**Ph 205a: "ADVANCED QUANTUM MECHANICS"**

Richard P. Feynman

### I. Time-Dependent Perturbation Theory

<table>
<thead>
<tr>
<th>A. First-Order Perturbation Theory</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Introduction</td>
<td>1</td>
</tr>
<tr>
<td>2. First Born Approximation</td>
<td>8</td>
</tr>
<tr>
<td>3. Space-limited Central Potential</td>
<td>12</td>
</tr>
<tr>
<td>4. Oscillating Perturbations</td>
<td>18</td>
</tr>
<tr>
<td>5. Interaction with a Quantum Oscillator</td>
<td>20</td>
</tr>
<tr>
<td>6. Nuclei in a Magnetic Field (NMR)</td>
<td>25</td>
</tr>
<tr>
<td>7. Interaction with a System of Oscillators</td>
<td>28</td>
</tr>
<tr>
<td>8. Atomic Fractions in a Crusty</td>
<td>31</td>
</tr>
<tr>
<td>10. Resonating of Classical Systems</td>
<td>45</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>B. Higher Order Time-Dependent Perturbation Theory</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Time-Dependent Perturbation</td>
<td>54</td>
</tr>
<tr>
<td>2. Conservation of Probability (Continuity)</td>
<td>59</td>
</tr>
<tr>
<td>3. Scattering of Light from an Atom</td>
<td>62</td>
</tr>
<tr>
<td>4. Roton Excitation Problem</td>
<td>74</td>
</tr>
<tr>
<td>5. Improvements to the Theory - Coupling with Continuum States</td>
<td>79</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>C. Alternative Formulations</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Evolution Operators U(t, t')</td>
<td>95</td>
</tr>
<tr>
<td>2. Integral Formulations</td>
<td>97</td>
</tr>
<tr>
<td>3. Some Properties of H -- Ordering Indices</td>
<td>98</td>
</tr>
<tr>
<td>4. Newman Series</td>
<td>101</td>
</tr>
<tr>
<td>5. Interpretation by Feynman Diagram</td>
<td>104</td>
</tr>
<tr>
<td>6. Physics of the hammock V</td>
<td>106</td>
</tr>
<tr>
<td>7. T-Matrix</td>
<td>110</td>
</tr>
<tr>
<td>8. Kohn-Sham Problem (Kohn-Sham, Pies)</td>
<td>114</td>
</tr>
</tbody>
</table>
II. Angular Momentum

A. Rotation Groups
   1) Rotation of States
   2) Construction of Angular Momentum Operators
      (Generators of Rotation Groups)
   3) Restrictions on the Eigenvalues of \( J \)

B. Combination of Angular Momentum
   1) Introduction
   2) Method 1
   3) Method 2
   4) Method 3

C. Another Example of Group Ideas
   1) Isotopic Spin
   2) The Eightfold Way

D. Calculation of Matrix Elements
   1) Example: Spin \( \frac{1}{2} \)
   2) General Procedure

III. The Quantum Theory of Solids

A. Introduction
   1) Types of Solids
   2) Review of Statistical Mechanics

B. Nuclear Vibrations in a Solid
   1) Construction of Hamiltonian
   2) Classical Harmonic Oscillator
3. Quantum Harmonic Oscillator 152
4. Elastic Neutron Scattering from Solids 154
5. Calculation of Matrix Elements of SHM 158
6. Creation and Annihilation Operators 162
7. Lattice Vibrations 166
8. Solution for Eigenfrequencies 174
9. Specific Heat 178
10. Continuum Approximation 187
11. Analogy with Quantum Electrodynamics 191

C. Electron Theory of Metals 195
1. Degenerate Electron Gas 200
2. Electron Motion in Periodic Potentials 203
   a. Weak potential approximation 205
   b. Strong potential approximation 208
3. Coulomb Interactions in Fermi Gas 210
4. Conductivity of Metals 211

D. Creation Operators for Electrons 214
1. Introduction 214
2. Electron-Electron Interactions 224
3. Theory of Holes 228

IV. Relativistic Quantum Mechanics 230

A. Introduction 235
1. Example of Coulomb-Scattering 236
2. Relativistic Mechanics 238

B. Dirac Equation 239
1. Motivation 239
2. Various Representations 241
3. Non-relativistic Form -- Spin 250
Ph 205a        ADVANCED QUANTUM MECHANICS

R.P. Feynman

I. Scattering

II. Solid State Physics

III. Relativistic Quantum Theory

Find a relativistically invariant S-equation.

TIME-DEPENDENT PERTURBATION THEORY

A. First-Order Perturbation Theory

1) The time evolution of a state is given by

\[ -\frac{i}{\hbar} \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \]  \hspace{1cm} (1)

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

\[ H(t) = H_0 + V(t) \]  \hspace{1cm} (2)

First consider the related problem for \( V = 0 \)

\[ -\frac{i}{\hbar} \frac{d}{dt} |\psi(t)\rangle = H_0 |\psi(t)\rangle \]  \hspace{1cm} (3)

*All problems are decided by 4, and are to be worked without reference to books.
*Here \( \hbar = c = 1 \)
Assume we can solve this by
\[ |\psi(t)\rangle = \sum_n c_n(t) |\phi_n\rangle \]
where the $|\phi_n\rangle$ are defined by the eigenvalue problem
\[ H_0 |\phi_n\rangle = E_n |\phi_n\rangle \]
and
\[ c_n(t) = \langle \phi_n | \psi(t) \rangle \]
If we plug our expansion (4) into (3) we find
\[ -i \frac{d}{dt} c_n(t) = E_n c_n(t) \]
on solving directly
\[ c_n(t) = a_n e^{-i E_n t} \]

Since this worked for $V(t) = 0$, suppose we try it again
for $V(t)$ small
\[ -i \frac{d}{dt} |\psi(t)\rangle = \left[ H_0 + V(t) \right] |\psi(t)\rangle \]
and write again
\[ |\psi(t)\rangle = \sum_n c_n(t) |\phi_n\rangle \]
Substitute into (8)
\[ \sum_n \langle \phi_n | -i c_n(t) |\phi_n\rangle = \sum_n \langle \phi_n | H_0 |\phi_n\rangle + \sum_n \langle c_n(t) | V(t) |\phi_n\rangle \]
Take the scalar product with \( \langle \phi_m \rangle \) and use orthogonality to find

\[
-\frac{i}{\hbar} \dot{C}_m(t) = E_m C_m(t) + \frac{\langle m | V(t) | n \rangle}{V_{mn}(t)} C_n(t)
\]

(11)

Note: \( V(t) \) is small, try a solution like

\[
C_m(t) = e^{-iE_m t} \chi_m(t)
\]

(12)

\[\text{Note: } |C_m(t)|^2 = |\chi_m(t)|^2 = \text{prob. of being in state } m \text{ at time } t\]

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

\[\text{Plug this into (11)}\]

\[
-\frac{i}{\hbar} \dot{\chi}_m(t) = \frac{\langle m | V(t) | n \rangle}{V_{mn}(t)} \chi_n(t) e^{i(E_n - E_m) t}
\]

(13)

\[
= \frac{\langle m | V(t) | n \rangle}{V_{mn}(t)} \chi_n(t)
\]

(14)

This is still exact and gives 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.,

$$\lambda_{lk} = \langle \phi_1 | V(t) | \phi_k \rangle = \int \langle \phi_1 | V(t') | \phi_k \rangle dt'$$

Claim: We can solve this problem for given $k$ and $l$, we can solve it for any $k$, $l$.

Thus our initial condition becomes

$$+ = 0: \quad \lambda_5(0) = \delta_{5k}$$

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

$$\lambda_k(t) = \lambda_k(0) - i \int_0^t \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \left[ \lambda_{5k}(0) - i \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \lambda_{5k}(t''') \lambda_{5l}(t''') dt'''' dt''' dt'' dt' \right] dt$$

$$= \lambda_k(0) - i \int_0^t \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \left[ \lambda_{5k}(0) - i \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \lambda_{5k}(t''') \lambda_{5l}(t''') dt'''' dt''' dt'' dt' \right] dt'' dt''' dt'''' dt'$$

$$+ (-i)^2 \int_0^t \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \lambda_{5k}(t''') \lambda_{5l}(t''') dt'''' dt''' dt'' dt'$$

$$+ (-i)^2 \int_0^t \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \lambda_{5k}(t''') \lambda_{5l}(t''') dt'''' dt''' dt'' dt'$$

$$+ (+i)^3 \int_0^t \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \lambda_{5k}(t''') \lambda_{5l}(t''') dt'''' dt''' dt'' dt'$$

$$+ \ldots$$
\[ \ldots + (-i)^N \int_0^T \int_0^T \ldots \int_0^T \ldots \sum_{n} \sum_{m} v_{mn}(t') \ldots v_{mn}(t) \sum_{n} \sum_{m} v_{mn}(t') \ldots v_{mn}(t) \nonumber \]

Now using our i.c. \( \chi_0(0) = \xi_{ek} \) in our general "solution" for \( \chi_{nk}(t) \):

\[ \chi_{nk} = \langle \xi_{ek} | V(t) | \eta_k \rangle \]

\[ = \chi_{ek}(t) \]

\[ = \xi_{ek} + (-i) \int_0^T \sum_{n} v_{nk}(t') \xi_{nn} dt' + (-i)^2 \int_0^T \int_0^T \sum_{n} \sum_{m} v_{mn}(t') v_{mn}(t) \xi_{nn} \xi_{mm} dt' \sum_{n} \sum_{m} v_{mn}(t') v_{mn}(t) \cdots \]

Now suppose our perturbation was constant, i.e. \( V(t) = V \). Then

\[ \chi_{mn}(t') = \sum_{n} v_{mn} e^{i (E_m - E_n) t'} \]

and from (16),

\[ \chi_{nk} = \xi_{ek} + (-i) \int_0^T \sum_{n} v_{nk} e^{i (E_n - E_k) t} dt + \ldots \]

\[ = \xi_{ek} - \frac{e^{i (E_n - E_k) t} - 1}{E_n - E_k} v_{ek} + \ldots \]
Thus
\[
\begin{cases}
\text{prob. } k \to 0 \\
\text{for } k \neq 0
\end{cases}
\]
\[= |\lambda_k|^2 \]
\[= 4 \sin^2 \left( \frac{E_0 - E_k}{2} \right) \frac{|V_{kn}|^2}{(E_0 - E_k)^2} + \ldots \]  

What is wrong with this?
SUMMARY TO DATE

Problem: \(-i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle\)

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

\[\Rightarrow H_0 |\phi_n\rangle = E_n |\phi_n\rangle\]

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

Then find

\[i \phi_n(t) = \sum_n \tilde{\phi}_{nn}(t) \phi_n(t)\]

where \(\tilde{\phi}_{nn}(t) = e^{iE_n t} \langle \phi_n | V(t) | \phi_n \rangle e^{-iE_n t}\)

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

Solution:

\[\phi_n(t_f) = \sum_n \tilde{\phi}_{nn}(t) \phi_n(t_i)\]  

That is, if \(\phi_n(t_i)\) is the coefficient \(n\) at initial time, then the coefficient \(n\) at final time is equal to the sum of each of the \(n\) initial values \(\phi_n(t_i)\) times the amplitude that the state will go into \(\phi_n(t_f)\) at final time. Evidently \(\tilde{\phi}_{nn}(t_f) = \tilde{\phi}_{nn}(t_i)\).

We found

\[\tilde{\phi}_{nn}(t_f) = \sum_n \tilde{\phi}_{nn}(t_i) e^{i(E_n - E_m) t_f} + \sum_{n \neq m} \tilde{\phi}_{nm}(t_i) V_{nm}(t_f) e^{i(E_n - E_m) t_f}

\[+ \sum_{n \neq m \neq k} \tilde{\phi}_{nk}(t_i) V_{nm}(t_f) V_{mk}(t_f) e^{i(E_n - E_m - E_k) t_f} + \cdots\]

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 $\Psi_m(t_f)$ and see what you can find out about $\Psi_m(t_i)$
iii.) check fact that total probability = 1. How does this affect now?
iv.) if $V(t)=V$, can we compare results to energy perturbation theory?
v.) make up several problems (messes, etc.) and work them

2.) The First Born Approximation

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

Return to the d.c. potential where

$$\Psi_m(t) = e^{-i(\hat{E}_m - \hat{E}_n)t} \Psi_m$$

We find from (20)

$$\lambda_{mn} = \frac{e^{-i(\hat{E}_m - \hat{E}_n)t_f} - e^{-i(\hat{E}_m - \hat{E}_n)t_i}}{(\hat{E}_m - \hat{E}_n)}$$

Last time we had

$$t_i = 0$$
$$t_f = T$$

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

$$\left| \lambda_{mn} \right|^2 = \frac{4 \sin^2 \left(\frac{\hat{E}_m - \hat{E}_n}{2}\right) T}{(\hat{E}_m - \hat{E}_n)^2} \left| \Psi_m \right|^2$$

(21)

Note this depends only on the relative time $T$, not on when we turn $V$ on.
Of course we can see that if $E_n - E_m$ is very large, Prob is very small.

Note if $m = n$, we get a $\text{Prob} \sim T^2 |V_{mn}|^2$ 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 notation (21) for $P_{nm}$ gets into trouble since it is too precise. We smear out our separation of the final state by a little and accept the probability of going into a range of states. Then

$$P_{nm} = \frac{4 \sin^2 \left(\frac{E_m - E_n}{2} \right)}{m} \leq \frac{4 \sin^2 \left(\frac{E_m - E_n}{2} \right)}{(E_m - E_n)^2} |V_{mn}|^2$$

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

in the limit $\to \lim$ and all of this contribution to the integral comes from near $E = E_n$:

$$\int_{-\infty}^{\infty} \frac{4 \sin^2 \left(\frac{E_m - E_n}{2} \right)}{E_m - E_n} d(E_m) = 2T \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = 2\pi T$$

Thus we can interpret the individual probabilities and rate as

$$\text{Rate} = \frac{P_{nm}}{\text{area}} = 2\pi \delta(E_m - E_n) |V_{mn}|^2$$

(22)

Fermi's Golden Rule

This doesn't always hold (less than 99.9% of the time), we can modify this to handle a continuous distribution of the initial states.
**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.

[Note as \( t_i \to -\infty, \ t_f \to +\infty \), the \( t_{\text{fin}} \) is frequently denoted by \( S_{\text{fin}} \) in the literature. Thus the origin of S-matrix terminology.]

For \( m \neq n \)

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

where \( \langle \phi_m | V(t) | \phi_n \rangle = V_{mn}(t) \)

But recall the Fourier transform is defined by

\[
\Phi(\omega) = \mathcal{F}\{\phi(t)\} = \int_{-\infty}^{\infty} e^{i\omega t} \phi(t) \, dt
\]

\[
\mathcal{F}^{-1}\{\Phi(\omega)\} = \int_{-\infty}^{\infty} e^{-i\omega t} \Phi(\omega) \, d\omega
\]
We could define the Fourier transform of an operator

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

Thus

\[ S_{mn} = -i \langle m | V^{\text{FT}}(\omega) | n \rangle \]

\[ \omega = E_m - E_n \]

---

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

---

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

\[ V^{\text{FT}}(\omega) = \frac{e^{i\omega t_t} - e^{i\omega t_f}}{i\omega} \]

which is what we found earlier. Thus we can adopt 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 constant-velocity 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

\[ \frac{d}{dt} \mathbf{r} = \frac{q}{m} \mathbf{E} + \frac{q}{m} \mathbf{v} \cdot \mathbf{B} \]

Here we write

\[ H = \frac{\mathbf{p}^2}{2m} + V(r) = \frac{\hbar^2}{2m} \nabla^2 + V(r) \]

Our unperturbed eigenfunctions satisfy the free-particle equation

\[ H_0 \Phi_n = \frac{\hbar^2}{2m} \nabla^2 \Phi_n \]

Thus we identify

\[ \Phi_n = k \]

\[ \Phi_m = k' \]

and in \( r \) representation

\[ \langle \mathbf{r} | k \rangle = \psi_k(r) = \frac{e^{i k \cdot r}}{\sqrt{\text{vol}}} \]

[Note we have used volume normalization of the plane wave: \( \psi_k(r) \).]

