minimum wavelength).

For a general problem we conclude that the solution should have a quite simple form: the first unit cell has some disturbance, and the same thing should appear in the next cell only slightly out of phase. $q_{N,s} = q'_s e^{i\vec{N}\cdot\vec{K}}$

Inserting this $\omega_a^2 q_r^1 e^{i\vec{N}\cdot\vec{K}} = \sum_{M,s} \Gamma_{r,s}(\vec{N}-\vec{M}) e^{i\vec{K}\cdot\vec{M}} q_s^1$

But $\sum_{N'} \Gamma_{r,s}(N') e^{i\vec{K}\cdot\vec{N}'} = \gamma_{r,s}(K)$ is just a Fourier transform of the $\Gamma_{r,s}$

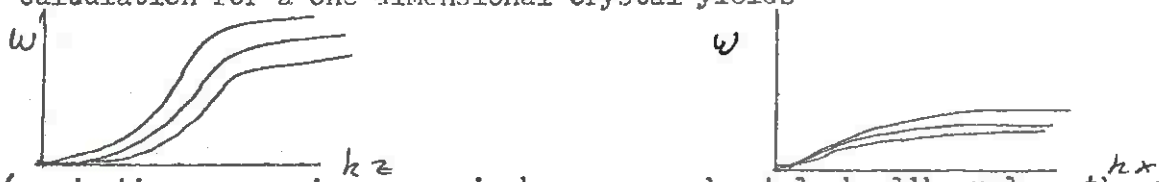
$$\boxed{\omega_B^2 q_r^1 = \sum_s \gamma_{r,s}(K) q_s^1}$$

In this form it is clear that it is only necessary to solve the determinant within a single cell - a problem of the same order of nagnitude as encountered in the case of polyatomic molecules, and one which can conceivably be done on the computer.

In computational problems, one should keep in mind that the spacings of k (box type

normalization) are $\frac{2\pi}{L_a}, \frac{2\pi}{L_b}, \frac{2\pi}{L_c}$. Any sum over k goes over naturally to an integral $\int \frac{d^3k \ (\text{volume})}{(2\pi)^3}$

For a three dimensional crystal with one atom per unit cell the simple generalization of our calculation for a one dimensional crystal yields

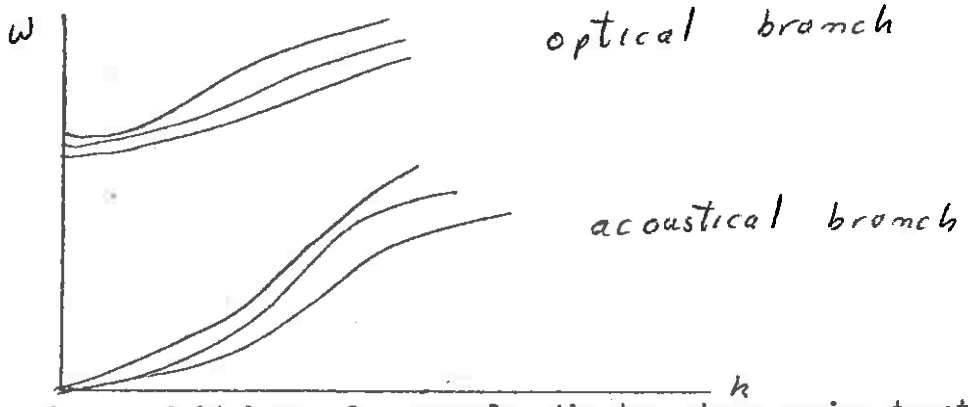


(projections on various axes in k space need not look alike unless the crystal is isotropic)

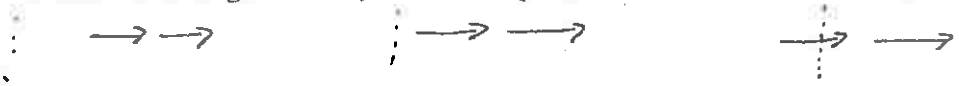
It is possible to prove that at k=0, $\omega \sim k^2$ for all cases of physical interest.

The three modes shown above can be approximately classified as 1 longitudinal mode and two transverse modes, although when the crystal is anisotropic there is no need for the sound vibrations in the longitudinal mode to be exactly along k, or for the transverse mode to be exactly transverse (compare propagation of polarized light in an anisotropic crystal)

If there are two atoms in the unit cell then the number of degrees of freedom is multiplied by 2 and analysis shows that there are indeed 6 possible modes of vibration. However, as k→0, it is not necessary that all frequencies go through zero. One finds in fact



In the acoustical branch one might have, for example, the two atoms moving together



with the pattern slightly displaced from cell to cell

For the optical branch they might move →← with a much higher frequency and hence energy, but the entire pattern may be only slightly displaced from cell to cell (this is what determines k)

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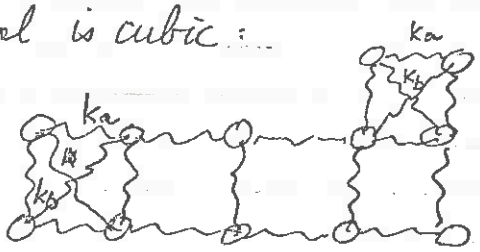
Additional Problems (Do one or more):

(1) Consider a one-dimensional line of atoms with spacing "a". Develop the theory of small vibrations in the limiting case $a \to 0$. (This is a special example of a one-dimensional quantum field).

(2) Find the frequency spectrum for the normal modes for a particular crystal, or find the specific heat of the crystal.

Simplest crystal is cubic:



Find the high frequency branch (optical modes) as well. Can you determine the elastic constants?

In the acoustical branch, $\omega \to 0$ as $k \to 0$ because the forces depend only on relative displacement of the nuclei, and $k \to 0$ corresponds to all the atoms moving together. On the other hand, $k \to 0$ can yield an electric dipole moment and this can act as a restoring force to generate frequencies $\neq 0$, and this is the optical branch. (As $k \to 0$, there are 3 optical and 3 acoustical frequencies).

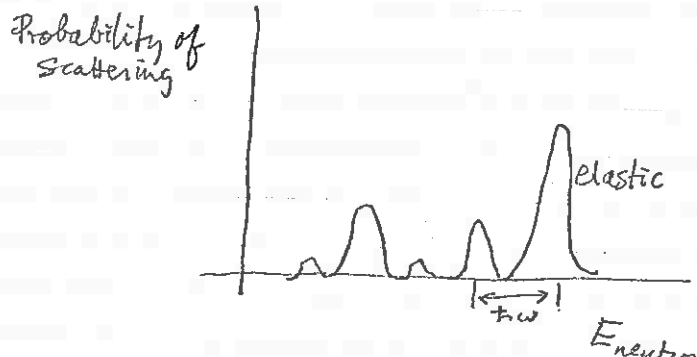
The coupling constants of lattice vibrations to external disturbances are needed for calculations. Experimentally, some of these are determined from elastic constants which are either measured or inferred from the speed of sound.

(3) Show how to find the elastic constants by measuring the speed of sound.

(4) Neutron Scattering Let $\underset{\sim}{P} = \underset{\sim}{P}_{out} - \underset{\sim}{P}_{in}$

Show that this will excite a mode of wavevector $\underset{\sim}{K}$ where

$\underset{\sim}{K} = \underset{\sim}{\rho} + \underset{\sim}{L}$ where $\underset{\sim}{L}$ is a reciprocal lattice vector. (see below)



The positions of the peaks are determined by the modes, and provide a means of measuring the frequencies of the modes.

Reciprocal Lattice:

$$\sum_k \longrightarrow \int \frac{d^3k}{(2\pi)^3} \text{(vol.)}$$

We are not usually interested in all $\underset{\sim}{k}$ values.

If the 3 fundamental translation vectors of the lattice are $\underset{\sim}{a}, \underset{\sim}{b}, \underset{\sim}{c}$, then the phase in the $\underset{\sim}{N}$ th cell is

$e^{i\underset{\sim}{K}\cdot\underset{\sim}{N}}$ for a mode with wave-vector $\underset{\sim}{K}$.

Now if $\underset{\sim}{K}' = \underset{\sim}{K} + \underset{\sim}{L}$

then $e^{i\underset{\sim}{K}'\cdot\underset{\sim}{N}} = e^{i\underset{\sim}{K}\cdot\underset{\sim}{N}}$ if $e^{i\underset{\sim}{N}\cdot\underset{\sim}{L}} = 1$

This will be insured if $\underset{\sim}{L} = \mathcal{L}_a \frac{\underset{\sim}{b}\times\underset{\sim}{c}}{|\underset{\sim}{a}\cdot\underset{\sim}{b}\times\underset{\sim}{c}|} + \mathcal{L}_b \frac{\underset{\sim}{c}\times\underset{\sim}{a}}{|\underset{\sim}{a}\cdot\underset{\sim}{b}\times\underset{\sim}{c}|} + \mathcal{L}_c \frac{\underset{\sim}{a}\times\underset{\sim}{b}}{|\underset{\sim}{a}\cdot\underset{\sim}{b}\times\underset{\sim}{c}|}$

where $\mathcal{L}_a = \underset{\sim}{L}\cdot\underset{\sim}{a} = 2\pi n_1$.

$\mathcal{L}_b = 2\pi n_2$, $\mathcal{L}_c = 2\pi n_3$ n_1, n_2, n_3 are integers.

$\mathcal{L}_a, \mathcal{L}_b, \mathcal{L}_c$ are the components of $\underline{\mathcal{L}}$ along the three directions perpendicular to the 3 planes formed by choosing 2 of the 3 vectors $\underline{a}, \underline{b}, \underline{c}$.

$$\mathcal{L}_a, \mathcal{L}_b, \mathcal{L}_c = 2\pi \text{ (integer)}$$

The set of all such $\underline{\mathcal{L}}$'s form a lattice, called the reciprocal lattice. The name 'reciprocal lattice' is justified by the fact that the reciprocal of lattice of the reciprocal lattice is the original lattice.
Construct the "Brillouin zone" from this.

Specific Heat of a Crystal due to Atomic Vibrations

Modes $\omega_\beta(k)$

At temperature T, $\quad U = \sum_\beta \sum_k \dfrac{\hbar\omega_\beta(k)}{e^{\frac{\hbar\omega_\beta(k)}{k_B T}} - 1}$ $\quad k_B$ = Boltzmann's constant

$$= V \sum_\beta \int_R \frac{d^3k}{(2\pi)^3} \frac{\hbar\omega_\beta}{e^{\frac{\hbar\omega_\beta}{k_B T}} - 1}$$

$$C_V = \frac{\partial U}{\partial T} = k_B V \sum_\beta \int_R \frac{d^3k}{(2\pi)^3} \left(\frac{\hbar\omega_\beta}{k_B T}\right)^2 \frac{e^{\hbar\omega_\beta/kT}}{\left(e^{\hbar\omega_\beta/kT} - 1\right)^2}$$

The integration $\int_R d^3k$ is only over a single cell in the reciprocal lattice. This is because the other cells give the same frequencies and energies of the harmonic oscillators of the atomic vibrations, and the avg. level of excitation of a particular oscillator depends only on the temperature.

The approximations made in obtaining C_V are not valid for metals or magnets. In metals there is non-negligible energy in the electronic motions, in magnets, there is energy in the spin orientations of the particles.

In many solids, the approximation that only phonons occur is a good one.

For high T, $kT > \hbar\omega_\alpha(\underline{k})$ for all α and $\underline{k}$

then $U \simeq kT \sum_{\text{Modes}} \int_R \frac{d^3k}{(2\pi)^3} V$

V = volume of unit cell $= |\underline{a}\cdot\underline{b}\times\underline{c}|$

$$\int \frac{d^3k}{(2\pi)^3} V = 1$$

$$\therefore U \simeq k_B T \,(\text{no. of modes}) = 3Nk_BT$$

N = no. of atoms in crystal

$$\therefore C_V = 3R \quad \text{per degree Kelvin per mole}$$
$$= 6 \text{ calories per deg. per mole} \quad \text{at high } T.$$

For low T: $\omega_\alpha(\underline{k}) = c_\alpha|\underline{k}|$; c_α depends slightly on direction of $\underline{k}$.
only 3 α's exist for low T – those for which $\omega_\alpha \to 0$ in acoustical branch

$$U = k_BT\, V \sum_\alpha \int \frac{d^3k}{(2\pi)^3} \left(\frac{\hbar c_\alpha k}{k_B T}\right) \frac{1}{\exp\left(\frac{\hbar c_\alpha k}{k_B T}\right) - 1}$$

Let $x = \dfrac{\hbar c_\alpha k}{k_B T}$

Then $U = k_B T \int \frac{d\Omega_k}{4\pi} \left(\frac{k_B T}{\hbar c_\alpha}\right)^3 \frac{1}{(2\pi^2)} \int_0 \frac{x^3 dx}{e^x - 1}$

only a small error is introduced if we take the upper limit as ∞, and then the integral $= \frac{\pi^4}{15}$

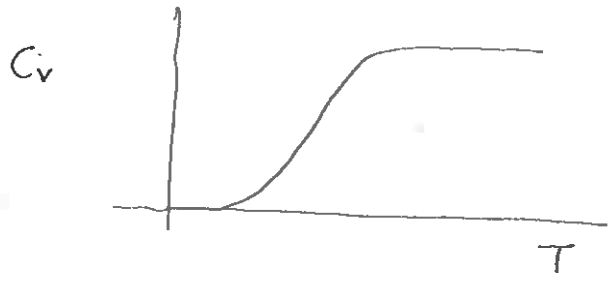
Then $U = (k_BT)^4 \frac{\pi^2}{10 c_0^3 \hbar^3}$, where $\frac{1}{c_0^3} = \frac{1}{3}\sum_{\alpha'} \frac{1}{c_{\alpha'}^3}$

$\therefore C_V \propto T^3$ as $T \to 0$.

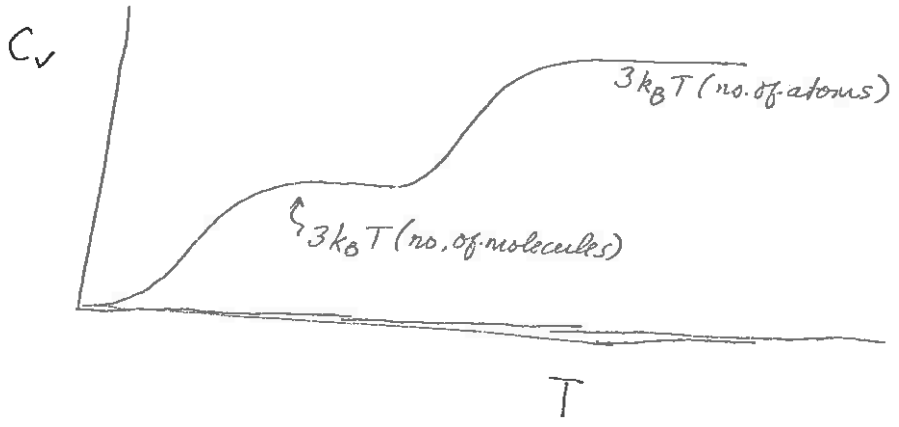
c_0 is some average speed of sound.

For very small T (say. 10^{-6} °K.), C_v no longer goes as T^3, and that is because of the discreteness of the modes. C_v then depends on the volume.

So the ideal specific heat curve looks like



We can see that for particular crystals C_v vs. T needn't be so simple. For example if we had a crystal in which strongly bound molecules are weakly ~~bound~~ bound to each other, then we would obtain



There is a theory due to Debye, and this consists of first writing

$$\omega_k = c_0 k \qquad \text{for all } k$$

and considering that there are 3 such modes.

Use the same c_0 for each mode because other approximations used are more severe.

Then $U = 3k_BT \int \frac{d^3k}{(2\pi)^3} \frac{\hbar c_0 k}{k_B T} \frac{1}{\exp\left(\frac{\hbar c_0 k}{k_B T}\right) - 1}$

Use the approximation of replacing the unit cell in the reciprocal lattice by a sphere of radius k_{max}.

Then $\int \frac{d^3k}{(2\pi)^3} \cdots \longrightarrow 4\pi \int_0^{K_{max}} dK \frac{K^2}{(2\pi)^3} \frac{\hbar c_0 K}{k_B T} \frac{1}{e^{\frac{\hbar k c_0}{k_B T}} - 1}$

and $U = \frac{(k_B T)^4}{(\hbar c_0)^3} \frac{3}{2\pi^2} \int_0^{\theta/T} \frac{x^3 dx}{e^x - 1}$ $\qquad \theta = \frac{K_{max} \hbar c_0}{k}$

For $T \longrightarrow 0$, we recover previous formula.

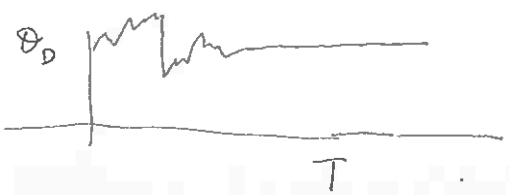
For $T >> \theta$, (θ is called the Debye temperature, it is a useful quantity to know in the case of a particular crystal.)

$U = \frac{k_B^4 T}{(\hbar c_0)^3} \frac{\theta^3}{2\pi^2} \Longrightarrow C_V$ = constant independent of T and independent of c_0.

Hard crystals coocash generally have high θ (diamond)
Soft crystals generally have low θ. (Argon)

This theory of specific heat has been widely abused. Rather than plotting C_V vs. T, with θ as an adjustable parameter, and comparing with experimental C_V vs. T, people have plotted θ_D vs. T as a way of reporting measurements of the specific heat.

One obtains in this manner foolish curves like



Problem: Evaluate $\sum_{n=0}^{\infty} \phi_n(x)\,\phi_n^*(x')\,e^{-iE_n t}$

where E_n is the energy and $\phi_n(x)$ the wavefunction for the n^{th} excited state of a harmonic oscillator with frequency ω.

Solution: $\phi_n(x) = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} e^{-x^2/2} H_n(x)$

where $H_n(x) = (-)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$

(A word of caution: different books use different normalizations for the Hermite polynomials. Our normalization is fixed by the normalization of $\phi_n(x)$ and the expression for $\phi_n(x)$ in terms of $H_n(x)$)

$$\therefore \Sigma = \sum_{n=0}^{\infty} \frac{e^{+x^2/2}}{\sqrt{\pi}} \frac{e^{+x'^2/2}}{2^n n!} \left(\frac{d^n}{dx^n} e^{x^2}\right)\left(\frac{d^n}{dx'^n} e^{-x'^2}\right) e^{-\frac{i\omega t}{2}} e^{-in\omega t}$$

$$\frac{d^n}{dx^n} e^{-x^2} = \frac{1}{\sqrt{2\pi}} \frac{d^n}{dx^n} \int_{-\infty}^{\infty} e^{ixy} e^{-y^2/4}\, dy$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (iy)^n e^{ixy} e^{-y^2/4}\, dy$$

$$\therefore \Sigma = \frac{e^{-\frac{i\omega t}{2}}}{2\pi^{3/2}} e^{x^2/2} e^{x'^2/2} \int_{-\infty}^{\infty} dy\, e^{ixy} e^{-y^2/4} \int_{-\infty}^{\infty} dy'\, e^{ix'y'} e^{-y'^2/4} \sum_{n=0}^{\infty} \frac{(-yy')^n}{2^n n!} e^{-in\omega t}$$

$$= \frac{e^{-\frac{i\omega t}{2}}}{2\pi^{3/2}} e^{x^2/2} e^{x'^2/2} \int_{-\infty}^{\infty} dy\, e^{ixy} e^{-y^2/4} \int_{-\infty}^{\infty} dy'\, e^{ix'y'} e^{-y'^2/4} \exp\left(\frac{-yy'}{2} e^{-i\omega t}\right)$$

The evaluation of the integrals is straightforward (though slightly tedious) the result is

$$\sum_{n=0}^{\infty} = \frac{2}{\sqrt{\pi}\,(1-e^{-2i\omega t})^{1/2}} \exp\left(\frac{x^2+x'^2}{2}(1+e^{2i\omega t}) + 2xx' e^{-i\omega t}\right)$$

Physics 2050

January 27, 30, 31

More on Neutron Scattering

The amplitude for the process takes the form

$$\left\langle e^{i\vec{k}_f\cdot\vec{r}} \left| \sum_i V_i(r_\alpha - R_i) \right| e^{i\vec{k}_i\cdot\vec{r}} \right\rangle$$

where the sum is over the lattice sites

V_i has different values for the different types of atoms involved

$$\sum_j \int e^{-i\vec{k}_f\cdot\vec{r} + i\vec{k}_i\cdot\vec{r}} \psi_f^* \psi_i V_j(r_\alpha - R_i)\, d^3r\, d^3R =$$

(if $\vec{P} = \vec{k}_i - \vec{k}_f$)

$$\langle f | \sum_j V_j(P) e^{i\vec{R}_j\cdot\vec{P}} | i \rangle$$

Provided the wavelength for $\vec{P}$ is long compared to other dimensions, the dipole approximation can be used to evaluate the integrals and $V_j(P)$ is approximately independent of $\vec{P}$

If the wavelength is comparable with the dimensions involved, then $V_j(P)$ is a form factor

If the final lattice state is the same as the initial state, the matrix element looks as follows: $\langle i | \sum e^{i\vec{P}\cdot\vec{q}_i} e^{i\vec{P}\cdot\vec{R}_0^i} | i \rangle$

where $\vec{q}_i$ is the oscillating coordinate and $\vec{R}_0^i$ is the equilibrium position

Hence we find $\sum_j V_j(P) e^{i\vec{P}\cdot\vec{R}_0^j} \langle i | e^{i\vec{P}\cdot\vec{q}_i} | i \rangle$

this was previously evaluated to give $e^{-P^2\langle q^2\rangle/2}$

It is obvious that if $\frac{\langle q^2\rangle}{d^2} \gg 1$, there will be almost no elastic scattering

The probability is then just

$$\left| \sum_j V_j(P) e^{i\vec{P}\cdot\vec{R}_0^j} \right|^2 e^{-P^2\langle q^2\rangle}$$

$V_j(r_\alpha - R_j)$ is the same for all atoms of a given type inside the crystal

Hence $V_j(P)$ is the same for all atoms of the type

thus we get $\sum_{\text{types}\,\alpha} V_\alpha(P) \sum_j e^{i\vec{P}\cdot\vec{R}_0^{j,\alpha}}$

for one type this is $V(P) \sum_{nml} e^{i[p_1 an + p_2 bm + p_3 cl]}$

where p_1, p_2, p_3 are the components along the directions in reciprocal lattice space

$$\sum_0^N e^{ip_1 an} = \left(1 - e^{ip_1 aN}\right)/\left(1 - e^{ip_1 a}\right)$$

Hence we arrive at $V(P)\left[\frac{1 - e^{ip_1 aN}}{1 - e^{ip_1 a}}\right]\left[\frac{1 - e^{ip_2 bM}}{1 - e^{ip_2 b}}\right]\left[\frac{1 - e^{ip_3 cL}}{1 - e^{ip_3 c}}\right]$

The absolute square gives

$$|V(P)|^2 e^{-P^2\langle q^2\rangle} \left[\frac{\sin^2 p_1 aN/2}{\sin^2 p_1 a/2}\right]\left[\frac{\sin^2 p_2 bM/2}{\sin^2 p_2 b/2}\right]\left[\frac{\sin^2 p_3 cL/2}{\sin^2 p_3 c/2}\right]$$

This approaches a product of δ functions as $N \to \infty$ $\left[\delta\left(\frac{P_{av}}{2} = [illegible]\pi\right)\right]$

Thus $\vec{P}$ must be a reciprocal lattice vector to have any appreciable contribution

Now consider the case of inelastic scattering

$$\sum_j V_j(\vec{P}) \langle f | e^{i\vec{P}\cdot\vec{q}_j} | i \rangle e^{i\vec{P}\cdot\vec{R}_j}$$

In general the crystal will make transitions to all sorts of final states. These final states are clustered close together in energy because the spacing of the k for the modes is so small.

Hence our plan of attack should be to

a) find the transition amplitude to a final state at energy E_0

$$T_{fi}(E_0) = \int \frac{d^3k_f}{(2\pi)^3} \delta(E_{k_f} - E_0) \langle f | e^{i\vec{P}\cdot\vec{q}_j} | i \rangle$$

b) Sum individual probabilities over E_0 to find the total probability

$$\sum_{E_0} |T_{fi}(E_0)|^2$$

Why this gives an answer with no hint of a diffraction pattern is left as an exercise to the student

Demonstration that the average energy lost by the neutron to the crystal is just the classical energy $\psi_{after} = e^{ipx}\psi_{before}$

$$\langle \psi_a^* | H | \psi_a \rangle - \langle \psi_b^* | H | \psi_b \rangle$$

$$H = p^2/2m + f_{m,\text{other momenta}} + V$$

$$\langle \psi_b^* | e^{-ip\cdot x} H e^{ip\cdot x} - H | \psi_b \rangle = \frac{P^2}{2m} + \vec{P} \cdot \langle \psi_b^* | \frac{\vec{p}}{2m} | \psi_b \rangle$$

because

$$p_{op}\left[e^{ipx} f(x)\right] = \hbar f(x) p_{number} e^{ipx} + e^{ipx}(p_{op}) f$$

Provided the mean momentum of the system is 0, the second term is zero. If there is mean momentum, we get a Doppler type correction

Question from the class: how do you calculate the probability of "recoilless emission" at finite temperature?

This involves sums of the form $\sum_n e^{-\beta n} |\langle m | e^{iPQ} | n \rangle|^2$

Feynman was unable to solve this problem in class and returned at the next meeting with the news that the answer he had predicted is probably incorrect

Beware: in doing the sums required for crystal statistical mechanics, one encounters the operators q_m = displacement $= \frac{1}{\sqrt{\eta}} \sum Q^{\kappa} e^{ikx}$

where η is the number of atoms

Do not use arguments based on the fact that $\frac{1}{\sqrt{\eta}}$ is a very small number, for you will almost always discover that there is a very large number of these to be added up.

(This is the way the answer suggested in previous notes was arrived at).

QUANTUM FIELD THEORY: Developed as the continuum limit of a line of oscillators

$$H = \sum_m \left[\frac{1}{2} p_m^2 + \frac{\alpha}{2} (q_m - q_{m+1})^2 \right]$$

$$Q_\kappa = \frac{1}{\sqrt{n}} \sum_m q_m e^{ik x_m}$$

where $x_m = am$ is the actual position in space of the atom

For long wavelengths $\omega^2 = 2\alpha (1 - \cos ka)$ becomes $\omega^2 \propto \alpha a^2 k^2$

ka small implies q_m may be replaced by the continuous $q(x)$

$$Q_\kappa = \int \frac{dx}{a} \frac{e^{ikx}}{\sqrt{\eta}} q(x)$$

defines the normal modes

Generally one redefines $Q' = \int dx\ e^{ikx} q(x)$

$$q(x) = \int Q'_\kappa \frac{dk}{2\pi} e^{-ik\cdot x}$$

Then the formula for the energy becomes

$$H = \int \left[\frac{1}{2} \left(\frac{\partial q(x)}{\partial t} \right)^2 \frac{dx}{a} + \frac{1}{2} \alpha a^2 \left(\frac{\partial q(x)}{\partial x} \right)^2 \frac{dx}{a} \right]$$

$\rho = 1/a$ is the density, because each atom had unit mass

This is not the Hamiltonian, in a strict sense. The standard Hamiltonian is a form in terms of $\pi(x)$ and $q(x)$. To get $\pi(x)$, set $\pi(x) = p_m a$

$$p_{m'} q_m - q_m p_{m'} = -i\hbar \delta_{mm'} \longrightarrow \pi(x) q(x') - q(x') \pi(x) = -i\hbar a \delta(x - x')$$

$$H = \int \frac{dx}{a} \left[\frac{\rho^2 \pi^2}{2} + \frac{c^2}{2} (\nabla q)^2 \right]$$

$q(x)$ & $\pi(x)$,

because they give a scalar operator for each value in x, are quantum mechanical scalar fields

Notice that our Hamiltonian is not expressed in normal form because of the $(\nabla q)^2$ terms

Before substituting the Q_k's, define a Fourier transform of the conjugate momentum

$$p\pi(x) = \int e^{-ikx} \frac{P(k)\,dk}{2\pi}$$

$$P(k_1)Q(k_2) - Q(k_2)P(k_1) = -i\delta(k_1 - k_2)$$

$$H = \int \frac{dk}{2\pi}\left[\frac{1}{2}P^2 + \frac{1}{2}k^2c^2Q(k)^2\right]$$

which is a normal mode form

Keep in mind that this is the form used for expansion of the Hamiltonian when we can't see the atoms, but only the waves.

This was the procedure followed for quantum electrodynamics. But we have no idea of the scale a; this may be why there are high energy difficulties with QED

In practice, of course, one works in three dimensions and must take into account the anisotropy of the crystal

At each point in space there is a displacement vector field, not just a scalar

$$KE = \frac{1}{2}\int \frac{\partial \vec{Q}}{\partial t} \cdot \frac{\partial \vec{Q}}{\partial t}\, d(vol)$$

$$PE = \frac{1}{2}\int c_{ijkl}\, e_{ij} e_{kl}\, dx$$

$$e_{ij} = \frac{1}{2}\left[\frac{\partial Q_i}{\partial x_j} + \frac{\partial Q_j}{\partial x_i}\right]$$

The tensor c_{ijkl} hides all the elastic constants of the crystal

For your amusement:

How many elastic constants are there for a general crystal? (21)

Show that there are three elastic constants for a cubic crystal

Show that an isotropic medium has only two elastic constants: the compression and shear moduli

Problem: Let p and q be the coordinates of a harmonic oscillator

Then $q(t)$ can be expressed in terms of $p(0)$ and $q(0)$

Find $[q(t_0), q(t_1)]$

(notice that changes of q with time look like momenta, so there is no reason for this commutator to be 0)

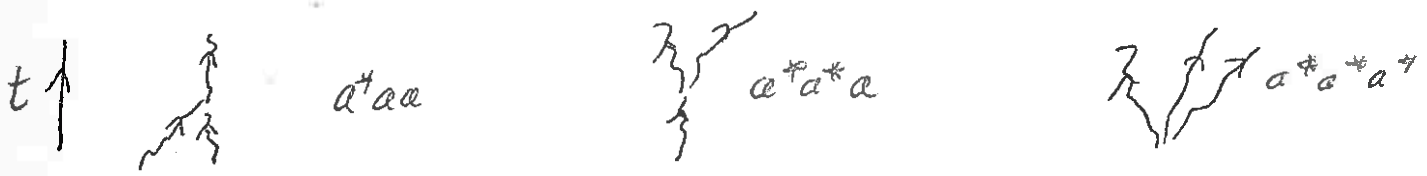
Hint: use the representation in which operators change with time

$$q(t) = U^{-1} q(0)\, U$$

PHONON INTERACTIONS

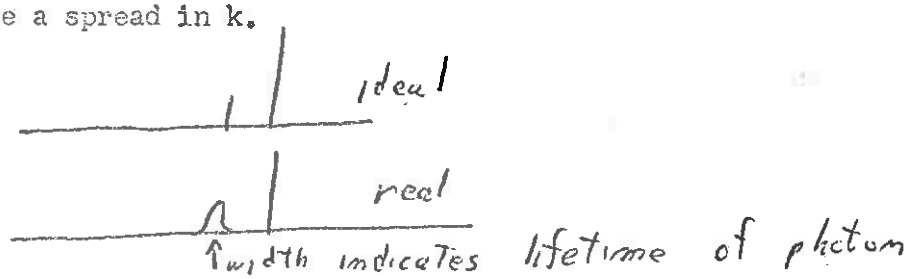
So far we have talked only about modes of vibration of an entire perfect crystal. Independent excitation of these can't possibly explain thermal conductivity. To get at thermal conductivity, it is necessary to realize that real phonons have a finite mean free path; hence they can diffuse.

Derivation of this mean free path depends on including higher order terms in the expansion of the potential: for example third order pieces in a and a^*. When the processes are virtual, it is possible to have contributions from all of these terms.



Problem: calculate the mean free life of a photon. Explain thermal conductivity on this basis.

This finite lifetime can be detected experimentally by neutron scattering. Recall that subsidiary peaks are spaced from the elastic peak by wave vector k. Finite lifetime implies that there will be a spread in k.



At the low k end of the spectrum, we can approximate reality by the previously developed continuum formalism, and try using $\left(\frac{\partial q}{\partial x}\right)^3$ as a perturbation.

We can, using the field expansion for soft phonons, write down and calculate diagrams for all sorts of processes. Phonon-phonon scattering, for example

There is, however, one large difference between this treatment of phonons and the corresponding treatment of photons. This comes in the definition of the momentum assigned to the quantum of excitation.

For a photon the momentum is well defined by its interactions with other particles. For a phonon, however, the wave number vector (which people like to call the momentum)

can be defined only up to a reciprocal lattice vector (because if $\vec{\mathbb{L}}$ is a reciprocal lattice vector, $e^{i\vec{x}\cdot\vec{\mathbb{L}}} = 1 \quad \forall \vec{x}$ indicating lattice sites in the crystal).

Thus the momentum conservation laws are not as cut and dried as in electron-photon interactions. With the k's all cut back to members of the first Brillouin zone, the law becomes $\vec{k}' + \vec{k}'' = \vec{k}''' + \vec{\mathbb{L}}$ for $\left.\begin{matrix} k''' \\ k' \\ k'' \end{matrix}\right\}$ vertex

For very small k, no $\vec{\mathbb{L}}$ will be required. If $\vec{\mathbb{L}}$ is required, the process is called an umklapp process.

Hence we may restate the above

Problem: Explain carefully how the umklapp prozessen give you finite thermal conductivity.

For very small k, due to lack of umklapp, there is an exponentially small thermal resistance. The formula written down in class was

$e^{-1/2T}$ [Energy at top of acoustical branch]

How is this obtained?

Problem:It is difficult to understand the idea of some process taking place at one atom in a lattice imparting a momentum to the entire crystal. Use the uncertainty principle to explain the recoil momentum of the whole crystal in (for example) the Mossbauer effect

Problem:invent a way to measure the momentum of a phonon

Asides:

i)For an amorphous medium there are quantities analogous to phonons, but they scatter very fast and very randomly

ii) For waves the simple minded rule of thumb

$$\frac{k}{\omega} = \frac{\text{momentum}}{\text{energy}}$$

will almost always give the same answers as more elaborate analyses

Problem:Influence of impurities on the properties of crystals

Take a low density (n) of atoms with different masses. Assum each flaw acts independently scattering phonons into other directions

$\sim 2\omega_{\vec{k}}$

As $T \to 0$, for density (n) , how does the thermal conductivity depend on T and how on (n) ?

(give just a power law dependence, since that would be the first thing you'd measure)

Ph 205b Week 5 Feb. 3, 6, 7

We found that we can treat the quantum-mechanical vibrations of a one dimensional line of atoms in the limit of zero spacing between atoms as a quantum field.

If p_n, q_n are the momentum and position operators respectively of the n^{th} atom, then the transition to the continuum is achieved by

$$q_n \longrightarrow q(x)$$

$$\frac{p_n}{a} \longrightarrow \pi(x) \quad , \quad a = \text{spacing between atoms in discrete core}$$

then $[q_n, p_m] = i\delta_{nm}$

$$\Longrightarrow [\pi(x), q(x')] = -i\delta(x-x') \quad \ldots\ldots (1)$$

In terms of $q(x)$, $\pi(x)$,

$$\text{kinetic energy} = \frac{1}{2}\int \left(\frac{\partial q}{\partial t}\right)^2 dx = \frac{1}{2}\int \pi^2(x)\,dx$$

$$\text{potential energy} = \frac{c^2}{2}\int \left(\frac{\partial q}{\partial x}\right)^2 dx$$

i.e., $$H = \frac{1}{2}\int \left\{\pi^2(x) + c^2\left(\frac{\partial q}{\partial x}\right)^2\right\} dx \quad \ldots\ldots (2)$$

Write $$q(x) = \sum_k \frac{1}{\sqrt{2\omega_k}}\left(a_k^* + a_{-k}\right) e^{-ikx}$$

$$\pi(x) = \sum_k i\frac{\sqrt{\omega_k}}{2}\left(a_k^* - a_{-k}\right) e^{-ikx} \quad \ldots\ldots (3)$$

then with the substitution

$$\sum_k \longrightarrow \frac{1}{(2\pi)^3}\int dk$$

the commutation (C.R.) rules of the a's are found to be:

$$[a_k, a_\ell^*] = \delta(k-\ell)$$
$$[a_k, a_\ell] = 0 = [a_k^*, a_\ell] \qquad \text{---- (4)}$$

One may verify the equivalence of (4) and (1), by using (4) and (3) to obtain the CR's of $\pi(x)$, $q(y)$:

$$q(x)\pi(y) - \pi(y)q(x)$$
$$= \sum_{k\ell} \frac{i}{2}\sqrt{\frac{\omega_\ell}{\omega_k}}\left\{(a_k^* + a_{-k})(a_\ell^* - a_{-\ell}) - (a_\ell^* - a_{-\ell})(a_k^* + a_{-k})\right\} e^{-ikx} e^{-i\ell y}$$
$$= \sum_k i\, e^{-ik(x-y)} = i\int \frac{dk}{2\pi} e^{-ik(x-y)}$$
$$= i\,\delta(x-y)$$

And clearly, $[q(x), q(y)] = 0 = [\pi(x), \pi(y)]$

The Hamiltonian may also be evaluated in terms of the a's. It is a simple matter to show

$$H = \frac{1}{2}\int \{\pi^2 + c^2(\nabla q)^2\}\, dx = \sum_k \hbar\omega_k (a_k^* a_k + 1/2)$$

To obtain the equations of motion, recall that for any operator A that does not depend explicitly upon the time

$$-i\dot{A} = [H, A]$$

So that $\dot{q}(y) = \frac{+i}{2}\int dx \left[\pi^2(x) + c^2\left(\frac{\partial q}{\partial x}\right)^2, q(y)\right]$

$$= \frac{+i}{2}\int dx \left[\pi^2(x)q(y) - \pi(x)q(y)\pi(x) + \pi(x)q(y)\pi(x) - q(y)\pi^2(x)\right]$$
$$= \frac{+i}{2}\int dx \left[\pi(x)(-i\delta(x-y)) + (-i\delta(x-y))\pi(x)\right]$$

or, $\dot{q}(y) = \pi(y)$ as expected

Also $\dot{\pi}(y) = i[H, \pi(y)]$

$= c^2 \frac{\partial^2 q}{\partial x^2}$ upon integrating by parts

For a 3 dimensional scalar field (only one disturbance at each point in space)

$$\dot{\pi} = c^2 \nabla^2 q = \ddot{q}$$

Vibrations of a three-dimensional solid:

There are 3 different disturbances (3 independent displacements) at each point — label by i.

then $[\pi_i(\underset{\sim}{x}), q_j(\underset{\sim}{y})] = -i\delta^3(\underset{\sim}{y} - \underset{\sim}{x})\,\delta_{ij}$

kinetic energy $= \frac{1}{2}\int \frac{\partial \vec{q}}{\partial t} \cdot \frac{\partial \vec{q}}{\partial t}\, d^3x$

potential energy $= \frac{1}{2}\int \sum_{ij,kl} c_{ij,kl} \frac{\partial q_i}{\partial x_j} \frac{\partial q_k}{\partial x_l}\, d^3x$

where the coefficients $c_{ij,kl}$ have are symmetric under any of the following interchanges

$i \leftrightarrow j$
$k \leftrightarrow l$
$ij \leftrightarrow kl$

This gives the following equations of motion

$$\ddot{q}_i = \sum_{jkl} c_{ij,kl} \frac{\partial^2}{\partial x_j \partial x_k} q_l(x)$$

The general case is rather formidable. A simpler case would be

$$\dot{\underset{\sim}{q}} = \lambda_1 \nabla^2 \underset{\sim}{q} + \lambda_2 \nabla(\nabla \cdot \underset{\sim}{q})$$

with λ_1, λ_2 being elastic constants characteristic of the solid.

Free Fields

In classical physics we obtain the equations of motion of a free field not by commuting the fields with the Hamiltonian, but from the action principle.

In general, $\mathcal{L} = \mathcal{L}(\phi_\alpha)$: $\mathcal{L}$ may depend on $\frac{\partial \phi_\alpha}{\partial x_k}, \phi_\alpha, \dot{\phi}_\alpha$.

then $S = \int \mathcal{L}\, d^4x$ is an extremum for arbitrary variations $\delta\phi_\alpha$ in the fields ϕ_α.

the Euler-Lagrange Equations are then

$$\frac{\partial \mathcal{L}}{\partial \phi_\alpha} = \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}_\alpha}\right) + \sum_k \frac{\partial}{\partial x_k}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \phi_\alpha}{\partial x_k}\right)}\right)$$

Example: For $\mathcal{L} = \frac{1}{2}\dot{\phi}^2 - \frac{c^2}{2}\left(\frac{\partial \phi}{\partial x}\right)^2$

the equation of motion is $\ddot{\phi} = c^2 \frac{\partial^2 \phi}{\partial x^2}$

For classical electromagnetism (free field),

$$\mathcal{L} = \frac{1}{2}(E^2 - B^2)$$

(in presence of sources, add $(\underset{\sim}{J} \cdot \underset{\sim}{A} - \rho\phi)$.)

Writing $\mathcal{L}$ in terms of $\underset{\sim}{A}$, ϕ, the action principle becomes

$$\frac{1}{2}\delta\int\left\{\left[\frac{\partial A}{\partial t}+\nabla\phi\right]^2-\left(\nabla\times A\right)^2\right\}d^3x=0$$

Expanding and integrating by parts

$$\delta\int\left\{\left(\frac{\partial A}{\partial t}\right)^2+(\nabla\phi)^2-2\phi\frac{\partial}{\partial t}\nabla\cdot A-(\nabla\times A)^2\right\}d^3x=0$$

Choose ~~gaaage~~ gauge so that $\nabla\cdot A=0$ (coulomb gauge)

integrating $(\nabla\phi)^2=-\nabla^2\phi+\nabla\cdot(\phi\nabla\phi)$ by parts and making use of the result $\nabla^2\phi=0$ for free fields as a shortcut

$$\delta\int\left[\left(\frac{\partial A}{\partial t}\right)^2-(\nabla\times A)^2\right]d^3x=0\implies(\partial_t^2-\nabla^2)\vec{A}=0$$

Let $\underset{\sim}{\pi}=\dfrac{\partial\underset{\sim}{A}}{\partial t}$

Then ~~the~~ the quantum mechanical condition is

$$[\pi_i(\underset{\sim}{x}),A_j(\underset{\sim}{y})]=-i\delta^3(\underset{\sim}{x}-\underset{\sim}{y})\delta_{ij}$$

and

$$H=\int\mathcal{H}d^3x=\frac{1}{2}\int\left\{(\vec{\pi}(x))^2+(\nabla\times A)^2\right\}d^3x$$

or, when sources are present

$$H=\frac{1}{2}\int\left\{\vec{\pi}^2+(\nabla\times A)^2+J\cdot A-\rho\phi\right\}d^3x$$

Problems (Do not hand in — no assignment this week)

① Derive Maxwell's Equations as operator equations from

$$\dot{\underset{\sim}{\Pi}} = i[H, \underset{\sim}{\Pi}]$$

$$\dot{\underset{\sim}{A}} = i[H, \underset{\sim}{A}]$$

② a. Evaluate $[A_\ell(\underset{\sim}{x},t), A_m(\underset{\sim}{x}',t')]$ for free fields.

b. Write $A_\ell(x) = \sum_{k,\alpha=1,2} \frac{1}{\sqrt{2\omega_k}} [a^\dagger_{k,\alpha} e_\ell e^{-ik\cdot x} + e^*_\ell a_{k,\alpha} e^{ik\cdot x}]$

and interpret the a's. (Find CR's, etc.)

Remarks:

In our treatment of elasticity, we began with real atoms (and the Schrodinger Equation), and deduced that in certain situations a quantum field-theoretic description held. In electromagnetism, on the other hand, we began by assuming a field structure. The question arises as to whether there exists a solid that imitates electrodynamics. The answer at present is no.

Historically, the wavelike properties of light caused people to treat light as the elastic vibrations of a solid, since that was where wavelike behaviour first arose. McCullough was the first to consider light independently of the model. His work was not recognized as correct till later because scientists' minds were so tuned to thinking of light in terms of the model that they couldn't accept it.

For amusement, consider the following:

In 3 dimensions, as everybody knows, there are 3 phases of matter — solid, liquid, gas. Does the same thing hold in 2 dimensions? There is some experimental evidence that this is not the case.

If you decide that there are only 2 phases, is the second the analog of the liquid or the solid phase of 3 dimensions? Elaborate — consider neutron scattering in two dimensions, for example.

Electrons in Metals

Let us work out the consequences of making the following wild approximations:

1) Disregard the potential at the electron due to the ion cores

2) Disregard electron – electron interactions.

Let there be N electrons in volume V. Density $n = N/V$. The electrons are taken to be independent except for the Pauli Exclusion Principle.

$$E = \frac{k^2}{2m}$$

3) All occupied states are within a sphere of radius $k_{max} (= K_f)$ in K-space.

$$\text{Then } N = \underbrace{2}_{\substack{\uparrow \\ \text{2 possible} \\ \text{spin orientations}}} \int \frac{d^3k}{(2\pi)^3} \text{ vol.} = \frac{2V}{(2\pi)^3} \frac{4\pi}{3} K_f^3$$

$$\therefore \quad n = \frac{K_f^3}{3\pi^2}$$

And the total energy

$$E = 2 \int_{\text{sphere}} \frac{d^3k}{(2\pi)^3} V \cdot \frac{k^2}{2m} = \frac{k_f^5 V}{10\pi^2 m}$$

This is a completely degenerate electron gas — electron gas at 0 temperature.

$$\text{Energy/unit volume} \propto n^{5/3}$$

Problems (Do one, due February 20)

1) Stars burn up. An ash remains which then contracts. What is the maximum size of the star? What is the distribution of mass inside a star that is smaller than the critical size (which corresponds to a critical mass M_c)? What happens if $M > M_c$.

— Use Newtonian Gravity.

Suggestions for a model:

$T = 0$ (this temperature assumption is not important)

no. of neutrons $\simeq$ no. of protons

Electrons get pushed up as the nucleons are pulled together, so that they are approximately free.

p = pressure, $\frac{dp}{dr} = \frac{G(\text{Mass inside radius } r)\rho}{r^2}$ $\qquad M(r) = \int_0^r \rho(r) r^2 dr\, 4\pi$

Find $p = p(\rho)$.

2) Weak magnetic field $\vec{B}$ on a system of electrons. Find the magnetic effect of the spins. (This is easy — phenomenon called Pauli paramagnetism)

Neglect the effect on the spins — there is an effect on the orbits.

Strong $\vec{B}$ — what happens?

Find energy E vs. field strength B. $\chi = \frac{\partial E}{\partial B}$ = magnetic susceptibility.

We obtained the energy of a system of free electrons. What is the wave-function $\psi(\underline{R}_1, \underline{R}_2 \ldots \underline{R}_i \ldots)$?

These are non-interacting e's. Consider electrons with spin "up"; wavefunction is

$$\psi = e^{i k_{\alpha_1} \cdot R_1} e^{i k_{\alpha_2} \cdot R_2} \cdots$$

Let there be N electrons with spin up, then the requirements of Pauli principle are satisfied if

$$\psi = \frac{1}{\sqrt{N!}} \sum_{\text{permutations } P} (-)^P \prod_i e^{i k_{\alpha_{P_i}} R_i}$$

where P is the permutation that takes α_i into α_{P_i}.

this can also be written as a (Slater) determinant:

$$\psi = \frac{1}{\sqrt{N!}} \det \begin{Bmatrix} \phi_{\alpha_1}(R_1) & \phi_{\alpha_1}(R_2) & \cdots & \phi_{\alpha_1}(R_n) \\ \phi_{\alpha_2}(R_1) & \phi_{\alpha_2}(R_2) & \cdots & \phi_{\alpha_2}(R_n) \\ \vdots & & & \\ \phi_{\alpha_n}(R_1) & \phi_{\alpha_n}(R_2) & \cdots & \end{Bmatrix}$$

Incidentally, all the ϕ_{α_k}'s are different — otherwise ψ would vanish.

What is the probability of finding an electron at R_b if we find one at $\underline{R}_a$? We expect this to be a function of $r = |\underline{R}_a - \underline{R}_b|$ only, starting at 0 for $r=0$ and levelling off to a constant as $r \to \infty$

Find instead the probability of finding one e at "a" and one electron at "b". This is proportional to finding the probability of finding one at "b"

when one has been found at "b"

Prob. (one e at "a"; one e at "b")

$$= \langle \psi | \sum_i \delta(\underline{R}_a - \underline{R}_i) \sum_j \delta(\underline{R}_b - \underline{R}_j) | \psi \rangle$$

Typical term in this matrix element is

$$\langle e^{i\underline{k}_{\alpha_1}\cdot\underline{R}_1} e^{i\underline{k}_{\alpha_2}\cdot\underline{R}_2} \cdots e^{i\underline{k}_{\alpha_n}\cdot\underline{R}_n} | \delta(\underline{R}_a - \underline{R}_1)\delta(\underline{R}_b - \underline{R}_2) | e^{i\underline{k}_{\beta_1}\cdot\underline{R}_1} e^{i\underline{k}_{\beta_2}\cdot\underline{R}_2} \cdots \rangle$$

integrating over all variables except $\underline{R}_1, \underline{R}_2$

Obtain either $\alpha_1 = \beta_1$, $\alpha_2 = \beta_2$

contribution to Matrix element = 1

or $\alpha_1 = \beta_2$, $\alpha_2 = \beta_1$

contribution to matrix element $= -e^{i(\underline{k}_{\alpha_2} - \underline{k}_{\alpha_1})\cdot(\underline{R}_a - \underline{R}_b)}$

$= -e^{i\underline{k}\cdot\underline{r}}$ $\quad \underline{k} = \underline{k}_{\alpha_2} - \underline{k}_{\alpha_1}$, $\quad \underline{r} = \underline{R}_a - \underline{R}_b$

So that probability $\propto \left| \int d^3k \, (e^{i\underline{k}\cdot\underline{r}} - 1) \right|^2$ Also, $|\underline{r}| = r = R$

integrate over k

K_f = fermi energy

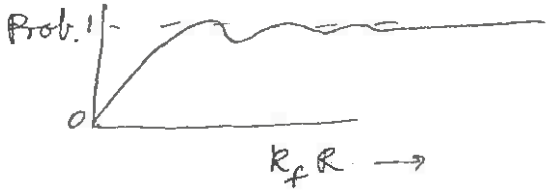
$$\text{Prob.} \propto \left| \int_0^{2K_f} \frac{4\pi}{} dk \left(1 - \frac{\sin kR}{kR}\right) k^2 \right|^2$$

notice that as $R \to 0$, prob. $\to 0$

Let $x = 2K_f R$

then prob. $\propto \left\{ 1 + \frac{3}{x^3}(x\cos x - \sin x) \right\}^2$

Normalize so that prob. $\to 1$ as $x \to \infty$



Ph 205b

February
~~January~~ 10,13,14

So far we have discussed the problems of putting electrons in a three dimensional box:a)how the exclusion principle governs the filling up of discrete energy levels and b)what the antisymmetrization of wave functions tells you about the form of the electron distribution. We now want to go into further properties of many electron systems. In order to understand the electrical conductivity properties of solids one must know what the energy levels of electrons inside them look like, and how they are populated as a function of temperature.

Hence the basic outline of the next few lectures is as follows:

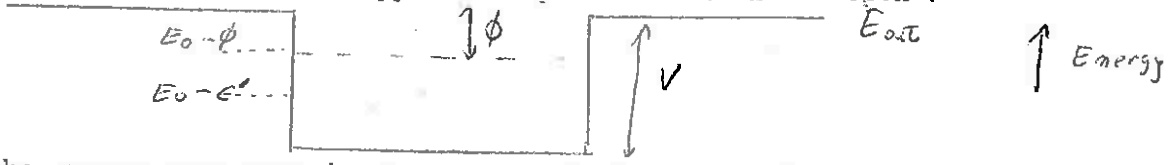
1)How is the quantum statistics of particles in a box affected by the fact that they are fermions with the exclusion principle acting ?

2)How can the theory of particles in a box be applied to electrons in a solid with periodic potential?

QUANTUM STATISTICS OF FERMIONS

Oversimplified explanation to get the picture

Assume a flock of fermions trapped in a potential well of depth V



Let ϕ_0 bethe energy necessary to remove a particle at the Fermi surface from the metal. Recall that we defined the Fermi energy to be the maximum energy reached by particles when they are thrown into a box a T=0 with regard to the exclusion principle. Thus any unoccupied state below the Fermi energy, or occupied state above it, implies an excitation of the system. The weighting factor in quantum statistics is $e^{-E/kT}$, where E is the excitation above ground state. Hence to compute this exponent we must measure energy levels relative to the Fermi surface.

$(E_0-\epsilon')-(E_0-\phi) = -\epsilon'+\phi$ Weighting factor is $e^{(\epsilon'-\phi)/kT}$

$\epsilon_f = E_0-\phi_0$ $\epsilon_a = E_0-\epsilon'$

$e^{(\epsilon'-\phi)/kT} = e^{-(\epsilon_a-\epsilon_f)/kT}$

More Accurate View

The above is not strictly correct - the energy levels should be measured relative to the chemical potential μ, not the Fermi energy. For metals near room temperature, the two are almost the same. At zero T the two are exactly the same. Unfortunately it is difficult to understand what the chemical potential is until the Fermi-Dirac statistics has been developed more fully. For the time being let ϕ_T be the energy necessary to remove some "average" electron from the metal; $\mu_T = V - \phi_T$; weighting factor $e^{-\beta(\epsilon_a - \mu_T)}$. We will soon discover just what is meant by "average" in this context; and that ϕ_T is just the work function of the metal involved.

Suppose that there are n_a^i particles in energy state n_a, for a given configuration i of the N electrons in the system. Then the probability of this configuration is $e^{-\beta \sum_a n_a^i \epsilon_a}$ $\Big| \sum n_a^i = N$ the net probability that the system is in some state is $\sum_{\substack{\text{configs} \\ \text{of } N \text{ particles}}} e^{-\beta \sum_a n_a^i \epsilon_a}$

It is extremely hard to do the sum, taking care of the constraint on the number of particles. Hence a mathematical device is used: write $\epsilon_a \to \epsilon_a - \mu$ for some μ and sum as if there were no constraint on the total number of particles in the system. μ is then picked to make the total number come out right. i.e. from now on all energies are written relative to μ and all sums are unrestricted. (Students who want to really understand what is going on here should trace this through by use of Lagrange multipliers - see a statistical mechanics text.)

Thus the normalization for all statistical quantities is written as $\sum_i e^{-\beta \sum_a n_a^i (\epsilon_a - \mu)} = e^{-\beta g}$

A bit of experimentation will show that if you have no constraint on the total number of particles then

$$\sum_{\substack{\text{configurations} \\ i}} e^{-\beta \sum_a n_a^i (\epsilon_a - \mu)} = \prod_a \left[\sum_{\substack{\text{configs} \\ i}} e^{-\beta (n_a^i)(\epsilon_a - \mu)} \right]$$

each configuration has either $n_a^i = 0$ or 1. Then this becomes $\prod_a \left[1 + e^{-\beta(\epsilon_a - \mu)} \right]$

From $e^{-\beta g} = \prod_a \left[1 + e^{-\beta(\epsilon_a - \mu)} \right]$

we find $g = -\frac{1}{\beta} \sum_a \ln \left[1 + e^{-\beta(\epsilon_a - \mu)} \right]$

The sum is then approximated by an integral. (Prove to yourselves that this is a good approximation and that we do not lose anything by setting $\epsilon_a = p^2/2m$ for the electron.

$$g = -\frac{1}{\beta} \int \ln \left[1 + e^{-\beta(p^2/2m - \mu)} \right] \cdot 2 \frac{d^3p}{(2\pi\hbar)^3} \cdot \text{Volume}$$

Phase space for electrons of momentum p. The 2 is because each direction of spin has its own

Calculation of Statistical Quantities

$\langle N \rangle$ = average number in the box = $\dfrac{\sum_i \left[\sum_a n_a^i \, e^{-\beta\left(\sum_a n_a^i\right)(\epsilon_a - \mu)} \right]}{\sum_i e^{-\beta \sum_a n_a^i (\epsilon_a - \mu)}}$

$$= \frac{1}{\beta} e^{\beta \mathcal{J}} \frac{\partial}{\partial \mu} e^{-\beta \mathcal{J}} = -\frac{\partial \mathcal{J}}{\partial \mu}$$

This shows how the number in the box is related to the chemical potential.

We can also calculate the density $\rho = \langle N \rangle / V$ and the average number in a given energy state

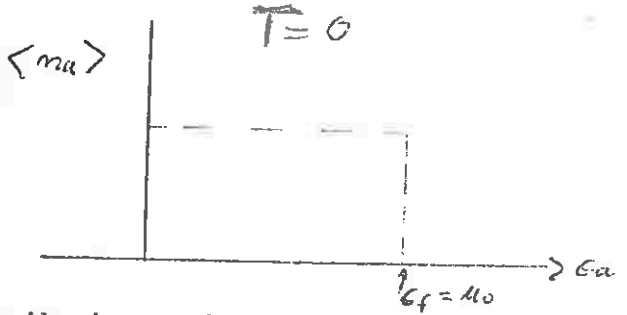
$$\langle n_a \rangle = \frac{\sum n_a^i e^{-\beta n_a^i (\epsilon_a - \mu)}}{\sum_i e^{-\beta (n_a^i)(\epsilon_a - \mu)}} = \frac{0 + e^{-\beta(\epsilon_a - \mu)}}{1 + e^{-\beta(\epsilon_a - \mu)}}$$

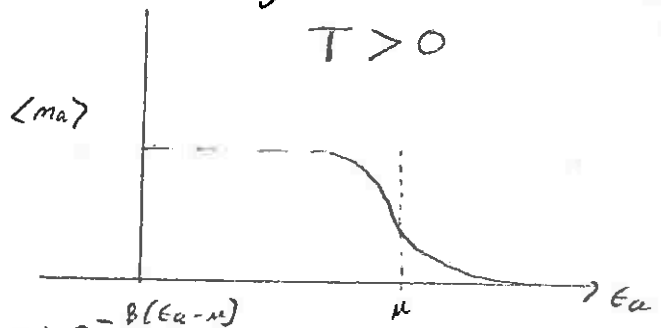
$$\boxed{\langle n_a \rangle = \frac{1}{1 + e^{\beta(\epsilon_a - \mu)}} = \left[1 + e^{\beta(\epsilon_a - \mu)} \right]^{-1}}$$

It is easy to remember the + sign in the denominator, because $\langle n_a \rangle$ must be a number between 0 and 1.

We can now define "average" energy as that energy at which $\langle n_a \rangle = \frac{1}{2}$. This defines $\mu_T + \rho$

Notice that if T=0 $\beta \to \infty$ $\quad \epsilon < \mu \Rightarrow e^{\beta(\epsilon_a - \mu)} = 1$; $\epsilon > 0 \Rightarrow e^{\beta(\epsilon_a - \mu)} \to \infty$

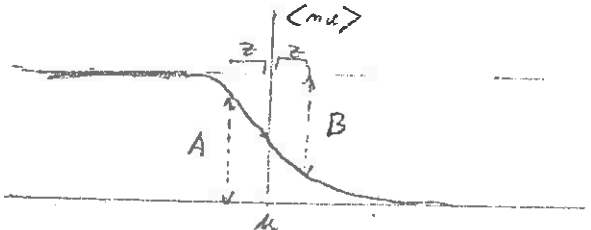




As the temperature gets higher and higher, $\langle n_a \rangle \sim \frac{1}{2} e^{-\beta(\epsilon_a - \mu)}$, which has the shape $e^{-\epsilon/kT}$ that you'd expect if you knew only about Maxwell-Boltzmann statistics

The curve is symmetric in the sense that the shape of the pieces above and below μ is the same

$$\frac{1}{1 + e^{\beta(\epsilon_a - \mu)}} = 1 - \frac{1}{1 + e^{\beta(\mu - \epsilon_a)}}$$



$|A| = |B|$

This will be useful in doing integrals.

PROBLEM(If you wish this can be handed in)

a) Density of states as a function of energy (plot this as T=0 and see what it looks like)

b) energy density as a function of T

c) pressure as a function of T

In order to do b) and c), it is necessary to do integrals of the form

$$I = \int_0^\infty \frac{g(\epsilon)\,d\epsilon}{1+e^{\beta(\epsilon-\mu)}} = \int_0^\infty f(\epsilon)\,d\epsilon$$

There is a handy way to get at these:

$$I = \int_0^\mu f(\epsilon) + \int_\mu^\infty f(\varepsilon) = \int_0^\mu g(\epsilon)d\epsilon - \int_0^\mu \frac{g(\epsilon)d\epsilon}{1+e^{\beta(\mu-\epsilon)}} + \int_\mu^\infty \frac{g(\varepsilon)d\varepsilon}{1+e^{\beta(\varepsilon-\mu)}}$$

$$\int_0^\mu \frac{g(\varepsilon)\,d\varepsilon}{1+e^{\beta(\mu-\varepsilon)}} = \frac{1}{\beta}\int_0^{\beta\mu} \frac{g(\mu-y/\beta)\,dy}{(1+e^y)} \;;\; \int_\mu^\infty \frac{g(\varepsilon)\,d\varepsilon}{1+e^{\beta(\varepsilon-\mu)}} = \frac{1}{\beta}\int_0^\infty \frac{g(\mu+x/\beta)\,dx}{1+e^x}$$

$$I = \int_0^\mu g(\varepsilon)\,d\varepsilon - \frac{1}{\beta}\int_0^{\beta\mu} \frac{g(\mu-y/\beta)\,dy}{1+e^y} + \frac{1}{\beta}\int_0^\infty \frac{g(\mu+x/\beta)\,dx}{1+e^x}$$

For most applications $\int_0^{\beta\mu} \approx \int_0^\infty$

$$g(\mu-y/\beta) \approx g(\mu) - y/\beta\, g'(\mu) \;;\; g(\mu+x/\beta) \approx g(\mu) + \frac{x}{\beta} g'(\mu)$$

To do $\int_0^\infty \frac{x\,dx}{1+e^x}$, expand $\frac{xe^{-x}}{1+e^{-x}}$ in a power series and sum. You should find

$$\int_0^\infty \frac{x\,dx}{1+e^x} = \pi^2/12$$

If you use these tricks in b), you should find that the total energy looks like

$$U = U_0 + \gamma T^2$$

then $$C_V = \frac{\partial U}{\partial T} = 2\gamma' T$$

Hence the specific heat of a metal takes the form

$C_V = 2\gamma' T + \alpha T^3$ lo T

$2\gamma' T + 3R$ hi T

in both cases the electron contribution is detectable.

If you go to temperatures that are too high, it is necessary to include higher terms in the expansion of $g(\varepsilon)$ and the result will have a different T dependence.

It is fun to see that this qualitative behavior can be found by quite simple basic arguments.

Electron contribution: At low T, we fill up all the states in k space to the Fermi surface. Then only those electrons within energy kT of the Fermi energy will be excited.

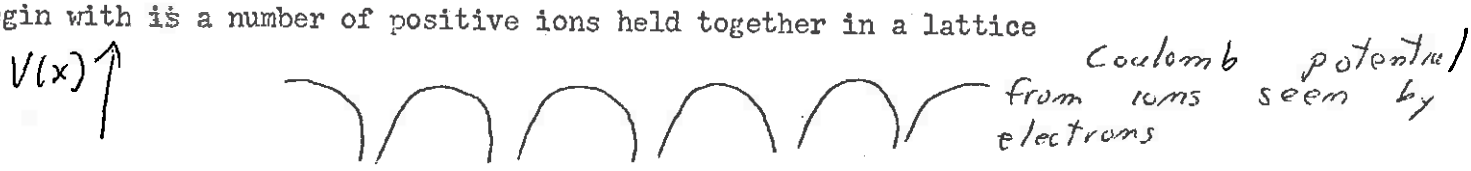
electrons in a spherical shell = $4\pi k^2 dk = 4\pi k E\, dE \approx 4\pi k_f \epsilon_f (kT)$

Phonon contribution: The number of phonons which will contribute to the specific hhat is the number of lattice vibrations that can be excited = all those up to $\hbar\omega = kT$

Look in k space for the phonons. We know have the whole volume of the sphere
$\sim k^3_{outside} \sim w^3_{highest} \sim T^3$

We have sketchily derived the basic effects of Fermi-Dirac statistics on the electron distribution within a box. For any reasonable T, most of the electrons are huddled in the states at the bottom of our potential well. The states just below the chemical potential energy are not fully populated: these particles are in the state above μ .

Now the point is to apply this box to the physical case of a solid. What we have to begin with is a number of positive ions held together in a lattice



The innermost electrons in the atoms will in general stay attached to the ions, and we can forget about them for the moment. Lets worry only about the outer electrons. These are much more loosely bound to the ions and are thus the ones which will best reflect the peculiar properties of solids.

Before we begin to do detailed calculations, lets try to understand what happens on a qualitative level. Most students have done the following problem at some time in elementary quantum mechanics courses:

Begin with 2 identical potential wells

Each alone has a certain set of energy levels, ϵ_a . Now consider the system of the two together and compute the energy levels of the systems as a function of r. One finds that for large r the levels are roughly those of the individual atoms; but as r decreases they tend to split - each into 2 new energy levels

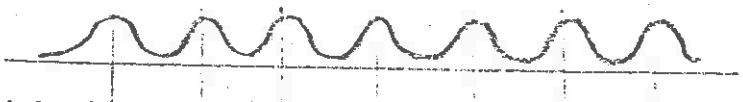
where the energy of the new levels depends on the symmetry of the new wave functions.

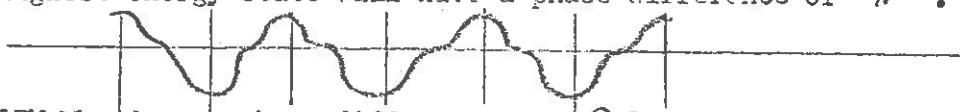
Repeating this with enough atoms, you can assemble a whole crystal lattice. Each of the atomic states characterized by n and l now splits into 2N levels.

spin # atoms

It happens that this splitting is so small that there is usually still space between the

resulting energy bands. 