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

Then

\[ H_0 |k\rangle = \frac{\hbar^2}{2m} |k\rangle = E_n |k\rangle \]
Now we can compute

\[ V_{mn} = \langle \psi_m | V | \psi_n \rangle = \langle \mathbf{k}_m | V | \mathbf{k}_n \rangle \]

\[ = \int_{\text{vol}} V^{\ast}_m (\mathbf{r}) V(\mathbf{r}) \psi_n(\mathbf{r}) \, d^3r \]

\[ = \int_{\text{vol}} e^{-i \mathbf{k}_m \cdot \mathbf{r}} V(\mathbf{r}) e^{i \mathbf{k}_n \cdot \mathbf{r}} \frac{d^3r}{(\text{vol})} \]

But we can define a 3-dimensional Fourier transform by

\[ V^{\text{FT}}(\mathbf{q}) = \int_{\text{vol}} e^{i \mathbf{q} \cdot \mathbf{r}} V(\mathbf{r}) \, d^3r \]

Thus

\[ V_{mn} = \frac{V^{\text{FT}}(\mathbf{k}_m - \mathbf{k}_n)}{\text{vol}} \]

Try to plug this back into our work and finish the problem. Find the apparent scattering cross-section [not easy]
Recall we had found

\[
\text{Rate at which a system intransformed from state in ten by a perturbation} = 2\pi \delta (E_n - E_m) |\langle m | V | n \rangle|^2
\]

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

\[
E_n = \frac{\hbar^2}{2m} \quad \phi_n = \frac{e^{i k_n r}}{\sqrt{\text{vol}}}
\]

Thus our matrix elements are

\[
V_{mn} = \frac{1}{\text{vol}} \int e^{-i \vec{k}_n \cdot \vec{r}} e^{i \vec{k}_m \cdot \vec{r}} V(r) \, d^3 r = \frac{1}{\text{vol}} V^T(q)
\]

\[
q = \vec{k}_n - \vec{k}_m
\]

**Example:** Coulomb potential \( V(r) = \frac{Ze^2}{r} \)

\[
V^T(q) = \int e^{i q \cdot r} \frac{Ze^2}{r} \, d^3 r = \frac{4\pi Ze^2}{q^2}
\]

\( q \) is charge, \( \frac{Ze^2}{q} = e^2, \quad \frac{e^2}{\hbar c} = \frac{1}{1370365} \)
Thus using (1)

\[
\text{Rate} \propto 8 \pi \left[ \frac{\hbar^2}{2m} \right] \frac{1}{(\text{vol})^2} |V_i(q)|^2
\]

Note the S-fun implies \(|\vec{k}| = |\vec{k}'| \Rightarrow \text{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

No. of states leaving \(\vec{k}\) in range \(d\vec{k}_x d\vec{k}_y d\vec{k}_z = \frac{d^3k}{(2\pi)^3}\)

Consider a rectangular box and quantize the wave function as shown

\[\sin(k_x x) \Rightarrow k_x L_x = n_x \pi\]

Thus

\[n_x \text{ of states in } d\vec{k}_x = \frac{d\vec{k}_x}{\frac{2\pi}{L_x}}\]

Thus

\[\text{No. of states in } \vec{k} = \frac{d\vec{k}}{\frac{2\pi}{L_x} \frac{2\pi}{L_y} \frac{2\pi}{L_z}} = \frac{d^3k}{(2\pi)^3}\]

But these are standing waves composed of two \(e^{i\vec{k}' \cdot \vec{r}}\) waves which come from periodic b.c. Thus factor of \(\frac{1}{2}\) gives the required expression.
Thus

\[ \text{Rate} = 2 \pi S \left[ \frac{k^2}{2m} - \frac{k^2}{2m} \right] \frac{d^3 k'}{\text{vol} \ (2\pi)^3} \left| V'(q) \right|^2 \]

(4)

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

Use

\[ \int S[S(x)] \phi(x) dx = \frac{\phi(x_0)}{f(x_0)} \]

(5)

where \( f(x_0) = 0 \)

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

\[ \text{Rate} = \frac{2\pi}{\text{vol}} \frac{k^2}{2m} \text{dS} \left| V'(q) \right|^2 \]

where \( q \to \bar{k} = \frac{\bar{q}}{m} \)

We now introduce the concept of a cross-section: imagine an effective area which includes the vol of \( U(x) \). If we use

\[ v = \frac{df}{dk} = \frac{k}{m} \]

in a time \( T \), particle moves \( vT \). Thus the effective volume is \( vT \).

But plane wave problem cc = \( \frac{1}{2} \) vol.

\[ \text{Prob} = \frac{cT}{\text{vol}} \quad \text{Rate} = \frac{\sigma v}{\text{vol}} \]
Thus

$$V d\Omega = \frac{m \hbar^2}{4\pi^2} d\varphi \left| V^T(q) \right|^2$$

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

Also $E$ and always appear with $\frac{1}{r}$. Also $2\pi\int \delta(E_n - E \eta)$, since $S$-fun involves $dE$.

**Example**: Coulomb case

$$V^T = \frac{4\pi ze^2}{\eta^2}$$

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

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

Thus

$$\frac{dV}{d\Omega} = \frac{1}{4\pi^2} \frac{m \hbar}{V} \frac{16\pi^2 z^2 e^4}{16(\sin^4 \theta) k^4}$$

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

- classical works if $\eta$ low, $V$ large
- first Born approx if $\eta$ high, $V$ low
4) Oscillating Perturbation

\[ P_{nm} = \left| \int_{t_i}^{t_f} \langle m | \sigma(t) | n \rangle dt \right|^2 \]

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

Then

\[ \langle m | \sigma(t) | n \rangle = e^{-i(\mathcal{E}_m - \mathcal{E}_n)t} Z_{\omega} \cos \omega t \langle m | V_0 | n \rangle \]

Upon integrating we find things like

\[ \left[ \frac{e^{-i(\mathcal{E}_m - \mathcal{E}_n - \mathcal{E}_\omega)t} + e^{i(\mathcal{E}_m - \mathcal{E}_n - \mathcal{E}_\omega)t}}{\mathcal{E}_m - \mathcal{E}_n - \mathcal{E}_\omega} \right]^2 + \left[ \frac{e^{-i(\mathcal{E}_m - \mathcal{E}_n + \mathcal{E}_\omega)t} - e^{i(\mathcal{E}_m - \mathcal{E}_n + \mathcal{E}_\omega)t}}{\mathcal{E}_m - \mathcal{E}_n + \mathcal{E}_\omega} \right]^2 \]

For large \( T \) we can show cross-terms \( \sim 0 \) upon proper averaging.

For continuum transitions

\[ \text{Rate} = 2\pi S(\mathcal{E}_m - \mathcal{E}_n - \mathcal{E}_\omega) |V_0|^2 + 2\pi S(\mathcal{E}_m - \mathcal{E}_n + \mathcal{E}_\omega) |V_0|^2 \]

---

**Problem:** Consider an H-atom in the ground state. Consider the proof of exciting this atom and emitting an electron when using an oscillating wave-like field. [Ignore any quantization or wave nature of field -- assume it is very strong]. Do as detailed as you can. Various directions, etc.
Comment: Say we wish to compute the rate of transitions between states \( m \), e.g.

\[
\text{Rate} \quad \underset{n \rightarrow (n', m)}{\rightarrow} \quad \text{Rate} \quad \underset{n \rightarrow m}{\rightarrow} \quad 2\pi S(E_{m} - E_{n}) |V_{nm}|^2
\]

\[
\rightarrow \int dE_{m} \rho(E_{m}) \int dE_{n} S(E_{m} - E_{n}) |V_{nm}|^2 = 2\pi \rho(E_{m}) |V_{nm}|^2
\]

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

Recall we had found

\[
\text{Rate} = 2\pi S(E_{m} - E_{n} + \hbar \omega) |V_{nm}|^2 + 2\pi S(E_{m} - E_{n} - \hbar \omega) |V_{nm}|^2
\]

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

Example: Consider an atom in an electric field

\[
V = (2\omega \sin \theta E_{0}) z
\]

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

\[
\text{Rate} \quad \underset{\text{ground}}{\rightarrow} \quad \underset{\text{excited}}{\rightarrow} \quad 2\pi S(E_{m} - E_{0} - \hbar \omega) |V_{nm}|^2 \frac{E_{0}^2}{2}\]
If we use white light, we must integrate. Use

\[ \Delta \propto \langle E^2 \rangle = 2E_0^2 \]

\[ \text{Intensity} \]

\[ \text{Rate} = 2\pi \sqrt{S(E_m - E_n - \hbar \omega)} \left| \frac{Z_{\text{nl}}}{2} \frac{\omega_n}{\Delta(\omega)} \right| \]

\[ = \frac{1}{Z_{\text{nl}}} \frac{\omega_n}{\Delta(\omega)} \quad \omega_n = E_m - E_0 \]

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).

\[ H = H_{\text{atom}} + H_{\text{osc}} + \mathbf{K}_g \]

\[ H_{\text{osc}} = \frac{\hat{p}^2}{2m} + \frac{1}{2} \mu \omega^2 \hat{q}^2 \]

Use

\[ \text{Rate} = 2\pi \sqrt{S(E_m - E_n)} \left| \frac{Z_{\text{nl}}}{2} \right|^2 \]

We want

\[ H_0 |\phi_n\rangle = E_n |\phi_n\rangle \]

Suppose we knew

\[ H_{\text{atom}} |X_a\rangle = |X_a\rangle \]
We know:
\[ H_{ac} |U_n> = \hbar \omega (N + \frac{1}{2}) |U_n> \]

Thus to find \( |\Phi_n> \) use the non-interaction of Hatom \& Hac to write:

\[ |\Phi_n> = |Xa> |U_n> \]

\[ E_{an} = \epsilon_a + \hbar \omega (N + \frac{1}{2}) \]

Now plug into our expression:

\[ R_{\Phi_n} \left( \frac{b^\dagger b}{N} \right) \]

\[ = 2\pi \Theta (E_{n_a} - E_{n_b}) |<\Phi_{n_b} | X_b | \Phi_{n_a}>|^2 \]

\[ = 2\pi \Theta (\epsilon_a - \epsilon_b + \hbar \omega (N + \frac{1}{2})) |<b|X_b|a>|^2 \text{Ker} |X_a> |U_n> |U_n> \]

To derive this:

\[ <\Phi_{n_b} | X_b | \Phi_{n_a}> = \int \Phi_{n_b}^* \chi^* (\mathbf{r}) \theta (\mathbf{r}) \Phi_{n_a} d^3 \mathbf{r} d\mathbf{q} \]

\[ = \int \chi_{n_b}^* (\mathbf{r}) \theta (\mathbf{r}) \Phi_{n_b}^* \Phi_{n_a} d^3 \mathbf{r} d\mathbf{q} \]

\[ = \int \left[ \int \chi_{n_b}^* (\mathbf{r}) \chi (\mathbf{r}) \chi_{n_b} (\mathbf{r}') d^3 \mathbf{r}' \right] \left[ \int \theta^* (\mathbf{q}) \theta (\mathbf{q}) d\mathbf{q} \right] \]

\[ = <\chi_{n_b} | \chi | \chi_{n_b}> <\theta | \theta | \theta> \]

\[ = <\chi_{n_b} | \chi | \chi_{n_b}> <\mathbf{U}_n | \mathbf{U}_n | \mathbf{U}_n> \]
Now we can show

\[ \langle N | g | N \rangle = 0 \quad \text{unless} \quad N = N + 1 \]

\[ \langle N+1 | g | N \rangle = \sqrt{\frac{N}{2N+1}} \frac{i}{\omega} \]

\[ \langle N-1 | g | N \rangle = \sqrt{\frac{N}{2N+1}} \frac{i}{\omega} \]

Thus

\[ \text{Rate}_{a \to b}^{N \to N+1} = 2\pi \delta (\varepsilon_a - \varepsilon_b - \hbar \omega) |k| \bar{a}_1^2 \frac{\hbar}{3\omega} (N+1) \]

\[ \text{Rate}_{a \to b}^{N \to N-1} = 2\pi \delta (\varepsilon_a - \varepsilon_b + \hbar \omega) |k| \bar{a}_1^2 \frac{\hbar}{3\omega} N \]

Comparison with Classical Perturbation

Here \( H = H_{\text{Heun}} + \chi q(t) \)

\[ q(t) = 2Q_0 \cos \omega t \]

and

\[ \text{Rate}_{a \to b}^{\chi} = 2\pi \delta (\varepsilon_a - \varepsilon_b - \hbar \omega) |k| \bar{a}_1^2 Q_0^2 \]

\[ \text{Rate}_{a \to b}^{\chi} = 2\pi \delta (\varepsilon_a - \varepsilon_b + \hbar \omega) |k| \bar{a}_1^2 Q_0^2 \]

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

\[ \text{classical: } \uparrow = \downarrow \quad \text{q.m.: } \uparrow > \downarrow \]
Try instead to compare with

\[ \langle \mu \delta^2 Q^2 \rangle_d = \frac{1}{2} \text{ excitation energy in oscillator} \]

Then the g.m. oscillator gives

Rate \( \alpha \to \beta \) (atom emits)

\[ \text{Rate} = \frac{2\pi}{\hbar} \delta (E_\alpha - E_\beta - \hbar \omega) \left| \langle E_\alpha \rangle \right|^2 \left[ \frac{1}{2} \langle Q^2 \rangle \right]_{\text{excitation}} + \frac{\hbar}{2\mu \omega} \]

Rate \( \beta \to \alpha \) (atom absorbs)

Thus all but the \( \hbar \omega \) 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 g.m. and classical fields.