Within a band the relative energies of the levels depend on the phase difference of the wave functions from one cell to the next. The lowest energy state will look something like  Phase difference = 0

The highest energy state will have a phase difference of π. 

PROBLEM: Why does a phase difference of δ always give the same energy as $-\delta$?

PROBLEM: From some sort of knowledge about the shapes of wave functions within a given cell, Plus phase differences from cell to cell, explain why for one band the energy versus k curve looks like  whereas for the next band it may look like  .

It also happens that within a given band the electrons feel a certain average potential due to the collection of ions and other electrons, which is as though the electrons were held in a box with this average potential. Thus the distribution among levels in the solid follows the laws of Fermi-Dirac statistics that we found above.

Now to get down to brass tacks, we go into the mathematics of wave functions for electrons in a periodic potential. Once again we find that taking advantage of the periodicity saves quite a bit of work.

Begin by writing down the Schrodinger equation for the system

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = \epsilon\psi(\vec{r})$$

$V(\vec{r}) = V(\vec{r}+\vec{N})$ where $\vec{N}$ is any lattice vector.

Substitute $\vec{r}' = \vec{r}+\vec{N}$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}+\vec{N})\right]\psi(\vec{r}+\vec{N}) = \epsilon\psi(\vec{r}+\vec{N})$$

$$\left[-\hbar^2/2m\,\nabla^2 + V(\vec{r})\right]\psi(\vec{r}+\vec{N}) = \epsilon\,\psi(\vec{r}+\vec{N})$$

Hence $\psi(\vec{r}+\vec{N})$ is a solution with the same energy as $\psi(\vec{r})$, for any lattice vector $\vec{N}$.

Define $\mathcal{U}(\vec{r}) = \sum_{\vec{N}} \psi(\vec{r}+\vec{N})e^{-i\vec{\kappa}\cdot\vec{N}}$

This is then a solution of the Schrodinger equation with the same energy as $\psi(\vec{r})$

It has the property $\mathcal{U}(\vec{r}+\vec{N}_0) = \mathcal{U}(\vec{r})e^{i\vec{\kappa}\cdot\vec{N}_0}$

Thus solutions of the Schrodinger equation with a periodic potential can be constructed to satisfy $\psi(\vec{r}+\vec{N}) = \psi(\vec{r})e^{i\vec{\kappa}\cdot\vec{N}}$ $\forall\,\vec{N}$

Then Floquet's theorem says that the solutions take the form $\psi(\vec{r}) = u(\vec{r})e^{i\vec{\kappa}\cdot\vec{r}}$

Expand the $u(\vec{r})$ in a Fourier series $u(\vec{r}) = \sum_{\vec{L}} A_{\vec{L}} e^{i\vec{L}\cdot\vec{r}}$

($\vec{L}$ is a vector in the reciprocal lattice space). Then plug this back into

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right] u(\vec{r}) e^{i\vec{K}\cdot\vec{r}} = \epsilon\, u(\vec{r}) e^{i\vec{K}\cdot\vec{r}}$$

We then find

$$\sum_{\vec{L}} \left[\frac{\hbar^2}{2m}(\vec{K}+\vec{L})^2 + V(\vec{r})\right] A_{\vec{L}} e^{i(\vec{L}+\vec{K})\cdot\vec{r}} = \epsilon \sum_{\vec{L}} A_{\vec{L}}\, u(\vec{r})\, e^{i(\vec{K}+\vec{L})\cdot\vec{r}}$$

Hence $$\left[\frac{\hbar^2}{2m}(\vec{K}+\vec{L})^2 - \epsilon\right] A_{\vec{L}} = -\sum_{\vec{L}''} V_{\vec{L}-\vec{L}''} A_{\vec{L}''}$$

The point is to solve this for the energy levels ϵ and the wave function pieces $A_{\vec{L}}$.

Up to this point we haven't made approximations. But, as usual, to get a solution it is necessary to approximate.

APPROXIMATION 1: Weak Binding

$V_{\vec{L}-\vec{L}'}$ small; $V_{\vec{0}} = 0$

This just sets the constant part of the potential equal to 0; we are just raising or lowering the overall scale.

First approximation to the wave function

Weak potential implies $\psi(x) \approx A_{\vec{0}}\, e^{i\vec{K}\cdot\vec{x}}$; $A_{\vec{L}} \approx 0 \quad \vec{L} \neq 0$

$$\left[\frac{\hbar^2}{2m}(\vec{K}+\vec{L})^2 - \epsilon\right] A_{\vec{L}} \approx -V_{\vec{L}} \qquad \vec{L} = 0 \Rightarrow \epsilon \approx \frac{\hbar^2 K^2}{2m}$$

$$\vec{L} \neq 0 \Rightarrow A_{\vec{L}} = \frac{-V_{\vec{L}}\, 2m/\hbar^2}{(\vec{K}+\vec{L})^2 - \vec{K}^2}$$

We can substitute this back to find the correction to ϵ_K

$$\epsilon = k^2/2m - \sum \frac{|V_L|^2\, 2m}{(K+L)^2 - K^2}$$

However for $\vec{L} \neq 0$ $(\vec{K}+\vec{L})^2 \approx \vec{K}^2 \Rightarrow$

$A_{\vec{L}}$ is large and not ≈ 0 as we assumed. Thus in this case the approximation breaks down and the analysis has to be redone.

The trouble comes for $2\vec{K}\cdot\vec{L} + \vec{L}^2 = 0 \qquad \vec{L}\cdot(\vec{K} + \vec{L}/2) = 0$

This equation defines a set of troublesome vectors $\perp \vec{L}$ - a plane of $\vec{K}$'s which goes through $-\vec{L}/2$

Hence each $\vec{L}$ gives a plane of singular points in k space. The set of all such planes divides k space up into Brillouin zones. Thus we see that at the edge of the Brillouin zone

the energy will probably deviate from $\hbar^2/2m$

To find out quantitatively what is happening, pick one particular L_1 $\ni$

$$(K+L_1)^2 - K^2 \sim V$$

Then A_0, A_{L_1} are not small, but all the other terms are. Returning to the original set of equations gives

$$\left[\frac{\hbar^2 K^2}{2m} - \epsilon\right] A_0 = -V_{-L_1} A_{L_1}$$

$$\left[\frac{\hbar^2}{2m}(K+L_1)^2 - \epsilon\right] A_{L_1} = -V_{L_1} A_0$$

($V_{-L}^{\dagger} = V_L$ to have a real potential) . Define $w(p) = p^2/2m$

Then equations can be solved only for

$$\epsilon = \frac{w(K+L_1)+w(K)}{2} \pm \sqrt{\left[\frac{w(K+L_1)-w(K)}{2}\right]^2 + |V_{L_1}|^2}$$

small $|V_{L_1}|^2 \Rightarrow$ $\epsilon = w(K) - |V_{L_1}|^2/[w(K+L_1)-w(K)]$

$$\epsilon = w(K+L_1) + |V_{L_1}|^2/[w(K+L_1)-w(K)]$$

Thus the edge of the zone leads to a gap in the energy curve

ASIDE: ONE DIMENSIONAL MODELS OF SOLIDS TO PLAY WITH

a) Cosine potential - leads to Mathieu's equation

b)  $\uparrow V(x)$

$\rightarrow x$

The Kronig-Penny model of a solid.

This is quite useful because you can vary the heights and widths of the holes and hence can see what happens if one of the atoms is different.

STRONG BINDING APPROXIMATION

Here the potential wells are taken as relatively deep and far apart.

If f(r) is the solution around one of the wells, try as a solution

$$\sum_N e^{i\vec{K}\cdot\vec{N}} f(|\vec{r}-\vec{N}|)$$

It there is only one atom per unit cell of a given kind,

$$V = \sum_N v(R-N) \; ; \; -\tfrac{1}{2m}\nabla^2 f + v(r) f = \epsilon_0 f$$

To get an idea of the energy levels, use the formula

$$\mathcal{E} = N/D = \int \psi^* H \psi \, dV \Big/ \int \psi^* \psi \, dV$$

$$D = \sum_{N N'} e^{i k \cdot (N - N')} \int f^*(r - N') f(r - N)\, d^3 r$$

$$= 1 + \sum_{N \neq N'} e^{i k \cdot (N - N')} \int f^*(r - N') f(r - N)\, d^3 r = 1 + \sum_M e^{i k \cdot M} I(M)$$

$$I(M) = \int f^*(r - M) f(r)\, d^3 r$$

should probably be computed for only those M corresponding to nearest neighbors

$$N = \sum_{N N'} e^{i k \cdot (N - N')} \int f^*(r - N') \underbrace{\left[\frac{-\hbar^2}{2m} \nabla^2 + \sum_\ell v(R - \ell) \right]}_{\epsilon_0 - v(r - N) + \sum_\ell v(r - \ell)} f(r - N)\, d^3 r$$

Then

$$\mathcal{E} = \epsilon_0 + N'/D$$

Define $$J(M) = \int f^*(R - M) [V(R) - v(R)] f(R)\, d^3 R$$

$$\mathcal{E} = \epsilon_0 + \left[\frac{J_0 + \sum_{M \neq 0} J(M) e^{i k \cdot M}}{1 + \sum_{M \neq 0} I(M) e^{i k \cdot M}} \right]$$

In practice it is difficult to get numbers out of this. However we can understand what is going on by assuming the J's go down so fast that only the nearest neighbors contribute. Then

$$\mathcal{E} = \epsilon_0 + \left\{ \frac{J_0 + 2 J_{100} [\cos k_x a + \cos k_y a + \cos k_z a]}{1 + 2 I_{00} [\cos k_x a + \cos k_y a + \cos k_z a]} \right\}$$

Physics 205b

February 24,27,28

CREATION AND ANNIHILATION OPERATORS FOR ELECTRONS

Up to this point we have been using a formalism in which bosons(photons, phonons, etc.) are described by creation and annihilation operators, while the electrons in the system havebbeen treated by standard wave function methods. One might expect that a certain elegance would result from use of a formalism which also contained creation and annihilation operators for fermions. However, the main reason for applying this language to electrons is not elegance, but rather the fact that certain phenomena,such as pair creation, seem much more reasonable when approached in this manner.

What we want is some sort of operator c such that $c^*_{k,i}$ creates an electron with momentum k in spin state i, and $c_{k,i}$ removes such an electron from the picture. (To simplify things, the spin index will be left out; any student who is confused by this should go through and reinsert all the indices.) If we had such an operator, we could write down interaction Hamiltonians which would in first order produce any desired process.

Example:

Electron k scatters to electron k' by absorbing phonon k

This is produced by an interaction like

$$\sum \Gamma_{k,\kappa,\kappa'} a_k c^*_{\kappa'} c_\kappa$$

However if this is part of a Hamiltonian operator, its Hermitian conjugate must be included also

$$\mathcal{H}^{int.} = \sum \Gamma_{k,\kappa,\kappa'} a_k c^*_{\kappa'} c_\kappa + \sum \Gamma^*_{k,\kappa,\kappa'} a^*_k c^*_\kappa c_{\kappa'}$$

Knowledge of the Γ's would then allow perturbation theory calculations of all sorts of processes, with $\mathcal{H}^{int.}$ as perturbation

To perform such calculations, one must know the properties of these c_κ's as operators To begin with, suppose a universe of one electron state. It can either be empty or filled with one electron. Hence we arrive at

$$\left.\begin{aligned} c^*|0\rangle &= |1\rangle \\ c^*|1\rangle &= 0 \end{aligned}\right\} \quad c^*c^* = 0$$

By taking the adjoint,

$$c|1\rangle = |0\rangle \qquad cc = 0$$

$\Rightarrow \qquad c|0\rangle = 0$

Similarly $\quad c\,c^* + c^* c = 1$

(test by applying to all possible states)

and $\quad c_i^* c_i = N_i \qquad$ (where N_i is either 0 or 1)

Puzzle: Suppose you know only that an operator c obeys

$c^* c^* = 0 \qquad c\,c = 0 \qquad c\,c^* + c^* c = 1$

Find a representation for the operator. Is it unique?

When the universe is expanded to include two electrons, a little bookkeeping becomes necessary. Let electron #1 be the one which is created first.

$c_a^* c_b^* |0\rangle = |a\,b\rangle$

means electron #1 is in state b; electron #2 is in state a.

The electron wave functions must be antisymmetric under interchange of electrons 1 and 2

$|a\,b\rangle = -|b\,a\rangle \Rightarrow \quad c_a^* c_b^* |0\rangle = -c_b^* c_a^* |0\rangle$

In fact the same relation holds for states other than the vacuum and we have the operator equations

$$c_a^* c_b^* = -c_b^* c_a^*$$

$$c_a c_b = -c_b c_a$$

The next thing to check is clearly $\quad c_a c_b^* \stackrel{?}{=} -c_b c_a^*$

There is a clever way to determine this:

The equation $c_c^* c_c + c_c c_c^* = 1$ must hold for the creation operator for any electron state. By the principle of superposition, if $|a\rangle$ and $|b\rangle$ are states, a perfectly allowable state is $\quad \alpha|a\rangle + \beta|b\rangle = |c\rangle \quad \ni \quad |\alpha|^2 + |\beta|^2 = 1$

$$c_c^* = \alpha c_a^* + \beta c_b^*$$

Hence

$$(\alpha c_a^* + \beta c_b^*)(\alpha^* c_a + \beta^* c_b) + (\alpha^* c_a + \beta^* c_b)(\alpha c_a^* + \beta c_b^*) = 1$$

Expand. Use $|\alpha|^2 + |\beta|^2 = 1$

Then

$$\beta\alpha^* c_b^* c_a + \alpha\beta^* c_a^* c_b + \beta^*\alpha\, c_b c_a^* + \alpha^*\beta\, c_a c_b^* = 0$$

$$c_b^* c_a + c_a c_b^* = 0$$

We thus have a set of anticommutation relations for fermions which parallel the commutation relations previously derived for bosons

$$[c_a, c_b]_+ = 0 \qquad [c_a, c_b^*]_+ = \delta_{ab} \quad \Big| \begin{array}{l} \text{if } a \neq b \\ \text{are} \\ \text{orthogonal} \end{array}$$

$$[c_a^*, c_b^*]_+ = 0$$

Exercise: figure out what these relations are if a and b are not orthogonal

Above we determined the operator $c_c^* = \alpha c_a^* + \beta c_b^*$ which creates an electron with amplitude α to be in state a and amplitude β to be in state b. Likewise, $c_\phi^* = \sum_p c_p^* \phi(p)$ creates an electron with amplitude $\phi(p)$ to have momentum p. This means its wave function must have the form $\sum_p \phi(p) e^{ip\cdot x} = \phi(x)$ And $c_\phi^* = \sum c_p^* \langle p|\phi\rangle$. If we symbolize the creation operator by $\langle \phi|$ then $c_\phi^* = \sum_p \langle \phi|p\rangle\langle p|\phi\rangle = \langle \phi|\phi\rangle$.

This sort of formalism makes it obvious that the manipulations performed here with operators are the same as usually performed with the states they create.

Let $\psi^*(x_0)$ be an operator which creates an electron at x_0. Then

$$\psi^*(x_0) = \sum \langle \phi|p\rangle\langle p|x_0\rangle = \sum_p c_p^* e^{-ip\cdot x_0}$$

$$\psi(x) = \int \frac{d^3p}{(2\pi)^3} e^{ip\cdot x} c_p$$

Exercise: using the properties of the c_p's, convince yourself that

$$\psi^*(x)\psi(y) + \psi(y)\psi^*(x) = \delta^3(x-y)$$

$$\psi^*(x)\psi^*(y) + \psi^*(y)\psi^*(x) = 0$$

These $\psi(x)$ operators are called field operators. Because $\psi^*(x) = \int \frac{d^3p}{(2\pi)^3} e^{-ip\cdot x} c_p^*$ and $c_\phi^* = \sum c_p^* \langle p|\phi\rangle$

Then $c_\phi^* = \int \underbrace{\psi^*(x)}_{\text{field op.}} \underbrace{\phi(x)}_{\text{wave fn}} d^3x$

The field operator may be thought of as just a device which changes wave functions into the corresponding operators.

These methods can equally well be applied to solid state physics. If $f_\kappa(R) = e^{ik\cdot R} u_\kappa(r)$ is the wave function for an electron of propagation vector k, then the operator which creates such a particle is $\varphi_\kappa^* = \int f_\kappa(R)\, \psi^*(R)\, d^3R$

Thus, for an arbitrary number of non-interacting electrons, the Hamiltonian of the system can be written as $\mathcal{H} = \sum \epsilon_\kappa n_\kappa = \sum \epsilon_\kappa \varphi_\kappa^* \varphi_\kappa$

But $\psi^* = \sum_k \varphi_\kappa^* f_\kappa^*(R)$ and if h is the Hamiltonian for the individual electron wave function, then $h\psi^* = \sum_k \varphi_\kappa^* h f_\kappa^*(R) = \sum_k \epsilon_\kappa \varphi_\kappa^* f_\kappa^*(R)$

$$\int \psi^* h \psi \, d^3x = \int d^3x \sum_k \sum_{k'} \epsilon_{k'} \varphi_k^* f_k^*(k) \varphi_{k'} f_{k'}(k)$$

$$= \Sigma_k \epsilon_k \varphi_k^* \varphi_k$$

Thus the Hamiltonian operator for the entire system can be expressed in terms of the Hamiltonian for an individual wave function and the field operator by

$$\mathcal{H} = \int \psi^*(x) h \psi(x) d^3x$$

Convince yourself that the creation operators for electrons must commute with all the operators for phonons. Then it is easy to see that a sample Hamiltonian for an interacting system of phonons and electrons might be written

$$\mathcal{H} = \Sigma_k \epsilon_k \varphi_k^* \varphi_k + \Sigma_k \hbar \omega_k a_k^* a_k$$

$$+ \sum_{k k' k} \left[\varphi_{k'}^* \varphi_k a_k \Gamma_{k,k',k} + \Gamma_{k,k',k}^* \varphi_k^* \varphi_{k'} a_k^* \right]$$

This formalism can be used to treat any system in which electrons interact only by exchange of phonons. If, in additiion to this, there is some direct electron-electron interaction, a further development is necessary.

If the electrons interact through some potential $V(R_1 - R_2)$ then the amplitude for scattering by this potential will be proportional to $v(Q) = \int V(R) e^{-i Q \cdot R} d^3R$ Then the definitions of the creation operators imply that the Hamiltonian should contain terms of the form

$$\sum_p (p^2/2m) c_p^* c_p + \sum v(Q) \delta(p_1 + p_2 - p_3 - p_4) c_{p_4}^* c_{p_3}^* c_{p_2} c_{p_1}$$

Use of the relation $c_p^* = \int e^{ip \cdot x} \chi^*(x) dx$

allows us to rewrite the interaction term as

$$\iint \psi^*(x) \psi^*(y) V(x-y) \psi(x) \psi(y) d^3x d^3y = \int \psi^*(x) \psi(x) V(0) d^3x$$

$$- \iint \psi^*(x) \psi(x) V(x-y) \psi^*(y) \psi(y) d^3x d^3y$$

To understand this, we compare it with the classical expression for interaction of two charge densities. $\epsilon_{classical} = \frac{1}{2} \iint \rho(x) V(x-y) \rho(y) d^3x d^3y$

By doing this we discover:

a) we should have defined the interaction as $\frac{1}{2} \sum v(Q) \delta(\ ) c_{p_4}^* c_{p_3}^* c_{p_2} c_{p_1}$

Else we count each interaction twice

b) There seems to be an extra term $\int \chi^*(x) \psi(x) V(0) d^3x$

This means that our quantum interaction contains no self-energy. This is exactly what we want (especially for things like a Coulomb potential where the self-energy

is infinite)

c) There is a difference of a - sign between the classical result and the one we found. But we can fix this just by permuting the fermion creation operators in the definition. So this is not serious or important.

Hence the Hamiltonian for a system of any number of electrons, interacting through the Coulomb potential, can be expressed as

$$H = \int \psi^*(x) \left[\frac{-\hbar^2}{2m} \left(\nabla - \frac{e}{c} A(x,t) \right)^2 + e\phi(x,t) \right] \psi(x)\, d^3x + \frac{1}{2} \iint \psi^*(x)\, \psi^*(y)\, \frac{e^2}{|\vec{x} - \vec{y}|}\, \psi(y)\, \psi(x)\, d^3x\, d^3y$$

where the ψ's are field operators.

With this Hamiltonian, the Schrödinger equation for such a system is

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi_0 = H \Psi_0$$

Notice that there is no reason for the solution Ψ_0 to be composed of a definite number of electrons. However, because this particular Hamiltonian commutes with the particle number operator $N = \int \psi^*(x)\, \psi(x)\, d^3x$ it is possible to choose solutions which do have the property $N \Psi_0 = n \Psi_0$ In general, this interaction will not mix subspaces with different n.

Moore, Hudson, Williams, Smith

Ph 205 b Mar. 3, 6, 7 Week 9

Let C_k^* be the operator that creates an electron in state k. Then $\{C_k, C_\ell^*\} = \delta_{k\ell}$ and $\{C_k, C_\ell\} = 0$.

A simple hamiltonian that permits discussion of electron scattering in a crystal is

$$H = \sum_k \epsilon_k C_k^* C_k + \sum_{kk'} \lambda_{kk'} C_k^* C_{k'}$$

An unfilled electron state in an energy band is called a "hole". Electron creation operators are hole destruction operators and vice-versa.

The formal identification is $C_k = b_k^*$, consequently

$$\{b_k, b_\ell^*\} = \delta_{k\ell} \quad , \quad \{b_k, b_\ell\} = 0.$$

Rewrite the hamiltonian:

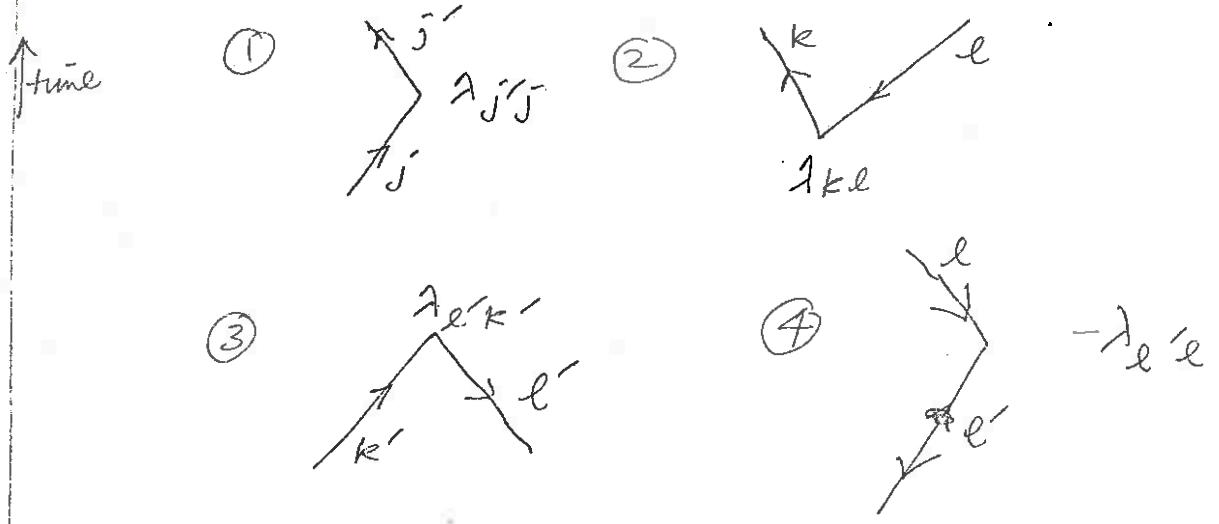
$$H = \sum_k \epsilon_k C_k^* C_k + \sum_\ell \epsilon_\ell b_\ell b_\ell^*$$
$$+ \sum_{kk'} \lambda_{kk'} C_k^* C_{k'} + \sum_{k\ell} \lambda_{k\ell} C_k^* b_\ell^*$$
$$+ \sum_{\ell' k'} \lambda_{\ell' k'} b_{\ell'} C_{k'} + \sum_{\ell' \ell} \lambda_{\ell' \ell} b_{\ell'} b_\ell^*$$

where the sum over all electron states k has been written as the sums over two sets of states.

$$\sum_\ell \epsilon_\ell b_\ell b_\ell^* = -\sum_\ell \epsilon_\ell b_\ell^* b_\ell + \sum_\ell \epsilon_\ell$$

the last term on the right is a zero point energy which may be neglected by changing the zero level of the energy

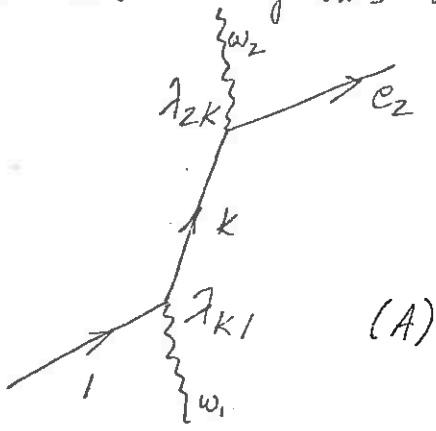
The 4 terms bilinear in the creation and destruction operators yield the following processes in first order:



Convention: An arrow pointing in the direction of increasing time indicates an electron; an arrow pointing in the direction of decreasing time indicates a hole.

2nd order contributions

Consider the following Hamiltonian 2 diagrams that contribute in 2nd order:



(A)

and

(B)

Now to conserve energy, in the initial state there is a phonon of energy ω_1 and in the final state there is a phonon of energy ω_2 where

$$\epsilon_1 + \omega_1 = \epsilon_2 + \omega_2$$

ϵ_1 = energy of electron 1, ϵ_2 = energy of electron 2.

From the perturbation theory of last term, the 2nd order contribution to the amplitude is

$$\sum_r \frac{\langle f|V|r\rangle\langle r|V|i\rangle}{E_i - E_r + i\varepsilon}, \quad \text{where the sum runs over all intermediate states } r.$$

Evaluating (A) and (B):

$$(A): \sum_k \frac{\langle 2|\lambda_{2k} c_2^* c_k|k\rangle\langle k|\lambda_{k1} c_k^* c_1|1\rangle}{E_1 - E_k + i\varepsilon}$$

$$= \sum_k \frac{\lambda_{2k}\lambda_{k1}}{\epsilon_1 + \omega_1 - \epsilon_k + i\varepsilon}$$

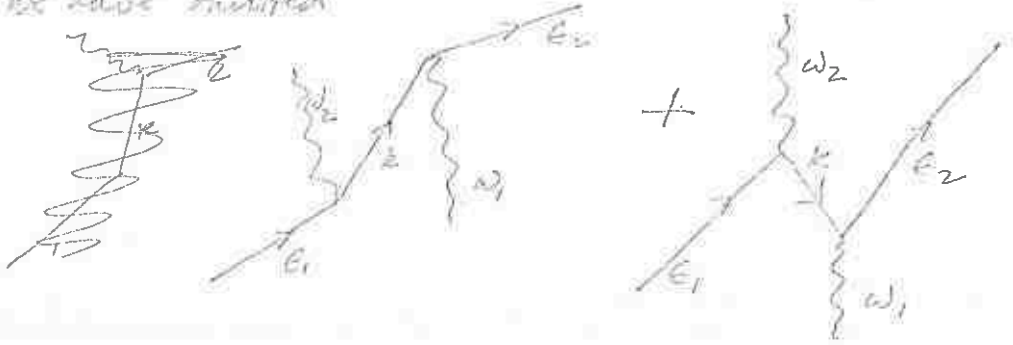
$$(B): \sum_k \frac{\langle 2|\lambda_{k1} b_k c_1|hole\, k, \epsilon_1, \epsilon_2\rangle\langle hole\, k, \epsilon_1, \epsilon_2|\lambda_{2k} c_2^* b_k^*|1\rangle}{\epsilon_1 + \omega_1 - (\epsilon_1 + \epsilon_2 + \omega_1 + \epsilon_2 - \epsilon_k) + i\varepsilon}$$

$$= \sum_k \frac{\langle 0|c_2 b_k c_1 b_k^* c_1^* c_2^*|0\rangle\langle 0|c_2 c_1 b_k c_2^* b_k^* c_1^*|0\rangle \lambda_{2k}\lambda_{k1}}{\epsilon_k - (\epsilon_2 + \omega_2) + i\varepsilon}$$

$$= -\sum_k \frac{\lambda_{2k}\lambda_{k1}}{\epsilon_k - \omega_1 - \epsilon_1 + i\varepsilon} = \sum_k \frac{\lambda_{2k}\lambda_{k1}}{\epsilon_1 + \omega_1 - \epsilon_k - i\varepsilon}$$

So that the contribution of (B) is the same as that of (A) except for the sign of $i\varepsilon$ in the denominator.

Notice that we have <u>not</u> evaluated the complete 2nd order amplitude as we have omitted



The contribution of the holes may be included as a modification of the propagator.

Let $\lambda_{k'k} = \int \phi_{k'}^*(x)\, \lambda(x)\, \phi_k(x)\, dx$

then the contribution of (A) may be written

$$\int dx_2\, dx_1\, dt_2\, dt_1 \quad \phi_2^*(x_2)\, \lambda(x_2)\, K_+(2,1)\, \lambda(x_1)\, \phi(x_1)$$

where $K_+(2,1) = \theta(t_2 - t_1) \sum_{\substack{\text{electrons} \\ k}} e^{-i\epsilon_k(t_2-t_1)}\, \phi_k^*(x_1)\, \phi_k(x_2)$

$$\theta(t_2 - t_1) = \begin{cases} 1 & t_2 > t_1 \\ 0 & t_2 < t_1 \end{cases}$$

if we define for $t_2 < t_1$

$$K_+(2,1) = -\sum_{\substack{k \\ \text{holes}}} e^{-i\epsilon_k(t_2-t_1)}\, \phi_k(x_2)\, \phi_k^*(x_1)$$

(A)+(B) may be written in the same form as (A) alone:

$$\int dx_2\, dx_1\, dt_2\, dt_1 \quad \phi_2^*(x_2)\, \lambda(x_2)\, K(2,1)\, \lambda(x_1)\, \phi(x_1)$$

Relativistic Quantum Mechanics

There is no known violation of the invariance principle of relativity. Two consequences of putting together relativity and quantum mechanics that are important in elementary particle theory are: (1) the existence of antiparticles. Moreover the dynamics of antiparticles are determined from ~~theory of~~ the dynamics of the corresponding particles. This is known as the CPT theorem.

(2) the connexion between spin and statistics, namely that integer spin particles obey Bose statistics and that half integer spin particles obey Fermi statistics. We will give a demonstration of this result later.

The Schrödinger Equation $H\psi = i\frac{\partial \psi}{\partial t}$ is unsymmetrical in its treatment of time and space.

Basically there are 3 ways of doing relativistic quantum mechanics:

(1) A method which is easy to understand, but in which the relativity is not manifestly obvious.

(2) A method which is less easy to understand, in which the relativity is obvious.

(3) Abstract, elegant way.

We will follow method (1). In some problems, approach (2) is simpler.

Maxwell's Equations are relativistically invariant, but their effect may be treated in a non-relativistic manner in some applications (Compton scattering, photoelectric effect).

Maxwell's Eq'ns may be derived from a Lagrangian L that gives the

$$\text{action} = \int\left[\left(-\nabla\phi - \frac{\partial A}{\partial t}\right)^2 - (\nabla \times A)^2\right] d^3x\, dt$$

Interaction with matter is handled by adding the additional term $\int j_\mu(x) A_\mu(x)\, d^3x$ to the Lagrangian.