**Problem:** Consider a cavity with E.H. wave as shown.

Also a d.c. Bo field in \( z \) direction. Interaction of atoms of

\[ H = \mu \cdot g \cdot (\mathbf{J} \cdot \mathbf{B}) \]

\[ = \mu \cdot g \cdot J_z B_0 + \mu \cdot g \cdot J_x B_x \]
Recall we had been considering

\[ H = H_{\text{atom}} + H_{\text{osc}} + \mathcal{V}_g \]

**Example:** Consider the nucleus of an atom in a solid as it interacts as the quantized oscillator.

We consider its interaction with an electron moving through a solid which is

\[ U(\vec{r} - \vec{R}_{\text{wider}}) \]

Locate the coordinate origin at the nucleus such that \( \vec{r} = q \cdot \vec{\varepsilon} \). Then we can linearize the interaction if \( q \) is small.

\[ U(\vec{r} - \vec{R}_{\text{wider}}) \sim U(\vec{r}_e) - \left( \frac{\partial U(\vec{r}_e)}{\partial \vec{z}} \right) q \]

We had found for the quantized oscillator interaction,

\[
\left| \frac{\partial \mathcal{E}}{\partial \mathcal{W}} \right| \sim \frac{\hbar}{2\nu \omega} (N+1) \]

\[ n \rightarrow m, \quad N \rightarrow N+1 \]

[Note: This assumes \( T \) is large such that the states assume a continuum]
6. Nucleus in a Magnetic Field in a Cavity [NHR]

Let \( \mathbf{B} = B_0 \hat{z} + B_x \hat{x} \) in cavity mode

Consider a typical cavity model

\[
\mathbf{A} = A_y \hat{y} = q(t) \sin k_z \mathbf{e}_y
\]

\[
E_y = \frac{\partial \mathbf{A}}{\partial t} \Rightarrow E_y = \dot{q}(t) \sin k_z
\]

\[
\mathbf{B} = \nabla \times \mathbf{A} \Rightarrow B_x = \frac{\partial A_y}{\partial z} = k q(t) \cos k_z
\]

Then

\[
H = g \mu_n (\mathbf{j} \cdot \mathbf{B}) = g \mu_n J_z B_0 + g \mu_n J_x (k \cos k_z) q(t)
\]

Now we know

\[
J_z = m_z, \quad m_z = -j, \ldots, j
\]

\[
\epsilon_{m_z} = g \mu_n B_0 m_z
\]

Thus we can calculate

\[
\text{Rate} = 2\pi \sum_{m_z = -m_z}^{m_z} \left[ g \mu_n B_0 (m_z-m_z) - \hbar c \right] \frac{\hbar}{2m_w} (N+1) \left| K_{m_z} J_x m_z \right|^2 (\hbar^2 \cos k_z)^2 \dot{q}(t)
\]
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,

$$\text{Energy} = \frac{\varepsilon_0}{2} \int (E^2 + c^2 B^2) \, d\text{Vol} = c_0 \text{Vol} \frac{1}{2} \left[ \frac{q^2}{2} + \frac{c^2 \varepsilon_0^2 q^2}{2} \right]$$

Now, the usual simple harmonic oscillator obeys

$$\text{Energy} = \frac{1}{2} \frac{\mu}{\omega^2} q^2 + \frac{\mu \omega^2}{2} q^2$$

Thus, we can identify $\omega = \omega_c$.

\[ [\mu q = \tilde{\varepsilon}] \]

$$\mu = \frac{c_0 \text{Vol}}{2} = c_0 \int (\sin^2 kz) \, d\text{Vol}$$

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

$$H_{\text{sc}} = \frac{p^2}{2\mu} + \frac{\mu \omega^2 q^2}{2} = -\frac{k^2}{2\mu} \frac{\partial^2}{\partial q^2} + \frac{\mu \omega^2}{2} q^2$$

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

**Example**: $H_{\text{sc}} \Psi = \gamma \Psi$ creates the usual SHO wave function.

If we consider $|\Psi|$, we can interpret it meaning that if we measured $\tilde{\varepsilon}$ when the cavity was empty, there would be a certain probability of finding $\tilde{\varepsilon}$ non-zero.
The energies are \( E_N = \hbar \omega (N + \frac{1}{2}) \).

We can either say that the qubit is in the 3rd excited state of the SHO or that we have 3 photons in the case of \( N = 3 \). Thus photons \( \equiv \) oscillator excited states.

Just remember however, \( \ell \) is not a position variable.

Now we also know:

\[
\langle m_z | J_\lambda | m_z' \rangle = \sqrt{j(j+1) - m_z(m_z \pm 1)} \quad \text{for } m_z' = m_z \pm 1
\]

\[
= 0 \quad \text{otherwise}
\]

Hence,

\[
\text{Rate} = 2\pi \delta (\omega_0 - \omega) \frac{\hbar (N+1)}{2(\varepsilon_{\text{SHO}})^2} \left( gN_{\text{qubit}} \right)^2 \left[ j(j+1) - m_z (m_z - 1) \right]
\]

\[
\omega_0 = gN_{\text{qubit}} \omega_{\text{Larmor}}
\]

\[
= \text{Larmor precession frequency}
\]

Thus no nuclear transitions unless cavity \( \omega \) is at the Larmor precession frequency, i.e. resonances [N.M.R.].

Note if the atom has only been in the field for a time \( T \),
we must go back to eqn. (2) on p. 8.
Interaction with a System of Oscillators

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

\[ H = H_{\text{atom}} + \sum \hat{H}_{\text{osc}_i} + \sum \hat{X}_i \hat{P}_i \]

\[ \hat{H}_{\text{osc}_i} = \frac{\partial^2}{\partial x_i^2} + \frac{m_i^2}{2} \hat{p}_i^2 \]

\[ V = \sum \hat{V}_i \]

Now return to the general theory.

Initial state \( n \): Atom in state \( a \), 1st exciton \( n_1 \), etc.

\[ |n\rangle = |n_1, n_2, n_3, \ldots \rangle \]

\[ H_0 |n\rangle = \left[ \epsilon_a + (n_1 + \frac{1}{2}) \hbar \omega + (n_2 + \frac{1}{2}) \hbar \omega + \cdots \right] |n\rangle \]

Final state \( m \): Atom \( b \), \( n_1, n_2, \ldots \)

\[ |m\rangle = |n_1, n_2, \ldots \rangle \]

Now to calculate the matrix element \( \langle m | V | n \rangle \)

\[ \langle m | V | n \rangle = \sum_i \langle m | V_i | n \rangle \]
Now note

\[ \langle \mathbf{m} | V_j | \mathbf{n} \rangle = \left\langle \frac{b_i}{n_i} \ldots | \chi_j(x) \psi_j \right| \frac{a_i}{n_i} \ldots \mathbf{n}, \mathbf{n} \right\rangle \]

\[ = 0 \text{ unless } N_i = N_{i+1}^i, \quad N_j = N_j^i + 1 \]

\[ = \langle b_i \mathbf{V}_j | a_i \rangle \frac{\hbar}{2 \mu_j \omega_j} (N_j + 1) \quad N_j = N_j + 1, \quad N_i = N_{i+1}^i \]
Problem: Consider states in He such that the energy as a function of momentum is

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

where \( \Delta \) and \( p_0 \) are constants. Now suppose

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

What is the prob. of emitting a photon of momentum \( \vec{k} \)?

\[ \vec{P} \rightarrow \vec{P}' = \vec{P} - \vec{k} \]

In terms of \( P_0, \Delta_0, d, \) and \( c_s \)? [Assume only longitudinal sound wave, 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

\[ H = H_0 + \sum_i \epsilon H_i \text{vac} + \sum_i \delta_i \]

where \( H_0 \text{vac} = \frac{P_i^2}{2\mu_i} + \delta_i \text{a} \gamma_i^2 \frac{\mu_i}{2} \)

Now we want the proof of \( \left| n, \ldots \right. \rightarrow \left| n, \ldots \right| \text{a} \)
We found

\[
\frac{\text{Rate}}{a \rightarrow b} = 2\pi S (E_a - E_b - \hbar \omega_j) |\langle b | \psi_j | a \rangle|^2 \frac{N_j + 1}{2 \mu_j \omega_j}
\]

\[
\frac{\text{Rate}}{a \rightarrow b} = 2\pi S (E_a - E_b + \hbar \omega_j) |\langle b | \psi_j | a \rangle|^2 \frac{N_j}{2 \mu_j \omega_j}
\]

Thus each oscillator interacts independently with the system of transitions; if we wanted just the rate of transition, regardless of which oscillator was involved, we need merely sum over the class of \( N_j \rightarrow N_j \pm 1 \) of the \( j \) oscillators.

8) Atomic Transitions in a Cavity

**Example:** We consider the probability that an atomic electron in state \( a \) radiates into an empty box. Since we may take the box as arbitrarily large, this is just the problem of an excited electron interacting with the \( E \times H \) field. It is our first real example of quantum electrodynamics -- although in the non-relativistic approximation.

\[
E_a - E_b = \hbar \omega \quad \text{and} \quad I
\]

Assume when the atom is in state \( a \), no photons in the box. When it falls into state \( b \), a photon of energy \( \hbar \omega \) 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

\[
\mathbf{A}(\mathbf{r}, t) = Q_1(t) \sin k_x x \mathbf{e}_x + Q_2(t) \sin k_y y \mathbf{e}_y + \ldots \\
+ \mathbf{k}_L = \mathbf{q}_L \mathbf{e}_z
\]

\[
\mathbf{A}(\mathbf{r}, t) = \sum \mathbf{A}_{\mathbf{k}, \mathbf{q}} \mathbf{e}^{-i \mathbf{k} \cdot \mathbf{r}}
\]

where \( \mathbf{k} \) is the wave vector
\( \mathbf{e} \) is the polarization vector
\( \mathbf{q} \) is the momentum vector

\[ \mathbf{k} \cdot \mathbf{e} = 0 \] (transverse mode)

Note: i.) we have chosen the scalar potential \( \Phi = 0 \)
ii.) we need a \( \mathbf{r} \times \mathbf{q} \). This introduces a \( \frac{1}{2} \) factor at the end.

Now to find the classical field, use Maxwells' equations to find

\[
\nabla^2 \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = 0
\]

Plug in (*) to find

\[
-k^2 c^2 Q \mathbf{e} \mathbf{e} - \mathbf{A} \mathbf{e} = 0
\]

Now to get the ged, find

\[
\mathbf{E} = \frac{\partial \mathbf{A}}{\partial t} = \sum \mathbf{A}_{\mathbf{k}, \mathbf{e}} \frac{\partial}{\partial t} \mathbf{e}^{-i \mathbf{k} \cdot \mathbf{r}}
\]

(harmonic oscillator of \( \omega \mathbf{e} = k \mathbf{e} \))
\[ \mathbf{B} = \nabla \times \mathbf{A} = \sum_{k, \ell} i \left( \mathbf{k} \times \mathbf{e} \right) Q_{k, \ell} e^{i \mathbf{k} \cdot \mathbf{r}} \]

Then

\[ \frac{\varepsilon_0}{2} \sqrt{\left( \mathbf{E}^2 + c^2 \mathbf{B}^2 \right) \text{dVol}} = \frac{\varepsilon_0 \text{Vol}}{2} \sum_{k, \ell} \left( \frac{\mathbf{q}_{k, \ell}^2}{\varepsilon_0} + \frac{k^2 c^2 \mathbf{q}_{k, \ell}^2}{\varepsilon_0} \right) \]

\[ \therefore \quad M_{k, \ell} = \frac{2}{\varepsilon_0 \text{Vol}} = \mu \]

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

\[ H_{\text{oscillators}} = \frac{1}{2} \sum_{k, \ell} \left[ \frac{\mathbf{p}_{k, \ell}^2}{2\mu} + \mu \left( \mathbf{q}_{k, \ell}^2 \right) \right] \]

\[ \mu = \frac{\varepsilon_0 \text{Vol}}{2} \]

Now

\[ H_{\text{atomic field}} = \frac{1}{2m} \left( \mathbf{p} - \mathbf{q} \mathbf{e} \mathbf{A} \right)^2 + \frac{q^2 \mathbf{z}}{4\pi \varepsilon_0 \mathbf{V}} + M \mathbf{e} \mathbf{B} + \cdots \quad \text{relativistic} \]

\[ = H_{\text{atom}} + \left[ -\frac{q \mathbf{e}}{2m} \left( \mathbf{p} \cdot \mathbf{A}(\mathbf{r}) + \mathbf{A}(\mathbf{r}) \cdot \mathbf{p} \right) + M \mathbf{e} \mathbf{B} \cdot (\mathbf{\nabla} \mathbf{A}) \right] \]

\[ + \frac{q^2 \mathbf{z}}{2m} \mathbf{A}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) + \cdots \]

Now if \( \mathbf{H} \) is small, we drop the \( \mathbf{A} \cdot \mathbf{A} \) term since it is 2nd order (and our perturbation theory is only to first order).
We find
\[ \hat{H}_\text{int} = \sum_{\tilde{r}, \tilde{\varepsilon}} \left\{ -\frac{q_e}{2\hbar} \left[ \hat{p} \hat{\varepsilon} e^{i \mathbf{k} \cdot \mathbf{r}} + e^{i \mathbf{k} \cdot \mathbf{r}} \hat{\varepsilon} \hat{p} \right] + \mu_e \hat{\sigma} \cdot (i \mathbf{k} \hat{\varepsilon}) e^{i \mathbf{k} \cdot \mathbf{r}} \right\} \chi_{\tilde{r}, \tilde{\varepsilon}} \]

We now want
\[ \text{Rate} \quad a \rightarrow b \]
\[ \text{Rate} = \frac{Z e^2}{2 \omega} \frac{N_j + 1}{2 \Omega} \]

\[ = 2 \pi S (\varepsilon_a - \varepsilon_b - \hbar \omega) | \langle b | \hat{\mathbf{k}} \frac{\mathbf{r}}{\hbar} | a \rangle |^2 \frac{N_j + 1}{2 \Omega} \frac{1}{2 \omega} \]}

[Taking into account \( \frac{1}{2} \) factor from \( \text{Re} \{ \beta \} \)]

\[ = 2 \pi S (\varepsilon_a - \varepsilon_b - \hbar \omega) | \langle b | \hat{\mathbf{k}} \frac{\mathbf{r}}{\hbar} | a \rangle |^2 \frac{1}{2 \omega} \]}

Show \( \hat{p} e^{i \mathbf{k} \cdot \mathbf{r}} = e^{i \mathbf{k} \cdot \mathbf{r}} (\hat{\mathbf{p}} + \frac{\mathbf{r}}{\hbar}) \) and then \( [\hat{\mathbf{p}}, \hat{\mathbf{A}}] = 0 \)

Also,
\[ \text{Rate} \quad a \rightarrow b \]
\[ \text{Rate} = \frac{Z e^2}{2 \omega} \frac{N_j + 1}{2 \Omega} \]

\[ \frac{1}{2 \omega} \]

The rate of emitting photons with \( \tilde{r}, \tilde{\varepsilon} \)

\[ \text{Rate} = \frac{Z e^2}{2 \omega} \frac{N_j + 1}{2 \Omega} \]

\[ \frac{1}{2 \omega} \]

\[ = 2 \pi S (\varepsilon_a - \varepsilon_b - \hbar \omega) \frac{4 \pi e^2}{\hbar \omega} | \langle b | \hat{\mathbf{k}} \frac{\mathbf{r}}{\hbar} | a \rangle |^2 \]

\[ \text{using} \quad \frac{q_e}{4 \pi e_0} = e^2 \]

\[ \text{and neglecting spin terms.} \]
Remember each time a photon couples with a system we get a $\frac{1}{\sqrt{\pi}} e^{-\epsilon^2}$ factor.

Now if we want the prob of transition to $d^3k$, we sum, passing in the limit to

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

If we integrate over constant $|k|$, we find

$$\text{Rate} = \frac{2\pi}{2\omega} \frac{d^3\omega}{(2\pi)^3} 4\pi e^2 |\langle b | \frac{e^{i\omega \cdot k}}{\omega} e^{i\epsilon} | a \rangle|^2$$

where $k = |k| = \epsilon_0 - \epsilon_1$

$$c = \frac{\hbar}{\epsilon} = 1$$
The Dipoic Approximation

We had found

\[ \text{Rate of emission of} \]

\[ \text{photon with} \ e^2 \]

\[ \text{atom} \ a \rightarrow b \]

\[ = 2\pi \delta(e_a-e_b-a) \frac{m e^2}{c} |<b| \hat{\vec{p}} \cdot \hat{\vec{e}} \mid a\rangle|^2 \frac{d^3 k}{2\omega (2\pi)^3} \]

The \( e^i k \cdot r \) factor accounts for phase interference from different parts of the atom. Now for light radiated

by atoms, typically \( kr \ll \frac{\alpha}{\lambda} \ll 1 \). Thus we approximate

\[ e^i k \cdot r \approx e^i k \cdot \hat{r}_{\text{atom}} \]

Now \( e^i k \cdot \hat{r}_{\text{atom}} \) is no longer an operator and can be carried into

of the matrix elements. This is called the "electric dipole approximation". [Note: it frequently does not work.]