In the ~~non-~~relativistic non-covariant coulomb guage $\nabla \cdot A = 0$, the interaction of charged particles through the electromagnetic field is equivalent to

(1) Instantaneous coulomb interaction $\frac{e^2}{r_{ij}}$

(2) $H = \sum_k \omega_k a_k^* a_k + \int j_\mu(x) A_\mu(x)\, dx + H_{matter}$

$$\underset{\sim}{A}(x) = \sum_{k,i} \frac{1}{\sqrt{2\omega_k}} \left[\underset{\sim}{\varepsilon}_{k,i} e^{ik\cdot x} a_{k,i} + \underset{\sim}{\varepsilon}^*_{k,i} e^{-ik\cdot x} a^*_{k,i} \right]$$

Let us write down the classical relativistic relations for particles.

$$E = m_0 \gamma \qquad \underset{\sim}{p} = m_0 \gamma \underset{\sim}{v} \quad , \qquad \gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2}$$

(c taken to be 1 from here on wherever convenient)

so $E^2 = p^2 + m_0^2$ omit the subscript — all masses referred to will be REST masses.

or $p_\mu^2 = m^2$ where $p_\mu = (E, \underset{\sim}{p})$

and if $A_\mu = (A_0, \underset{\sim}{A})$, $B_\mu = (B_0, \underset{\sim}{B})$

then $A \cdot B = A_\mu B_\mu = A_0 B_0 - \underset{\sim}{A} \cdot \underset{\sim}{B}$

Definition: $\delta_{\mu\nu} = \begin{cases} 0 & \mu \neq \nu \\ 1 & \mu = \nu = 0 \\ -1 & \mu = \nu = 1, 2, \text{or } 3 \end{cases}$

Let $\nabla_\mu = \left(\frac{\partial}{\partial t}, \frac{-\partial}{\partial x}, \frac{-\partial}{\partial y}, \frac{-\partial}{\partial z}\right) = \left(\frac{\partial}{\partial t}, -\underset{\sim}{\nabla}\right)$ (Notice the minus sign in the definition of ∇_μ)

Another useful vector is $x_\mu = (t, \underset{\sim}{x})$

Non-relativistically the phase of a free particle of momentum $\underline{k}$ frequency (energy) ω is

$$e^{i(\underline{k}\cdot\underline{x} - Et)} \quad \text{or} \quad e^{i(\underline{k}\cdot\underline{x} - \omega t)}$$

This may be written as a Lorentz invariant as

$$e^{-ip\cdot x}$$

we will take this over to the relativistic case (first done by de Broglie)

Then, using the relativistic expression: $\omega = \sqrt{k^2 + m^2}$

we obtain $\frac{d\omega}{dk} = v_{group} = \frac{dE}{dp} = v_{classical} = \frac{p}{E}$

The Schrodinger eq'n is of first order in time and permits the principle of superposition which we want to retain. Let us look for a relativistic wave equation that is first order in time

$E = \sqrt{p^2 + m^2}$ suggests

$i\frac{\partial \psi}{\partial t} = \sqrt{m^2 - \nabla^2}\,\psi$ which, horrible as it looks, can be made to work out

But the equation in the presence of an external field:

$$(i\partial_t - eA_0)\psi = \sqrt{m^2 - (\underline{\nabla} - ie\underline{A})^2}\,\psi$$

presents difficulties.

a second-order equation suggests itself

$$\left[(i\partial_t - eA_0)^2 - (-i\underline{\nabla} - e\underline{A})^2\right]\psi = m^2\psi$$

This is a serious contender for a relativistic wave equation. There are possible difficulties:

① Does it conserve probability?
② Does it reduce to a correct nonrelativistic equation? (in the non-relativistic limit)
③ Energy levels of the hydrogen atom.
④ Does it violate causality?

Problem (Due first week next term): Test out one of these questions.

The most serious test is ③ — the others are basically theoretical prejudices.

The Dirac Equation

Dirac looked for an equation of the form $H\psi = i\frac{\partial \psi}{\partial t}$, where he permitted the wave-function ψ to have several components, and the Hamiltonian was permitted to be a matrix operator on these components.

Guessed $$H = \alpha_x \frac{1}{i}\frac{\partial}{\partial x} + \alpha_y \frac{1}{i}\frac{\partial}{\partial y} + \alpha_z \frac{1}{i}\frac{\partial}{\partial z} + \beta m$$

where $\underset{\sim}{\alpha}, \beta$ are matrices.

i.e., $$H = \underset{\sim}{\alpha} \cdot \underset{\sim}{p} + \beta m \qquad \underset{\sim}{\alpha}, \beta \text{ hermitean}$$

with an external field present,

$$H = \underset{\sim}{\alpha} \cdot (\underset{\sim}{p} - e\underline{A}) + \beta m \qquad \underset{\sim}{p} = -i\underset{\sim}{\nabla}$$

and $$i\frac{\partial}{\partial t} \longrightarrow i\frac{\partial}{\partial t} - e\phi$$

Look for a sol'n of the form $\psi = u e^{-ik\cdot x}$ (free particle)

then u satisfies the equation

$$E u = (\underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta m) u$$

$$\therefore \quad E^2 u = (\underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta m)^2 u$$

$$E^2 = k_1^2 + k_2^2 + k_3^2 + m^2$$

$$\Longrightarrow \quad \alpha_x^2 = 1 = \alpha_y^2 = \alpha_z^2$$

$$\alpha_x\alpha_y + \alpha_y\alpha_x = 0, \text{ etc.}$$

$$\beta\alpha_x + \alpha_x\beta = 0$$

and $\quad \beta^2 = 1$

in 4 dimensions an explicit set of α's and β that satisfy these equations is

$$\alpha_x = \begin{pmatrix} 0&0&0&1\\ 0&0&1&0\\ 0&1&0&0\\ 1&0&0&0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$$

$$\alpha_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} \qquad \alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$$

where $\sigma_x, \sigma_y, \sigma_z$ are the usual Pauli spin matrices.

I : 2×2 identity matrix
0 : 2×2 zero matrix

Write the 4 component wavefunction

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} e^{-ikx} \quad \text{as} \quad \begin{pmatrix} u_a \\ u_b \end{pmatrix} e^{-ikx}$$

where u_a, u_b are 2 component objects

in an external field $\left(i\frac{\partial}{\partial t} - e\phi\right)\psi = \underset{\sim}{\alpha}\cdot\left(\frac{1}{i}\underset{\sim}{\nabla} - e\underset{\sim}{A}\right)\psi + \beta m\psi$

"multiply" by β: $\beta\left(i\frac{\partial}{\partial t} - e\phi\right) + \beta\underset{\sim}{\alpha}\cdot\left(i\underset{\sim}{\nabla} + e\underset{\sim}{A}\right)\psi = m\psi$

Define another set of matrices: $\gamma_0 = \gamma_t = \beta$

$\underset{\sim}{\gamma} = \beta\underset{\sim}{\alpha}$

Then the equation becomes

$$\gamma_\mu\left(i\nabla_\mu - eA_\mu\right)\psi = m\psi$$

where $\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu}$

These commutation rules are invariant under Lorentz transformations

Let $\psi = \begin{pmatrix}\psi_a\\ \psi_b\end{pmatrix}$

then $\left(\frac{-\hbar}{i}\frac{\partial}{\partial t} - e\phi\right)\psi_a = \underset{\sim}{\sigma}\cdot\left(\frac{1}{i}\underset{\sim}{\nabla} - e\underset{\sim}{A}\right)\psi_b + m\psi_a$

and

$$\left(\frac{-1}{i}\frac{\partial}{\partial t} - e\phi\right)\psi_b = \underset{\sim}{\sigma}\cdot\left(\frac{1}{i}\underset{\sim}{\nabla} - e\underset{\sim}{A}\right)\psi_a - m\psi_b$$

For a neutrino equations are

$$-\frac{1}{i}\frac{\partial}{\partial t}\psi_a = \sigma\cdot\left(\frac{1}{i}\underset{\sim}{\nabla}\right)\psi_b$$

$$-\frac{1}{i}\frac{\partial}{\partial t}\psi_b = \sigma\cdot\left(\frac{1}{i}\underset{\sim}{\nabla}\right)\psi_a$$

PHYSICS 205c

Week 1

DIRAC EQUATION

$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi \qquad H = \beta m + eV + \vec{\alpha}\cdot(\vec{p} - \frac{e}{c}\vec{A})$

where

in order to a) have an equation linear in time derivatives and

b) have time and space derivatives enter on an equal footing

It is found that in order for this to work, different α_i must anticommute, and $\alpha_i\beta = -\beta\alpha_i$ One representation of these commutation relations is

$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$

Hence if ψ is written in the form of a pair of 2 component spinors $\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$ then the Dirac equation gives a set of 2 coupled equations for the two component spinors.

Because H is Hermitian, $\frac{\partial}{\partial t}$ is antihermitian and

$\frac{\partial}{\partial t}\int \psi^\dagger\psi\, dvol = \int\left[\frac{\partial\psi^\dagger}{\partial t}\psi + \psi^\dagger\frac{\partial\psi}{\partial t}\right] dvol = \int\left[-\psi^\dagger\frac{\partial\psi}{\partial t} + \psi^\dagger\frac{\partial\psi}{\partial t}\right] dvol = 0$

Thus $\psi^\dagger\psi$ can be thought of as a probability density

Expectation values take the usual form $\langle\alpha\rangle = \int\psi^\dagger\alpha\psi\, dvol$

Notice that none of the answers will change if we change the representation (i.e. if we pick some different form which satisfies the commutation relations) for the $\vec{\alpha}$ and β matrices. Then the new representation can be related to the old as follows: $SS^\dagger = 1 \qquad \psi' = S\psi \qquad \psi'^\dagger = \psi^\dagger S^{-1}$

$\alpha' = S\alpha S^{-1} \qquad \beta' = S\beta S^{-1}$

check: $\alpha'\psi' = S\alpha S^{-1} S\psi = S(\alpha\psi)$

$\alpha'\beta' = S(\alpha\beta)S^{-1}$

Change of representation sometimes makes the physics more transparent. For example, the Dirac equation written in terms of ψ_a and ψ_b looks like $(\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A})$

$(E - eV)\psi_a - \vec{\sigma}\cdot\vec{\pi}\,\psi_b = m\psi_a$

$(E - eV)\psi_b - \vec{\sigma}\cdot\vec{\pi}\,\psi_a = -m\psi_b$

for $\psi_s = \psi_a + \psi_b \qquad \psi_d = \psi_a - \psi_b$

these may be rewritten as

$(E - eV)\psi_s - \vec{\sigma}\cdot\vec{\pi}\,\psi_d = m\psi_d$

$(E - eV)\psi_d + \vec{\sigma}\cdot\vec{\pi}\,\psi_s = m\psi_s$

$$(E-eV+\vec{\sigma}\cdot\vec{\pi})(E-eV-\vec{\sigma}\cdot\vec{\pi})\psi_s = m^2\psi_s$$

$$(E-eV-\vec{\sigma}\cdot\vec{\pi})(E-eV+\vec{\sigma}\cdot\vec{\pi})\psi_d = m^2\psi_d$$

Thus in this representation it is easy to uncouple the equations (although the equation has become quadratic in the energy rather than linear, in the process).

Because the electron in β decay is created as pure ψ_s, this is the natural representation to use to calculate the effects of electromagnetism on it as it shoots out of the nucleus.

CHANGE OF NOTATION

To make the equation more obviously similar in time and space components, multiply through by β

$$\left\{\beta\left[-\frac{\hbar}{i}\frac{\partial}{\partial t} - eV\right] - \beta\vec{\alpha}\cdot\left(\vec{p} - \tfrac{e}{c}\vec{A}\right)\right\}\psi = m\psi$$

Define $\gamma_0 = \beta$ $\quad \vec{\gamma} = \beta\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}$

because $p_0 = -\frac{\hbar}{i}\frac{\partial}{\partial t}$ we can write

$$\left[\gamma_0(p^0 - eV) - \vec{\gamma}\cdot\left(\vec{p} - \tfrac{e}{c}\vec{A}\right)\right]\psi = m\psi$$

For any four vector $\vec{B}$, define $\not{B} = B_0\gamma_0 - \vec{B}\cdot\vec{\gamma}$

then the Dirac equation takes the form

$$\boxed{\left(\not{p} - \tfrac{e}{c}\not{A} - m\right)\psi = 0}$$

i.e. because $p_0 = i\hbar\frac{\partial}{\partial t}$, $\vec{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ define $\nabla_\mu = \left(\hbar\frac{\partial}{\partial t}, -\hbar\frac{\partial}{\partial x}\right)$

then $\left(i\not{\nabla} - \tfrac{e}{c}\not{A}\right)\psi = m\psi$

SOLUTIONS OF THE DIRAC EQUATION

a) Particle at rest, no field $\quad \vec{p} = 0\,;\ \vec{A} = 0$

$$(p_0\gamma_0 - m)\psi = 0 \Rightarrow \begin{pmatrix} E-m & 0 \\ 0 & -(E+m) \end{pmatrix}\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = 0$$

For ψ_a, E=m $\quad \psi_a = \begin{pmatrix} \phi \\ 0 \end{pmatrix} e^{-imt}$

For ψ_b, E=-m $\quad \psi_b = \begin{pmatrix} 0 \\ \chi \end{pmatrix} e^{imt}$

Here ϕ and χ can be any 2 component spinor ($\begin{pmatrix} a \\ b \end{pmatrix}$ for general constants a and b)

b) No field, particle moving

It is much easier to solve the problem in momentum space. Then one can always Fourier transform back by multiplying by $e^{-iEt + i\vec{p}\cdot\vec{x}}$

$$(\not{p} - m)\psi = 0$$

$$(E-m)\phi - \vec{p}\cdot\vec{\sigma}\chi = 0$$

$$\vec{p}\cdot\vec{\sigma}\phi - (E+m)\chi = 0$$

solution i) $$\chi = \left(\frac{\vec{p}\cdot\vec{\sigma}}{E+m}\right)\phi$$

$$\psi = \begin{pmatrix} \phi \\ \frac{\vec{p}\cdot\vec{\sigma}}{E+m}\phi \end{pmatrix}$$

By substituting this back we see that

$$(E-m)\phi - \frac{\vec{p}\cdot\vec{\sigma}\,\vec{p}\cdot\vec{\sigma}}{E+m}\phi = 0 \qquad E^2 = p^2 + m^2$$

Hence in position space

$$\chi = \begin{pmatrix} \phi \\ \frac{\vec{\sigma}\cdot\vec{p}}{E+m}\phi \end{pmatrix} e^{i(\pm\sqrt{p^2+m^2}\,t) + i\vec{p}\cdot\vec{x}}$$

Choose the sign such that as $\vec{p}\to 0$, this approaches $\begin{pmatrix}\phi\\0\end{pmatrix} e^{-imt}$

$$\chi = \begin{pmatrix} \phi \\ \frac{\vec{p}\cdot\vec{\sigma}}{(E+m)}\phi \end{pmatrix} e^{-i\sqrt{p^2+m^2}\,t + i\vec{p}\cdot\vec{x}}$$

solution ii) $$\phi = \frac{\vec{p}\cdot\vec{\sigma}\,\chi}{E-m}$$

Here again $E^2 = m^2 + p^2$, but we choose the square root such that as $\vec{p}\to 0$, the solution approaches $\begin{pmatrix}0\\\chi\end{pmatrix} e^{imt}$

Thus we get $$\begin{pmatrix} -\frac{\vec{p}\cdot\vec{\sigma}\,\chi}{m+\sqrt{p^2+m^2}} \\ \chi \end{pmatrix} e^{i\sqrt{p^2+m^2}\,t + i\vec{p}\cdot\vec{x}}$$

or, if $\vec{p}' = -\vec{p}$, $$\begin{pmatrix} \frac{\vec{p}'\cdot\vec{\sigma}\,\chi}{m+\sqrt{p^2+m^2}} \\ \chi \end{pmatrix} e^{i\sqrt{p^2+m^2}\,t - i\vec{p}'\cdot\vec{x}}$$

which is sometimes written $$\begin{pmatrix} \frac{\vec{p}'\cdot\vec{\sigma}}{E+m}\chi \\ \chi \end{pmatrix} e^{-(-iEt + i\vec{p}'\cdot\vec{x})}$$

Thus if we associate this second solution with $\vec{p}'$, it looks just like the first solution except that the "large" and "small" components of the spinor have been interchanged, and there is an overall - sign in the exponent. Some people like to think of this - sign as a reversal of x and t; this at least is a mnemonic.

For the moment, ignore the problem of normalizing these,

It is much more complicated to find solutions for $\vec{A}\neq 0$. For the present, lets forget about this and just try to understand the nonrelativistic limit of the Dirac equation in a field

$(\not{p} - e/c \not{A} - m)\chi = 0$ reduces to the set of coupled equations

$$(E - m - e/c V)\phi - (\vec{p} - e/c \vec{A})\cdot\vec{\sigma}\,\chi = 0$$

$$\vec{\sigma}\cdot(\vec{p} - e/c \vec{A})\,\phi - (E + m - e/c V)\chi = 0$$

$$\chi = \left(\frac{1}{E + m - e/c V}\right)\vec{\sigma}\cdot(\vec{p} - e/c \vec{A})\phi$$

Substitute this into the first equation. It is important to preserve the order of operators, because the $\vec{p}$ and E are differential operators which don't commute with $\vec{A}$

$$(E - m - e/c V)\phi = (\vec{p} - e/c \vec{A})\cdot\vec{\sigma}\,\frac{1}{(E + m - e/c V)}\,\vec{\sigma}\cdot(\vec{p} - e/c \vec{A})\phi$$

Use $E \equiv m + W$

$$\frac{1}{2m + w - e/c V} \approx \frac{1}{2m} - \frac{(w - e/c V)}{(2m)^2}$$

$$(w - e/c V)\phi = \frac{1}{2m}\vec{\sigma}\cdot\vec{\pi}\,\vec{\sigma}\cdot\vec{\pi}\,\phi - \frac{\vec{\sigma}\cdot\vec{\pi}}{(2m)^2}(w - e/c V)\vec{\sigma}\cdot\vec{\pi}\,\phi$$

Rewrite the equation by adding and subtracting the same thing on both sides

$$\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right](w - V')\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]\phi = \frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2\phi +$$

$$+ \frac{1}{8m^2}\left[(\vec{\sigma}\cdot\vec{\pi})^2(w - V') - 2\,\vec{\sigma}\cdot\vec{\pi}\,(w - V')\vec{\sigma}\cdot\vec{\pi} + (w - V')(\vec{\sigma}\cdot\vec{\pi})^2\right]\phi$$

To really be able to consider the non-relativistic limit, we should write everything in terms of a non-relativistic wave function. ϕ is not the non-relativistic wave function in the case where the fields are present. Define $\boxtimes = \left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right]\phi$

Then to lowest non-trivial order $\phi = \boxtimes - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\boxtimes$

hence $\chi^\dagger\psi = \phi^\dagger\phi + \chi^\dagger\chi \approx \phi^\dagger\phi\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{4m^2}\right] \approx \boxtimes^\dagger\boxtimes$

$\boxtimes$ contains the major effects of the "small" components as well as the large ones. Thus we can think of $\boxtimes$ as a non-relativistic wave function and imagine the problem of finding the energy eigenvalues to be the same as that of minimizing

$$\frac{\int \boxtimes^\dagger (\text{mess})\,\boxtimes\, d\text{vol}}{\int \boxtimes^\dagger \boxtimes\, d\text{vol}}$$

Upon substituting this expression for ϕ we obtain an equation of the form

$$\left[1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\right](w - V')\,\boxtimes = (\text{Glotch})$$

which we unravel again to first order by

$$(w - V')\,\boxtimes \approx \text{Glotch} - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2}\,\text{Glotch}$$

Keeping lowest order terms, we arrive at

$$(w - V')\,\boxtimes = \frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2\,\boxtimes - \frac{(\vec{\sigma}\cdot\vec{\pi})^4}{8m^3}\,\boxtimes$$

$$+ \frac{1}{8m^2}\left\{(\vec{\sigma}\cdot\vec{\pi})^2(w - V') - 2\,\vec{\sigma}\cdot\vec{\pi}\,(w - V')\vec{\sigma}\cdot\vec{\pi} + (w - V')(\vec{\sigma}\cdot\vec{\pi})^2\right\}\boxtimes$$

For any two operators A and B,

$$A^2B - 2ABA + BA^2 = [A,[A,B]]$$

set $A = \vec{\sigma}\cdot\vec{\pi}$ $\qquad B = W - V'$

Calculate $[\vec{\sigma}\cdot\vec{\pi},\ E - M - eV] = [\vec{\sigma}\cdot(\vec{p} - \tfrac{e}{c}\vec{A}),\ E - m - eV]$

Assume for simplicity that $\frac{\partial \vec{A}}{\partial t} = 0$ (This is not necessary. For fun and practice try working the whole mess through without assuming this)

Thus we get $-e[\vec{\sigma}\cdot\vec{p}, V] = -e\sigma_i[p_i, V] = -ie\vec{\sigma}\cdot\vec{E}$

$$\{\ \} = [\vec{\sigma}\cdot\vec{\pi}, -ie\vec{\sigma}\cdot\vec{E}]$$

$$= -ie[\vec{\sigma}\cdot\vec{p}, \vec{\sigma}\cdot\vec{E}] + i\frac{e^2}{c}(\vec{\sigma}\cdot\vec{A}\,\vec{\sigma}\cdot\vec{E} - \vec{\sigma}\cdot\vec{E}\,\vec{\sigma}\cdot\vec{A})$$

use $\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\vec{b} = \vec{a}\cdot\vec{b} + i\vec{\sigma}\cdot(\vec{a}\times\vec{b})$

$$[\vec{\sigma}\cdot\vec{A}, \vec{\sigma}\cdot\vec{E}] = 2i\vec{\sigma}\cdot(\vec{A}\times\vec{E})$$

$$[\vec{\sigma}\cdot\vec{p}, \vec{\sigma}\cdot\vec{E}] = -i\vec{\nabla}\cdot\vec{E} + i\vec{\sigma}\cdot(\vec{p}\times\vec{E}) - i\vec{\sigma}\cdot(\vec{E}\times\vec{p})$$

$$\vec{\sigma}\cdot(\vec{p}\times\vec{E})f = \varepsilon_{ijk}\sigma^i p^j E_k f$$

$$= -\vec{\sigma}\cdot(\vec{E}\times\vec{p})f + \frac{\sigma^i}{i}\left[\frac{\partial E_k}{\partial x^j} - \frac{\partial E_j}{\partial x^k}\right]f$$

But $E_k = -\frac{\partial\phi}{\partial x^k}$; $\therefore\ \vec{p}\times\vec{E} = -\vec{E}\times\vec{p}$

and

$$-ie[\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}] = -e[\vec{\nabla}\cdot\vec{E} + 2\vec{\sigma}\cdot(\vec{E}\times\vec{\pi})]$$

In similar fashion we calculate

$$\vec{\sigma}\cdot\vec{\pi}\,\vec{\sigma}\cdot\vec{\pi} = \vec{\pi}\cdot\vec{\pi} + i\vec{\sigma}\cdot(\vec{\pi}\times\vec{\pi})$$

$$\vec{\pi}\times\vec{\pi} = \frac{ei}{c}\vec{\nabla}\times\vec{A} = i\frac{e}{c}\vec{B}$$

Hence we obtain (to lowest order)

$$W\boxed{\ } = V'\boxed{\ } + \frac{1}{2M}(\vec{\pi}\cdot\vec{\pi})\boxed{\ } - \frac{e}{2M}\vec{\sigma}\cdot\vec{B}\boxed{\ } - \frac{(\vec{p}\cdot\vec{p})^2}{8M^3}\boxed{\ }$$

$$-\frac{e}{8M^2}\{\vec{\nabla}\cdot\vec{E} + 2\vec{\sigma}\cdot(\vec{E}\times\vec{\pi})\}\boxed{\ }$$

The individual terms can now be interpreted

- V' — ordinary potential energy
- $\frac{\vec{\pi}\cdot\vec{\pi}}{2M}$ — non-relativistic kinetic energy
- $-\frac{e}{2M}\vec{\sigma}\cdot\vec{B}$ — Pauli spin effect (magnetic moment $\frac{-e\vec{\sigma}}{2M}$ due to spin)
- $-\frac{(\vec{p}\cdot\vec{p})^2}{8M^2}$ — first relativistic correction to the kinetic energy

$$\left(\sqrt{p^2+M^2} = m\sqrt{1+p^2/m^2} = m\left[1 + \tfrac{1}{2}p^2/m^2 - \tfrac{1}{8}p^4/m^4 \cdots\right]\right.$$

We are left only with the term $\frac{-e}{2M}\left\{\frac{\vec{\nabla}\cdot\vec{E}}{4M} + \frac{\vec{\sigma}\cdot(\vec{E}\times\vec{\pi})}{2M}\right\}$ (A)

$\frac{\vec{p}-\frac{e}{c}\vec{A}}{m}$ is like $\vec{v}$

a particle in motion in an electric field sees a magnetic field

$$-\frac{\vec{v}\times\vec{E}}{c} = \vec{E}\times\frac{\vec{\pi}}{m}$$

Then the energy of interaction of the electron's spin magnetic moment with this field will be $-\frac{e}{2m}\frac{\vec{\sigma}\cdot(\vec{E}\times\vec{\pi})}{m}$

This looks like the term found above but differs from it by a factor of 2 (see below)

(Another way to get the same result is to recall that a moving magnetic moment produces an electric dipole moment of the form $-\vec{\mu}\times\vec{v}$ which then interacts with the electric field via $-(\vec{\mu}\times\vec{v})\cdot\vec{E}$)

Within an atom, the electric field of the nucleus has the form $\vec{r}/r^3$

Then $\vec{\sigma}\cdot(\vec{v}\times\vec{E}) \sim \frac{Ze^2}{4M^2}\frac{(\vec{r}\times\vec{p})\cdot\vec{\sigma}}{r^3}$

$\vec{r}\times\vec{p}=\vec{L}$, the orbital angular momentum

$\vec{L}\cdot\vec{\sigma}/r^3$ produces $\vec{L}\cdot\vec{\sigma}\left\langle 1/r^3\right\rangle$

$\vec{L}\cdot\vec{\sigma} = 2\vec{L}\cdot\vec{S} = j(j+1) - \ell(\ell+1) - s(s+1)$ splits apart energy levels of different j

$\vec{L}\cdot\vec{\sigma}$ is, however, 0 for L=0 states

But for $\vec{E} = Ze\vec{R}/r^3$, $\vec{\nabla}\cdot\vec{E} = 4\pi Ze\,\delta(r)$

This contributes only to s states (the only ones which are non-zero at the origin)

Thus the combination of terms in $\{\ \}$ can be thought of as a spin-orbit contribution, for every l.

Not all spin $\frac{1}{2}$ particles found in nature have magnetic moments equal to the Dirac moment $e/2m$. In fact only the electron and the muon appear to obey the unmodified Dirac equation (in any approximation). To account for these "anomalous" magnetic moments, an additional term is added to the original equation (Pauli's idea). Of course, you could add lots of different terms to the original equation and still have it remain Lorentz covariant, but it is conventional to choose a particular form which accounts for the observations (and introduces as few derivatives as possible. This second criterion will become reasonable in a month or two when we study various divergences)

The new equation is

$$\left[\not{p} - e\not{A} - \mu/2\, \sigma_{\mu\nu} F^{\mu\nu} - m\right]\psi = 0$$

where $\sigma_{\mu\nu} = \frac{i}{2}\left[\gamma^\mu, \gamma^\nu\right]$

$$F_{\mu\nu} = \frac{\partial}{\partial x_\mu} A_\nu - \frac{\partial}{\partial x_\nu} A_\mu$$

Figure out how to work this through to a non-relativistic equation and show that (up to a possible - sign)

$$w\boxed{\ } = V'\boxed{\ } + \frac{1}{2m}(\vec{\pi}\cdot\vec{\pi})\boxed{\ } + (\mu - e/2m)\vec{\sigma}\cdot\vec{B}\boxed{\ } - \frac{(\vec{p}\cdot\vec{p})^2}{8m^3}\boxed{\ }$$

$$+ \frac{1}{2}(\mu - e/4m)\{\vec{\nabla}\cdot\vec{E} + 2\vec{\sigma}\cdot(\vec{E}\times\vec{\pi})\}\boxed{\ }$$

This form shows that the factor of 2 which we previously had trouble with in the term is not really an overall multiplier. Rather there are two effects

$$\frac{1}{2}(\mu - e/2m)\{\ \} + \frac{1}{2}\frac{e}{4m}\{\ \}$$

This part was explained above

The second term is called the Thomas term. Its presence may be understood as follows:

We calculated the effect on the electron due to precession of the spin magnetic moment in the magnetic field seen instantaneously. This would be ok if the electron were an inertial frame. But it is constantly being accelerated by a force proportional to the charge. Thus we must correct for this (since the acceleration is not proportional to magnetic moment, we don't expect the correction term to involve μ).

The correction is actually calculated in the Ph 209 book. You might be able to find a dimpler and clearer explanation of the numbers on your own.

When the magnetic moments of the electron and muon are actually measured, they are found to be slightly different from $e/2m$. The discrepancy can, however, be completely accounted for by considering quantum effects of the electromagnetic field.

The anomalous magnetic moments of other spin $\frac{1}{2}$ particles are presumably due to their interactions with mesons. One way of looking at the situation is to say that the physical proton (neutron, lambda, etc.) is made up of an ideal Dirac proton plus a lot of mesons, which are continually being emitted and absorbed. These mesonic interactions alter the Dirac moment to its anomalous value. At present there is no good (i.e. precise) way to theoretically calculate anomalous moments

Ph 205c Week 2

Anomalous magnetic moment of the electron:

An electron is described by a wave-function ψ that satisfies the Dirac Equation:

$$\gamma_\mu (i D_\mu - e A_\mu)\psi = m\psi \quad \ldots\ldots\ldots \quad (1)$$

Where $A_\mu = A_\mu^{\text{total}}$ is made up of an external field $A_\mu^{\text{ext.}}$ together with A'_μ, the field due to the electron itself.

$$A_\mu = A_\mu^{\text{ext}} + A'_\mu$$

Classically, an electron trajectory satisfies $m \frac{d^2 x_\nu}{ds^2} = v_\mu F_{\mu\nu}$

where $F_{\mu\nu} = F_{\mu\nu}^{\text{ext.}} + F'_{\mu\nu}$

then $m \frac{d^2 x_\nu}{ds^2} - v_\mu F'_{\mu\nu} = v_\mu F_{\mu\nu}^{\text{ext.}}$

and the term $v_\mu F'_{\mu\nu}$ is called the force of radiation resistance

Equation (1) with $A_\mu = A_\mu^{\text{ext.}}$ is analogous to the classical equation in which the force of radiation resistance is neglected

If we put the full A_μ instead of $A_\mu^{\text{ext.}}$ into eq. (1) we expect to obtain the anomalous magnetic moment of the electron as a term in the non-relativistic ~~reduction of eq. (1)~~ hamiltonian derived from eq. (1). The term would look like

$$\frac{e}{2m} g \underset{\sim}{\sigma} \cdot \underset{\sim}{B}^{\text{ext}}$$

where the anomalous moment g is determined from the radiation resistance. The calculation of this quantity using standard techniques yields divergences which may be evaded by the method of "mass and charge renormalization."

One compares the calculated value of the anomalous moment with experiment by observing the hyperfine structure of the energy levels of atomic hydrogen. One also wants to correct for effects due to a space charge distribution within the proton when making the comparison.

There is no experiment today that absolutely requires a modification of the scheme outlined above.

Problems

(1) In the non-relativistic, hamiltonian reduction of the Dirac Equation with the Pauli term there appeared the term

$$\frac{e}{8m} \nabla \cdot E$$

which came mathematically from $[\sigma \cdot p, \sigma \cdot E]$.
Explain the physical origin of the term.

(2) For entertainment, you might try to examine the Dirac Equation in Hamiltonian form with

$$H_D = \underset{\sim}{\alpha} \cdot (\underset{\sim}{p} - e\underset{\sim}{A}) + \beta m$$

and using the operator equation of motion

$$\dot{O} = i[H, O] \text{ , evaluate } \dot{\underset{\sim}{x}} \text{ and } \dot{\underset{\sim}{p}}.$$

Find the velocity operator for the Dirac electron.

(3) How many different matrices can you make from products of α's and β. (The purpose of this exercise is to gain familiarity with the commutation laws).

Solutions to the Dirac Equation for a Free Particle

Let $\Psi = e^{-i(Et - p\cdot x)} \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$; $\psi = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$

Then with our choice of $\underset{\sim}{\alpha} = \begin{pmatrix} 0 & \underset{\sim}{\sigma} \\ \underset{\sim}{\sigma} & 0 \end{pmatrix}$, $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ the Dirac Equation becomes

$$(E+m)\psi_b = \sigma\cdot p\, \psi_a$$
$$(E-m)\psi_a = \sigma\cdot p\, \psi_b$$

$$(E^2 - m^2)\psi_a = (E+m)\sigma\cdot p\, \psi_b = \sigma\cdot p\,(E+m)\psi_b = \underset{\sim}{p}^2 \psi_a$$

so that $E^2 = m^2 + p^2$ or $\psi = 0$.

$$\Rightarrow E = \pm E_p \quad \text{where} \quad E_p = +\sqrt{p^2+m^2}.$$

A. For $E = E_p$ $\qquad \psi_b = \dfrac{\sigma\cdot p}{m+E_p}\psi_a$

Let us choose our axes so that p is in $\hat{z}$ direction.

Spin up (positive helicity) then $\sigma_z \psi_a = +\psi_a = \gamma\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\qquad$ γ = some number chosen for convenient normalization

$$\text{then } \psi_b = \frac{p\sigma_z}{m+E_p}\psi_a = \frac{\gamma p}{E_p+m}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Choosing the normalization $\psi^\dagger\psi = \psi_b^*\psi_b + \psi_a^*\psi_a = 1$

$$\text{we have } \gamma^{-1} = \sqrt{\frac{2E}{E+m}} \quad \text{or} \quad \gamma = \sqrt{\frac{E+m}{2E}}$$

$$\text{or} \quad \psi = \sqrt{\frac{E+m}{2E}}\begin{pmatrix} 1 \\ 0 \\ \frac{p}{E_p+m} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2E_p}}\begin{pmatrix} \sqrt{E_p+m} \\ 0 \\ \sqrt{E_p-m} \\ 0 \end{pmatrix}$$

Spin down (negative helicity) $\quad \sigma_z \psi_a = -\psi_a$

then $\sigma_z \psi_b = -\psi_b$

and $$\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} 0 \\ \sqrt{E_p+m} \\ 0 \\ -\sqrt{E_p+m} \end{pmatrix}$$

Now, if we want an eigenstate of σ_x instead of σ_z, we try $\quad \sigma_x \psi_a = \psi_a \qquad \psi_a = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

but then $\psi_b = \frac{p}{\sqrt{2}(E_p+m)}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ is not an eigenstate of σ_x.