Thus we can find

\[ \text{Rate into} \ a \rightarrow b = \frac{4\pi e^2}{2\omega} \frac{k^2 \delta(\omega)}{(2\pi)^3} \mid <b| \hat{\vec{p}} \cdot \hat{\vec{e}} \mid a\rangle \mid^2 \]

Now if we consider \( \hat{\vec{p}} \cdot \hat{\vec{e}} = p_z \), then

\[ <b| \hat{\vec{p}} \cdot \hat{\vec{e}} |a\rangle = <b|H_z \hat{\vec{e}} |a\rangle = \frac{(e_0-e_a)}{\omega} <b| \hat{\vec{e}} |a\rangle \]

Thus

\[ \text{Rate} = 2m^2 \frac{\omega^2}{c^2} |<b| \hat{\vec{e}} |a\rangle|^2 \frac{d^3 k}{4\pi} \]

Note all of this is exact within 1st order perturbation theory for non-relativistic theory.
Example: $2p \rightarrow 1s$

$$l = 0 \quad (\omega \theta \sim z) \quad \langle b|l|x\rangle = 0 \quad \langle b|y|a\rangle = 0 \quad \langle b|z|a\rangle \neq 0$$

Then

$$\text{Rate} = 2\omega^2 e^2 \left| \langle b|z|a\rangle \right|^2 \frac{e^2 \omega}{4\pi}$$

Now noting

The polarization out of page will vary.

Now

$$\text{Rate} \quad \propto \left| \langle b|z|a\rangle \right|^2$$

any direction

any polarization

Then

$$\text{Energy loss} \quad \propto \frac{4\omega^4}{3c^3} \left( \text{matrix element of dipole moment} \right)^2$$
We now compare this to a small classical oscillating dipole

\[ z = 2z_0 \cos \omega t \]

Dipole moment = \( 2eZ_0 \cos \omega t \)

\[ (\text{Dipole moment})^2 = 2(eZ_0)^2 \]

\[ \frac{\text{Energy radiated}}{2e} = \frac{2}{8} \frac{\omega^4}{c^3} (\text{Dipole moment})^2 \]

This is close to the quantum answer except for a factor \( Z \).

Thus an atom in empty space radiates as a dipole provided we use

\[ (\text{Dipole moment classical})^2 = 2 | \text{Dipole matrix element - 0, 0, 1} |^2 \]

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

We proceed for an atom radiating in a general cavity with holes in it. [with perfect walls here].

Assume the atom dimmings << size of cavity. Now surround the cavity by an resonance box. This has various modes [although very complicated]. For the indicated geometry the modes resemble...
The superposition of these modes inside the box, make 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 needn't worry about reflection from the wall.

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

\[
\text{Rate} = 2\pi S(\epsilon_0 - \epsilon_0 - k\omega) \left| \langle b | \Psi_i | a \rangle \right|^2 \frac{1}{2\epsilon_0 \omega},
\]

Now \( \text{Hint} = \int \vec{A}(\vec{r}) \cdot \hat{z} \)

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

Thus

\[
\text{Rate} = \sum_i 2\pi S(\epsilon_0 - \epsilon_0 - k\omega) \frac{\left| \Phi_i(\vec{r}) \right|^2}{2\epsilon_0 \omega} |j_{ab}|^2
\]

We will compare this to a classical problem.

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

\[
\frac{\partial^2 \vec{A}}{\partial t^2} - \nabla^2 \vec{A} = J(\vec{r}) = S(\vec{r} - \vec{r}_0) J
\]

Now we \( \vec{A} = \sum \Phi_i(t) \hat{z} \Phi_i(\vec{r}) \) and plug in to find

\[
\sum (\dddot{\Phi}_i + \omega^2 \Phi_i) \Phi_i(\vec{r}) = S(\vec{r} - \vec{r}_0) J(t)
\]
From orthogonality

\[ q_i'' + \omega^2 q_i = \Phi_i(r) j(t) \]  

If \( j(t) \) varies as \( e^{j\omega t} \) then the electric field varies as \( E_0 e^{j\omega t} \)

\[ E_0 = z(\omega) j_0 \]

where \( z(\omega) \) is the impedance

Using \( E_0 = \sum q_i(r) \Phi_i(r) \)

we find, solving \((*)\), that

\[ E_0 = j_0 \sum \frac{1}{\omega^2 - \omega^2} \Phi_i(r)^2 \frac{j_0}{z(\omega)} \]

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

\[ \text{Rate}_{a \to b} = \frac{2\pi}{2\pi} \sum (\delta (a - b - n\omega_i) | \langle k | j | a \rangle |^2 | \Phi_i(r) |^2 \frac{1}{2\pi \omega_i} \]

Claim: \( \text{Rate}_{a \to b} = \frac{2}{n \omega_{ab}} \left[ \text{Re} \{z(\omega_{ab})\} \right] | \langle k | j | a \rangle |^2 \)
Proof: If we return to (1),
\[ f(\omega) = j\omega \leq \frac{1}{\omega_0^2 - \omega} \phi^2(\omega) \]

we realize we have no prescription for \( \lim_{\omega \to \omega_0} f(\omega) \).

Thus we use the analogy of a damped oscillator:
\[ \ddot{q} + \omega_0^2 q + \gamma \dot{q} = j\omega_0 \cdot \omega_0^2 \]

or \( (-\omega^2 + \omega_0^2 + j\omega)q = j\omega_0 \)

\[ q = \frac{j\omega_0}{\omega_0^2 - \omega^2 + j\omega} \]

we see that we can apply the condition of causality and the initial condition if \( q = 0 \) for \( t \leq 0^- \). To claim we should write 0/0

\[ q_x = \frac{1}{\omega_0^2 - (\omega - i\epsilon)^2} \phi_x(\omega_0) j\omega \]

Thus we assume no free waves on i.c. before returning our oscillator, we eventually take him. Note this is just like turning off the interaction” at \( \epsilon = 0^- \) in scattering problems.

Before continuing, we need a little more with first,
Detour

Cauchy Principal Values and Generalized Functions (a la Feynman)

It is convenient to take as a prescription

\[ \lim_{\varepsilon \to 0} \frac{1}{x+i\varepsilon} = \text{P.V.} \left( \frac{1}{x} \right) - i\pi \delta(x) \]  \hspace{1cm} (3)

[Note we also might have specified]

\[ \lim_{\varepsilon \to 0} \frac{1}{x+i\varepsilon} = \text{P.V.} \left( \frac{1}{x} \right) + i\pi \delta(x) \]

or

\[ \lim_{\varepsilon \to 0} \frac{1}{x+i\varepsilon} = \text{P.V.} \left( \frac{1}{x} \right) \]

More generally

\[ \lim_{\varepsilon \to 0} \frac{1}{x+i\varepsilon} = \text{P.V.} \left( \frac{1}{x} \right) + \lambda \delta(x) \]

To "justify" (3), note

\[ \frac{1}{x+i\varepsilon} = \frac{x-i\varepsilon}{x^2+\varepsilon^2} = \frac{x}{x^2+\varepsilon^2} - i \frac{\varepsilon}{x^2+\varepsilon^2} \]

The first term resembles

Now

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

By keeping equal distances we get cancellation.
For the second term

\[ \int_{-\infty}^{\infty} \frac{e^{ix}}{x^2 + \varepsilon} \, dx = i \pi \]

By definition

\[ \int_{-\infty}^{\infty} e^{i|x|} \, dx = f(0) \]

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

**EXAMPLE:** Consider the Fourier transform of a step function

\[ \int_{-\infty}^{t=0} e^{-ix^2} \, dt \]

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

\[ \int_{0}^{\infty} e^{-ix^2} \, dx = \lim_{\varepsilon \to 0} \int_{0}^{\infty} e^{-ix^2 + \varepsilon} \, dx \]

\[ = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left( \frac{-1}{x-i\varepsilon} \right) = \lim_{\varepsilon \to 0} \frac{-1}{i\varepsilon} \]

Note that how we take our prescription affects the inverse transform.
Returning now to our problem, we find

\[ \mathfrak{f}(\omega) = i\Omega \sum_{i} \frac{|\phi_i|^2}{\omega_i^2 - \omega^2 + 2i\omega} \]

\[ = i\Omega \sum_{i} \text{P.V.} \frac{1}{\omega_i^2 - \omega^2} |\phi_i|^2 + i\Omega \left( \text{P.V.} \sum_{i} \delta(\omega_i^2 - \omega^2) |\phi_i|^2 \right) \]

Note this is very close to our q.m. result. When we take 

\[ \text{Re} \{ \mathfrak{f}(\omega) \} \]

we get the result

\[ \text{Rate} = \frac{2}{\hbar^2} \left[ \text{Re} \{ \mathfrak{f}(\omega) \} \right] |\langle b | j | a \rangle|^2 \]

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

\[ |\text{down} \rangle \rightarrow |\langle a | j | a \rangle| = \frac{\hbar}{\epsilon} |\langle a | j | c \rangle| = \frac{\hbar}{\epsilon} |\langle a | j | c \rangle|^2 \]

\[ = |\langle a | j | b \rangle|^2 + |\langle b | j | a \rangle|^2 \]

\[ |\text{up} \rangle \]
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

\[
\text{Rate}_{a \rightarrow b} = \frac{Z}{\hbar} \text{Re} \left\{ Z(\omega) \right\} |\langle a | \hat{J} | b \rangle|^2
\]

But for a perfect cavity the rate of transition with the energy going into the excitation of a well-defined mode \( \phi_0 \) is

\[
\text{Rate}_{a \rightarrow b} = 2\pi S(\omega_b - \omega_b) |\langle a | \hat{J} | b \rangle|^2 |\phi_0(r)\rangle \frac{\hbar}{2\omega_b}
\]

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

\[
Z(\omega) = \lim_{\epsilon \to 0} \frac{i\omega}{\omega^2 - \omega_0^2 + i\epsilon \omega_b} |\phi_0(r)\rangle^2
\]

\[
= \omega S(\omega^2 - \omega_0^2) |\phi_0(r)\rangle^2
\]

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

\[
Z(\omega) = \frac{i\omega}{\omega^2 - \omega_0^2 + i\epsilon \omega_b} |\phi_0(r)\rangle^2 = \frac{i\omega}{2\omega_b(\Delta \omega) + i\epsilon \omega_b}
\]

Thus

\[
\text{Rate}_{a \rightarrow b} = \frac{2\pi}{\Delta \omega} \left( \frac{k^2}{2} \right) |\langle a | \hat{J} | b \rangle|^2 |\phi_0(r)\rangle^2 \frac{\hbar}{2\omega_b}
\]
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 1929. 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

\[ \dot{B} = \nabla \times \dot{A} \]  \hspace{1cm} (4)

\[ \dot{E} = -\nabla \phi + \frac{\dot{A}}{c^2} \]  \hspace{1cm} (5)

\[ \nabla \cdot \dot{E} = \frac{\dot{\rho}}{\epsilon_0} \]  \hspace{1cm} (6)

\[ \nabla \times \dot{B} = \frac{\dot{\rho}}{\epsilon_0} + \frac{\dot{E}}{c^2} \]  \hspace{1cm} (7)

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

\[ \dot{A}' = \dot{A} + \nabla \chi \]

It was customary to take a Lorentz gauge

\[ \nabla \cdot \dot{A} = \frac{\dot{\rho}}{\epsilon_0} \]

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 Lorenz 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

\[ \nabla \cdot \mathbf{A} = 0 \]

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

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

\[ \nabla^2 \phi = \frac{\rho}{\varepsilon_0} \]

Thus the scalar potential \( \phi \) is always determined by

\[ \phi(1) = \sqrt{\frac{Q(2)}{4\pi \varepsilon_0 R^2}} \]

(8)

Thus using \( \varepsilon^2 \) is exact in the 2-eggs. All we need to know
now is how \( \varepsilon^2 \) falls in the \( \mathbf{A} \). But (8) \( \Rightarrow \) disturbances
propagate at infinite speed. Oh, well, "Damn the torpedoes,
full-speed ahead!!"
Use (4) in (7)
\[ \nabla \times (\nabla \times \mathbf{A}) - \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla \frac{\partial \mathbf{\Phi}}{\partial t} = \frac{\mathbf{j}}{\varepsilon_0} \]

or
\[ \nabla^2 \mathbf{A} - \frac{\partial^2 \mathbf{A}}{\partial t^2} = \frac{\mathbf{j}}{\varepsilon_0} - \nabla (\frac{\partial \mathbf{\Phi}}{\partial t}) \]  

But
\[ \frac{\partial \mathbf{\Phi}}{\partial t} = \int \frac{\partial \mathbf{\phi}}{\partial t} d\mathbf{r}_2 \]

Then
\[ \nabla \cdot \mathbf{j} = \frac{\partial \mathbf{\Phi}}{\partial t} \Rightarrow \frac{\partial \mathbf{\Phi}}{\partial t} = \sqrt{\frac{\nabla \cdot \mathbf{j}(\mathbf{r}_2) d\mathbf{r}_2}{4 \pi \varepsilon_0 \varepsilon_r}} \]

Thus \( \mathbf{A} \) is completely determined by the current. This means we take into account the transverse part of the current so that \( \nabla \times \mathbf{A} = 0 \).

Now expand everything in plane waves
\[ \mathbf{J}(\mathbf{r}, t) = \sum \mathbf{J}_k(t) e^{i \mathbf{k} \cdot \mathbf{r}} \]
\[ \mathbf{A}(\mathbf{r}, t) = \sum \mathbf{A}_k(t) e^{i \mathbf{k} \cdot \mathbf{r}} \]
Now then from (9), (10), (11)

\[ \frac{d^2 \hat{A}(k, t) + \hbar^2 c^2}{dt^2} \hat{A}(k, t) = \frac{i}{\hbar} \hat{J}_{\text{even}}(k, t) \]

where \( \hat{J}_{\text{even}} = \hat{J}(k, t) - \frac{(k \cdot \tilde{J}) \tilde{J}}{k^2} \)

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 $\nabla \cdot A = 0$. We found the basic equations to then be

$$\nabla^2 \varphi(r, t) = \varphi(r, t) \frac{1}{\epsilon_0}$$

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

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

We solve immediately for

$$\varphi(r, t) = \int \frac{\varphi(r', t') \, dV_2}{4\pi \epsilon_0 |r - r'|}$$

This indicates one rule for quantization:

1) Use the instantaneous Coulomb-potential 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 $A$.

To find this classically, we use Fourier transforms (momentum space):

$$\tilde{\varphi}(k, t) = \int e^{-i k \cdot r} \varphi(r, t) \, d^3 r$$
Also \( \Phi(k,t) = \mathcal{F}\{\tilde{\phi}(p,t)\} \)

\[ \Phi(k,t) = \mathcal{F}\{\phi(p,t)\} \]

\[ P(k,t) = \mathcal{F}\{p(p,t)\} \]

Transforming our equations, the gauge becomes

\[ \mathbf{k} \cdot \mathbf{A}(k,t) = 0 \]

which the other equations are

\[ k^2 \Phi = P \]

\[ \frac{\partial^2}{\partial t^2} \mathbf{A}(k,t) + k^2 c^2 \mathbf{A}(k,t) = i \mathbf{A}(k,t) - \frac{\mathbf{k}}{\mathbf{k}^2} \left( \frac{\partial \Phi}{\partial t} \right) \]

\[ i \mathbf{k} \cdot \mathbf{A} = -\frac{\partial P}{\partial t} \]

We can see \( \frac{\partial \Phi}{\partial t} = \frac{1}{k^2 c^2} \frac{\partial P}{\partial t} = -i \frac{\mathbf{k}}{k^2} \frac{\partial P}{\partial t} \)

Thus we get

\[ \frac{\partial^2}{\partial t^2} + k^2 c^2 \mathbf{A} = \frac{1}{c_0} \left( \mathbf{f} - \mathbf{k} \cdot \left( \frac{\Phi}{k^2} \right) \right) \]

(1)
We could expand $\hat{a}$ in two transverse polarization modes

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

$$\hat{e}_1 \cdot \hat{e}_2 = 0, \quad \hat{e}_1 \cdot \hat{e}_1 = 1, \quad \hat{e}_2 \cdot \hat{e}_2 = 0$$

Plugging this into (\S)

$$\hat{e}_1 \left( \frac{\partial^2 \alpha_1(\vec{k}, t)}{\partial t^2} + k^2 \alpha_1(\vec{k}, t) \right) + \hat{e}_2 \left( \frac{\partial^2 \alpha_2(\vec{k}, t)}{\partial t^2} + k^2 \alpha_2(\vec{k}, t) \right) = \frac{1}{\varepsilon_0} \hat{J}$$

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

$$\frac{\partial^2 \alpha_1(\vec{k}, t)}{\partial t^2} + k^2 \alpha_1(\vec{k}, t) = \frac{\hat{e}_i \cdot \hat{J}}{\varepsilon_0}$$

$$\frac{\partial^2 \alpha_2(\vec{k}, t)}{\partial t^2} + k^2 \alpha_2(\vec{k}, t) = \frac{\hat{e}_i \cdot \hat{J}}{\varepsilon_0}$$

Thus the current along $\hat{e}_i$ feeds the $\alpha_i$ mode, the $\hat{e}_j$ current feeds the $\alpha_j$ mode. Here $\hat{e}_i \cdot \hat{J}$ is the projection of the current in the $\alpha_i$ direction. The $(i,j)$

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

Now to get QUANTUM ELECTRODYNAMICS

1.) Use the instantaneous Coulomb potential $E = \frac{e_i e_j}{r_{ij}}$ in the $S$-eqns.