This is because the operator $\begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}$ does not commute with the hamiltonian. Only the operator $\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$ commutes with H when the momentum is in the z direction.

The explicit form of the 4×4 matrices that represent the spin operators are $\begin{pmatrix} \underline{\sigma} & 0 \\ 0 & \underline{\sigma} \end{pmatrix}$ with our choice of $\underline{\alpha}$, β, and

more generally, $$\sigma_x = -i\alpha_y\alpha_z$$
$$\sigma_y = -i\alpha_z\alpha_x$$
$$\sigma_z = -i\alpha_x\alpha_y$$

Momentum in arbitrary direction

Suppose the spherical angles describing the direction of $\vec{p}$ relative to fixed coordinate axes are θ, ϕ. Then $\sigma\cdot p\, \psi_+ = p\, \psi_+$ where $\psi_+ = \begin{pmatrix} \cos\theta/2\, e^{-i\phi/2} \\ \sin\theta/2\, e^{i\phi/2} \end{pmatrix}$

Then $\psi_a = \psi_+$ and $\psi = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} \sqrt{E_p+m}\cos\theta/2\, e^{-i\phi/2} \\ \sqrt{E_p+m}\sin\theta/2\, e^{i\phi/2} \\ \sqrt{E_p-m}\cos\theta/2\, e^{i\phi/2} \\ \sqrt{E_p-m}\sin\theta/2\, e^{-i\phi/2} \end{pmatrix}$

(positive helicity spinor)

and negative helicity spinor is $\psi = \frac{1}{\sqrt{2E}} \begin{pmatrix} -\sqrt{E+m}\sin\theta/2\, e^{-i\phi/2} \\ +\sqrt{E+m}\cos\theta/2\, e^{i\phi/2} \\ +\sqrt{E-m}\sin\theta/2\, e^{-i\phi/2} \\ -\sqrt{E-m}\cos\theta/2\, e^{+i\phi/2} \end{pmatrix}$

B. For $E = -E_p$

let $\vec{p}$ be in $\hat{z}$ direction. For helicity $(h) = +$, $\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} -\sqrt{E_p-m} \\ 0 \\ \sqrt{E_p+m} \\ 0 \end{pmatrix}$

$h = -$, $\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} 0 \\ \sqrt{E_p-m} \\ 0 \\ \sqrt{E_p+m} \end{pmatrix}$

Dirac proposed that the negative energy states exist, but, in a "vacuum" are all filled with electrons. This invites the interesting possibility that a photon will excite an electron from a negative energy state to a positive energy state. The appearance of an electron with positive energy and the disappearance of an electron with negative energy from the negative-energy sea of electrons is physically the same as the creation of an electron and a positron, both with positive energy.

Example of the use of solutions of the Dirac Equation — Scattering in a Coulomb Potential (first Born approximation)

The scattering cross section 6 is given by

$$6 v_{in} = 2\pi\, 6(E_f - E_i)\, d^3 p_f \; |M|^2_{if}$$

$$\mathcal{M}_{fi} = \int \psi_f^* V(x)\, \psi_i(x)\, d^3x$$

$$\psi_f(x) = e^{i(\underset{\sim}{p}_2 \cdot \underset{\sim}{x} - E_p t)} u$$

$$\mathcal{M} = \int u_2^\dagger e^{i(\underset{\sim}{p}_1 - \underset{\sim}{p}_2)\cdot \underset{\sim}{x}} \frac{Ze^2}{r} u_1\, d^3x$$

$$= (u_2^\dagger u_1)\, \frac{4\pi Ze^2}{Q^2} \qquad \underset{\sim}{Q} = \underset{\sim}{p}_1 - \underset{\sim}{p}_2$$

$\delta(E_f - E_i)$ insures that $|\underset{\sim}{p}_1| = |\underset{\sim}{p}_2| = p$

then,

$$6\sigma_1 = 2\pi \frac{d\Omega}{(2\pi)^3} \int dp'\, \delta(\sqrt{p'^2+m^2} - \sqrt{p_1^2+m^2})\, p'^2 dp' \left(\frac{4\pi Ze^2}{Q^2}\right)^2 |u_2^\dagger u_1|^2$$

$$= (2\pi)^{-2} p\, (16\pi^2) \frac{Z^2e^4}{Q^4} E_p\, d\Omega\, |(u_2^\dagger u_1)|^2$$

$$\frac{6}{\sim}_1(\theta) = \frac{4Z^2e^4 (m^2+p^2) |(u_2^\dagger u_1)|^2}{16 p^4 \sin^4\theta/2}$$

We must still evaluate $u_2^\dagger u_1$.

There are 4 cases: $h = +$ $\longrightarrow$ $h=+$ or $h=-$

$h = -$ $\longrightarrow$ $h=+$ or $h=-$

u_1: $h=+$, $u_1 = \begin{pmatrix} \sqrt{E+m} \\ 0 \\ \sqrt{E-m} \\ 0 \end{pmatrix} \frac{1}{\sqrt{2E}}$, $h=-$, $u_1 = \frac{1}{\sqrt{2E}} \begin{pmatrix} 0 \\ \sqrt{E+m} \\ 0 \\ -\sqrt{E-m} \end{pmatrix}$

u_2: $h=+$, $u_2 = \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{E+m}\cos\theta/2 \\ \sqrt{E+m}\sin\theta/2 \\ \sqrt{E-m}\cos\theta/2 \\ \sqrt{E-m}\sin\theta/2 \end{pmatrix}$; $h=-$ $u_2 = \frac{1}{\sqrt{2E}} \begin{pmatrix} -\sqrt{E+m}\sin\theta/2 \\ \sqrt{E+m}\cos\theta/2 \\ \sqrt{E-m}\sin\theta/2 \\ -\sqrt{E-m}\cos\theta/2 \end{pmatrix}$

$h=+ \to h=+, \quad u_2^\dagger u_1 = \cos\theta/2$

$h=+ \to h=-, \quad u_2^\dagger u_1 = -\frac{m}{E}\sin\theta/2$

$h=- \to h=-, \quad u_2^\dagger u_1 = \cos\theta/2$

$h=- \to h=+, \quad u_2^\dagger u_1 = \frac{m}{E}\sin\theta/2$

If the helicity of the incoming electron is +, then the scattering cross section is

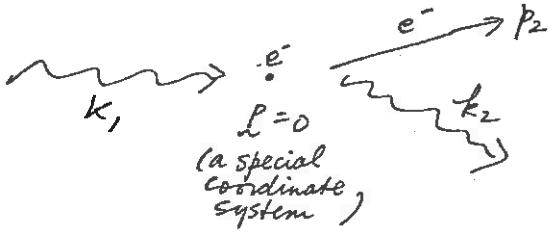
$$\frac{Z^2e^4\,(m^2+p^2)}{4p^4\sin^4\theta/2}\left(\cos^2\theta/2 + \frac{m^2}{E^2}\sin^2\theta/2\right)$$

$$= \frac{Z^2e^4}{4p^4\sin^4\theta/2}\underbrace{\left(E^2\cos^2\theta/2 + m^2\sin^2\theta/2\right)}_{=\,1+p^2\cos^2\theta/2}$$

The cross-section is the same with incoming electron of $h=-$, and also the same as the cross-section for scattering unpolarized electrons.

Problem: Calculate the cross-section for the Compton Effect using the solutions of the Dirac equation for a free particle and perturbation theory.

Compton effect: incoming photon k_1, incoming electron p_1 $\longrightarrow$ outgoing photon k_2, outgoing electron p_2



PH 205c

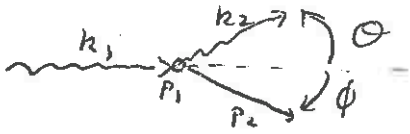
April 10,11,14

CALCULATION OF THE COMPTON EFFECT

$\gamma + e^- \to \gamma + e^-$

(notice that the process $\gamma + e^- \to e^-$ can't be a real process, because it is impossible to conserve energy and momentum. Hence Compton scattering is the simplest process involving electrons and photons)

Choose to work this in the lab system



(wiggly lines are photons; straight ones are electrons)

Write down all the 4 vectors (A_0, A_x, A_y, A_z) associated with the problem:

$p_1 = (m, 0, 0, 0)$

$k_1 = \omega_1 (1, 0, 0, 1)$

$k_2 = \omega_2 (1, \sin\theta, 0, \cos\theta)$

$p_2 = (E_2, -p_2 \sin\phi, 0, p_2 \cos\phi)$

Final state quantities are constrained by

$\vec{p}_1 + \vec{k}_1 = \vec{p}_2 + \vec{k}_2$ energy-momentum conservation

$\vec{p}_2^{\,2} = m^2 = (\vec{p}_1 + \vec{k}_1 - \vec{k}_2)^2 = m^2 + 2p_1 \cdot k - 2p_1 \cdot k_2 - 2k_1 \cdot k_2$

This gives the well known formula for change of ray frequency

$*$ $\qquad 1 - \cos\theta = \frac{m}{\omega_2} - \frac{m}{\omega_1}$

Must also consider the possible polarizations of the γ ray

$\perp$ plane of scattering $(0,0,1,0)$

possible for both e_1 and e_2

$\parallel$ plane of scattering

use $e \cdot k = 0$ to get possibilities

$e_1 = (0, 1, 0, 0)$

$e_2 = (0, \cos\theta, 0, -\sin\theta)$

The cross section formula we are about to derive was first obtained by Klein and Nishina. When they did it, it was considered a difficult and complicated problem; with the computational tricks to be taught in this course plus a little practice the average Ph 205 student will be able to complete problems of this

difficulty in less than $\frac{1}{2}$ hour.

Probability of transition/sec = $2\pi \delta(E_{out} - E_{in}) \frac{d^3k_2}{(2\pi)^3} |\mathcal{M}|^2$

(Notice: this formula always holds, relativistic kinematics or no relativistic kinematics. It is the change in the way you write E inside the δ function which changes the ultimate form for the phase space)

$H = \beta m + \vec{\alpha}\cdot(\vec{p} - e/c\,\vec{A}) = H_0 + H_{int}$; $H_{int} = -e/c\,\vec{\alpha}\cdot\vec{A}$

(notice that Dirac theory contains no $\vec{A}\cdot\vec{A}$ terms)

$\vec{A} = \sum_{i,k} \frac{1}{\sqrt{2\omega}} \left[a^i_k * \hat{e}^i_k e^{ik\cdot x} + a^i_k \hat{e}^i_k e^{-ik\cdot x} \right]$

↖ sum is over 2 different possible polarizations for each k

Since Compton scattering requires the annihilation of one photon and the creation of another, the first contribution in perturbation theory comes from second order.

$Prob/sec = 2\pi \delta(\sqrt{m^2 + (\vec{k}_1 - \vec{k}_2)^2} + \omega_2 - m - \omega_1) \frac{k_2^2 dk_2\, d\Omega_2}{(2\pi)^3} |\mathcal{M}|^2$

If we cancel the δ function against dk_2 we get an angular distribution for the emitted photons; if we cancel it against $d\Omega_2$ we get a frequency spectrum (these are of course related by *)

Generally one measures angular distributions.

use $\delta(f(x)) = \frac{\delta(x-a)\,dx}{|f'(a)|}$ if f=0 at x=a

Here $f(k_2) = \sqrt{m^2 + \omega_1^2 + \omega_2^2 - 2\omega_1\omega_2\cos\theta} + \omega_2 - m - \omega_1$

$f'(k_2) = \frac{\omega_2 - \omega_1\cos\theta}{E_2} + 1$

This must be evaluated at $\omega_2 = m + \omega_1 - E_2$

$f'(a) = \frac{\omega_1 m}{\omega_2 E_2}$

Thus

$Prob/sec = \sigma c = \frac{\omega_2^3 E_2}{m\omega_1 (2\pi)^2} d\Omega_2 |\mathcal{M}|^2 =$ cross section * relative velocity

where $E_2 = m + \omega_1 - \omega_2$ and $1 - \cos\theta = \frac{m}{\omega_2} - \frac{m}{\omega_1}$

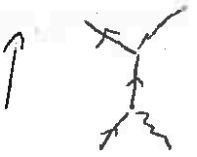
allow one to get the whole mess solely in terms of the angles and incident energy

Now for the matrix element! From first term we recall that there are two contributions to the second order matrix element

A: first annihilate γ_1, then create γ_2

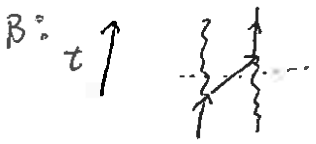
$\frac{\sqrt{2\omega_1 2\omega_2}}{e^2} A = \sum_i \frac{\langle 2 | \vec{\alpha}\cdot\hat{e}_2^* e^{-i\vec{k}_2\cdot\vec{x}} | i \rangle \langle i | \vec{\alpha}\cdot\hat{e}_1 e^{i\vec{k}_1\cdot\vec{x}} | 1 \rangle}{E_1 + \omega_1 - E_i}$

set $a_1 = \vec{\alpha}\cdot\hat{e}_1$, etc.

A: 

B: first create γ_2, then annihilate γ_1

$$\frac{\sqrt{w_1 w_2}}{e^2} B = \sum_j \frac{\langle 2|a_1 e^{i\vec{k}_1\cdot\vec{x}}|j\rangle\langle j|a_2 e^{-i\vec{k}_2\cdot\vec{x}}|1\rangle}{E_1 + w_1 - (E_j + w_1 + w_2)}$$

B: 

$|E_i| = \sqrt{p_i^2 + m^2}$, from the way we got the formula

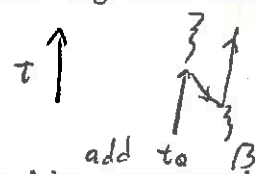
All that remains is to stick in the wave functions and get the numbers. Each electron wave function has the form $ue^{ip\cdot x}$, where u is a 4 component spinor. Everyone knows what to do with the $e^{ip\cdot x}$ pieces (integral over x just gives momentum conservation) so we forget about this for now and concentrate on the matrix part.

Each of the sums must be split into a sum over positive energy intermediate states and over negative energy states

$$A = \sum_{\substack{2\,\text{spins}\\ +\,\text{energy}}} \frac{\langle u_2|a_2|u_i\rangle\langle u_i|a_1|u_1\rangle}{E_1 + w_1 - |E_i| - i\varepsilon} + \sum_{\substack{2\,\text{spins}\\ -\,\text{energy}}} \frac{\langle u_2|a_2|u_i\rangle\langle u_i|a_1|u_1\rangle}{E_1 + w_1 + |E_i| - i\varepsilon}$$

$$B = \sum_{+\,\text{energy}} \frac{\langle u_2|a_1|u_j\rangle\langle u_j|a_2|u_1\rangle}{E_1 - w_2 - |E_j| - i\varepsilon} + \sum_{-\,\text{energy}} \frac{\langle u_2|a_1|u_j\rangle\langle u_j|a_2|u_1\rangle}{E_1 - w_2 + |E_j| - i\varepsilon}$$

Keep in mind that the states j have different momentum from those labelled i. Physically, however, we do not allow the possibility of negative energy states. We do have the new possibility of pair creation. This means we should eliminate all sums over negative energy states and add in terms for diagrams like



The idea expressed in terms of hole theory is as follows:

You can't knock an electron into a negative energy state, because they are full. However, a photon <u>can</u> excite an electron out of one of these states, leaving a hole in the sea. Then the next photon can make one of the electrons drop back into the negative energy state.

New term to be added to B has energy denominator

$$E_1 + w_1 - (E_1 + |E_k| + E_2) - i\varepsilon = -(E_1 - w_2 + |E_k|) - i\varepsilon$$

But overall contribution must be multiplied by a - sign relative to the first term in B because of the following argument

We should really put in our matrix element the grand wave function of all electrons in the world, even though the Hamiltonian acts only on one particular electron. The incident g.w.f. is the same for both pictures. But B_2 differs from B_1 in the final state, because in B_1 the final state is the same electron as initially whereas in B_2 the initial electron has been exchanged for one in the sea. The g.w.f. is totally antisymmetric under interchange of any two electrons.

qed

Hence the only overall change is in the sign of the $i\epsilon$ contribution to the denominator

$$\frac{\sqrt{2\omega_1 2\omega_2}}{e^2} A = \sum \frac{\langle u_2|\alpha_2|u_i\rangle\langle u_i|\alpha_1|u_1\rangle}{E_1+\omega_1-|E_i|-i\epsilon} + \sum \frac{\langle u_2|\alpha_2|u_i\rangle\langle u_i|\alpha_1|u_1\rangle}{E_1+\omega_1-|E_i|+i\epsilon}$$

$$\frac{\sqrt{2\omega_1 2\omega_2}}{e^2} B = \sum \frac{\langle u_2|\alpha_1|u_j\rangle\langle u_j|\alpha_2|u_1\rangle}{E_1-\omega_2-|E_j|-i\epsilon} + \sum \frac{\langle u_2|\alpha_1|u_j\rangle\langle u_j|\alpha_2|u_1\rangle}{E_1-\omega_2-|E_j|+i\epsilon}$$

When the arrow on the solid line is running backward in time you have a positron (hole)

It is possible (although difficult!) to do an experiment in which all the spins of incident and final particles are polarized. However, one must always sum over the spins of the internal states. When one contemplates just how many matrix elements have to be summed if the external particles are unpolarized, the problem that faced Klein and Nishina becomes quite clear.

Casimir invented an improvement to do the sum over intermediate states

$$\sum_i (u_2^* \alpha_2 u_i)(u_i^* \alpha_1 u_1) = \sum_i (v^*)_\alpha (u_i)_\alpha (u_i^*)_\beta (w)_\beta$$

$$= v^* \lambda^+ w$$

where

$$\lambda^+_{\alpha\beta} = \sum_{+\text{ energies}} (u_i)_\alpha (u_i^*)_\beta$$

Explicit computation with the u's shows that

$$\lambda^+ = \frac{1}{2E}\left[E + m\beta + \vec{\alpha}\cdot\vec{p}\right]$$

$$\lambda^- = \frac{1}{2|E|}\left[|E| - m\beta - \vec{\alpha}\cdot\vec{p}\right]$$

These can be obtained more simply:

$$\sum_{\text{all states}} u_i u_i^+ = \overleftrightarrow{1}$$

$$\sum_{+\text{ energies}} u_2^* \frac{N(H+|E_i|)}{2E_i} u_i u_i^* M u_1 = \sum_{\text{all energies}} u_2^* \frac{N(H+|E_i|)}{2E_i} u_i u_i^* M u_1$$

$$= u_2^* \frac{N(H+|E_i|)}{2E_i} M u_1$$

Likewise $\lambda^- = \frac{H - |E_i|}{2E_i} = \frac{|E_i| - H}{2|E_i|}$

We thus see that any summover positive energy intermediate states is got by inserting λ^+; similarly for λ^- and negative energy intermediate states.

Hence we have

$$A = \frac{u_2^* \alpha_2 (|E_i| + m\beta + \vec{\alpha}\cdot\vec{p}_i)\alpha_1 u_1}{2|E_i|(E_1 + \omega_1 - |E_i|)} + \frac{u_2^* \alpha_2 (|E_i| - m\beta - \vec{\alpha}\cdot\vec{p}_i)\alpha_1 u_1}{2|E_i|(E_1 + \omega_1 + |E_i|)}$$

$$= \frac{u_2^* \alpha_2 \{E_1 + \omega_1 + m\beta + \vec{\alpha}\cdot(\vec{p}_1 + \vec{k}_1)\}\alpha_1 u_1}{(E_1 + \omega_1)^2 - (\vec{p}_1 + \vec{k}_1)^2 - m^2} = \frac{u_2^* \alpha_2 [\not{p}_1 + \not{k}_1 + M]\beta\alpha_1 u_1}{(\vec{p}_1 + \vec{k}_1)^2 - m^2}$$

Define $u^*\beta = \bar{u}$

Thus if $u^* = (u_1^*, u_2^*, u_3^*, u_4^*)$ then $\bar{u} = (u_1^*, u_2^*, -u_3^*, -u_4^*)$

The final form for our A matrix element is then

$$\frac{\bar{u}_2 \not{\varepsilon}_2 (\not{p}_1 + \not{k}_1 + M) \not{\varepsilon}_1 u_1}{(p_1 + k_1)^2 - m^2}$$

Likewise B is

$$\frac{\bar{u}_2 \not{\varepsilon}_1 (\not{p}_1 - \not{k}_2 + M) \not{\varepsilon}_2 u_1}{(p_1 - k_2)^2 - m^2}$$

Feynman's contribution was to arrive at this stage and then figure out rules by which you could write these answers down without going through all the intermediate steps.

Aside #1: Effect of two time inversions on a spin J system

$$T^2 |J = n + 1/2\rangle = -1 |\ \rangle \qquad (n \in +\text{integer})$$
$$T^2 |J = n\rangle = +1 |\ \rangle$$

How to find answer:

from elementary q. mech.

a) $T|J, m\rangle = \text{phase}\ |J, -m\rangle$

b) $T(\alpha|1\rangle + \beta|2\rangle) = \alpha^* T|1\rangle + \beta^* T|2\rangle$

c) Integral spin, mass $\neq 0 \Rightarrow \exists$ state $\ni S_z = 0$

$T|0\rangle = e^{i\delta}|0\rangle$

$T^2|0\rangle = e^{-i\delta} T|0\rangle = |0\rangle$

d) Half integral spin

$T|+\rangle = e^{i\delta}|-\rangle \qquad T|-\rangle = e^{i\delta'}|+\rangle$

$\frac{1}{\sqrt{2}} T[|+\rangle + |-\rangle]$ must be spin down in x direction

$$= \frac{e^{i\phi}}{\sqrt{2}}[|+\rangle - |-\rangle] = \frac{1}{\sqrt{2}}[e^{i\delta}|-\rangle + e^{i\delta'}|+\rangle]$$

$$= \frac{1}{\sqrt{2}} e^{i\delta'}[|+\rangle + e^{i(\delta - \delta')}|-\rangle]$$

$$\Rightarrow e^{i(\delta - \delta')} = -1$$

$T^2|+\rangle = T(e^{i\delta}|-\rangle) = e^{-i\delta}e^{i\delta}|+\rangle = -|+\rangle$

Aside #2: Because the electron has only two possible helicities, it should be possible to describe it by just a 2 component wave function, rather than a 4 component one. One way to do this is to start with the two component wave function for an electron at rest and then transform it to the desired momentum.

For a state at rest $|0,i\rangle$ where i describes the spin state

$$e^{i\upsilon N_x}|0,i\rangle = |m\sinh\upsilon, 0, 0; i\rangle = |3\ \text{momentum}; i\rangle$$

The general "boost" operator has the form $e^{i\upsilon\vec{N}\cdot\vec{a}}$

Other operators work as expected

$$P_z|p_x,p_y,p_z;i\rangle = p_z|p_x,p_y,p_z;i\rangle$$

$$\tanh\upsilon = p/E \qquad \sinh\upsilon = p/m$$

defines the parameter v for the transformation

$$P_t|0;i\rangle = m|0;i\rangle$$

The operator $P_t^2 - P_x^2 - P_y^2 - P_z^2$ is an invariant for a given representation

Hence every state can be described in terms of a momentum and a spin state at rest.

The generators of the transformation can be written

$$J_z = i\left[p_x\frac{\partial}{\partial p_y} - p_y\frac{\partial}{\partial p_x}\right] + j_z \longrightarrow (\text{intrinsic spin})$$

$$N_z = i\left[p_z\frac{\partial}{\partial p_x} - p_x\frac{\partial}{\partial p_z}\right] + \left[\frac{\vec{J}\times\vec{p}}{E+m}\right]_z$$

The most general wave function can then be written in the form

$$|\psi\rangle = \sum_p \left(a_{p+}|p^+\rangle + a_{p-}|p^-\rangle\right)$$

and the most general scattering operator can be put as

$$f(p_1,p_2) + \vec{\sigma}\cdot\vec{\vec{F}}(\vec{p}_1,\vec{p}_2)$$

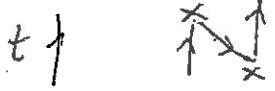
For fun, figure out from conventional theory and/or this theory why the two component scattering amplitude operator in a scalar potential would take the form

$$\frac{(E_1+m)(E_2+m) - \vec{p}_1\cdot\vec{p}_2 + i\vec{\sigma}\cdot(\vec{p}_1\times\vec{p}_2)}{\sqrt{2m(E_1+m)\ 2m(E_2+m)}}$$

and in a pseudoscalar potential would look like

$$\frac{\vec{\sigma}\cdot\vec{p}_1(E_2+m) - \vec{\sigma}\cdot\vec{p}_2(E_1+m)}{\sqrt{2m(E_1+m)\ 2m(E_2+m)}}$$

Question: If you scatter twice in a scalar potential according to the graph



can you prove from the amplitude resulting that electron and positron must have opposite intrinsic parity?

Week 4 - Part II Ph 205c

Differential cross-section for Compton Scattering in lab ($\vec{p}_1 = 0$):

$$d\sigma = \frac{1}{16 m E_2 \omega_1 \omega_2} \frac{1}{(2\pi)^2} |M|^2 \omega_2^2 \frac{E_2 \, d\Omega}{m + 2\omega \sin^2\theta/2} \quad ; \quad d\Omega = d\Omega_\theta = \text{solid angle of outgoing photon.}$$

$$= \frac{d\Omega}{64\pi^2} \frac{\omega_2}{m\omega_1} \frac{|M|^2}{m + 2\omega \sin^2\theta/2}$$

ω_1 = energy of incoming γ
ω_2 = energy of outgoing γ
E_2 = energy of outgoing e^-

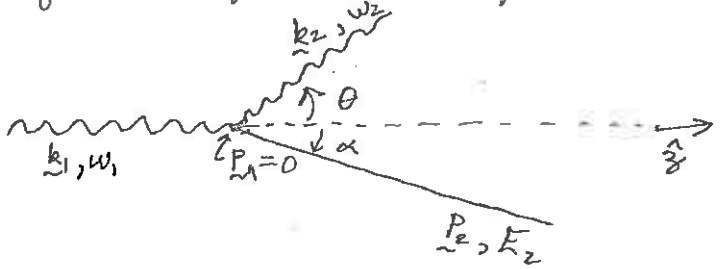
From kinematics, $\frac{\omega_2}{\omega_1} = \frac{m}{m + 2\omega \sin^2\theta/2}$

$$\therefore \quad \left.\frac{d\sigma}{d\Omega}\right]_{lab} = \frac{1}{64\pi^2} \frac{|M|^2}{m^2} \frac{\omega_2^2}{\omega_1^2} \qquad \cdots (1)$$

This cross-section refers to a definite process in which the initial and final states are completely ~~specified~~ defined "pure" states.

Now there are 2 possible helicities for the electron in the initial state, as well as 2 possible helicites for the electron in the final stake. In addition, there are 2 possible polarization states for the photon in both the initial and final states. There are, therefore, 16 polarized differential amplitudes M that occur in Compton scattering.

Kinematics of scattering in the lab system



Initial state spinors (Recall: normalization is 2E particles/unit volume)

$$u_1 = u_{1+} = \sqrt{2m} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{or} \quad u_1 = u_- = \sqrt{2m} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Final state spinors:

$$u_2 = u_{2+} = \begin{pmatrix} \sqrt{E+m}\cos\alpha/2 \\ -\sqrt{E+m}\sin\alpha/2 \\ \sqrt{E-m}\cos\alpha/2 \\ -\sqrt{E-m}\sin\alpha/2 \end{pmatrix}, \quad \text{or} \quad u_2 = u_{2-} = \begin{pmatrix} \sqrt{E+m}\sin\alpha/2 \\ \sqrt{E+m}\cos\alpha/2 \\ -\sqrt{E-m}\sin\alpha/2 \\ -\sqrt{E-m}\cos\alpha/2 \end{pmatrix}$$

$$\bar{u}_{2-} = \left(\sqrt{E+m}\,\delta, \sqrt{E+m}\,\Gamma, \sqrt{E-m}\,\delta, \sqrt{E-m}\,\Gamma\right)$$

$$\bar{u}_{2+} = \left(\sqrt{E+m}\,\Gamma, -\sqrt{E+m}\,\delta, -\sqrt{E-m}\,\Gamma, \sqrt{E-m}\,\delta\right)$$

where $\boxed{\delta = \sin\alpha/2 \quad \Gamma = \cos\alpha/2}$

There are 2 possibilities for e_1, the polarization of the incoming γ

(i) polarized in plane of scattering, $e_1 = (1, 0, 0; 0) = e_{1a}$ (x, y, z; t)

(ii) polarized perpendicular to plane of scattering $e_1 = (0, 1, 0; 0) = e_{1b}$

similarly for e_2:

(i) in plane of scattering $e_2 = (\cos\theta, 0, -\sin\theta; 0) = e_{2a}$

(ii) perpendicular to the plane of scatt., $e_2 = (0, 1, 0; 0) = e_{2b}$

Now we carry out the computation of $\mathcal{M}$ for the 16 different processes:

In each case, we have

$$\frac{\mathcal{M}}{4\pi e^2} = \frac{\bar{u}_2 \not{e}_2 (\not{p}_1 + \not{k}_1 + m) \not{e}_1 u_1}{(p_1 + k_1)^2 - m^2} + \frac{\bar{u}_2 \not{e}_1 (\not{p}_1 - \not{k}_2 + m) \not{e}_2 u_1}{(p_1 - k_2)^2 - m^2}$$

$$= \bar{u}_2 \left(\frac{\not{e}_2 \not{k}_1 \not{e}_1}{2m\omega_1} + \frac{\not{e}_1 \not{k}_2 \not{e}_2}{2m\omega_2} \right) u_1$$

since $\not{p}_1 \not{e}_1 = -\not{e}_1 \not{p}_1$

$\not{p}_1 \not{e}_2 = -\not{e}_2 \not{p}_1$

$$\not{k}_1 = \omega_1 (\gamma_t - \gamma_z)$$

$$\not{k}_2 = \omega_2 (\gamma_t - \gamma_z \cos\theta - \gamma_x \sin\theta)$$

Case 1: $u_1 = u_{1+}$ $\quad u_2 = u_{2+}$
$e_1 = e_{1a}$ $\quad e_2 = e_{2a}$

$C = \cos\theta$
$S = \sin\theta$

Then $-\not{e}_1 = \not{\gamma}_x \quad = x$
$-\not{e}_2 = \not{\gamma}_x C - \not{\gamma}_z S \quad = xC - zS$

according to the abbreviations:

$\not{\gamma}_x \to x$
$\not{\gamma}_y \to y$
$\not{\gamma}_z \to z$
$\not{\gamma}_t \to t$

Then $M_1 \times \frac{2m}{4\pi e^2} = \bar{u}_2 \left[(xC - zS)(t - z) x + x (t - zC - xS)(xC - zS) \right] u_1$

$= \bar{u}_2 \left[tC - zC - txzS - xS + tC + txzS - zC^2 - xzCS + xzCS - zS^2 \right] u_1$

where repeated use has been made of the commutation rules for the γ's: $xt + tx = 0$

$x^2 = -1$, etc.

$= \bar{u}_2 \left[2tC - xS - z(1+C) \right] u_1$

To evaluate $[2tC - xS - z(1+C)]u_1$, we make use of the table of γ-matrices on page 4.

Obtain $M_1 \times \frac{2m}{4\pi e^2} = \bar{u}_2 \begin{pmatrix} 2C \\ 0 \\ 1+C \\ S \end{pmatrix} \sqrt{2m} = \sqrt{2m} \begin{pmatrix} \sqrt{E+m}\,\Gamma, & -\sqrt{E+m}\,\sigma, & -\sqrt{E-m}\,\Gamma, & \sqrt{E-m}\,\sigma \end{pmatrix} \begin{pmatrix} 2C \\ 0 \\ 1+C \\ S \end{pmatrix}$

$M_1 \frac{\sqrt{2m}}{4\pi e^2} = 2\sqrt{E+m}\, C\Gamma + \sqrt{E-m}\,(\sigma S - \Gamma C) - \Gamma\sqrt{E-m}$

$= 2\sqrt{E+m}\cos\theta\cos\alpha/2 - \sqrt{E-m}\cos(\theta + \alpha/2) - \sqrt{E-m}\cos\alpha/2$

or, $M_1 = \frac{4\pi e^2}{\sqrt{2m}} \left(2\sqrt{E+m}\cos\theta\cos\alpha/2 - \sqrt{E-m}\cos(\theta+\alpha/2) - \sqrt{E-m}\cos\alpha/2 \right)$

Table of Independent γ-matrices :

We write this out in a particular representation defined by

$$\underset{\sim}{\alpha} = \begin{pmatrix} 0 & \underset{\sim}{\sigma} \\ \underset{\sim}{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Then $\underset{\sim}{\gamma} = \beta\underset{\sim}{\alpha} = \begin{pmatrix} 0 & \underset{\sim}{\sigma} \\ -\underset{\sim}{\sigma} & 0 \end{pmatrix}$ $\qquad \gamma_t = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\gamma_x\gamma_y = -i\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$$

$$\gamma_y\gamma_z = \begin{pmatrix} -i\sigma_x & 0 \\ 0 & -i\sigma_x \end{pmatrix} \qquad \gamma_5 = \gamma_x\gamma_y\gamma_z\gamma_t = +i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\gamma_z\gamma_x = \begin{pmatrix} -i\sigma_y & 0 \\ 0 & -i\sigma_y \end{pmatrix}$$

$$\gamma_t\gamma_x = \alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$$

$$\gamma_t\gamma_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}$$

$$\gamma_t\gamma_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}$$

$$\gamma_5\gamma_x = \begin{pmatrix} -i\sigma_x & 0 \\ 0 & i\sigma_x \end{pmatrix} = \gamma_t\gamma_y\gamma_z$$

$$\gamma_5\gamma_y = \begin{pmatrix} -i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix} = \gamma_t\gamma_z\gamma_x$$

$$\gamma_5\gamma_z = \begin{pmatrix} -i\sigma_z & 0 \\ 0 & i\sigma_z \end{pmatrix} = \gamma_t\gamma_x\gamma_y$$

$$\gamma_5\gamma_t = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix} = \gamma_x\gamma_y\gamma_z$$

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

2. $u_{1+} \longrightarrow u_{2+}$ $\quad -\not{q} = \gamma_x$
$e_{1a} \longrightarrow e_{2b}$ $\quad -\not{q}_2 = \gamma_y$

$$\mathcal{M}_2 \times \frac{2m}{4\pi e^2} = \bar{u}_2 \{ y(t-z)x + x(t-zC-xS)y \} u_1$$

$$= \bar{u}_2 \{ \cancel{txy} - xyz - \cancel{txy} + xyzC + yS \} u_1$$

$$= \sqrt{2m}\,\bar{u}_2 \begin{pmatrix} 0 \\ 0 \\ i(C-1) \\ -iS \end{pmatrix} = i\sqrt{E+m}\{\Gamma - \Gamma C - GS\}$$

$$\mathcal{M}_2 \frac{\sqrt{2m}}{4\pi e^2} = i\sqrt{E-m}\{\cos\alpha/2 - \cos(\theta - \alpha/2)\}$$

3. $u_{1+} \longrightarrow u_{2-}$ $\quad -\not{q}_1 = \gamma_x$
$e_1 = e_{1a} \longrightarrow e_2 = e_{2a}$ $\quad -\not{q}_2 = \gamma_x C - \gamma_z S$

$$\mathcal{M}_3 \frac{2m}{4\pi e^2} = \bar{u}_2 \{ (xC - zS)(t-z)x + x(t-zC-xS)(xC-zS) \} u_1$$

$$= \bar{u}_2 \{ tC - zC - txzS - xS + tC - zC^2 + xCS + txzS \\ - xCS - zS^2 \} u_1$$

$$= \bar{u}_2 (2tC - z - zC - xS) u_1$$

$$\mathcal{M}_3 \frac{\sqrt{2m}}{4\pi e^2} = \bar{u}_2 \begin{pmatrix} 2C \\ 0 \\ 1+C \\ S \end{pmatrix} = \{ 2\sqrt{E+m}\cos\theta \sin\alpha/2 + \sqrt{E-m}\sin(\theta + \alpha/2) + \sqrt{E-m}\sin\alpha/2 \}$$

4. $u_{1+} \longrightarrow u_{2-}$
$e_{1a} \longrightarrow e_{2b}$, as in case 2, $\mathcal{M} \times \frac{2m}{4\pi e^2} = \bar{u}_2 (xyz(C-1) + yS) u_1$

$$\mathcal{M} \frac{\sqrt{2m}}{4\pi e^2} = -i\sqrt{E-m}\{\sin(\theta - \alpha/2) + \sin\alpha/2\}$$

5. $u_{1-} \longrightarrow u_{2-}$
$e_{1a} \longrightarrow e_{2a}$

$$\mathcal{M}_5 \frac{\sqrt{2m}}{4\pi e^2} = \{ 2\sqrt{E+m}\cos\theta\cos\alpha/2 - \sqrt{E-m}\cos(\theta + \alpha/2) - \sqrt{E-m}\cos\alpha/2 \}$$

Notice that $M_5 = M_1$. This can be seen to be a consequence of the invariance of the coupling $j_\mu A_\mu$ under the parity transformation P.

Under P, $\vec{S}$ (spin), like $\vec{l}$ (orbital ang. mom.) is invariant. $\vec{p}$, however, changes sign, so $\vec{S}\cdot\vec{p}$ also changes sign and we have the result that the helicity of an electron changes sign under parity.

From the form of the amplitude, it is obvious that reversing the directions of polarization of both photons leaves the lowest order amplitude invariant.

Putting these together, we see that

$$M_1\begin{pmatrix} u_{1+}\to u_{2+} \\ e_{1a}\to e_{2a}\end{pmatrix} = M\begin{pmatrix} u_{1-}\to u_{2-} \\ -e_{1a}\to -e_{2a}\end{pmatrix} = M_5\begin{pmatrix} u_{1-}\to u_{2-} \\ e_{1a}\to e_{2a}\end{pmatrix}$$

Similarly, $$M_6\begin{pmatrix} u_{1-}\to u_{2-} \\ e_{1a}\to e_{2b}\end{pmatrix} = M_2\begin{pmatrix} u_{1+}\to u_{2+} \\ e_{1a}\to e_{2b}\end{pmatrix}$$

$$M_7\begin{pmatrix} u_{1-}\to u_{2+} \\ e_{1a}\to e_{2a}\end{pmatrix} = M_3\begin{pmatrix} u_{1+}\to u_{2-} \\ e_{1a}\to e_{2a}\end{pmatrix}$$

$$M_8\begin{pmatrix} u_{1-}\to u_{2+} \\ e_{1a}\to e_{2b}\end{pmatrix} = M_4\begin{pmatrix} u_{1+}\to u_{2-} \\ e_{1a}\to e_{2b}\end{pmatrix}$$

9. $\quad u_{1+}\to u_{2+} \qquad -\phi_1 = \gamma_y$
$\quad e_{1b}\to e_{2b} \qquad -\phi_2 = \gamma_4$

$$M_9\,\frac{\sqrt{2m}}{4\pi e^2} = \left\{2\sqrt{E+m}\cos\alpha/2 - \sqrt{E-m}\cos\alpha/2 - \sqrt{E-m}\cos(\theta+\alpha/2)\right\}$$

10. $\quad u_{1+}\to u_{2+} \qquad -\phi_1 = y$
$\quad e_{1b}\to e_{2a} \qquad -\phi_2 = xC - zS$

$$M_{10}\,\frac{\sqrt{2m}}{4\pi e^2} = \frac{1}{\sqrt{2m}}\,\bar{u}_2\,(xyzC - yS - xyz)\,u_1 = i\sqrt{E-m}\left(\cos\alpha/2 - \cos(\theta+\alpha/2)\right)$$

11. $u_{1-} \to u_{2-}$
$e_{1b} \to e_{2b}$ By parity $M_{11} = M_9$

12. $u_{1-} \to u_{2-}$
$e_{1b} \to e_{2a}$ By parity $M_{12} = M_{10}$

13. $u_{1+} \to u_{2-}$
$e_{1b} \to e_{2b}$

14. $u_{1-} \to u_{2+}$
$e_{1b} \to e_{2b}$

$$M_{13} = M_{14}$$

$$\frac{\sqrt{2m}}{4\pi e^2} M_{13} = 2\sqrt{E+m}\sin\alpha/2 + \sqrt{E-m}\sin\alpha/2 + \sqrt{E-m}\sin(\theta+\alpha/2)$$

15. $u_{1+} \to u_{2-}$
$e_{1b} \to e_{2a}$

16. $u_{1-} \to u_{2+}$
$e_{1b} \to e_{2a}$

$$M_{15} = M_{16}$$

$$\frac{\sqrt{2m}}{4\pi e^2} M_{15} = \frac{1}{\sqrt{2m}} \bar{u}_2 (xyzC - yS - xyz) u_1 \qquad (\text{same form as } 10.)$$

~~$= i\sqrt{E-m}(\cos\alpha/2 - \cos(\theta+\alpha/2))$~~

$$= i\left(\sqrt{E+m}\sin(\theta+\alpha/2) - \sqrt{E-m}\sin\alpha/2\right)$$

The various polarized cross sections are obtained by the replacement $M \to M_k$, $k = 1, 2, \ldots 16$ in Equation (1).

PH 205c

April 24,25,28

In this section we will work out the matrix elements from standard nonrelativistic perturbation theory, using all the field theory learned to date. Despite the fact that none of the intermediate steps look relativistically invariant, the answer will appear in a relativistically invariant form. We will then formulate rules for writing down the relativistically invariant form at once from the diagrams, and will never again work through the mess that is displayed below.

$$\mathcal{H} = \underbrace{\frac{1}{8\pi}\int (E^2+B^2)\,d(vol)}_{\text{Energy of Free Electromagnetic Field}} + \int \psi^*(x)\left[\beta m + e\phi(x) + \vec{\alpha}\cdot\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}\right)\right]\psi(x)\,d^3x$$

where the ψ's are operators which create and annihilate electrons

This may be broken down further into the energy of the free electron-positron field $\int \psi^*(x)\left[\beta m + \vec{\alpha}\cdot\frac{\hbar}{i}\vec{\nabla}\right]\psi(x)\,d^3x$

and a term which represents the interaction between the electric field and the matter fields $e\int \psi^*(x)\left[\phi(x) - \vec{\alpha}\cdot\vec{A}\right]\psi(x)\,d^3x = \int j_\mu(x) A_\mu(x)\,d^3x$

where $j_\mu = e\,\psi^*\beta\gamma_\mu\psi = e\,\overline{\psi}(x)\,\gamma_\mu\,\psi(x)$

and it is important to keep in mind that each of ψ, ψ^*, A_μ is linear in the appropriate creation operators.

Now we ruin the manifest covariance in order to relate pieces to previously learned physics.

Choose a gauge such that $\vec{\nabla}\cdot\vec{A} = 0$, $\nabla^2\phi = \rho$

(a point charge has $\phi(r') = \frac{e}{d} = \int \frac{\rho(r)\,d^3r}{|r'-r|}$

$j_0(x) = \rho = e\,\psi^*(x)\psi(x)$

Thus the $e\int \psi^*\phi(x)\,\psi(x)\,d^3x$ term can be written

$$\frac{e^2}{2}\int \frac{\psi^*(x)\psi(x)\,\psi^*(y)\psi(y)\,d^3x\,d^3y}{r_{xy}} \quad \text{up to } \infty$$

and we have managed to express this piece of the interaction without use of photon creation and annihilation operators. The ∞ mentioned above comes from the δ function in the anti-commutation relations for $\psi^*(x)$ and $\psi(y)$. It is a self energy term, of the type discussed before in this course. The thing to notice here is that this infinity seems to involve only spatial coordinates and

thus is not obviously relativistically covariant (in another system the self energy subtracted might be different). This was one of the difficulties of formulating the theory this way. Later on in this course the removal of certain relativistically covariant infinities will be discussed.

Then the interaction of the electron-positron field with photons is given by $-e \int \psi^*(x)\, \vec{\alpha}\, \psi(x) \cdot \vec{A}(x)\, d^3x$

where $\vec{A}(x) = \sum_{i,\kappa} \sqrt{\frac{4\pi}{2\omega_\kappa}} \left[\vec{e}_{i,\kappa}\, a_{\kappa i}\, e^{ik\cdot x} + \vec{e}^{\,*}_{i,\kappa}\, a^*_{\kappa i}\, e^{-ik\cdot x} \right]$

where $\vec{e}_{i,\kappa}$ is the polarization vector for a photon of polarization type i (helicity ± 1) and $\psi(x) = \sum_{p,\ell} u_{p,\ell}\, c_{p,\ell}\, e^{ip\cdot x}$

$u_{p,\ell}$ is a 4 component spinor for a solution of the Dirac equation of momentum p, type ℓ (ℓ runs over 4 possibilities - positive energy spin up and spin down, and negative energy spin up and spin down)

$$(\beta m + \vec{\alpha}\cdot\vec{p})\, u_{p,\ell} = \mathcal{E}\, u_{p,\ell}$$

$\mathcal{E} = +E_+ = \sqrt{m^2+p^2}$ or $\mathcal{E} = -E_+ = -\sqrt{m^2+p^2}$

Likewise $\psi^* = \sum_{p,\ell} c^*_{p,\ell}\, u^*_{p,\ell}\, e^{-ip\cdot x}$

Change notation:

let $u_{p\kappa}$ stand for those solutions such that $\mathcal{E} = +E_{p,\kappa}$

where κ is a spin index with two possible values

$v_{pj} = u_{-p\ell}$ for those solutions with $\mathcal{E} = -E_p$

Then we have $(\beta m + \vec{\alpha}\cdot\vec{p})\, u_{p\kappa} = E_p\, u_{p\kappa}$

$$(\beta m - \vec{\alpha}\cdot\vec{p})\, v_{pj} = -E_p\, v_{pj}$$

And the free Hamiltonian takes the form

$$H_{el,pos} = \sum_{p,\ell} \mathcal{E}_p\, c^*_{p,\ell}\, c_{p,\ell} = \sum_{p,\kappa} E_p \left[c^*_{p\kappa}\, c_{p\kappa} - c^*_{pj}\, c_{pj} \right]$$

where $c_{p'\ell'}\, c^*_{p\ell} + c^*_{p\ell}\, c_{p'\ell'} = \delta_{pp'}\, \delta_{\ell\ell'}$

In accordance with our new terminology for the spinors, define a new terminology for the annihilation operators of negative energy states

If $c_{p\kappa}$ annihilates an electron of momentum p, spin type k, then $c_{pj} = d^\dagger_{-pj}$ creates a positron with momentum -p.

Then $H_{free} = \sum E_p \left[c^*_{p\kappa}\, c_{p\kappa} + d^*_{p\kappa}\, d_{p\kappa} \right] - \underbrace{\sum E_p}_{\text{another } p}$

This is the energy of the full sea of negative energy states. We measure relative energies away from it.

Now $\psi = \sum_{p,\kappa} \left[c_{p,\kappa}\, u_{p\kappa}\, e^{i p\cdot x} + d^*_{p\kappa}\, v_{p\kappa}\, e^{-ip\cdot x} \right]$

notice that creation of positron in initial state (i.e. annihilation of positron in final state) gives a column vector $v_{p\kappa}$ whereas annihilation of electron in final state (by ψ^*) gives a row vector $\bar{u}_{p\kappa}$

Hence a positron in the initial state leads to $\bar{v}$ on the left side of the matrix element, whereas an electron in the initial state leads to u on the right side of the matrix element.

Use this to expand out the interaction Hamiltonian

$$-e \int \psi^*(x)\, \vec{\alpha}\, \psi(x) \cdot \vec{A}(x)\, d^3x$$

$$\vec{A} = \sum \sqrt{\frac{4\pi}{2\omega_\kappa}} \left[\vec{e}_{i\kappa}\, a_{\kappa i}\, e^{ik\cdot x} + \vec{e}^{\,*}_{i\kappa}\, a^*_{\kappa i}\, e^{-ik\cdot x} \right]$$

$$\psi = \sum \left[c_{p\kappa}\, u_{p\kappa}\, e^{ip\cdot x} + d^*_{p\kappa}\, v_{p\kappa}\, e^{-ip\cdot x} \right]$$

to obtain

$$\sum_{\text{all}} -e \sqrt{\frac{4\pi}{2\omega_\kappa}} \int \left[c^*_{p_1} u^*_{p_1} e^{-ip\cdot x} + d_{p_1} v^*_{p_1} e^{ip\cdot x} \right] \left[\vec{e}_{i\kappa}\cdot\vec{\alpha}\, a_{\kappa i}\, e^{ik\cdot x} + \vec{e}^{\,*}_{i\kappa}\cdot\vec{\alpha}\, a^*_{\kappa i}\, e^{-ik\cdot x} \right] \times \left[c_{p'_1} u_{p'_1} e^{ip'\cdot x} + d^*_{p'_1} v_{p'_1} e^{-ip'\cdot x} \right]$$

In every case the spatial integration will give only a δ function of the momenta (because the exponentials are the only functions of x present)

We then obtain a sum of the following pieces:

$$\sqrt{\frac{4\pi e^2}{2\omega_\kappa}}\; c^*_{p_1}\, a_{\kappa i}\, c_{p'_1}\; u^*_{p_1}\, \vec{e}_{i\kappa}\cdot\vec{\alpha}\, u_{p'_1}\, \delta(-p+\kappa+p')$$

$$\sqrt{\frac{4\pi e^2}{2\omega_\kappa}}\; c^*_{p_1}\, a_{\kappa i}\, d^*_{p'_1}\; u^*_{p_1}\, \vec{e}_{i\kappa}\cdot\vec{\alpha}\, v_{p'_1}\, \delta(-p+k-p')$$

$$\sqrt{\frac{4\pi e^2}{2\omega_\kappa}}\; c^*_{p_1}\, a^*_{\kappa i}\, c_{p'_1}\; u^*_{p_1}\, \vec{e}^{\,*}_{i\kappa}\cdot\vec{\alpha}\, u_{p'_1}\, \delta(p+k-p')$$

$$\sqrt{\frac{4\pi e^2}{2\omega_\kappa}}\; c^*_{p_1}\, a^*_{\kappa i}\, d^*_{p'_1}\; u^*_{p_1}\, \vec{e}^{\,*}_{i\kappa}\cdot\vec{\alpha}\, v_{p'_1}\, \delta(p+k+p')$$

$$\sqrt{\frac{4\pi e^2}{2\omega_k}}\; d_{p\ell}\, a_{ki}\, c_{p'\ell'}\, v_{p\ell}^{*}\, \vec{e}_{ik}\cdot\vec{\alpha}\, u_{p'\ell'}\, \delta(p+k+p')$$

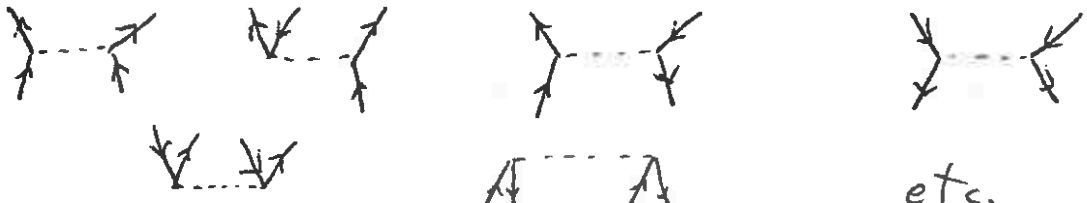
$$\sqrt{\frac{4\pi e^2}{2\omega_k}}\; d_{p\ell}\, a_{ki}^{*}\, c_{p'\ell'}\, v_{p\ell}^{*}\, \vec{e}_{ik}^{\,*}\cdot\vec{\alpha}\, u_{p'\ell'}\, \delta(p-k+p')$$

$$\sqrt{\frac{4\pi e^2}{2\omega_k}}\; d_{p\ell}\, a_{ki}\, d_{p'\ell'}^{\dagger}\, v_{p\ell}^{*}\, \vec{e}_{ik}\cdot\vec{\alpha}\, v_{p'\ell'}\, \delta(p+k-p')$$

$$\sqrt{\frac{4\pi e^2}{2\omega_k}}\; d_{p\ell}\, a_{ki}^{\dagger}\, d_{p'\ell'}^{\dagger}\, v_{p\ell}^{*}\, \vec{e}_{ik}^{\,*}\cdot\vec{\alpha}\, v_{p'\ell'}\, \delta(p-k-p')$$

The arrows show which is the entrance state and which the exit state in the matrix element. In writing a matrix element down from a picture start at the beginning of the arrow and the right of the matrix element; then follow the arrows and move to the left in the matrix element, putting in interaction matrices and spinors as they arise. Any line which points backwards in time belongs to a positron; those which point forward in time belong to electrons (It is best not to put arrows on boson lines except possibly to remind yourself of the sign of the momentum)

The 16 terms which arise from the Coulomb interaction can also be expressed in terms of pictures, even though the intermediate lines weren't obtained by explicit creation and annihilation operators.

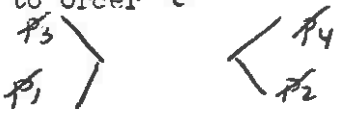


For fun and practice with the operator anti-commutation relations, see what the equation of motion $i\frac{\partial \psi}{\partial t} = \mathcal{H}\psi - \psi\mathcal{H}$ tells you about the operator ψ

Previously we obtained the electron propagator to be $\frac{1}{\not{p} - m}$

It should be possible to obtain the photon propagator from the pieces of matrix element above

Consider scattering to order e^2



for $\not{q} = \not{p}_3 - \not{p}_1$ $\quad q_\mu = (q_t, Q, 0, 0)$ the contributions are

1) Coulomb interaction $\frac{4\pi e^2}{Q^2} (u_3^\dagger u_1)(u_4^\dagger u_2)$

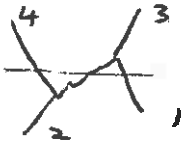
2) Virtual transverse photons

$$\sum_{\text{Internal polarizations}} \frac{\frac{4\pi e^2}{2\omega_q} (u_4^\dagger \vec{\alpha}\cdot\hat{e} u_2)(u_3^\dagger \vec{\alpha}\cdot\hat{e} u_1)}{(E_1 + E_2) - (E_3 + E_2 + \omega_q) + i\varepsilon}$$

from

$$\sum_{\text{Internal polarizations}} \frac{4\pi e^2}{2\omega_q} \frac{(u_3^\dagger \vec{\alpha}\cdot\hat{e} u_1)(u_4^\dagger \vec{\alpha}\cdot\hat{e}^* u_2)}{(E_1 + E_2) - (E_4 + E_1 + \omega_q) + i\varepsilon}$$

from



Notice that if there were 3 directions of polarization (two $\perp \hat{q}$ and one $\parallel \hat{q}$)

then $\sum_{\text{all 3 } i} (\vec{A}\cdot\hat{e}_i)(\vec{B}\cdot\hat{e}_i) = \vec{A}\cdot\vec{B}$

Hence $\sum_{\text{Transverse}} (\vec{A}\cdot\hat{e}_i)(\vec{B}\cdot\hat{e}_i) = \vec{A}\cdot\vec{B} - \vec{A}\cdot\hat{q}\,\vec{B}\cdot\hat{q}$

Thus combination of the two transversely polarized pieces gives

$$\left(\frac{4\pi e^2}{2\omega_q}\right)\left[(u_4^\dagger \vec{\alpha} u_2)\cdot(u_3^\dagger \vec{\alpha} u_1) - \frac{(u_4^\dagger \vec{\alpha}\cdot\vec{Q} u_2)}{Q}\frac{(u_3^\dagger \vec{\alpha}\cdot\vec{Q} u_1)}{Q}\right]\left[\frac{1}{E_1 - E_3 - \omega_q + i\varepsilon} + \frac{1}{E_2 - E_4 - \omega_q + i\varepsilon}\right]$$

But $\frac{1}{E_1 - E_3 - \omega_q} + \frac{1}{E_2 - E_4 - \omega_q} = \frac{2\omega_q}{\vec{q}^2}$

Hence the sum of all these terms gives

$$4\pi e^2 \left\{ \frac{1}{\vec{q}^2}(\bar{u}_4 \vec{\gamma} u_2)\cdot(\bar{u}_3 \vec{\gamma} u_1) + \frac{1}{Q^2}(\bar{u}_3 \gamma_0 u_1)(\bar{u}_4 \gamma_0 u_2) - \frac{(\bar{u}_3 \vec{\gamma}\cdot\vec{Q} u_1)(\bar{u}_4 \vec{\gamma}\cdot\vec{Q} u_2)}{\vec{q}^2 Q^2} \right\}$$

But $q_\mu \bar{u}_4 \gamma_\mu u_2 = \bar{u}_4 (\not{p}_2 - \not{p}_4) u_2 = \bar{u}_4 (m - m) u_2 = 0$

(current conservation)

Hence $\bar{u}_4 \vec{\gamma}\cdot\vec{Q} u_2 = q_t \bar{u}_4 \gamma_0 u_2$

and we arrive at

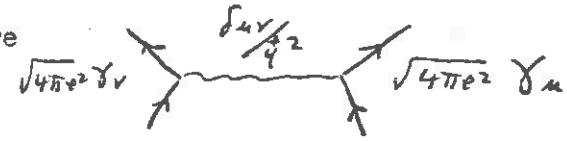
$$4\pi e^2 \left\{ -\frac{(\bar{u}_4 \gamma_\mu u_2)(\bar{u}_3 \gamma_\mu u_1)}{\vec{q}^2} + \frac{(\bar{u}_4 \gamma_0 u_2)(\bar{u}_3 \gamma_0 u_1)}{\vec{q}^2} + \frac{(\bar{u}_3 \gamma_0 u_1)(\bar{u}_4 \gamma_0 u_2)}{Q^2} - \frac{q_t^2 (\bar{u}_4 \gamma_0 u_2)(\bar{u}_3 \gamma_0 u_1)}{Q^2 \vec{q}^2} \right\}$$

But $\frac{1}{\vec{q}^2} + \frac{1}{Q^2} - \frac{q_t^2}{Q^2 \vec{q}^2} = 0$

Hence we have shown that all the lowest order interactions due to charge coalesce into one manifestly covariant matrix element

$$-\frac{4\pi e^2}{q^2}(\bar{u}_4\gamma_\mu u_2)(\bar{u}_3\gamma_\mu u_1)$$

which can be symbolized by the picture



For the charge current $j_\mu = \bar{u}_3\gamma_\mu u_1$, we have

$$\Box A_\mu = j_\mu \qquad A_\mu = \frac{1}{q^2} j_\mu$$

Interaction with $j_\mu' = \bar{u}_4\gamma_\mu u_2$ is by means of $j_\mu' A_\mu = j_\mu' \frac{1}{q^2} j_\mu$

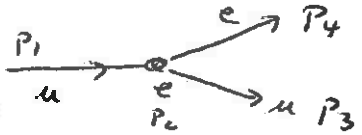
It is especially important to remember that when you use these rules with the propagators $\frac{1}{\not p - m}$ or $\frac{1}{q^2}$, it is no longer necessary to draw two graphs which differ by time ordering

It is only necessary to draw one graph  . This is <u>always</u> the convention used in applications.

<u>Applications and Discussion</u>

It happens that μ mesons obey (to the best of our present knowledge) exactly the same equations as electrons, with only the mass changed.

Suppose a stationary electron target, with μ particles shot in (in the lab frame). The μ and e will scatter into new momentum states because of the interaction of their charges



Rate = $\sigma v_\mu =$

$$(2\pi)^4\delta(p_4+p_3-p_2-p_1)\,(2\pi)\delta(p_3^2-\mu^2)\,(2\pi)\delta(p_4^2-m^2)\,\frac{d^4p_4}{(2\pi)^4}\,\frac{d^4p_3}{(2\pi)^4}\,\frac{1}{2m_e}\,\frac{1}{2E_{\mu m}}\,|M|^2$$

The δ functions may then be unraveled against the differentials in any order you find convenient (hint: the answer is usually pretty messy no matter what order you use, but there may be fewer messy steps in one sequence than in another)

Because the μ and electron have the same interaction with the electromagnetic field, we can write down the matrix element by using the same rules as for electron-

electron scattering

$$\frac{(4\pi e^2)\,(\overbrace{\bar{u}_3\gamma_\mu u_1}^{\mu})\,(\overbrace{\bar{u}_4\gamma_\mu u_2}^{e})}{(p_2-p_4)^2}$$

$\not{p}_3 u_3 = \mu u_3$
$\not{p}_2 u_2 = m_e u_2$

It is easy to see that the largest contributions to the cross section come from $p_2 \approx p_4$ (forward scattering in the center of mass system). When $\vec{q}^2$ is small, the interaction radius (the Fourier transform conjugate of $\sqrt{q^2}$) is large. This means most of the cross section is obtained from cases where the particles aren't close together. Hence this is not a good experiment to do if you want to test the laws of electrodynamics - we know already that they work fine for large separations because this is the classical limit. What we want to examine closely is whether the laws break down when the particles get close together. This would be found by looking at large $\vec{q}^2$ behavior of the matrix element. But $\vec{q}^2$ for this particular experiment is extremely small even for high energy μ's

Question: if it were possible to have a target of μ's and shoot electrons at them, would it be easier to explore the large $\vec{q}^2$ limit?

For education: is it true that to lowest order the scattering of $\mu^+ e^-$ can be obtained from the scattering of $\mu^- e^-$ by the replacement $\not{p}_{\mu+} = -\not{p}_{\mu-}$? Why?

One of the most precise experiments to date along this line is the scattering $e^- p \to e^- p$. Here the matrix element is again proportional to $\frac{J_\mu \cdot \bar{u}_4 \gamma_\mu u_2}{(p_2-p_4)^2}$, where J_μ now represents the electromagnetic current of the proton. It can be shown that the most general form of J_μ is

$$J_\mu = \bar{u}_3 \left[e F_1 \gamma_\mu + F_2 (\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu) q^\nu \right] u_1$$

where u_3 and u_1 are nucleon plane wave spinors and F_1 and F_2 are assumed for theoretical reasons to be functions only of the exchanged 4 momentum transfer squared ($\vec{q}^2$)

(Justify this form for J_μ by fiddling with others)

It is found empirically that both F_1 and F_2 have the shape $\frac{K_{1,2}}{(\vec{q}^2 - x^2)^2}$ where x^2

is a universal constant. One could, therefore, get the same result just by modifying the photon propagator. It is now considered more acceptable to ascribe the form factors F_i to mesonic substructure of the nucleons, rather than to a breakdown of qed.

Week 4 – Part II Ph 205c

Differential cross-section for Compton Scattering in lab ($\vec{p}_1 = 0$):

$$d\sigma = \frac{1}{16 m E_2 \omega_1 \omega_2} \frac{1}{(2\pi)^2} |M|^2 \omega_2^2 \frac{E_2 \, d\Omega}{m + 2\omega \sin^2\theta/2} \quad ; \quad d\Omega = d\Omega_\theta = \text{solid angle of outgoing photon.}$$

$$= \frac{d\Omega}{64\pi^2} \frac{\omega_2}{m\omega_1} \frac{|M|^2}{m + 2\omega \sin^2\theta/2}$$

ω_1 = energy of incoming γ
ω_2 = energy of outgoing γ
E_2 = energy of outgoing e^-

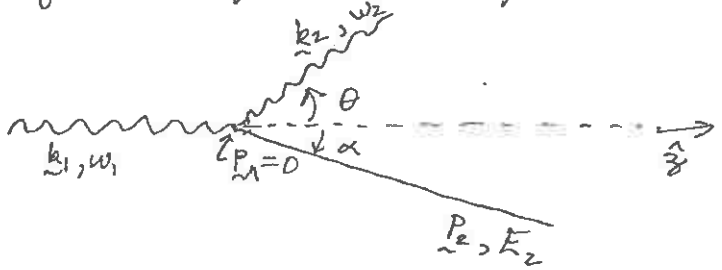
From kinematics, $\frac{\omega_2}{\omega_1} = \frac{m}{m + 2\omega \sin^2\theta/2}$

$$\therefore \left.\frac{d\sigma}{d\Omega}\right]_{lab} = \frac{1}{64\pi^2} \frac{|M|^2}{m^2} \frac{\omega_2^2}{\omega_1^2} \quad \cdots (1)$$

This cross-section refers to a definite process in which the initial and final states are completely ~~specified~~ defined "pure" states.

Now there are 2 possible helicities for the electron in the initial state, as well as 2 possible helicites for the electron in the final state. In addition, there are 2 possible polarization states for the photon in both the initial and final states. There are, therefore, 16 polarized differential amplitudes M that occur in Compton scattering.