2.) Put (**) into the form of quantum oscillators
DETOUR: More Feynman quide and dirty methods.

Say we want to evaluate

\[
\int e^{-i \mathbf{Q} \cdot \mathbf{r}} \phi(\mathbf{r}) \, d\text{Vol}
\]

We work backwards. Consider

\[\nabla^2 \left( \frac{1}{r} \right) = 4\pi \delta(\mathbf{r})\]

If we take the \( \mathbb{F} \{ \nabla^2 (\frac{1}{r}) \} = \mathbb{F} \{ \frac{1}{r} \} = 4\pi \mathbb{F} \{ \delta(\mathbf{r}) \} = 4\pi\]

\[
\Rightarrow \int e^{-i \mathbf{Q} \cdot \mathbf{r}} \left( \frac{1}{r} \right) \, d\text{Vol} = \frac{4\pi}{Q^2}
\]

Now consider

\[(\nabla^2 - m^2) \phi = 4\pi \delta(\mathbf{r})\]

From Yukawa, \( \phi \sim e^{-mr}/r \)

Thus

\[
\int e^{-i \mathbf{Q} \cdot \mathbf{r}} \frac{e^{-mr}}{r} \, d^3 \mathbf{r} = \frac{4\pi}{Q^2 + m^2}
\]

"Whatever I can remember are my axioms!"
Problem 3: For a long time astrophysicists wondered about continuum radiation from various nebulae. Some of this was due to synchrotron radiation. But not all. Consider an H atom (neglect spin)

\[ 2s \quad 2p \quad \text{done something here, but neglected} \]

If you wish

\[ 1s \]

Now we know \( 2s \rightarrow 1s \) transitions with one photon emitted are forbidden. However, these transitions can be induced by collisions or an electric field. However, in intergalactic 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 sums 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 using two laser beams to interact in H gas.]
B. Second-Order Time-Dependent Perturbation Theory

Recall we had

\[ S_{mn} = S_{mn} - i \int_{0}^{\infty} \mathcal{V}_{mn}(t) \, dt + (i)^2 \sum_{k_1, k_2 \neq m} \int_{0}^{\infty} \mathcal{V}_{mk_1}(t_1) \mathcal{V}_{k_1n}(t_2) \, dt_1 \, dt_2 + \cdots \]

where \( \mathcal{V}_{mn}(t) = \langle \Phi_m | \mathcal{V} | \Phi_n \rangle \)

1. Time-Independent Perturbation \( \mathcal{V} \)

\[ V(t) = 0 \quad t < 0 \]

\[ = V \quad 0 \leq t \leq T \]

\[ = 0 \quad t > T \]

A long calculation then finds

\[ S_{mn} = S_{mn} - V_{mn} \left[ \frac{i (E_m - E_n) T}{(E_m - E_n)^2} \right] + \sum_{k_1, k_2 \neq m} \frac{V_{mk_1} V_{k_1n}}{(E_k - E_n)} \left[ \frac{e^{i(E_m-E_n)T}}{(E_m - E_n)} - \frac{e^{-i(E_m-E_n)T}}{(E_m - E_n)} \right] \]

\[ + V_{mn} V_{mn} \left[ \frac{e^{i(E_m-E_n)T}}{(E_m - E_n)} - \frac{1}{(E_m - E_n)} \right] + V_{mn} V_{mn} \left[ \frac{1 - i(E_m-E_n)T}{(E_m - E_n)^2} \right] \]
We now calculate $S_{\nu\nu}$, the amplitude to remain in the same state as time goes on

$$S_{\nu\nu} = 1 - iT V_{\nu\nu} - \frac{T^2}{2} V_{\nu\nu}^2 - iT \sum \frac{V_{\nu\mu} V_{\mu\nu}}{(E_{\nu} - E_{\mu})} + \sum \frac{(V_{\nu\mu})^2}{(E_{\nu} - E_{\mu})^2} \left[ e^{i(E_{\nu} - E_{\mu})T} - 1 \right]$$

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

$$E_{\nu} = E_{\mu} + V_{\nu\mu} + \sum \frac{V_{\nu\mu} V_{\mu\nu}}{(E_{\nu} - E_{\mu})}$$

(Shift in level $\nu$)

Now the state in various times as $e^{iE_{\nu}t}$. But our TDPT has taken out $e^{-iE_{\nu}t}$, e.g.

$$e^{-iE_{\nu}t} e^{iE_{\mu}t} = e^{-i(E_{\nu} - E_{\mu})t} \left[ e^{i\text{shift}} \right]$$

If we plug this in and take into account that when turning off $V$ we are left exactly in the right state, we get the above expression for $S_{\nu\nu}$. 
Comment: This rather involved lecture was presented by one of the physics department substituting for Tegeman.

Review: We were considering

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

We expand $|\psi(t)\rangle$ in states of the unperturbed $H_0$, $|\phi_n\rangle$. Using the summation convention throughout,

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

Now to put into "interaction picture": assume

$$c_n \sim e^{-i\omega_nt} \chi_n$$

Then find

$$i \chi_n = \nabla_n \chi_n$$
where $\nabla_n = V_n(t) e^{i(\omega_n - \omega_n)t}$

If we integrate this equation, we can expand

$$\chi = e^{-i \int V(t) dt} \chi_0(t)$$

using $\chi_0(t) = \sum_n \chi_n(0)$

to find

$$\mu_{nm} = \mu_{nm} - i \int \nabla_{nm} dt + \int \int \nabla_{nm}(t_1, t_2) \chi_n(t_1) \chi_m(t_2) dt_1 dt_2 + \ldots$$

$$\mu_{nm} > \mu_{nm}$$
Example: Consider tritium decay as example of $V = 0 + \zeta$

\[ \phi_0, \phi_0 \]

Also assume electron should 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

$\phi_0 = a_0 \chi_0$

where $|a_0|^2$ is the prob.

Consider a 2-state system

We can solve this problem by stationary perturbation theory.

Note:

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

"T.D.P.T."
Now consider $S_{mm}$

$$S_{mm} = 1 - iT V_{mm} - \frac{T^2}{2} V_{mm}^2$$

$$-i T \sum_{k} \frac{V_{mk} V_{km}}{E_k - E_m} + \sum_{k} \frac{(V_{mk})^2}{(E_k - E_m)^2} \left[ e^{-i(E_k - E_m)T} - 1 \right]$$

Note we can write this as

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

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

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

$$= 1 - \sum_{k} \frac{4 \sin^2(E_m - E_k) T_k}{(E_m - E_k)^2} |V_{mk}|^2$$

(first order TDPT for transition prob.)
2) Conservation of Probability (Unitarity)

\[ t=0: \quad \psi_n(0) = 1, \quad \psi_m = 0 \quad m \neq n \]

\[ t=T: \quad \psi_m(T) = S_{mn} \psi_n(0) \]

Now, for all \( t \),

\[ \sum_n |\psi_m|^2 = 1 \]

so

\[ \psi_n^*(0) S_{mn} S_{np} \psi_p(0) = \psi_n^*(T) \psi_n(T) \]

\[ = \psi_n^*(0) \psi_n(0) \text{ postulate} \]

In matrix notation, this implies

\[ \chi^* S^*T S \chi = \chi^* \chi \]

\[ \Rightarrow \quad S^*T S = 1 \]

or

\[ S^*T S = 0 \]

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).]
Physically, an extremely powerful principle. To apply it further, we define the T matrix by

$$S = 1 + 2i \mathbf{T}$$

Thus, we can find our new unitarity condition

$$S^* S = (1 - 2i \mathbf{T}^+) (1 + 2i \mathbf{T}) = 1$$

$$= 1 - 2i (\mathbf{T} \mathbf{T}^+) - (2i)^2 \mathbf{T}^+ \mathbf{T} = 1$$

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

\textbf{Applications:}

a.) Optical Theorem:

Consider scattering $A + B \rightarrow A + B$

$\Rightarrow \quad C + D \rightarrow C' + D' + E'$

To find the transition probability for forward elastic scattering, we look $T_{ii}$ (state 0 to state 0)

$$\frac{T_{ii} - T_{ii}^*}{2i} = T_{ii}^+ T_{ii}$$

$$\therefore \quad \text{Im} \{T_{ii}\} = T_{ii}^* T_{ii} = \sum \left| T_{in} \right|^2 = (\ ) C_T$$

Note how similar this looks to our TDPT.
abs. note

\[ |T_{\text{II}}| > \text{Im} \{ T_{\text{II}} \} > T_{\text{II}} T_{\text{II}}^* = |T_{\text{II}}|^2 \]

b.) Final State Theorem: (Watson)

Known: \( ^0\pi N \rightarrow ^0\pi N \quad l = 0 \) (s-wave)

Want to examine \( ^2\Sigma N \rightarrow ^1\Sigma N \)

From time reversal we know \( T \) is symmetric.

\[ \text{Im} \{ T_{l=2} \} = T_{\text{II}}^* T_{l=2} + T_{l=2}^* T_{l=2} \]

If we assume \( ^0 \) intermediate state is dominant (\( ^2 \) process is second order), then

\[ \Rightarrow \text{phase} \ (T_{\text{II}}) = \text{phase} \ (T_{l=2}) \]
3) Scattering of Light from an Atom

Classically one develops Thomson scattering.

By examining the terms in \( \frac{e^2}{4\pi\varepsilon_0} \) 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

\[ \mathbf{J}(\mathbf{r}, t) = \mathbf{\nabla} \times \left( \frac{\hbar}{i\hbar m} \mathbf{\nabla} \psi \right) + \left( \frac{\hbar}{j\hbar m} \mathbf{\nabla} \psi \right) \times \psi \]

and then use

\[ \Box^2 \mathbf{A} = \mathbf{J}(\mathbf{r}, t) \]

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

\[ \psi(\mathbf{r}, t) = \sum_n \phi_n(\mathbf{r}) e^{-iEt} \]
Then

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

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

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

Thus if \( C_n = 0 \), all in the m-state so no spontaneous emission.

Point: if we think the other people are frequently going down the same dreams.

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

\[ \frac{\partial \psi}{\partial t} = (\mathcal{H} + V) \psi \]

We can do it if we use both incoming and outgoing waves (advanced and retarded potentials).
The problem is that we have been dealing with the EM field classically. The Nth N difference is needed for spontaneous emission.

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

$$\hat{A} = \sum_{\text{e}} \hat{Q}_e e^{i k_e} \hat{e}$$

Find

$$\hat{H} = \hat{S} \left[ \frac{1}{2} \hat{p}^2 + \frac{\mu_i}{2} Q_i^2 \right] + \psi_i Q_i \psi_j$$

Use

$$\hat{H}_{\text{atom}} = \frac{1}{2m} (\hat{p} - \frac{\xi}{c} \hat{A}) \cdot (\hat{p} - \frac{\xi}{c} \hat{A}) + eV$$

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

Thus

$$\frac{1}{2m} \hat{A}(\vec{r}) \cdot \hat{A}(\vec{r}) = \frac{1}{2m} \sum_{\text{e}} \sum_{\text{e}'} \langle \text{e} \vert \text{e}' \rangle Q_e Q_{e'} e^{i(k_e + k_{e'}) \cdot \vec{r}}$$

Thus we suspect

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

$$| M_{ij} | = \frac{\xi}{2} \langle b \hat{e}_b \vert Q_i Q_j C_j(\tau) \vert a, \hat{e} \rangle$$

$$= \frac{\varepsilon_1 \varepsilon_2}{2m} \langle b \hat{e}_b | e^{i \hat{e}_b \cdot \vec{r}} \hat{A}(\vec{r}) \rangle \sqrt{\frac{\hbar}{2m \omega_1}} \sqrt{\frac{\hbar}{2m \omega_2}}$$

Note: $\varepsilon_1 \varepsilon_2 = 0$, no scattering.
Part 2: Feynman's Approach

We were considering the scattering of photons off of atoms.

initial state: 1 atom in a, one photon of $|\vec{k}_1, \vec{\omega}_1\rangle$  
energy $\epsilon_a + \omega_1$

final state: 1 atom in b, one photon of $|\vec{k}_2, \vec{\omega}_2\rangle$  
energy $\epsilon_b + \omega_2$

We had suggested that the scattering rate could be represented by:

$$Rate = 2\pi S(E_f - E_i) \left| \langle f | M | i \rangle \right|^2$$

We will show later that:

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

Study this series, calculate higher terms, and interpret.

Now:

$$H = \frac{p^2}{2m} + V(r) + \frac{\mu}{2} \left( \frac{\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}}{2m} \right) + \frac{q^2}{2m} \frac{\vec{A} \cdot \vec{A}}{2m} + H_{\text{interaction}}$$

Now we expand:

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

[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 $\mathbf{A}\cdot\mathbf{A}$ term since it gave rise to a direct coupling between photon $k_1$ and photon $k_2$. We found

$$\langle f|N|l_i \rangle = \frac{\alpha_a \alpha_b}{\sqrt{2} \epsilon_1 \epsilon_2 \sqrt{\epsilon_1 \epsilon_2}} \langle b|e^{i(k_1-k_2) \cdot r_{1g}} \rangle$$

But classically we found terms like $\frac{\alpha_e}{\omega_2^2 \omega_1^2}$. Why don't we get this by our q.m.?

We forget that indirect coupling of photons through intermediate states is also possible, order like $\mathbf{A}\cdot\mathbf{A}$. We must then consider the probability that a photon interacts with the decay $\mathbf{p}\cdot\mathbf{A}$ and then the other re-admits a new photon against $\mathbf{p}\cdot\mathbf{A}$. This will involve the

$$\frac{\langle f|\mathbf{v}|l_i \rangle}{\epsilon_1 - E_1 + i\gamma}$$

Now our $\mathbf{V}$ is

$$\mathbf{V} = \sum_i \alpha_a \frac{\epsilon_e e^{i\mathbf{k}_1 \cdot \mathbf{r}_1}}{m} \mathbf{Q}_{i a}$$

Now what intermediate states are possible? Certainly not all. Only those states for which $\langle k|\mathbf{v}|l_i \rangle$ exist. (Equation (9).) One must see where one can get from initial state via the perturbation. Only one $\alpha$ in Hint, so one photon process are all that are possible.
Initial state atom inc, all oscillators zero except \( \tilde{b}, \tilde{e} \)

Possibly intermediate

1. atom inc, all oscillators zero
2. atom inc, photon in \( \tilde{b} \), photon in \( \tilde{c} \)
3. atom inc, 2 photons in \( \tilde{b} \)

Energy

\[ E_a + \omega_1 \]
\[ E_c \]
\[ E_c + \omega_3 + \omega_1 \]
\[ E_c + 2\omega_1 \]

Restrict to calculate the matrix elements \( \langle k|V|i \rangle \) using the dummy approach [don't consider \( \langle f|V|i \rangle \) yet]

\[ \langle k|V|i \rangle_0 = \frac{q_d \langle b | \frac{1}{m} \hat{p}^2 | a \rangle e^{i k_0 \tilde{e}} | a \rangle}{\sqrt{2 \mu a}} \]

\[ \langle k|V|i \rangle_1 = \frac{q_d \langle b | \frac{1}{m} \hat{p}^2 | a \rangle e^{-i k_0 \tilde{b}} | a \rangle}{\sqrt{2 \mu a}} \]

\[ \langle k|V|i \rangle_2 = \frac{q_d \langle b | \frac{1}{m} \hat{p}^2 | a \rangle e^{-i k_0 \tilde{e}} | a \rangle}{\sqrt{2 \mu a}} \]

Note that when a photon is eaten, \( e^{-i k_0 \tilde{b}} \), and when it is spit out, \( e^{-i k_0 \tilde{b}} \). Now for \( \langle f|V|i \rangle \)

\[ \langle f|V|i \rangle_0 = \frac{q_d \langle b | \frac{1}{m} \hat{p}^2 | c \rangle e^{-i k_0 \tilde{b}} | c \rangle}{\sqrt{2 \mu a}} \]

\[ \langle f|V|i \rangle_1 = \frac{q_d \langle b | \frac{1}{m} \hat{p}^2 | c \rangle e^{i k_0 \tilde{e}} | c \rangle}{\sqrt{2 \mu a}} \quad \text{[with } \tilde{b}_3 \text{ unit of } \tilde{b}_2 \text{]} \]

\[ \langle f|V|i \rangle_0 = 0 \quad \text{unless } \tilde{b}_2 = \tilde{b}_1, \text{ but we want consider forward scattering} \]

[Do it yourself]
Thus we find finally

\[
\langle \sin \theta \rangle = i \left\{ \frac{e_1 \epsilon_2}{\sqrt{\omega_1 \omega_2}} \langle \mathbf{b} | e^{i(k_1 - k_2) \cdot \mathbf{r}} | \mathbf{a} \rangle + \sum_{c} \frac{q_c^2}{\sqrt{\omega_1 \omega_2 \omega_3 \omega_4}} \langle \mathbf{b} | \frac{\mathbf{p}}{\omega_c} e^{-i \mathbf{k}_c \cdot \mathbf{r}} | \mathbf{c} \rangle \langle \mathbf{c} | \frac{\mathbf{p}}{\omega_c} e^{i \mathbf{k}_c \cdot \mathbf{r}} | \mathbf{a} \rangle \right. \\
+ \left. \sum_{c} \frac{q_c^2}{\sqrt{\omega_1 \omega_2 \omega_3 \omega_4}} \langle \mathbf{b} | \frac{\mathbf{p}}{\omega_c} e^{i \mathbf{k}_c \cdot \mathbf{r}} | \mathbf{c} \rangle \langle \mathbf{c} | \frac{\mathbf{p}}{\omega_c} e^{-i \mathbf{k}_c \cdot \mathbf{r}} | \mathbf{a} \rangle \right\}
\]

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

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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 last contributor."]

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How to explain violation of energy conservation in long-np penetration to inquisitive students: must use apparatus to measure the effect and then uncertainty principle falls you up.
[If you don't like this explanation just ask them to invent a physical experiment which shows a paradox.]

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, "we"-diagrams]

normal process

[Diagram of a normal process with labels a, b, c, and k\textsubscript{1}, k\textsubscript{2}.]

[Diagram showing a process where the photon is emitted before absorption.]
Problem: Derive a more detailed theory for the S-matrix (use matrix algebra or such) - definition, more terms, etc. Maybe just properties of S-matrix (time reversal).

Special Properties of Light Scattering:

We had found

\[ R_{\text{scat}} = 2\pi \delta(\varepsilon_a + \omega_{\text{in}} - \varepsilon_b - \omega_{\text{out}}) \frac{4\pi e^2}{(2\pi)^3} \frac{\alpha^2}{2\omega_{\text{in}} \omega_{\text{out}}} |\mathbf{M}|^2 \]

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

\[ \mathbf{M} = \sum_c \frac{\langle \mathbf{b}_1 \mathbf{c}_1 | \mathbf{e}^{-i\mathbf{k}_1 \cdot \mathbf{r}} | \mathbf{c} \rangle \langle \mathbf{c} | \mathbf{\hat{p}}_m \mathbf{e}^{i\mathbf{k}_2 \cdot \mathbf{r}} | \mathbf{a} \rangle}{\varepsilon_c - \varepsilon_a - \omega_1 + i\eta} \]

\[ + \sum_c \frac{\langle \mathbf{b}_1 \mathbf{c}_1 | \mathbf{e}^{i\mathbf{k}_1 \cdot \mathbf{r}} | \mathbf{c} \rangle \langle \mathbf{c} | \mathbf{\hat{p}}_m \mathbf{e}^{-i\mathbf{k}_2 \cdot \mathbf{r}} | \mathbf{a} \rangle}{\varepsilon_c - \varepsilon_a + \omega_2 + i\eta} \]

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

See what the rules are for complex \( \mathbf{\hat{e}}_1, \mathbf{\hat{e}}_2 \) (circularly polarized light).

Consider atomic systems with more than one electron. Include spin.
Note that the outgoing photon may leave a shifted frequency $\omega$, and thus the atom is excited. In oxygen, the electronic levels are largely spaced. However molecular levels are close, thus some scattering [Raman scattering -- made Raman the hero of Indian and Indian science known to the world]

We consider now elastic scattering from $H$-atom

$$\varepsilon_a + k_1 \rightarrow \varepsilon_a + k_2$$

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

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

$$k_1 \hat{r} \rightarrow 0$$

and find

$$M = \frac{\langle a|\hat{p}\hat{c}|c\rangle \langle c|\hat{p}\hat{c}|a\rangle}{\varepsilon_c - \varepsilon_a - \omega + i\gamma}$$

$$+ \frac{\langle a|\hat{p}\hat{c}|c\rangle \langle c|\hat{p}\hat{c}|a\rangle}{\varepsilon_c - \varepsilon_a + \omega + i\gamma}$$

$$+ \frac{1}{\mu} \langle a|11a\rangle \langle \hat{c}_1, \hat{c}_2 \rangle$$
Note

\[ \omega \sim E_2 - E_1 \]

we find resonant scattering for \( \omega \) near level energy difference and we can see a very large scattering.

Thus

\[ \langle c \left| \frac{\hat{p}}{m} \right| d \rangle = i \langle c | H \hat{x} - \hat{x} H | d \rangle \]

\[ = i (\varepsilon_c - \varepsilon_d) \langle c | \hat{x} | d \rangle \]

Then

\[ M = \sum_{c} \frac{i (\varepsilon_a - \varepsilon_c) \langle a | \hat{x} | c \rangle \langle c | \hat{x} | d \rangle}{\varepsilon_c - \varepsilon_a - \omega} \]

\[ - \sum_{c} \frac{i (\varepsilon_a - \varepsilon_c) \langle a | \hat{x} | c \rangle \langle c | \hat{x} | d \rangle}{\varepsilon_c - \varepsilon_a + \omega} \]

\[ + \frac{1}{m} \langle a | a \rangle (\hat{e}_1, \hat{e}_2) \]

\[ = -i \omega \sum_{c} \left\{ \frac{\langle a | \hat{x} | c \rangle \langle c | \hat{x} | a \rangle}{\varepsilon_c - \varepsilon_a - \omega} + \frac{\langle a | \hat{x} | c \rangle \langle c | \hat{x} | a \rangle}{\varepsilon_c - \varepsilon_a + \omega} \right\} \]

\[ - i \sum_{c} \left\{ \langle a | \hat{x} | c \rangle \langle c | \hat{x} | a \rangle - \langle a | \hat{x} | c \rangle \langle c | \hat{x} | a \rangle \right\} \]

\[ + \frac{1}{m} \langle a | a \rangle (\hat{e}_1, \hat{e}_2) \]
Now use the matrix product
\[ \xi < a | A | c > < c | B | b > = < a | A B | b > \]

Our second term becomes
\[ - i \left\{ < a | (\hat{x} \cdot \hat{e}_2) (\frac{\hat{p}_z \cdot \hat{e}_1}{m}) | a > - < a | (\frac{\hat{p}_z \cdot \hat{e}_1}{m}) (\hat{x} \cdot \hat{e}_2) | a > \right\} \]

Now \[ p_y - q_x = \frac{\hbar}{i} \]
\[ = - \frac{\hbar}{m} < a | a > (\hat{e}_1 \cdot \hat{e}_2) \]
and cancels the third term.

Follow some about sum rule
\[ \frac{\xi}{\hbar} \left| X_{mk} \right|^2 (E_n - E_k) = \frac{\hbar}{m} \]

If we had also done the \[ < c | \hat{p}_z \cdot \hat{e}_1 | a > \] we would have arrived
\[ \leq (\xi_0 - \xi_a) \left| < a | X_1 | c > \right|^2 = \frac{1}{m} \]
In the first term in (*), we see that for small 
|c - E - \omega|, one \sim \omega. Then we can drop \omega. 
Thus sum rules are very useful.

4) Roton Excitation Problem:

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

Here allow the density to vary,

\[ \epsilon(p) = \Delta + \frac{1}{2m} (p - p_0)^2 + d(p - \xi) \]

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

The amplitude for finding the roton at x can be taken to be

\[ \psi(r) = e^{i \hat{r} \cdot \hat{r}} \]

\[ \psi(x) \sim e^{i \hat{r} \cdot \hat{r}} \Phi(x) \]

Thus we take

**Initial state**: roton \( \hat{r} \)

**Final state**: roton \( \hat{r} \), phonon \( k \)

Phonons are to absorb what phonons are to light. Expect sound modes
Classical

**Displacement \( \vec{u} \)**

\[
\vec{u}(x,t) = \sum_k \frac{\xi_k}{k} \Phi_k(x) e^{i k \cdot \vec{r}} \frac{\vec{k}}{|k|}
\]

**Kinetic energy**

\[
T = \int V (\frac{\partial \vec{u}}{\partial t})^2 dx dt = \frac{1}{2} p_0 \sum_k \frac{\xi_k^2}{k^2} (\dot{Q}_k)^2
\]

**Potential energy**

\[
V = \frac{\Lambda}{2} (p - p_0)^2
\]

**Displacement change**

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

\[
= \Delta x + \Delta x \frac{\partial u}{\partial x}
\]

\[
\rho \Delta \xi = \rho_0 \Delta x
\]

\[
\frac{\rho}{p} = 1 + D \cdot \vec{u} \quad \Rightarrow \quad \rho_0 = \rho + \rho_0 \nabla \cdot \vec{u}
\]

\[
V = \frac{\Lambda}{2} \left[ (\rho_0 \nabla \cdot \vec{u})^2 \right] = \frac{\Lambda}{2} p_0^2 \sum_k Q_k^2 \frac{k^2}{k}
\]

**Total energy**

\[
E = \sum_k \frac{\rho_0}{2} \left( Q_k^2 + \gamma \rho_0 k^2 Q_k^2 \right)
\]

**Now** \( \omega = \omega_0 \) \quad \therefore \quad \gamma = \frac{\omega_0^2}{\rho_0} \)
Quantum:

Set $Q_k$ become quantum oscillators

$$H = \sum_k \left( \frac{p_k^2}{2\hbar} + \frac{p_k^2 Q_k^2}{2} \right)$$

Thus

$$H = H_{\text{free}} + H_{\text{conf}} + H_{\text{int}}$$

$$= \varepsilon(p) + \sum_k \left( \frac{p_k^2}{2\hbar} + \frac{p_k^2 Q_k^2}{2} \right) + d (\rho(x) - \rho)$$

$$H_{\text{int}} = \int \rho_0 \sum_k Q_k e^{ik \cdot \hat{r}}$$

Then

$$\text{Rate}_{\rho \to \rho', k} = 2\pi \delta (\varepsilon(p') + \hbar k c - \varepsilon(p)) \left| M \right|^2 \frac{d^3 k}{(2\pi)^3}$$

Now

$$M = \langle \rho', \hat{k} | \frac{d}{d \rho} \rho_0 \begin{cases} Q_k e^{ik \cdot \hat{r}} | \rho, 0 \rangle \end{cases}$$

$$= \frac{d \rho_0}{\sqrt{2 \rho_0 \omega_\rho}} \langle \rho' | e^{i \hat{k} \cdot \hat{r}} | \rho \rangle$$
\[
\langle \phi' e^{i\hat{\mathbf{p}}' \cdot \mathbf{r}} | \phi \rangle = \int e^{-i\mathbf{p}' \cdot \mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{r}} e^{i\mathbf{p} \cdot \mathbf{r}} d^3r
\]

\[
= \delta(\mathbf{p}' - (\mathbf{p} - \mathbf{k}))
\]

Conservation of momentum

\[
\text{Rate} = 2\pi \delta(\epsilon(\mathbf{p}') + \mathbf{p} \cdot \mathbf{k} - \epsilon(\mathbf{p})) \frac{d^2k^2}{2p_0^2k_c} \frac{\hbar^2 k_c}{(2\pi)^3}
\]

Consider first forward emission

\[
\mathbf{p} \quad \rightarrow \quad \frac{\mathbf{p}'}{\mathbf{k}} \quad \epsilon(\mathbf{p})
\]

No good

Thus a critical \( \rho \) below which we cannot emit phonons

\[
\frac{\partial \epsilon(\rho)}{\partial p_x} \bigg|_{p_x = \rho} = c_0
\]
In any system with $e = e(p)$

\[
\frac{de}{dp} = \nu_{\text{group}}
\]

**Proof:** \[\Delta e = F \Delta x \quad F = \frac{\Delta p}{\Delta t}\]

\[\frac{\Delta e}{\Delta t} = \frac{\Delta p}{\Delta t} \nu\]

\[\frac{\Delta e}{\Delta p} = \nu\]

Thus, velocity of motion must exceed speed of sound $c_s$ to have plasma emission [same as Compton radiation]
5) Some Improvements to our Theory

We had found things like

\[ 0 \leq \frac{\langle 0 | \hat{D}_1 | 0 \rangle \langle 0 | \hat{D}_2 | 0 \rangle}{\epsilon - \epsilon_a - \omega_1} \]

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

\[ m (\dot{x} + 2\omega_0 \dot{x} + \omega_0^2 x) = E \]

This gives a broadening of the resonance.

\[ \frac{1}{\omega_0^2 \omega^2 + i \omega \omega_0} \sim \frac{1}{2\omega_0 (\omega - \omega_0 + i \frac{1}{\gamma})} \]

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

\[ n \equiv \{ k \} \]

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 $\delta m(t)$, the amplitude that we will find the system in state $m$ at time $t$. We found

$$i \delta m(t) = \sum_n V_{mn} \chi_n(t) \chi_n(t)$$

$$= \sum_n V_{mn} e^{i(\delta n - E_n)t} \chi_n(t)$$

(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

$$i \delta n(t) = \left( \begin{array}{c} \text{terms relating states other than } n \text{ to the continuum} \\ \text{state other than } n \text{ to the continuum} \end{array} \right) + \sum_k V_{nk} e^{i(\delta n - E_n)t} b_k(t)$$

(2)

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

$$i b_k(t) = V_{kn} e^{i(\delta n - E_n)t} \chi_n(t)$$

(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

$$b_k(t) = -i \int_0^t V_{kn} e^{i(\delta n - E_n)t} \chi_n(t') dt'$$

Substitute this into (2) to find

$$i \delta n(t) = \left( \text{other terms} \right) - i \int_0^t \sum_k |V_{kn}|^2 e^{i(\delta n - E_n)t} \chi_n(t') dt'$$

(4)
We now rewrite equation in terms of the $\nu_k$'s above. We have removed details of the $\nu_k$. We only retain its affect on the actual process we are interested in.