Kinematics of scattering in the lab system



Initial state spinors (Recall: normalization is 2E particles/unit volume)

$$u_1 = u_{1+} = \sqrt{2m} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{or} \quad u_1 = u_- = \sqrt{2m} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Final state spinors:

$$u_2 = u_{2+} = \begin{pmatrix} \sqrt{E+m}\cos\alpha/2 \\ -\sqrt{E+m}\sin\alpha/2 \\ \sqrt{E-m}\cos\alpha/2 \\ -\sqrt{E-m}\sin\alpha/2 \end{pmatrix}, \text{ or } u_2 = u_{2-} = \begin{pmatrix} \sqrt{E+m}\sin\alpha/2 \\ \sqrt{E+m}\cos\alpha/2 \\ -\sqrt{E-m}\sin\alpha/2 \\ -\sqrt{E-m}\cos\alpha/2 \end{pmatrix}$$

$$\bar{u}_{2-} = (\sqrt{E+m}\,\delta, \sqrt{E+m}\,\Gamma, \sqrt{E-m}\,\delta, \sqrt{E-m}\,\Gamma)$$

$$\bar{u}_{2+} = (\sqrt{E+m}\,\Gamma, -\sqrt{E+m}\,\delta, -\sqrt{E-m}\,\Gamma, \sqrt{E-m}\,\delta)$$

where $\boxed{\delta = \sin\alpha/2 \quad \Gamma = \cos\alpha/2}$

There are 2 possibilities for e_1, the polarization of the incoming γ

(i) polarized in plane of scattering, $e_1 = (1,0,0,0) = e_{1a}$ (components x, y, z, t)

(ii) polarized perpendicular to plane of scattering $e_1 = (0,1,0,0) = e_{1b}$

similarly for e_2:

(i) in plane of scattering $e_2 = (\cos\theta, 0, -\sin\theta, 0) = e_{2a}$

(ii) perpendicular to the plane of scatt.; $e_2 = (0,1,0,0) = e_{2b}$

Now we carry out the computation of M for the 16 different processes:

In each case, we have

$$\frac{M}{4\pi e^2} = \frac{\bar{u}_2 \not{e}_2 (\not{p}_1 + \not{k}_1 + m)\not{e}_1 u_1}{(p_1+k_1)^2 - m^2} + \frac{\bar{u}_2 \not{e}_1 (\not{p}_1 - \not{k}_2 + m)\not{e}_2 u_1}{(p_1-k_2)^2 - m^2}$$

$$= \bar{u}_2 \left(\frac{\not{e}_2 \not{k}_1 \not{e}_1}{2mw_1} + \frac{\not{e}_1 \not{k}_2 \not{e}_2}{2mw_2} \right) u_1 \qquad \text{since } \not{p}_1 \not{e}_1 = -\not{e}_1 \not{p}_1, \quad \not{p}_1 \not{e}_2 = -\not{e}_2 \not{p}_1$$

$$\not{k}_1 = w_1(\gamma_t - \gamma_z)$$

$$\not{k}_2 = w_2(\gamma_t - \gamma_z\cos\theta - \gamma_x\sin\theta)$$

Case 1: $u_1 = u_{1+}$ $\quad u_2 = u_{2+}$
$e_1 = e_{1a}$ $\quad e_2 = e_{2a}$

$\boxed{C = \cos\theta \quad S = \sin\theta}$

Then $-\not{e}_1 = \not{\gamma}_x = x$
$-\not{e}_2 = \not{\gamma}_x C - \not{\gamma}_z S = xC - zS$

according to the abbreviations:

$\not{\gamma}_x \to x$
$\not{\gamma}_y \to y$
$\not{\gamma}_z \to z$
$\not{\gamma}_t \to t$

Then $M_1 \times \frac{2m}{4\pi e^2} = \bar{u}_2 \left[(xC - zS)(t - z)x + x(t - zC - xS)(xC - zS) \right] u_1$

$= \bar{u}_2 \left[tC - zC - txzS - xS + tC + txzS - zC^2 - xzCS + xzCS - zS^2 \right] u_1$

where repeated use has been made of the commutation rules for the γ's: $xt + tx = 0$

$x^2 = -1$, etc.

$= \bar{u}_2 \left[2tC - xS - z(1+C) \right] u_1$

To evaluate $[2tC - xS - z(1+C)]u_1$, we make use of the table of γ-matrices on page 4.

obtain $M_1 \times \frac{2m}{4\pi e^2} = \bar{u}_2 \begin{pmatrix} 2C \\ 0 \\ 1+C \\ S \end{pmatrix} \sqrt{2m} = \sqrt{2m} \left(\sqrt{E+m}\,\Gamma, -\sqrt{E+m}\,\sigma, -\sqrt{E-m}\,\Gamma, \sqrt{E-m}\,\sigma \right) \begin{pmatrix} 2C \\ 0 \\ 1+C \\ S \end{pmatrix}$

$M_1 \frac{\sqrt{2m}}{4\pi e^2} = 2\sqrt{E+m}\,C\Gamma + \sqrt{E-m}(\sigma S - \Gamma C) - \Gamma\sqrt{E-m}$

$= 2\sqrt{E+m}\cos\theta\cos\alpha/2 - \sqrt{E-m}\cos(\theta + \alpha/2) - \sqrt{E-m}\cos\alpha/2$

or, $M_1 = \frac{4\pi e^2}{\sqrt{2m}} \left(2\sqrt{E+m}\cos\theta\cos\alpha/2 - \sqrt{E-m}\cos(\theta+\alpha/2) - \sqrt{E-m}\cos\alpha/2 \right)$

Table of Independent γ-matrices :

We write this out in a particular representation defined by

$$\underset{\sim}{\alpha} = \begin{pmatrix} 0 & \underset{\sim}{\varepsilon} \\ \underset{\sim}{\varepsilon} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Then $\underset{\sim}{\gamma} = \beta \underset{\sim}{\alpha} = \begin{pmatrix} 0 & \underset{\sim}{\varepsilon} \\ -\underset{\sim}{\varepsilon} & 0 \end{pmatrix}$ $\qquad \gamma_t = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\gamma_x \gamma_y = -i \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$$

$$\gamma_y \gamma_z = \begin{pmatrix} -i\sigma_x & 0 \\ 0 & -i\sigma_x \end{pmatrix} \qquad \gamma_5 = \gamma_x \gamma_y \gamma_z \gamma_t = +i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\gamma_z \gamma_x = \begin{pmatrix} -i\sigma_y & 0 \\ 0 & -i\sigma_y \end{pmatrix}$$

$$\gamma_t \gamma_x = \alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$$

$$\gamma_t \gamma_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}$$

$$\gamma_t \gamma_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}$$

$$\gamma_5 \gamma_x = \begin{pmatrix} -i\sigma_x & 0 \\ 0 & i\sigma_x \end{pmatrix} = \gamma_t \gamma_y \gamma_z$$

$$\gamma_5 \gamma_y = \begin{pmatrix} -i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix} = \gamma_t \gamma_z \gamma_x$$

$$\gamma_5 \gamma_z = \begin{pmatrix} -i\sigma_z & 0 \\ 0 & i\sigma_z \end{pmatrix} = \gamma_t \gamma_x \gamma_y$$

$$\gamma_5 \gamma_t = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix} = \gamma_x \gamma_y \gamma_z$$

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

2. $u_{1+} \longrightarrow u_{2+}$ $\quad -\phi = \gamma_x$

$e_{1a} \longrightarrow e_{2b}$ $\quad -\phi_2 = \gamma_y$

$$M_2 \times \frac{2m}{4\pi e^2} = \bar{u}_2 \{ y(t-z)x + x(t-zC-xS)y \} u_1$$

$$= \bar{u}_2 \{ txy - xyz - txy + xyzC + yS \} u_1$$

$$= \sqrt{2m}\bar{u}_2 \begin{pmatrix} 0 \\ 0 \\ i(C-1) \\ -iS \end{pmatrix} = i\sqrt{E+m}\{ \Gamma - \Gamma C - GS \}$$

$$M_2 \frac{\sqrt{2m}}{4\pi e^2} = i\sqrt{E-m}\{ \cos\alpha/2 - \cos(\theta - \alpha/2) \}$$

3. $u_{1+} \longrightarrow u_{2-}$ $\quad -\phi_1 = \gamma_x$

$e_1 = e_{1a} \longrightarrow e_2 = e_{2a}$ $\quad -\phi_2 = \gamma_x C - \gamma_z S$

$$M_3 \frac{2m}{4\pi e^2} = \bar{u}_2 \{ (xC - zS)(t-z)x + x(t-zC-xS)(xC-zS) \} u_1$$

$$= \bar{u}_2 \{ tC - zC - txzS - xS + tC - zC^2 + xCS + txzS \\ - xCS - zS^2 \} u_1$$

$$= \bar{u}_2 (2tC - z - zC - xS) u_1$$

$$M_3 \frac{\sqrt{2m}}{4\pi e^2} = \bar{u}_2 \begin{pmatrix} 2C \\ 0 \\ 1+C \\ S \end{pmatrix} = \{ 2\sqrt{E+m}\cos\theta\sin\alpha/2 + \sqrt{E-m}\sin(\theta+\alpha/2) + \sqrt{E-m}\sin\alpha/2 \}$$

4. $u_{1+} \rightarrow u_{2-}$

$e_{1a} \rightarrow e_{2b}$, as in case 2, $M \times \frac{2m}{4\pi e^2} = \bar{u}_2 (xyz(c-1) + yS) u_1$

$$M_4 \frac{\sqrt{2m}}{4\pi e^2} = -i\sqrt{E-m}\{ \sin(\theta - \alpha/2) + \sin\alpha/2 \}$$

5. $u_{1-} \rightarrow u_{2-}$

$e_{1a} \rightarrow e_{2a}$

$$M_5 \frac{\sqrt{2m}}{4\pi e^2} = \{ 2\sqrt{E+m}\cos\theta\cos\alpha/2 - \sqrt{E-m}\cos(\theta+\alpha/2) - \sqrt{E-m}\cos\alpha/2 \}$$

Notice that $M_5 = M_1$. This can be seen to be a consequence of the invariance of the coupling $j^\mu A_\mu$ under the parity transformation P.

Under P, $\vec{S}$ (spin), like $\vec{l}$ (orbital ang. mom.) is invariant. $\vec{p}$, however, changes sign, so $\vec{S}\cdot\vec{p}$ also changes sign and we have the result that the helicity of an electron changes sign under parity.

From the form of the amplitude, it is obvious that reversing the directions of polarization of both photons leaves the lowest order amplitude invariant.

Putting these together, we see that

$$M_1\begin{pmatrix} u_{1+} \to u_{2+} \\ e_{1a} \to e_{2a} \end{pmatrix} = M\begin{pmatrix} u_{1-} \to u_{2-} \\ -e_{1a} \to -e_{2a} \end{pmatrix} = M_5\begin{pmatrix} u_{1-} \to u_{2-} \\ e_{1a} \to e_{2a} \end{pmatrix}$$

Similarly, $M_6\begin{pmatrix} u_{1-} \to u_{2-} \\ e_{1a} \to e_{2b} \end{pmatrix} = M_2\begin{pmatrix} u_{1+} \to u_{2+} \\ e_{1a} \to e_{2b} \end{pmatrix}$

$$M_7\begin{pmatrix} u_{1-} \to u_{2+} \\ e_{1a} \to e_{2a} \end{pmatrix} = M_3\begin{pmatrix} u_{1+} \to u_{2-} \\ e_{1a} \to e_{2a} \end{pmatrix}$$

$$M_8\begin{pmatrix} u_{1-} \to u_{2+} \\ e_{1a} \to e_{2b} \end{pmatrix} = M_4\begin{pmatrix} u_{1+} \to u_{2-} \\ e_{1a} \to e_{2b} \end{pmatrix}$$

9. $\begin{matrix} u_{1+} \to u_{2+} \\ e_{1b} \to e_{2b} \end{matrix}$ $\quad \begin{matrix} -\phi_1 = \gamma_y \\ -\phi_2 = \gamma_4 \end{matrix}$

$$M_9 \frac{\sqrt{2m}}{4\pi e^2} = \left\{ 2\sqrt{E+m}\cos\tfrac{\alpha}{2} - \sqrt{E-m}\cos\tfrac{\alpha}{2} - \sqrt{E-m}\cos\left(\theta+\tfrac{\alpha}{2}\right) \right\}$$

10. $\begin{matrix} u_{1+} \to u_{2+} \\ e_{1b} \to e_{2a} \end{matrix}$ $\quad \begin{matrix} -\phi_1 = y \\ -\phi_2 = xC - zS \end{matrix}$

$$M_{10} \frac{\sqrt{2m}}{4\pi e^2} = \frac{1}{\sqrt{2m}}\, \bar{u}_2 (xyz\,C - y\,S - xyz)\, u_1 = i\sqrt{E-m}\left(\cos\tfrac{\alpha}{2} - \cos\left(\theta+\tfrac{\alpha}{2}\right)\right)$$

11. $u_{1-} \to u_{2-}$
$e_{1b} \to e_{2b}$ By parity $M_{11} = M_9$

12. $u_{1-} \to u_{2-}$
$e_{1b} \to e_{2a}$ By parity $M_{12} = M_{10}$

13. $u_{1+} \to u_{2-}$
$e_{1b} \to e_{2b}$

14. $u_{1-} \to u_{2+}$
$e_{1b} \to e_{2b}$

$$M_{13} = M_{14}$$

$$\frac{\sqrt{2m}}{4\pi e^2} M_{13} = 2\sqrt{E+m}\sin\alpha/2 + \sqrt{E-m}\sin\alpha/2 + \sqrt{E-m}\sin(\theta+\alpha/2)$$

15. $u_{1+} \to u_{2-}$
$e_{1b} \to e_{2a}$

16. $u_{1-} \to u_{2+}$
$e_{1b} \to e_{2a}$

$$M_{15} = M_{16}$$

$$\frac{\sqrt{2m}}{4\pi e^2} M_{15} = \frac{1}{\sqrt{2m}} \bar{u}_2 (xyzC - yS - xyz) u_1 \qquad (\text{same form as } 10.)$$

~~$= i\sqrt{E-m}(\cos\alpha/2 - \cos(\theta+\alpha/2))$~~

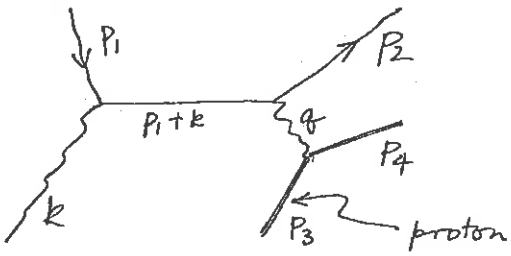
$$= i\left(\sqrt{E+m}\sin(\theta+\alpha/2) - \sqrt{E-m}\sin\alpha/2\right)$$

The various polarized cross sections are obtained by the replacement $M \to M_k$, $k = 1, 2, \ldots 16$ in Equation (1).

Week 6 May 1, 2, 5 Ph 205c

Pair production in matter

A photon may create an $e^- e^+$ pair in the presence of a proton according to the following diagram:



p_1 = 4 momentum of e^+
p_2 = 4 momentum of e^-

The piece of the matrix element that is represented by this diagram is

$$(\sqrt{4\pi e^2})^3 J_\mu \frac{1}{q^2} \bar{u}_2 \gamma_\mu \frac{1}{\not{p}_1 + \not{k} - m} \not{\epsilon} u_1$$

where J_μ = matrix element of the electromagnetic current operator taken between the initial and final free proton states.

From general arguments of relativity and charge and parity conservation, it can be shown that if spinor solutions of the free particle Dirac Equation are used to describe the free proton, then

$$J_\mu = e\bar{u}_4 \left\{ \gamma_\mu F_1(q^2) + \frac{1}{4M} q_\nu [\gamma_\nu, \gamma_\mu] F_2(q^2) \right\} u_3$$

$$= e\bar{u}_4 \left\{ \gamma_\mu F_1 + \frac{1}{4M} [\not{q}, \gamma_\mu] F_2 \right\} u_3$$

The threshold behavior of F_1 and F_2, that is $F_1(0)$, $F_2(0)$, may be determined in terms of the charge and magnetic moment of the proton by considering the

non-relativistic limit of the coupling of this J_μ to an external static field $A_\mu = (\phi, \vec{A})$, and identifying terms in the classical formula

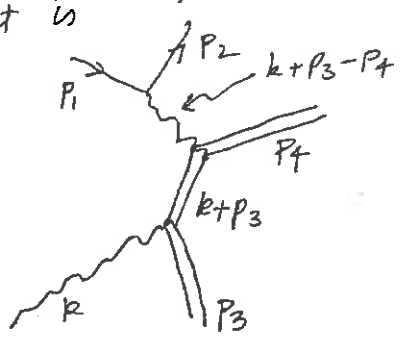
$$H_I^{NR} = e\phi + \vec{\mu}\cdot\vec{B}$$

In this manner, one obtains

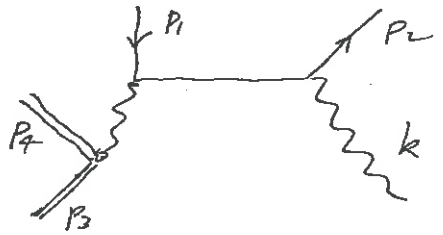
$$F_1(0) = 1$$
$$\mu = \frac{e}{2M}\left(F_1(0) + F_2(0)\right)$$

$\Rightarrow$ $F_2(0)$ is the anomalous magnetic moment of the proton, in nuclear magnetons.

In lowest order there is another diagram that must be considered for the process: $\gamma + p \to \gamma + p + e^+ + e^-$, and that is

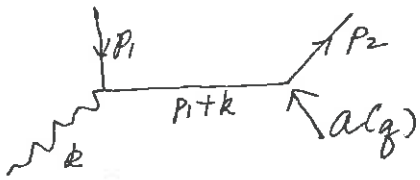


and a third diagram



If we neglect the recoil of the nucleus — that is, if we treat the nucleus as an external, static coulomb field, we have only two diagrams in lowest order

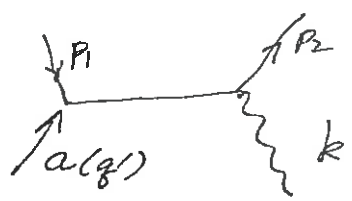
I.



$$p_2 = p_1 + k + q$$

or $q = p_2 - p_1 - k$

II.



$$q' = q = p_2 - p_1 - k$$

The amplitudes associated with these diagrams, M_I, M_{II} are

$$M_I = \bar{u}_2 \not{A}(q) \frac{1}{\not{p}_1 + \not{k} - m} \not{\epsilon} u_1 \sqrt{4\pi e^2}$$

and $$M_{II} = \bar{u}_2 \not{\epsilon} \frac{1}{\not{p}_2 - \not{k} - m} \not{A}(q) u_1 \sqrt{4\pi e^2}$$

where $$a_\mu(q) = \int A_\mu(x) e^{iqx} dx$$

$$A_\mu = \left(\frac{Ze^2}{R}, 0\right)$$

$$\therefore \not{A}(q) = \gamma_t 2\pi \int \frac{Ze^2}{R} \delta(q_t) e^{-i\vec{Q}\cdot\vec{R}}$$

$$= 2\pi \delta(q_t) Ze^2 \times \frac{4\pi}{Q^2} \gamma_t$$

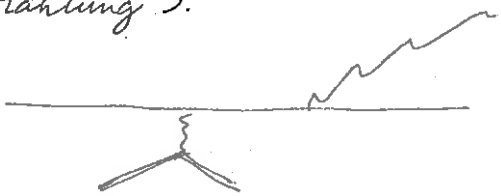
If we took into consideration the effect of electron shielding of the field of the nucleus by $V(R) = \frac{Ze^2}{R} e^{-br}$

we'd obtain

$$\not{A}(q) = 2\pi\delta(q_t) \frac{4\pi e^2 Z}{Q^2 + 1/b^2} \gamma_t$$

Substituting $\not{A}$ into $M_I + M_{II}$, and taking the absolute square, ~~squaring~~, and multiplying by the appropriate kinematical factors we obtain the cross-section for pair production in the field of a nucleus. The result is an ugly mess which is discussed in Heitler, Quantum Theory of Radiation §26. One simple result is that if the e^+e^- pair are produced with relativistic energies, they are created primarily in the forward direction within the cone defined by the angle $\theta \sim \frac{m}{k}$. For smaller energies, the effect is less marked.

Another phenomenon of considerable interest is the emission of a photon by an electron in the field of a nucleus ("Bremsstrahlung").



The matrix element for this process has the same form as that for pair production by a photon in the field of a nucleus.

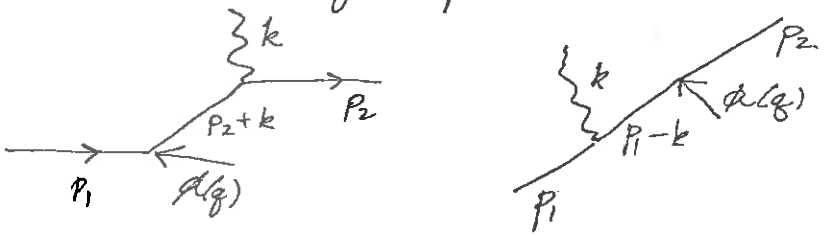
γ's create pairs which emit γ's by bremsstrahlung, which in turn create pairs, ... thus creating a "shower"

<u>The "common sense" infinity of quantum electrodynamics</u>

It is not possible for scattering to take place without the emission of photons. That is because the field far away from the charge must change if the particle is deflected. It can change only if photons are emitted.

There is some interest, therefore, in an approximate formula for bremsstrahlung with the emission of low frequency photons.

Consider the emission of one photon. The relevant diagrams are



$$\text{Rate} = 2\pi\,\delta(E_2+\omega-E_1)\,\frac{d^3p_2}{(2\pi)^3\,2E_1\,2E_2}\,\frac{d^3k}{2\omega\,(2\pi)^3}\,|M|^2$$

$$M = \left\{\bar{u}_2\not{\epsilon}\,\frac{1}{\not{p}_2+\not{k}-m}\,\not{A}\,u_1 + \bar{u}_2\not{A}\,\frac{1}{\not{p}_1-\not{k}-m}\,\not{\epsilon}\,u_1\right\}\sqrt{4\pi e^2}$$

$$M = \bar{u}_2 \left\{ \not{e} \frac{(\not{p}_2 + \not{k} + m)\not{a}}{2p_2 \cdot k} + \not{a} \frac{(\not{p}_1 - \not{k} + m)\not{e}}{-2p_1 \cdot k} \right\} u_1 \sqrt{4\pi e^2}$$

we are interested only in low-energy photons, so the two terms with arrows above them are small compared to the other terms in the expression, and can be neglected to an accuracy of the order $\frac{k}{m}$.

then $M = \bar{u}_2 \left(\frac{-\not{p}_2\not{e} + 2p_2 \cdot e + \not{e}\not{k}}{2p_2 \cdot k} \right) \not{a} u_1 + \bar{u}_2 \not{a} u_1 \frac{2p_1 \cdot e}{-2p_1 \cdot k}$

(The X's indicate terms that cancel)

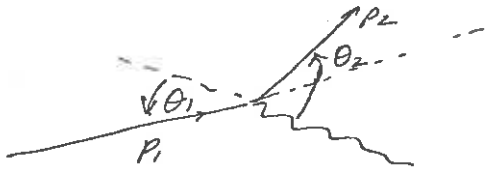
$$= \bar{u}_2 \not{a} u_1 \left(\frac{p_2 \cdot e}{p_2 \cdot k} - \frac{p_1 \cdot e}{p_1 \cdot k} \right) \sqrt{4\pi e^2}$$

$$\therefore \text{Rate} = 2\pi \delta(E_f - E_i) \underbrace{\frac{d^3 p_2}{(2\pi)^3 2E_2 2E_1} |\bar{u}_2 \not{a}(q) u_1|^2 \left\{ \omega \left(\frac{p_2 \cdot e}{p_2 \cdot k} - \frac{p_1 \cdot e}{p_1 \cdot k} \right) \right\}^2 4\pi e^2}_{A} \times \frac{d\omega}{\omega} \frac{d\Omega_2}{2(2\pi)^3}$$

A is the probability of scattering with no photons emitted, in lowest order.

to the approximation we've made $q \simeq p_2 - p_1$

The term $\{\ \}$ may be simplified



$$p_1 \cdot k = E_1 \omega - p_1 \omega \cos\theta_1 = \omega E_1 (1 - v_1 \cos\theta_1)$$

$$\{\ \} = \frac{v_1 \cdot e}{1 - v_1 \cos\theta_1} - \frac{v_2 \cdot e}{1 - v_2 \cos\theta_2} = \frac{v_1 \sin\theta_1}{1 - v_1 \cos\theta_1} - \frac{v_2 \sin\theta_2}{1 - v_2 \cos\theta_2}$$

$= 0$ if $\vec{e}$ is perpendicular to the plane of scattering.

$\therefore$ photons polarized in the plane of the collision.

Energy/unit time emitted in range dw

= Same formula (without the factor of $\frac{1}{w}$)

which is the same as the classical expression

Problem: Two soft photon emission (k, l)
Show that rate = Probability of scattering with emission of no photons
× probability of emitting one photon (k)
× probability of emitting other photon (l)
there is also a factor of $\frac{1}{2}$ from statistics.

(i.e., show that the two photons are emitted with statistically independent probabilities)

Classical case: A classical charged particle moves with uniform velocity and is suddenly deflected. What is the radiation like?

Let the trajectory in space time be represented parametrically by the functions $z_\mu(\alpha)$

the current density

$$j_\mu(x) = e\int \delta^4(x - z(\alpha))\, \dot{z}_\mu(\alpha)\, d\alpha$$

vector potential satisfies the equation

$$\Box A_\mu(x) = j_\mu(x)$$

Take the fourier transform of both sides

$$k^2 a_\mu(k) = \int e^{-ikx} j_\mu(x)\, d^4x$$

$$= \int e^{-ikx} \int \dot{z}_\mu(\alpha)\, \delta^4(x - z(\alpha))\, d\alpha\, d^4x$$

$$= \int e^{-ik\cdot z(\alpha)} \dot{z}(\alpha)\, d\alpha = j_\mu(k)$$

Let the deflection take place at $\alpha = 0$, then

$\alpha < 0 \qquad Z_\mu(\alpha) = p_{1\mu}\alpha$

$\alpha > 0 \qquad Z_\mu(\alpha) = p_{2\mu}\alpha$

then $j_\mu(k) = \int_{-\infty}^{0} p_{1\mu} e^{-ik\cdot p_1 \alpha} d\alpha + \int_0^{\infty} p_{2\mu} e^{-ik\cdot p_2 \alpha} d\alpha$

$= i\left(\frac{p_{1\mu}}{p_1\cdot k} - \frac{p_{2\mu}}{p_2\cdot k}\right)$, so $a_\mu(k) = \frac{i}{k^2}\left(\frac{p_{1\mu}}{p_1\cdot k} - \frac{p_{2\mu}}{p_2\cdot k}\right)$

This gives the classical expected energy in $d\omega = e^2 C(\omega) d\omega$

= mean energy liberated in $d\omega$ quantum-mechanically

mean no. of photons emitted $= e^2 C(\omega)\frac{d\omega}{\omega}$

Emission of many soft photons:

Rate for one photon emission $= A\left[\omega\left(\frac{v_1 \sin\theta_1}{1 - v_1\cos\theta_1} - \frac{v_2 \sin\theta_2}{1 - v_2\cos\theta_2}\right)\right]^2 \frac{d\Omega_\omega d\omega}{(2\pi)^3 \omega} 4\pi e^2$

Now to the same order in e^2, the cross-section for emitting no photons is

$$\sigma = \sigma_A(C+1)$$

σ_A = x section corresponding to rate A

Where C is a correction factor that comes from the interference term between the two diagrams

and

which is of $\mathcal{O}(e^2 A)$

i.e., $C = \mathcal{O}(e^2)$

σ for 1 photon emission $= \sigma_A \times (1+C) \times \left(\frac{d\omega}{\omega} f(\theta_1) d\Omega_1\right)$

σ for 2 photon emission $= \sigma_A \times (1+C)\frac{1}{2}\left(\frac{d\omega_1}{\omega_1} f(\theta_1) d\Omega_1\right)\left(\frac{d\omega_2}{\omega_2} f(\theta_2) d\Omega_2\right)$

σ for 3 photon emission $= \sigma_A (1+C)\frac{1}{3!}\left(\frac{d\omega_1}{\omega_1} f(\theta_1) d\Omega_1\right)\left(\frac{d\omega_2}{\omega_2} f(\theta_2) d\Omega_2\right)\left(\frac{d\omega_3}{\omega_3} f(\theta_3) d\Omega_3\right)$

etc.

$$\therefore \sigma_{\substack{\text{scattering with} \\ \text{any no. of } \gamma\text{'s emitted}}} = \sigma_A C' e^{\int \frac{d\omega}{\omega} f(\theta) d\Omega}$$

The divergence ("infared catastrophe") comes from the the fact that the integral in the exponential doesn't converge.

However $C' = e^{-\int_0 \frac{d\omega}{\omega} f(\theta) d\Omega}$ is the contribution of the low energy virtual photons, so $\sigma_{scatt.}$ is finite

The analysis implies that $\sigma_{no\ photons} = \sigma_A C' = 0$

Experimentally, there is an energy Δ such that photons with a total energy $< \Delta$ are not observed. So we measure σ of emitting no photon with energy $> \Delta$

$$\sigma_{(E(\gamma)<\Delta)} = \sigma_{no\ photon} + \sigma_{\substack{one\ photon \\ \omega_1 < \Delta}} + \sigma_{\substack{2\gamma's \\ \omega_1+\omega_2<\Delta}} + \cdots .$$

$$= \sigma_A C' \left(1 + \int_\varepsilon^\Delta \frac{d\omega}{\omega} f + \frac{1}{2} \int_\varepsilon^{\Delta-\omega_2} d\omega_1 \int_\varepsilon^{\omega_2} d\omega_2' \underbrace{f(\omega_1) f(\omega_2')}_{\omega_1, \omega_2'} + \cdots \right)$$

$$= \sigma_A e^{-\int_\varepsilon^\Delta \frac{d\omega}{\omega} f} \left(1 + \frac{2\alpha}{\pi} \log \Delta/\varepsilon + \frac{1}{2}\left(\frac{2\alpha}{\pi}\right)^2 (\log \Delta/\varepsilon)^2 + \cdots \right)$$

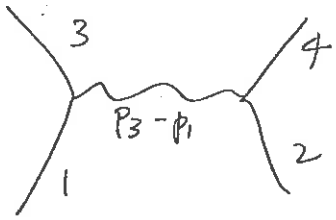
$$= \sigma_A e^{-\frac{2\alpha}{\pi}(\log \frac{m}{\varepsilon} - \log \Delta/\varepsilon)}$$

$$= \sigma_A e^{-\frac{2\alpha}{\pi} \log m/\Delta} = \sigma_A \left(\frac{m}{\Delta}\right)^{-2\alpha/\pi}$$

this can be a large correction

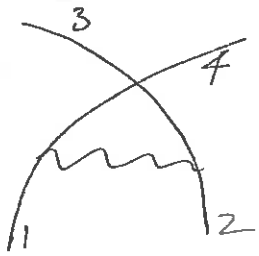
we will show later how to calculate C'.

Additional rules for calculating diagrams: $e^- - e^-$ scattering



$$\mathcal{M}_A = (\sqrt{4\pi e^2})^2 \frac{\bar{u}_4 \gamma_\mu u_2 \; \bar{u}_3 \gamma_\mu u_1}{(p_1 - p_3)^2} = A$$

A is the full amplitude for $e^- - \mu^-$ scattering but not for $e^- - e^-$ scattering because there is the exchange possibility:



$$\mathcal{M}_B = -(\sqrt{4\pi e^2})^2 \frac{\bar{u}_4 \gamma_\mu u_1 \; \bar{u}_3 \gamma_\mu u_2}{(p_1 - p_4)^2}$$

The minus sign in this contribution to the amplitude comes from the rule of Fermi statistics for electrons, because B differs from A only in that the two outgoing electrons are interchanged.

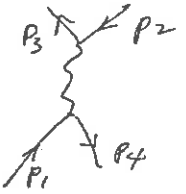
$e^- - e^+$ scattering

$-p_4$ = 4 momentum of incoming e^+

The matrix element is the same as A above.

What corresponds to the exchange diagram for $e^- - e^-$ scattering?

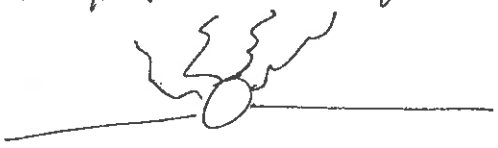
The analog is the annihilation diagram



This is the same as the first diagram rotated 90° together with the exchange of two electron exit lines (3 and 4) $\Longrightarrow$ relative minus sign in the amplitude.

That this additional term in the $e^- e^+$ amplitude is present has been checked experimentally to better than 10% by observations of the energy level spectrum of positronium. The "annihilation force" causes a shift in the energy levels from those expected on the basis of pure coulomb attraction.

A technique for calculating unpolarized cross-sections:



single incoming
and single outgoing electron

$$\text{Rate} = \ldots |\bar{u}_2 N u_1|^2$$

Suppose the incoming particle is unpolarized and the spin of the final particle is not measured

$$\text{then rate} = \ldots \sum_{\substack{\text{spins} \\ 1,2}} |\bar{u}_2 N u_1|^2 = \ldots \sum \bar{u}_2 N u_1 (\bar{u}_2 N u_1)^*$$

Let $\bar{N}$ be defined by $(\bar{g} N f)^* = (\bar{f} \bar{N} g)$ (it is easy to see $\bar{N} = \gamma_t N^\dagger \gamma_t$)

$$\text{then rate} = \ldots \sum_{\text{spins } 1,2} \overbrace{|\bar{u}_2 N u_1|^2}^{X}$$

$$X = \sum_{\substack{\text{spin 1} \\ \text{spin 2}}} (\bar{u}_2 N u_1)(\bar{u}_1 \bar{N} u_2) = \sum_{\substack{\text{spin 1} \\ \text{spin 2}}} \bar{u}_2 N \frac{\not{p}_1 + m}{2m} u_1 \bar{u}_1 \bar{N} u_2$$

$$= \sum_{\substack{\text{spin 2}, \\ r=1}}^{r=4} \bar{u}_2 N \frac{\not{p}_1 + m}{2m} u_r \bar{u}_r \bar{N} u_2 \qquad \text{since } (\not{p}_1 + m) u_3 = 0 = (\not{p}_1 + m) u_4$$

$$\text{Now } \sum_{r=1}^{4} u_r \bar{u}_r = 2m I \quad , \; I = \text{identity matrix}$$

$$\text{So } X = \sum_{\text{spin 2}} \bar{u}_2 N \frac{\not{p}_1 + m}{\cancel{2p_1}} \bar{N} u_2 = \sum_{r=1}^{4} \bar{u}_r N \frac{\not{p}_1 + m}{\cancel{2p_1}} \bar{N} \frac{\not{p}_2 + m}{2m} u_r$$

$$= \text{trace}\left(N \frac{(\not{p}_1 + m)}{\cancel{(p_1 + m)}} \bar{N} (\not{p}_2 + m) \right)$$

Aids: $\text{Tr } I = 4$, $\text{Tr } \gamma_\mu = 0$, $\text{Tr } \gamma_x \gamma_y = 0$, Tr (product of any 3 γ's) $= 0$, $\text{Tr } \gamma_5 = 0$.