Now assume the $\nu_k$'s vary slowly and

$$\nu_k(t) \sim \nu_k(t')$$

we also consider time-independent perturbations and note,

$$\int_{-\infty}^{\infty} \frac{1}{e^{-iu} - e^{-iu'}} = \frac{1}{\epsilon + i(E_n - E_k)}$$

we can write (4) as

$$i \dot{\nu}(t) = (\text{other terms}) - \left[ \sum_{k} \frac{\epsilon |\nu_k|^2}{E_n - E_k - i\epsilon} \right] \nu_k(t)$$

Now define

$$\lim_{\epsilon \to 0} \sum_{k} \frac{\epsilon |\nu_k|^2}{E_n - E_k - i\epsilon} = \Delta_n + i \frac{\Gamma_n}{2}$$

so that (5) becomes

$$i \dot{\nu}(t) = (\text{other terms}) - (\Delta_n + i \frac{\Gamma_n}{2}) \nu(t)$$

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

$$\nu(t) = \nu(0) e^{(\Delta_n + i \frac{\Gamma_n}{2})t}$$

But recall $$\nu(t) = C(t) e^{E_k t}$$
Thus, \[ C_n(t) = e^{-i(En - \Delta n)t} e^{-\frac{\Gamma_n t}{2}}. \]

We can see from this special case that the continuum interaction shifts the levels by \( \Delta n \) [for example, all levels of the S-枝 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 \( \frac{1}{\Gamma_n} \).

In the remainder of our analysis we will forget the small shift correction \( \Delta n \) for a bit. The important physical effect for us is \( \Gamma_n \), the line width.

We now return to calculating \( \Gamma_n \) and \( \Delta n \) from \( (6) \).

Recall

\[ \lim_{\epsilon \to 0} \frac{1}{x+i\epsilon} = \text{PV.} \left( \frac{1}{x} \right) - i\pi S(x) \]

We then find

\[ \Delta n = \text{PV.} \int_{-\infty}^{\infty} \frac{\omega_{nl}^2}{E_n - E_k} \]

(similar to 2nd order perturbation theory result)

\[ \Gamma_n = 2\pi \int_{-\infty}^{\infty} \omega_{nl}^2 S(E_k - E_n) \]

Note: to go from state \( n \) to anything (all \( k \))

\[ \text{[Sustains with} \quad \hbar \frac{d}{dt} n = -\Gamma_n P_n \text{]} \]
To generalize these results we recognize that we get a $\Gamma_j$ for each type of continuum (a decay, B decay, etc... each decay channel).

**Example:** Sight emission by an atom which itself can disintegrate

$$n \quad m \quad \text{both } n \text{ and } m \text{ can disintegrate}$$

Let the atom initially be in state $n$, i.e. $a_n(0) = 1$.

The analogue to (5) becomes

$$a_n(t) = -i \nu_{nm}(t) a_m(t) - \frac{\Gamma_m}{2} a_n(t) \quad (5a)$$

$$a_m(t) = -i \nu_{nm}(t) a_n(t) - \frac{\Gamma_n}{2} a_m(t) \quad (5b)$$

Where we have ignored $\Delta n$ and $\Delta m$. Ignoring $\nu_{nm}$ in (5a), we can solve directly for

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

We can then substitute this into (5b) to find

$$a_m(t) = e^{-\frac{\Gamma_n}{2} t} \int_0^t (-i \nu_{nm}(t)) e^{-\frac{\Gamma_m}{2} (t - t')} e^{\frac{\Gamma_n}{2} t'} dt'$$

Set $V = \text{const}$, $\nu_{nm} = V_{nm} e^{-i(En-Em)t}$

Thus

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

Suppose

state 1: atom in a

state 2: atom in b, photon c

If we use

\[ \int_0^\infty \frac{dx}{x^2 + \frac{\Gamma_n}{4}} = \frac{\pi}{\Gamma_n} \quad \int_0^\infty \frac{dx}{x^2 + \frac{\Gamma_m}{4}} \cos xt = \frac{\pi}{\Gamma_m} e^{-\frac{\Gamma_m}{2} t} \]

we can find

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

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

We can then think of the following problems ("decay bounds")

\[ \dot{P}_n(t) = -\Gamma_n P_n(t) \]
\[ \dot{\rho}_n(t) = r P_n(t) - \Gamma_n \rho_n(t) \]
PROBLEM: In string interactions, Goldhaber and Mandelstam cooked up quantities called strangeness $\Delta S$.

Example:

$$\pi^- + p \rightarrow \Lambda^0 + K^0$$

\[ S = 0 \quad S = 0 \quad S = -1 \quad S = 1 \]

or

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

\[ S = 0 \quad S = 0 \quad S = 1 \quad S = -1 \]

To distinguish, we note that in matter,

$$K^0 + p \rightarrow \Lambda^0 + \pi^+$$

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

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

Example:

$$K^0 \rightarrow \pi^+ + \pi^- \quad 10^{-10} \text{ sec} \quad \text{(mean life of decay)}$$

and

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

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. Goldhaber and Mandelstam found that for two states decaying into some continuum, the ratio of finding a $K$ decays exponentially. Find out how they did this 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 look at

\[ \kappa^0 \rightarrow \pi^- + \mu^+ + \nu \]

\[ \bar{\kappa}^0 \rightarrow \pi^+ + \mu^- + \bar{\nu} \]

which makes a more realistic problem

But need \( \langle 0 \rangle \sim \langle \rangle = \langle \bar{\rangle} \rangle \)

We return to our formulation 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, and must be regarded as an interaction with a continuum of states, one of which was our earlier definite energy state. Thus, the theory of degenerate perturbation theory.

We had introduced these concepts by writing

\[
i \dot{a}_m = \sum_n V_{mn}(t) a_n(t) + \sum_k M_{nk} b_k(t) e^{-i(E_n - E_k)t}
\]

\[
i \dot{b}_k = \sum_m M_{km} e^{i(E_k - E_m)t} a_m(t)
\]

We want to ignore the details of the \( b_k \)'s and worry only about the \( a_m \)'s. We found

\[
\dot{a}_m = -i \sum_n V_{nm}(t) a_n(t) - \sum_k M_{kn} e^{i(E_k - E_n)t} a_n(t) dt' + \sum_k M_{kn} e^{i(E_k - E_n)t} a_n(t') dt' \]
We are not interested in the last term since it would affect us very much (no "secular" or resonance effects), so we will ignore it.

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

$$a_n = -i \sum_{m} v_{m n}(t) a_m(t) - i \left( \Delta_n - i \frac{\Gamma_n}{2} \right) a_n(t)$$

where

$$\Delta_n - i \frac{\Gamma_n}{2} = \sum_{k} \frac{|M_{k n}|^2}{E_n - E_k + i \epsilon}$$

$$\Gamma_n = 2\pi \sum_{k} S(E_k - E_n) |M_{k n}|^2$$

If we ignore the shift $\Delta_n$, we find

$$a_n = -i \sum_{m} v_{m n}(t) a_m(t) - \frac{\Gamma_n}{2} a_n(t)$$

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

$$P_{\text{dis}} = \sum_{k} b_{k n}^* b_{k n}$$

Can show

$$P_{\text{dis}} = \Gamma_n |a_n(t)|^2$$

[Shaw 7]
Last time we were considering an example

\[ a, \Gamma_a \]

\[ \text{state: atomic population} \]

\[ b, \Gamma_b \]

\[ \text{state: atomic, electron} \]

\[ \alpha_m = -i \, V_{mn} \, e^{i(E_m - E_n)t} \, a_n(t) - \Gamma_m/2 \, a_m(t) \]

\[ \alpha_n = -\Gamma_n/2 \, a_n(t) \]

Can do this only to first order, by first solving

\[ a_n(t) = a_n(0) e^{-\Gamma_n t} = e^{-\Gamma_n t} \quad a_n(0) = 1 \]

Can then find

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

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

Now \[ E_m - E_n = \epsilon_0 + \omega - \epsilon_a = \omega - \omega_0 = \nu \] frequency difference from energy levels.

\[ \Gamma_m = \Gamma_0, \quad \Gamma_m = \Gamma_a \]
But we want prob. of finding photon of \( \nu \) and don't need to worry about what happens to state \( b \).

\[ P_\nu(t) = P_m(t) + P_{\text{decays}} \]

and

\[ P_{\text{decays}} = \Gamma_b P_m \]

Recall

\[ P_m = \text{probability of photon emission of frequency } \omega_0 + \nu = \omega \text{ and atom in } b \]

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

\[ P_\nu = \text{probability that some photon of } \nu \text{ is present} \]

Thus

\[ P_\nu(t) = P_m(t) + P_{\text{decays}}(t) \]

Look at

\[ P_\nu(\infty) = P_m(\infty) + P_{\text{decays}}(\infty) \]

Now \( P_m(\infty) = 0 \) \([\text{atom certainly has decayed by } t = \infty]\)

\[ P_{\text{decays}} = \int_0^\infty P_m(t) \, dt \]

from (1)

Thus

\[ P_\nu(\infty) = \Gamma_b \left| V_{mn} \right|^2 \frac{1}{2^{1/2} \left( \frac{\lambda_0 - \lambda}{2} \right)^3} \left[ \frac{1}{\Gamma_a} + \frac{1}{\Gamma_b} - \frac{2 \left( \frac{\lambda_0 + \lambda}{2} \right)}{\nu^2 + \left( \frac{\lambda_0 + \lambda}{2} \right)^2} \right] \]
Thus
\[ P_v(t) = \frac{|V_{tm}|^2 (\Gamma_a + \Gamma_b)}{\Gamma_a} \left[ \frac{1}{v^2 + \left( \frac{\Gamma_a + \Gamma_b}{2} \right)^2} \right] \]

"Lorentzian" or "Breit-Wigner" line shape

Note if our instruments aren't very accurate, this looks like
\[ P_v(t) \sim 2\pi \frac{|V_{tm}|^2 S(v)}{\Gamma_a} \]

Thus the probability of any photon of any \( v \) can be found by summing over \( n \) (or integrating \( \mathcal{E} \) over \( v \))

\[ P = \sum_{m} P_v(t) \sim \int P_v(t) \, dv = \frac{2\pi |V_{tm}|^2 S(v)}{\Gamma_a} \]

---

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

Rate of emission = \( 2\pi |V_{tm}|^2 S(v) \) \[ \text{Prob. to be in upperstate} \]

\[ e^{-\Gamma_a t} \]

Total rate of emission = \( \int \text{Rate} \, dt = \frac{2\pi |V_{tm}|^2 S(v)}{\Gamma_a} \)

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

Quite a few people use (3) to say that the line shape depends \( S(v) \) or Lorentzian but decays as \( e^{-\Gamma_a t} \). However, this is incorrect as we can see by considering a special case of
transitions to a stable state b

\[ P_a(t) = P_m = |V_m|^2 \left( 1 + e^{-\frac{\Gamma_a t}{2}} - e^{-\frac{\Gamma_a t}{2}} \cos \omega t \right) \]

\[ \frac{\Gamma_a}{2} \]

\[ \Gamma_b = 0 \]

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.

\[ a = 0 \]

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

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

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

\[ \dot{a}_k = -i V_{ki} a_i(t) e^{-i(E_k - E_i)t} - \frac{\Gamma_k a_k}{2} \]
Zero-order: $a_i = 1$

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

$$= -iV_{ki} \left[ e^{i(E_k-E_i) T} - e^{-\frac{\Pi k}{2}} \right]$$

We then find

$$a_j = -i \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Pi k}{2}} \int_0^T \left[ e^{-i(E_k-E_j) t} e^{i(E_k-E_j) T} e^{-\frac{\Pi k}{2}} e^{-i(E_k-E_j) t} \right] dt$$

$$= \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Pi k}{2}} \int_0^T e^{i(E_j-E_i) t} dt$$

$$= \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Pi k}{2}} \left[ e^{i(E_j-E_i) T} - 1 \right]$$

Thus we find

$$a_j(T) = \left\{ V_{ji} + \sum_k \left[ \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Pi k}{2}} \right] \right\} \int_0^T e^{i(E_j-E_i) t} dt$$

$$= V_{ji} + \sum_k \left[ \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Pi k}{2}} \right]$$

Thus

$$P_{jk} = \text{Im} \left| M_{ji} \right|^2 \frac{\sin^2(E_j-E_i) T/2}{(E_j-E_i)^2}$$

Rate:

$$= 2n S(E_i - E_j) \left| M_{ji} \right|^2$$

where

$$M_{ji} = V_{ji} + \sum_k \left[ \frac{V_{jk} V_{ki}}{E_k - E_i - i\frac{\Pi k}{2}} \right]$$

(replaces $e$ in our limit)
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 leave a $\Gamma$ (line resistance in circuit theory).

\[ \sum_{m \neq n} \sum_{k} \frac{V_{mk} V_{kn}}{E_k - E_n} \left( \frac{e^{i(E_n - E_k)T}}{E_n - E_k} - 1 \right) - \frac{e^{i(E_n - E_k)T}}{E_n - E_k} \left( \frac{e^{i(E_n - E_k)T}}{E_n - E_k} - 1 \right) \]

Look in Hibbs and Feynman, p.154 to get

\[ \sum_{m \neq n} \sum_{k} \frac{V_{mk} V_{kn}}{E_k - E_n - i\varepsilon} \]
Trichias & Quinn Rules

\[ \langle a l x 1 k \rangle < k l x lb \rangle = \langle a 1 x H x lb \rangle \]

\[ \langle a l x 1 k \rangle < k l x lb \rangle \quad \text{in} \quad e \text{m} + \theta \]

\[ = \langle a 1 x \frac{1}{H + Q} x lb \rangle \]

\[ \text{very hard to invert however} \]

Hints to get back to c

\[ c^2 / hc = \frac{1}{137} \]

[all theoretical physicists does before 137]

Length & time are equivalent units

\[ \text{Life time} = \frac{\text{Length}}{c} \]

\[ \frac{1}{\text{Length}} = \frac{1}{\text{time}} = \text{Energy} = \text{momentum} = \text{mass} \]

Now \[ \frac{1}{\text{time}} = \text{energy} \]

\[ \text{mass} = \frac{4 \pi c^2}{\text{length}} \]
c. ALTERNATIVE FORMULATIONS

Today we write the perturbation theory in different forms (not important, just 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 define

\[ i \frac{d|\psi(t_b)\rangle}{dt_a} = H(t_a) |\psi(t_a)\rangle \]

Thus

\[ i \frac{dU(t_b, t_a)}{dt_b} = H(t_b) U(t_b, t_a) \]

subject to \( U(t_a, t_a) = I \)

Sometimes we use

\[ S = \lim_{t_a \to -\infty} \lim_{t_b \to \infty} U(t_b, t_a) \]

although strictly speaking, the limit doesn't exist.

More trouble than it's worth, however.
Suppose $H$ is independent of time

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

What is the operation? Several possible (and equivalent) definitions:

1. If $H\Phi = E\Phi$, then
   $$e^{-iHT}\Phi = e^{-iET}\Phi$$

2. Power series expansion of $e^{-iHT}$

3. Define by differential equation

If $\Phi_n$ are basis states of $H(\Phi_n) = E_n(\Phi_n)$, 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

$$U = \sum_{m,n} \langle \Phi_m|\langle \Phi_m|U|\Phi_n\rangle\langle \Phi_n|$$

$$= \sum_{n} \langle \Phi_n|e^{-iE_n(t_b - t_a)}\langle \Phi_n|$$

Useful if we can find $\Phi_n$. 
2) Integral Formulations

We can now write a Hamiltonian in another representation, say $x$-representation:

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

If $H$ is constant,

$$\mathcal{K}(x'; x, T) = \sum_m \phi_m(x') \phi_m^*(x) e^{-i E_m T}$$

Thus

$$\psi(x', t_b) = \sqrt{\mathcal{K}(x', x; T)} \psi(x, t_a) dx$$

For many cases, $\mathcal{K}(x', x; T)$ can be named [free particle gives]

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

[the diffusion kernel]

Can sum for anything that has a form only up to quadratic order.
3) Some properties of $U$

$$U(t_0, t_a) = U(t_b, t_c) U(t_c, t_a) \quad t_a < t_c < t_0 \quad (\star)$$

[Diagonalization in Hilbert space, so obvious]

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

[But relation not complete]

Phys. Rev. 84, 108 (1951) adds an ordering index

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

where $U_{i+1} \lessgtr U_i$

Thus if you want $BA_2$, write $A_2 B$ or $BA_2$.