PH 205c

May 8,9,12

INTENSITY DISTRIBUTION OF BREMSTRAHLUNG RADIATION

Consider the factor $\frac{p_1 \cdot e}{p_1 \cdot k} - \frac{p_2 \cdot e}{p_2 \cdot k}$, which may be interepreted as the probability that an electron emit a soft photon of momentum k in going from momentum p_1 to momentum p_2

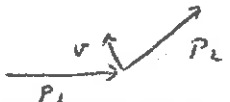
$$p_1 \cdot k = k[E_1 - p_1 \cos\theta_1]$$

$$p_1 \cdot e = -p_{1x} e_x - p_{1y} e_y = p_1 \sin\theta$$

Hence we obtain a function of shape

$$\frac{v_1 \sin\theta_1}{1 - v_1 \cos\theta_1} - \frac{v_2 \sin\theta_2}{1 - v_2 \cos\theta_2}$$

A non-relativistic interpretation of this is to examine the electron before and after

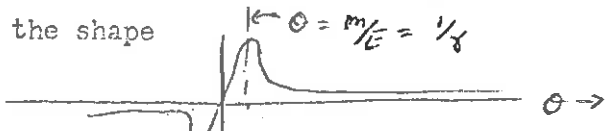


The electron is accelerated in the direction Δv by the scattering, and hence must emit light. Detailed comparison of the above result with classical results (see Jackson, around p. 472) is left as a exercise for the student.

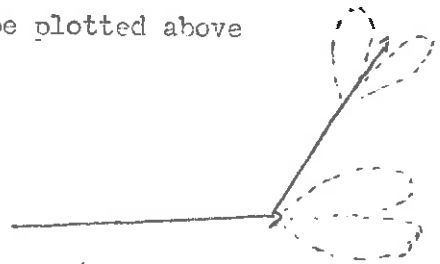
In the highly relativistic region, where $v_1 \sim c$, $p = \sqrt{E^2 - m^2} \to E - \frac{m^2}{2E}$

Thus $\frac{p \sin\theta}{E - p\cos\theta} \to \frac{E\theta}{\frac{E}{2}\left[\theta^2 + \frac{m^2}{E^2}\right]} \sim \frac{\theta}{\theta^2 + \left(\frac{m}{E}\right)^2}$

This takes on the shape



When the deflection angle due to scattering is big compared to $1/\gamma$, then either one or the other of the above terms is big, and the radiation emitted takes on the shape plotted above



For small angle scattering the shape gets more complicated

Notice that if you emit two identical particles, some care must be taken in obtaining a final answer.

Suppose you wish to measure the differential cross section and total rate for a process in which 2 photons are emitted, along with some other stuff. Assume you have one photon counter.

Every time any photon hits the counter, it records a count. For each such count, the other photon could have gone anywhere. Thus the rate measured by the counter when it is placed at angle Ω_1 is $\frac{d\sigma}{d\Omega_1}$ - the differential cross section for particle 1, where we define particle 1 as the one that hit the counter.

That is, the answer got by integrating the familiar expression over Ω_2 gives the cross section to measure the emission of some photon into angle $d\Omega_1$. We have no way of telling whether this is the "red" photon or the "blue" one in the Feynman diagram, and we don't care.

If we now integrate over angles Ω_1, we are summing cases like

where 1 and 2 have been assigned simply on the basis of the counter position. These cases are indistinguishable.

To get a total rate, all we want is the probability that the reaction went. $\int \frac{d\sigma}{d\Omega_1 d\Omega_2} d\Omega_1 d\Omega_2$ gives twice this probability. Hence, in obtaining a total rate, we must divide the final integral by $n!$, where n is the number of indistinguishabl particles in the final state.

MORE ABOUT THE DIRAC EQUATION

Velocity in Dirac language

$$H = \beta m + \vec{\alpha} \cdot (\vec{p} - \vec{A}) + V \quad \Rightarrow \quad \dot{x} = i [H, x] = \alpha_x$$

Hence one would like to find some interpretaion for α_x in terms of particle velocity

However, $\alpha_x^2 = 1$; thus the eigenvalues are ± 1, and this seems to imply that a measurement of the velocity in the x direction would yield $\pm c$

This has caused some concern.

Diracis explanation:

To measure the velocity, you must measure the position twice. But the first accurate measurement of position would make the momentum totally uncertain, and thus you would measure c.

A measurement of average velocity, given by $v^2 = \left(\frac{x_{t+T} - x_t}{T}\right)^2$ would give roughly $\left(\frac{p}{\sqrt{p^2+m^2}}\right)^2$ if $T > \hbar/m$ (can you show this?) but measurement of the instantaneous value would come out wrong.

Feynman's explanation

Dirac's logic is wrong. For $[\alpha_x, p_x] = 0$ implies they can be measured simultaneously. If one fumbles around, one finds that it is indeed possible to construct a solution of the Dirac equation which has a definite eigenvalue of α_x and p_x ; but such a solution does not have a definite energy. In order to be a solution with definite momentum p, it must have energy $\pm\sqrt{p^2+m^2}$. Hence the solution in question must be some mixture of electron and positron.

Given that the system must have a certain net charge, the Dirac equation can describe systems with one electron or one electron and pair(s); thus α_x is not necessarily a single particle operator and might better be thought of as a sort of current density

The commutators of such operators as $\alpha_x\alpha_y\alpha_z$, $\beta\alpha_x\alpha_y\alpha_z$ etc. with the Hamiltonian have not been completely explored.

RELATIVISTIC INVARIANCE OF DIRAC EQUATION

So far we have calculated all answers with a given set of γ matrices. But we have assigned a Lorentz index to these matrices and treated them like a 4 vector. How, then, do we know we are using the right γ's ? Why don't we use some $\gamma_\nu' = a_\nu{}^\mu \gamma_\mu$ with the transformation $a_\nu{}^\mu$ depending on the frame of the problem?

A clever answer to this is to say that if you read your Dirac equation off some moving system with a telescope, it wouldn't change anything. This argument, however, doesn't get to the core of the problem. The explanation of this apparent paradox is that γ_μ and $a_\mu{}^\nu \gamma_\nu$ are related by an equivalence transformation. Provided they are used with solutions of the Dirac equation that are transformed in the same way, all answers will be independent of the representation used.

To discover in general the conditions that we have the same physics with different matrices

$$[\gamma_\mu(i\nabla_\mu - A_\mu) + m]\psi = 0$$

Define $\psi'' = S\psi$, where S is a matrix of constants

Then $[\gamma_\mu''(i\nabla_\mu - A_\mu) + m]\psi'' = 0$ will be equivalent to the above

if $S\gamma_\mu S^{-1} = \gamma_\mu''$ $\qquad \gamma_\mu = S^{-1}\gamma_\mu'' S$

This sort of transformation preserves all algebraic relations between the matrices (in particular their commutation relations)

However, we must demand one more thing in order that the physics be unchanged.

Matrix elements must also be preserved. $\bar{\psi} A \psi = \bar{\psi}'' A'' \psi''$

Hence $\bar{S} = \gamma_0 S^\dagger \gamma_0$ must equal S^{-1}

Then an equivalence transformation by any S such that $\bar{S} = S^{-1}$ leaves ~~anything~~ every thing unchanged.

Relativistic Adjoints

$(\bar{f} M g)^\dagger = \bar{g} \bar{M} f$ defines $\bar{M} = \beta M^\dagger \beta$

For matrices A, B, C and constants α ,

$\overline{(\alpha AB\cdots C)} = \alpha^* \bar{C} \cdots \bar{B}\bar{A}$ $\qquad \bar{\gamma}_\mu = \gamma_\mu$

Hence the relativistic adjoint of any number of γ matrices is got simply by reversing their order

EXAMPLES of Useful Equivalence Transformations

1) Define w by $v/c = \tanh w$

Then the velocity transformations assume a form similar to that for rotations

For the velocity transform in z direction,

$$\gamma_z \to (\cosh w)\gamma_z - \gamma_t \sinh w$$
$$\gamma_x \to \gamma_x$$
$$\gamma_y \to \gamma_y$$
$$\gamma_t \to (\cosh w)\gamma_t - (\sinh w)\gamma_z$$

If $S = e^{w/2 \gamma_t \gamma_z}$, then $S^{-1} = e^{-w/2 \gamma_t \gamma_z} = \bar{S}$

$$\bar{S} = \gamma_0 S^\dagger \gamma_0 = \gamma_0 e^{-w/2 \gamma_z^\dagger \gamma_t^\dagger} \gamma_0 = e^{-w/2 \gamma_0 \gamma_z^\dagger \gamma_t^\dagger \gamma_0} = e^{-w/2 \gamma_t \gamma_z}$$

using $e^A = 1 + A + \frac{1}{2} A\cdot A + \frac{1}{3!} A\cdot A\cdot A + \cdots$

Expansion shows that

$$S = \cosh w/2 + \gamma_t \gamma_z \sinh w/2$$
$$S^{-1} = \cosh w/2 - \gamma_t \gamma_z \sinh w/2$$

2) Show that the corresponding rotation operator is $S = e^{\theta/2 \gamma_x \gamma_y}$

Then

$$\psi'(x,y,z,t) = e^{\theta/2\,\gamma_x\gamma_y}\,\psi(x\cos\theta+y\sin\theta,\,-x\sin\theta+y\cos\theta,\,z,t)$$

$$\overset{\text{1st order}}{\approx} (1+i J_z\theta)\psi \quad\Rightarrow\quad J_z = L_z + \tfrac{1}{2}\sigma_z$$

(work through the algebra to get some familiarity)

Using this definition of $\vec{J}$, one can show for the Dirac equation that if there is no vector potential, and if $V(\vec{r}) = V(r)$, then angular momentum is a constant of the motion

PROBLEM: See how much you can get from the non-relativistic point of view of the formula

$$2m\Delta m = (\text{const})\, e^2 4\pi \int \frac{[\bar{u}\gamma_\mu(\not p - \not k + m)\gamma_\mu u]}{\{(p-k)^2 - m^2\}\,(2\pi)^4\,k^2}\, d^4k$$

for the correction in mass of an electron of momentum p due to second order interactions with the electromagnetic field

Hint: If you start with transverse waves you will get only the γ_t piece. There is also a longitudinal contribution to the self energy, which looks like e^2/r_{ii}

COMPUTATIONAL AIDS

Spin summations for electrons and positrons

$$\sum_{\substack{\text{spins of } u_1 \\ \text{for + energy} \\ \text{states}}} \bar{u}_3 A u_1 \bar{u}_1 B u_2 = \sum_{\substack{\text{all } u_1 \\ \text{states}}} \bar{u}_3 A(\not p_1 + m) u_1 \bar{u}_1 B u_2 = \bar{u}_3 A(\not p_1 + m) B u_2$$

Thus

$$\sum_{u_1 \text{ spins}} |\bar{u}_2 M u_1|^2 = \bar{u}_2 M(\not p_1 + m)\bar{M} u_2$$

$$\sum_{u_2 \text{ spins}} \bar{u}_2 M(\not p_1 + m)\bar{M} u_2 = \mathrm{Tr}\,[M(\not p_1 + m)\bar{M}(\not p_2 + m)]$$

To calculate the traces:

$$\mathrm{Tr}\,1 = 4 \qquad \mathrm{Tr}\,\gamma_x = 0$$

Trace of any odd number of γ's is 0

Terminology $\mathrm{Trace}(X) = \mathrm{Spur}(X)$

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA) \qquad \mathrm{Tr}(ABC) = \mathrm{Tr}(BCA)$$

$$\mathrm{Sp}\,\not a \not b = 4\,a\cdot b \qquad \mathrm{Sp}\,\not a = 0 = \mathrm{Sp}(\not a \not b \not c)$$

$$\mathrm{Sp}(\not a \not b \not c \not d) = 4[a\cdot b\, c\cdot d - a\cdot c\, b\cdot d + a\cdot d\, b\cdot c]$$

Always try to use the Dirac equation $\not p u = mu \qquad \not p v = -mv$

to reduce the number of γ matrices in the matrix element before taking traces

There are tricks for taking traces of any number of γ matrices, but in practice even 6 γ matrices in a row lead to headaches. If you find you have to take traces of more than 4 γ's, it is worth trying to find some simplification. One helpful thing in problems involving photons is

Summing over Polarizations

Suppose you get something like

$$\sum_{\substack{\text{light} \\ \text{polarizations}}} Sp[\ \cdots\ \not{e}_1\ \sim\ \not{e}_1\ \cdots\ ]$$

Provided you have not used special properties of e_1 in some gauge (like assuming it has no time component) then the summation over transverse directions of the light can be replaced by

$$\not{e}_1 \sim \not{e}_1 \longrightarrow \gamma_\mu \sim \gamma_\mu$$

where summation is implied (also multiply the mess by -1)

Reason:

Gauge invariance implies that replacing e_1 by k_1 should give 0. If

$e_1 \leftrightarrow (0, e_x, e_y, 0)$ then $k_1 = (k, 0, 0, k)$

and gauge invariance says

$$k[(\gamma_t \sim \gamma_t) - (\gamma_z \sim \gamma_z)] = 0$$

Hence $\gamma_\mu \sim \gamma_\mu$ boils down to $-\{(\gamma_x \sim \gamma_x) + (\gamma_y \sim \gamma_y)\}$

which is what you expect from the property $\sum_{\substack{\text{polarizations} \\ j}} e^j_i e^j_k = \delta_{ik}$

(i and k are spacelike)

Once the quantity is in the form

$$\cdots \gamma_\mu \cdots \gamma_\mu \cdots$$

one then uses $\gamma_\mu \gamma_\mu = 4$

$\gamma_\mu \not{a} \gamma_\mu = -2 \not{a}$

$\gamma_\mu \not{a} \not{b} \gamma_\mu = 4\, a \cdot b$

Thus each summation over photon polarizations reduces the number of γ matrices in the trace by 2

SUMMARY OF RULES

$$\text{Prob. of } \frac{\text{Transition}}{\text{sec}} = 2\pi \rho(E) \prod_{in} \left(\frac{1}{2E_i}\right) \prod_{out} \left(\frac{1}{2E_i}\right) |\mathcal{M}|^2$$

$$= (2\pi)^4 \delta^4(p_{in} - p_{out}) \left[\prod_{out} (2\pi)\, \delta(p_i^2 - m_i^2)\, \frac{d^4 p_i}{(2\pi)^4}\right] \prod_{in} \left(\frac{1}{2E_i}\right) |\mathcal{M}|^2$$

where $\mathcal{M}$ is a relativistically invariant matrix

Using the normalization $\bar{u} u = 2m$ $\qquad e_\mu e_\mu = -1$

gives as the sum over states $Sp\{(\not{p}_1 + m)\, \mathcal{M}\, (\not{p}_2 + m)\, \bar{\mathcal{M}}\}$

Calculation of $\mathcal{M}\mathcal{M}$

Electron propagator $\frac{i}{\not p - m + i\varepsilon}$

Photon propagator $\frac{-i}{k^2 + i\varepsilon}$

Spin 0 meson propagator $\frac{i}{p^2 - m^2 + i\varepsilon}$

Couplings:

Fermions to a real photon $-i \not\epsilon \sqrt{4\pi e^2}$

Fermions to a potential $\not A(q) = \int e^{-iq\cdot x} \not A(x) d^3x$

To a virtual photon $(-i\sqrt{4\pi e^2})\gamma_\mu \quad \cdots \quad \gamma_\mu (-i\sqrt{4\pi e^2})$

To pseudoscalar meson $\sqrt{4\pi g^2}\ \gamma_5 \quad \cdots \quad \gamma_5 \sqrt{4\pi g^2}$

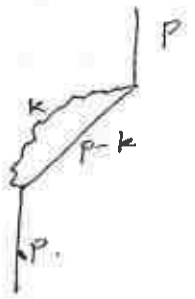
To scalar meson $\sqrt{4\pi g^2} \quad \cdots \quad \sqrt{4\pi g^2}$

For a closed loop of electrons, the rule is $-\mathrm{Sp}$.

If there is an indeterminate momentum, sum by $\int \frac{d^4p}{(2\pi)^4}$

Week 8 May 15, 16 Ph 205c

The correction to the energy of a free electron due to the interaction of the electron with its own electromagnetic field is represented in lowest order perturbation theory by the diagram



and this corresponds to

$$\Delta E^2 = 4\pi e^2 \int \bar{u}\,\gamma_\mu \frac{1}{\not p - \not k - m}\,\gamma_\mu\, u\, \frac{d^4k}{(2\pi)^4 k^2}$$

$$= \frac{4\pi e^2}{(2\pi)^4}\int \bar{u}\,\gamma_\mu \frac{[\not p - \not k + m]}{(p-k)^2 - m^2 + i\varepsilon}\gamma_\mu\, u\, \frac{d^4k}{k^2 + i\varepsilon}$$

This formula may be obtained from the expression for the second order correction to the energy of a state in ordinary perturbation theory:

$$\Delta E_i = \sum_n \frac{H'_{in} H'_{ni}}{E_i - E_n}\,, \quad \text{with } H' = \text{perturbation} = e(\underline{\alpha}\cdot\underline{A} - \phi) \text{ in our case}$$

ΔE^2 will turn out to be logarithmically divergent

$$\Delta E^2 = \frac{4\pi e^2}{(2\pi)^4}\int \bar{u}\,\frac{1}{k^2 + i\varepsilon}\,\frac{(-2\not p + 2\not k + 4m)}{(p-k)^2 - m^2 + i\varepsilon}\,u\; d^4k$$

$$= \frac{4\pi e^2}{(2\pi)^4}\int \frac{(-4m^2 + 4p\cdot k + 8m^2)}{(k^2 + i\varepsilon)\,[(p-k)^2 - m^2 + i\varepsilon]}\,d^4k$$

since $\bar{u}\gamma_\mu u = \frac{p_\mu}{m}\bar{u}u$

For the correction to the rest energy, put $\vec{p} = 0$

Then $p \cdot k = \omega m$

$$(p-k)^2 = k^2 + m^2 - 2\omega m$$

and

$$\Delta m^2 = \frac{4\pi e^2}{(2\pi)^4} \times 4 \int d^4k \; \frac{m(m+\omega)}{(\omega^2 - K^2 + i\varepsilon)(\omega^2 - K^2 - 2\omega m + i\varepsilon)} \qquad K = |\underline{k}|$$

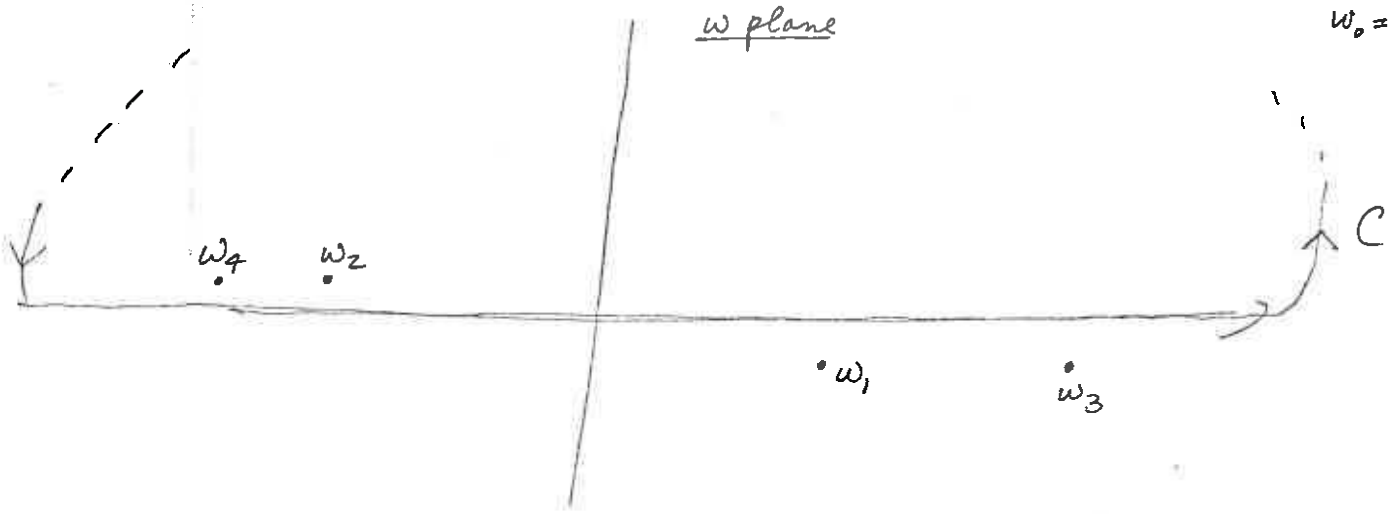
$$= \frac{e^2}{\pi^3} \int_{-\infty}^{\infty} d\omega \int_0^{\infty} 4\pi K^2 dK \; \frac{m(m+\omega)}{(\omega^2 - K^2 + i\varepsilon)(\omega^2 - K^2 - 2\omega m + i\varepsilon)}$$

The integrand has poles as a function of ω at

$$\omega = K - i\varepsilon = \omega_1 \qquad \omega = m + \sqrt{K^2 + m^2} - i\varepsilon = \omega_0 + m = \omega_3$$

$$\omega = -K + i\varepsilon = \omega_2 \qquad \omega = -\sqrt{K^2 + m^2} + m + i\varepsilon = -\omega_0 + m = \omega_4$$

$$\omega_0 = \sqrt{K^2 + m^2}$$



$$\int_{-\infty}^{\infty} d\omega \; \frac{m+\omega}{(\omega - m - \omega_0)(\omega - m + \omega_0)(\omega - \omega_1)(\omega - \omega_2)} = \int_C d\omega \; \frac{m+\omega}{(\underbrace{\omega - m - \omega_0}_{(\omega-\omega_3)})(\underbrace{\omega - m + \omega_0}_{(\omega-\omega_4)})(\omega-\omega_1)(\omega-\omega_2)}$$

where C is the contour shown.

The contribution from the large semicircle vanishes in the limit of infinite radius.

$$\int_C = 2\pi i \,(\text{Sum of residues of poles of integrand inside } C)$$

$$= 2\pi i \left\{ \frac{m-K}{(-2K)\left[\sqrt{K^2+m^2}-m-K\right]\left[-\sqrt{K^2+m^2}-m-K\right]} \right\} \leftarrow \text{res. at } \omega_2$$

$$+ 2\pi i \left\{ \frac{2m-\sqrt{K^2+m^2}}{(-2\sqrt{K^2+m^2})\left[m-K-\sqrt{K^2+m^2}\right]\left[K+m-\sqrt{K^2+m^2}\right]} \right\} \leftarrow \text{res. at } \omega_4$$

$$= 2\pi i \left\{ \frac{K-m}{4K^2m} + \frac{1-\frac{2m}{\sqrt{K^2+m^2}}}{-4m\left(\sqrt{K^2+m^2}-m\right)} \right\}$$

$$2m\Delta m = \frac{e^2}{\pi^2} \times 4m \times 2\pi i \int_0^\infty dK \left\{ \frac{K-m}{4m} - \frac{K^2}{4m} \frac{\left(1-\frac{2m}{\sqrt{K^2+m^2}}\right)}{\sqrt{K^2+m^2}-m} \right\}$$

$$= \frac{2e^2 i}{\pi} \int_0^\infty I(K)\,dK$$

for small K, $I(K)$ is regular.

For large K, $I(K) \simeq K - m - \dfrac{K\left(1-\frac{2m}{K}+\frac{m^3}{K^3}\right)}{\left(1-\frac{m}{K}+\frac{1}{2}\frac{m^2}{K^2}+\cdots\right)}$

$$I(K) \simeq K - m - K\left(1-\frac{2m}{K}\right)\left(1+\frac{m}{K}+\frac{m^2}{2K^2}\right)$$

$$\simeq K - m - K\left(1-\frac{m}{K}-\frac{3m^2}{2K^2}\right) = \frac{3m^2}{2K}$$

∴ If we integrate from 0 to Λ, then the leading term in Λ is

$$\frac{2e^2 i}{\pi} \cdot \frac{3m^2}{2} \log \Lambda$$

which is, as we asserted, logarithmically infinite.

Of course, other cutoff procedures are possible, and we consider now one in more detail.

The cutoff procedure we will adopt is relativistically invariant. It consists of modifying the photon propagator at high energies.

i.e., replace $\frac{1}{k^2}$ by $C(k^2)\frac{1}{k^2}$

where $C(k^2) \longrightarrow 1$ when $k^2 << \Lambda^2$

Λ = cutoff

we choose $C(k^2) = \frac{-\Lambda^2}{k^2-\Lambda^2} \longrightarrow \frac{1}{k^2}$ as $k^2 \to \infty$.

Suppose now that with this cutoff all integrals are convergent (they are not). If the answer for a problem depends on Λ, we consider that we don't know the answer. But if as $\Lambda \to \infty$, a finite limit ensues, then we consider the answer known in quantum electrodynamics.

Discussion of the infinite correction to the electron mass

m_D, the mass that appears in the Dirac Equation is not the physical mass of the electron, because there are corrections to m_D due to the interaction of the electron with the electromagnetic field.

theoretically, $m^2_{exp.} = m_D^2 + \frac{3e^2}{\pi} m_D^2 \left(\log \frac{1}{m} + \frac{3}{8}\right) + O(e^4)$

The problem is of course that $\Delta m^2 = \infty$

m_{exp} is the experimental, measured mass.

Aside: If you look at the mass difference between the neutral and charged pion in the same way, you will obtain a quadratically divergent infinity.

The electromagnetic structure of the pion is simply not known.

Let's look at a problem that we can solve in higher order.

Calculate the shift in ~~one~~ a particular energy level of the hydrogen atom due to the possibility of virtual emission and reabsorption of a photon ~~characteristic~~ by the electron.

obtain $\Delta E_n = E_1 + \frac{i\Gamma_1}{2}$

E_1, Γ_1 are real — Γ_1 gives the lifetime of the state (rate of disintigration)

ground state:

$$Re\ \Delta E_a = E_1 = \Delta m_D + \frac{me^4}{8\pi^2}$$

the infinite correction to m_D to obtain m_{exp}

If you re-express the energy ~~wrong~~ in terms of the physical mass (m_{exp}) rather than m_D, then the correction is finite as $\Lambda \to \infty$.

There are ways of by-passing the infinities such as dispersion theory but at the present time there is no method that is uniformly better than any other method for dealing with higher order corrections in qed.

Theory of β Decay:

Ref. PR 109, 193 (1958), Feyman & Gell-Mann

There are 2 different kinds of neutrinos: ν_e, ν_μ

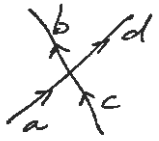
Muon decay occurs as: $\mu \longrightarrow e + \bar{\nu}_e + \nu_\mu$

The neutrinos are massless and obey Dirac's equation. $\not{p} u_\nu = 0$, $p_\nu^2 = 0$

Muon decay, β decay, and other process are described by the weak coupling.

$$\text{Rate} = \ldots\ldots |M|^2$$

where M is derived from a 4 particle point interaction



$a + c \longrightarrow b + d$

$$\mathcal{M} = G\sqrt{8}\,(\bar{u}_d \gamma_\mu a u_c)(\bar{u}_b \gamma_\mu a u_a) = G\sqrt{8}\,(\bar{d}c)(\bar{b}a)$$

abbreviated notation

$\sqrt{8}$ is there for historical reasons

$$a = \frac{1 + i\gamma_5}{2}$$

G is a constant with dimensions: $G M_p^2 = 1.01 \pm .01 \times 10^{-5}$

M_p = mass of proton

For particular weak processes, one must pick a, b, c, d suitably.

For μ decay: $(\bar{e}\nu_e)(\bar{\nu}_\mu \mu)$

and that is the same as for $\nu_e + \mu \longrightarrow \nu_\mu + e$

Problem: Calculate the shape of the energy spectrum in μ decay.

Aside: There is the IVB (intermediate vector boson) theory which says that ~~proto~~ $\mu + \nu_e \to e + \nu_\mu$, for example, is

i.e., that the interaction is mediated by a vector boson, but that the point interaction description is a good approximation because the IVB (called the W particle) is massive, and therefore corresponds to a short range force

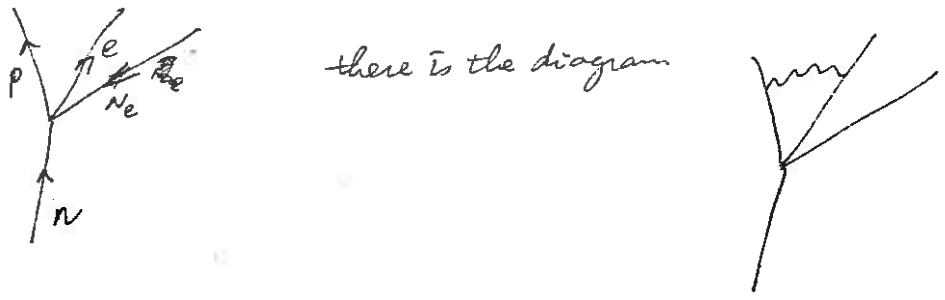
The interaction is written $G\sqrt{8}\, J_\mu^\dagger J_\mu$

where $J_\mu = (\bar{e}\nu_\mu \gamma_\mu a \nu_\mu) + (\bar{\nu}_e \gamma_\mu a e) + J_\mu^{\text{hadrons}}$

J_μ^{hadron} = weak current of strongly interacting particles ($n, p, \pi, K, \Lambda, \ldots$)

Problem: Calculate the rate of any weak process that interests you.

Aside: One can also do electromagnetic corrections to weak processes. For example, in ~~p decay~~ neutron β decay



there is the diagram

Returning now to the problem of infinities in qed, we write

$$\frac{C(k^2)}{k^2} = \frac{-\Lambda^2}{(k^2-\Lambda^2)\,k^2} = \frac{1}{k^2} - \frac{1}{k^2-\Lambda^2}$$

the first term is the one obtained from a massless photon
the second is obtain from a photon of mass Λ that couples to an imaginary charge. The charge is imaginary because what was $4\pi e^2$ is now $-4\pi e^2$. The imaginary charge implies that the hamiltonian is non-hermitean, and so unitarity is violated.

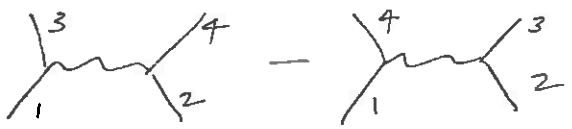
In the limit $\Lambda \to \infty$, things seem to be OK, but that has never been proved.

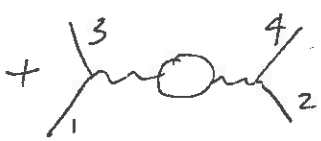
I do not believe that everything has been straightened out. The evaders always have a weak point in their arguments where they cannot prove anything.

Question: Is the final answer consistent with unitarity?

The procedures $\left\{ \begin{matrix} m_0 \to m_{exp.} \\ \frac{1}{k^2} \to \frac{C(k^2)}{k^2} \end{matrix} \right\}$ in all calculations ~~does~~ do ~~not straighten~~ not straighten out all infinities

Ex. e-e scattering in 4th order

$M =$  $-$

$+$  $-$ 

The 4th order diagrams give a contribution $e^2\left(1+e^2 \log\frac{\Lambda'}{m_0}\right)\gamma_\mu \cdots \gamma_\mu$

If then we identify

$$e^2_{exp} = e^2_{th}\left(1 + e^2_{th} \log \frac{\Lambda'}{m_e} + \dots\right)$$

and say that e^2_{exp} = observed charge

e_{th} = unrenormalized ("theoretical") charge

we once again have an infinite renormalization.

If now we find the rate, in any order, of a process

$$\text{Rate} = \Gamma(m_0, e_{th}, \Lambda, \Lambda') = G(m_{exp.}, e_{exp.}, \Lambda, \Lambda')$$

then $\lim_{\substack{\Lambda\to\infty \\ \Lambda'\to\infty}} G(m_{exp}, e_{exp}, \Lambda, \Lambda')$ exists.

The process of finding $m_{exp} = m_{exp}(m_0, \Lambda)$

and $e_{exp} = e_{exp}(e_{th}, \Lambda')$

is known as mass and charge renormalization.