Ex: old: \[ \nabla x (U_x U) \]

new: \[ \nabla x (U_x U) \]

New using

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

\[ U(t_b, t_a) = \lim_{\Delta t \to 0} \prod_{N=1}^{N \to \infty} e^{-i H(t_{\nu}) \Delta t} e^{-i H(t_{\nu-1}) \Delta t} \ldots e^{-i H(t_0) \Delta t} \]

\[ = \lim_{\Delta t \to 0} e^{-i \int_{t_0}^{t_b} H(t) \, dt} \]

Instead use

\[ U(t_b, t_a) = e^{-\int_{t_a}^{t_b} H(t) \, dt} \]

[Not used a good use for this yet, but feels it will come in handy somewhere]

Now from conservation of probability and causality

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

\[ \Rightarrow U \text{ is a unitary operator} \]
Try to extend definition of $U$ such that

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

Suppose things in future come affect past, then

Use non-unitary ans (*) distinct world. However, we can fix (*) up with some new variables. Maybe causality isn't correct.

Ex: EM field can be turned out leaving only partially

variables. Use highly retarded and advanced interactions.

Teylmann got stuck 3/4 through. Threat out differential

equation approach (he did get a "prize" for it,

however). D.E.'s are not useful relativistically,

All he did was use consider

$$H = (H^{(1)} + H^{(3)}) + \text{coulomb}$$

in

$$U = e^{-i\int H_1 \, dt} = e^{-i\int (H^{(1)} + H^{(3)}) \, dt} + e^{-i\int \frac{\vec{e}^2}{r_{13}-r_{14}} \, dt}$$

($$1-\frac{r_{13}}{c^2}$$)

Doesn't quite work.
Recall we had defined:

\[ U(t_b, t_a) : \quad i \frac{dU}{dt_b} = H(t_b) U \]

\[ U(t_a, t_a) = 1 \]  \hspace{1cm} (1)

4.) Neumann Series

If \( H \) independent of time,

\[ U(t_b, t_a) = e^{-iH(t_b-t_a)} \]

\[ = \sum_n \langle \Phi_n | e^{-iE_n(t_b-t_a)} | \Phi_n \rangle \]  \hspace{1cm} (2)

We can integrate (1) and use (2) to write:

\[ U(t_b, t_a) = U_0(t_b, t_a) - i \int_{t_b}^{t_a} U_0(t_b, t) V(t) U(t, t_a) dt \]  \hspace{1cm} (3)

By iteration we can set up the Neumann series

\[ U(t_b, t_a) = U_0(t_b, t_a) - i \int_{t_b}^{t_a} U_0(t_b, t) V(t) U_0(t_a, t) dt + \]

\[ + (-i)^2 \int_{t_2}^{t_b} U_0(t_b, t_1) V(t_1) U_0(t_1, t_2) V(t_2) U_0(t_2, t_a) dt_1 dt_2 dt_1 \]

\[ t_b < t_2 < t_1 < t_a \]  \hspace{1cm} (4)
One can prove the convergence of this series but why care? "If it doesn't converge, it doesn't work, and we don't use it?"

Now let $H_0$ be small and simple enough 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

$$U(t_b,t_a) = e^{-iH_0(t_b-t_a)} - i\int e^{-iH_0(t_b-t_1)} e^{-iH_0(t_1-t_a)} dt_1 + \ldots$$

Now consider $\langle m | U | n \rangle$. Note

$$e^{-iH_0^+ | n \rangle} = e^{-iE_n^+ | n \rangle}$$

Thus our series becomes

$$\langle m | U | n \rangle = \sum_n e^{-iE_n(t_b-t_a)} - i\int e^{-iE_n(t_b-t_1)} \langle m | V(t_1) | n \rangle e^{-iE_n(t_1-t_a)} dt_1,$$

$$+ (i)^2 \int e^{-iE_n(t_b-t_1)} \langle m | V(t_1) e^{-iH_0(t_1-t_2)} V(t_2) | n \rangle \cdot e^{-iE_n(t_2-t_a)} dt_1 dt_2$$

Use $\langle m | A B | n \rangle = \sum_k \langle m | A k \rangle \langle k | B | n \rangle$
Thus write
\[ \langle m | V(t_1) e^{-iH_0 (t_1 - t_2)} V(t_2) | n \rangle = \sum_{b, l} \langle m | V(t_1) | b, l \rangle \langle b, l | e^{-iH_0 (t_1 - t_2)} V(t_2) | n \rangle e^{-iE_b (t_1 - t_2)} S_{b, l} \]

Thus the third term becomes
\[ (-i)^2 \sum_{b} \sum_{l} e^{-iE_b(t_0 - t_1)} \langle m | V(t_1) | b, l \rangle e^{-iE_b(t_1 - t_2)} \langle b, l | V(t_2) | n \rangle e^{-iE_b(t_2 - t_3)} \]

Now make change of variable, recalculating
\[ e^{iE_b t_0} e^{-iE_b t_3} \langle m | U | n \rangle \]. Realizing this, we can recognize our earlier series.

Frequently people refer to using
\[ V(t) = e^{i(E_b - E_n) t} V(t) \]

as the "interaction representation." Only a matter of convenience in "one-up-mandship."
5. Interpretation by Feynman diagrams

\[ \begin{align*}
&U_0(t_0, t_1) V(t_1) U_0(t_1, t_2) V(t_2) U_0(t_2, t_3) U_0(t_3, t_4) V(t_4) U_0(t_4, t_5) U_0(t_5, t_6) V(t_6) \\
&+ \sqrt{\omega(t_0, t_1) V(t_1) U_0(t_1, t_2) V(t_2) U_0(t_2, t_3) U_0(t_3, t_4) V(t_4) U_0(t_4, t_5) U_0(t_5, t_6) V(t_6)}
\end{align*} \]

\[ (-i)^2 \int U_0(t_0, t_1) V(t_1) U_0(t_1, t_2) V(t_2) U_0(t_2, t_3) \, dt_1 \, dt_2 \]

\[ t_0 > t_1 > t_2 > t_a \]

Disturbance \( V \) can act on system any number of times. In all these series the amplitude to be scattered is 
\[ -i V(t_1) \]. Thus an interpretation of \( V(t_1) \) is seen here. We can see how these amplitudes add up.

Sometimes some people call \( U_0 \) the propagator. Feynman first calls \( V \) the scatterer.

**EXAMPLE:** Consider three \( V \)'s, \( V_A \) \& \( V_B \). But only interested in first order in \( V_A \), first order in \( V_B \).

\[ \sqrt{U_0(t_0, t_1) V(t_1) U_0(t_1, t_2) V(t_2) U_0(t_2, t_3) V(t_3) U_0(t_3, t_4) V(t_4) U_0(t_4, t_5) U_0(t_5, t_6) V(t_6)} \]

\[ t_1 < t_2 \]
Can we have $y$?

Instead reverse $B/A$ to pick up a second term

$$t_1 > t_2$$

Actually, this scheme isn't really dead in relativistic theory. Thus represents pair production, for instance. Need a new type of perturbation instead.

However, need a more general definition.

Comments:

1. Must add all terms together — find phase interference.

2. To define $U_0$ for negative time,

$$U_0(t_2, t_1) = 0 \quad t_2 < t_1$$

Then restrictions on integration are automatic.
\[ U(t_b, t_a) = U_0(t_b, t_a) - 2 \int U_0(t_b, t_1) V(t_1) U_0(t_1, t_2) dt_1 \]

\[ + (i)^2 \int U_0(t_b, t_2) V(t_2) U(t_2, t_1) V(t_1) U(t_1, t_a) dt_1 dt_2 \]

\[ U_0(t_1, t_2) \text{ propagation} \]

\[ V(t_1) \text{ scattering amplitude per unit time} \]

\[ U_{mn} = \delta_{mn} - i \int e^{-i(E_m - E_n)t} V_{mn} dt \]

\[ + (i)^2 \int e^{-i(E_m - E_n)t_1} V_{mn} e^{-i(E_n - E_l) t_2} V_{lm} dt_1 dt_2 \]

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

\[ H = \frac{\hbar^2}{2m} \sum_{j=1}^{23} \nabla_j^2 + \sum_{j=1}^{23} V(r_j) \]

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 then consider 1 as the correction to our approximation. In this sense it is physical. "Everything is approximate."

To understand bound states, we operate again and again. Thus we need the infinite series. Thus should attempt to analyze. For try by consider free p; e with \( V = \text{coupled interaction} \). Once we group bound states in \( H_0 \) then we can apply perturbation of \( O(e^2) \) for EM interactions.

\[ e^2 = \frac{1}{137} \] makes the treatment of QED feasible by this series. For many, \( e^2 = 10 \), and series does not converge. \[ \text{Field theory means perturbation theory} \] could try expansion in \( e^2 \). People don't know where to make zero approximation. Note close enough to experience.

Problems may look the same but have different numbers such that the same method won't work for both. Diff. 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 for real physics — not vice versa.

[Don't conclude we don't understand superconductivity because BCS theory doesn't apply to modern structure.]

Don't copy methods. Think first. Decide what approximation will work for your problem, then think up a method.
Examples:

Propagator in state of energy $E_k$ is $\xi E_k(t_2-t_1)$

Scattering amplitude $= -i V_{mn}$

To find second order term

\[ (-i)^2 \int e^{-iE_0(t_0-t_2)} V_{mk} e^{-iE_k(t_2-t_1)} V_{kn} e^{-iE_n(t_1-t_0)} d^4x_1 d^4x_2 \]

There is also a space representation

Look for first order ray

\[ -i \int V_0(x_0, x_1, t_0-t_1) V(x_1) V_0(x_1, x_2, t_1-t_0) dx_1 \]
Still a third method, [interaction representation]

Prop. n is $S_{\text{nu}} = 1$

Beatt. amplitude $= -i V_{\text{nu}} e^{i(E_{\text{n}} - E_{\text{nu}}) \tau}$

Now recall

$U_{\text{nu}} e^{i(E_{\text{nu}} - E_{\text{nu}}) \tau} = S_{\text{nu}} - i \int_{0}^{T} e^{-i(E_{\text{n}} - E_{\text{nu}}) \tau} V_{\text{nu}} d\tau$

We can use a shortcut by integrating over the difference assuming it is effective only over a finite time. Then we are left with

$S_{\text{nu}} + (-i) \int_{0}^{T} e^{-i(E_{\text{n}} - E_{\text{nu}}) \tau} \left[ V_{\text{nu}} + V_{\text{nu}}^{\dagger} \frac{1}{E_{\text{n}} - E_{\text{nu}} - i\epsilon} V_{\text{nu}} \right. + V_{\text{nu}} V_{\text{nu}}^{\dagger} \frac{1}{E_{\text{n}} - E_{\text{nu}} - i\epsilon} \left. V_{\text{nu}} + \ldots \right]$

Thus

$\text{Rate} = 2\pi S \left| (E_{\text{n}} - E_{\text{nu}}) \right| T_{\text{nu}}$
7) **T- MATRIX**

We have found

\[ \text{Rate} \propto = 2 \pi g \left| E_n - E_n \right| \left| T_{nn} \right|^2 \quad \text{Golden Rule} \# 2 \]

\[ T_{nn} = V_{mn} + \sum_k V_{mk} \frac{1}{E_n - E_{k+1}} V_{kn} + \sum_k V_{mk} \frac{1}{E_n - E_{k+1}} V_{kn} \frac{1}{E_n - E_{k+1}} V_{kn} \quad \text{Golden Rule} \# 1 \]

These can again be written in different forms. First note for \( E = E_n \),

\[ T = V + V \frac{1}{E - H_{101}} V + V \frac{1}{E - H_{101}} V \frac{1}{E - H_{101}} V + \ldots \quad (3) \]

where we have defined \( f(H_0) \phi_k = f(E_n) \phi_k \)

\[ \begin{bmatrix} f(H_0) \end{bmatrix}_{\phi_k} = f(E_n) \begin{bmatrix} \phi_k \end{bmatrix} \]

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.

**A and B are operators**

\[ \frac{1}{A + B} = \frac{1}{A} - \frac{1}{A} A B \frac{1}{A} + \frac{1}{A} A B \frac{1}{A} A B \frac{1}{A} - \ldots \]

**Proof:** Set \( X = \frac{1}{A + B} \) show \( (A + B)X = 1 \)

\[ AX = 1 - B \frac{1}{A} + B \frac{1}{A} B \frac{1}{A} - \ldots = 1 - B \left( \frac{1}{A} - \frac{1}{A} \right) \frac{1}{A} - \ldots \]

\[ = 1 - BX \Rightarrow (A + B)X = 1 \]
Now write

\[ T = V + V W(E) V \]

where

\[ W(E) = \frac{1}{E-H_{0}+i\epsilon} + \frac{1}{E-H_{0}+i\epsilon} V \frac{1}{E-H_{0}+i\epsilon} V + \cdots \]

\[ = \frac{1}{E-H_{0}+i\epsilon} = \frac{1}{E-H+i\epsilon} \]

\[ T(E) = V + V \frac{1}{E-H+i\epsilon} V \]

\[ = (H-H_{0}) + (H-H_{0}) \frac{1}{E-H+i\epsilon} (H-H_{0}) \]

Now suppose we want to study \( \frac{1}{Q} \). This means

\[ \frac{1}{Q} |\chi_n\rangle = \frac{1}{Q_n} |\chi_n\rangle \]

so

\[ \frac{1}{Q} = \sum_n \langle \chi_n | \chi_n \rangle \frac{1}{Q_n} <\chi_n| \]

Thus

\[ \frac{1}{E-H+i\epsilon} = \sum_n \langle \chi_n | \chi_n \rangle \frac{1}{E-E_n+i\epsilon} <\chi_n| \]

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 $H = H(t)$,

$$U(T) = e^{-iHT}$$

Now consider the Fourier transform

$$\sqrt{\int_{-\infty}^{\infty} e^{iET} U(T) dT} = iW(E)$$

But note:

$$-i\int_{-\infty}^{\infty} e^{i(E-H)T} dT = \frac{1}{E-H+i\gamma} = W(E)$$

Thus $W(E) = \mathcal{F}\{U(T)\}$

---

We have been considering $H = H_0 + V$. But now consider

**Example:** \[A + B \rightarrow C + D\], e.g. \(\text{He}^+ + H \rightarrow p + \text{He}\)

Write

$$H = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + \frac{e_1 e_x}{v_{1x}} + \frac{e_2 e_x}{v_{2x}} + \frac{e_1 e_y}{v_{1y}} + \frac{e_2 e_y}{v_{2y}}$$

$$+ \frac{p_{x1}^2}{2m_{x1}} + \frac{p_{y1}^2}{2m_{y1}} + \frac{e_{x1}}{v_{x1}} + \frac{e_{y1}}{v_{y1}}$$

Hence

$$H = H_0 + V$$

where

$$H_0 = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + \frac{e_1 e_x}{v_{1x}}$$

$$V = \frac{e_{x1}}{v_{x1}} + \frac{e_{y1}}{v_{y1}} + \frac{e_{x2}}{v_{x2}} + \frac{e_{y2}}{v_{y2}}$$

$$+ \frac{p_{x1}^2}{2m_{x1}} + \frac{p_{y1}^2}{2m_{y1}} + \frac{e_{x1}}{v_{x1}}$$
\[ H = H_{\Pi} + V_{\Pi} \]

\[ H_{\Pi} = \left( \frac{p_y^2}{2m_y} \right) + \left( \frac{p_x^2}{2m_x} + \frac{e_x e_1}{V_{1y}} + \frac{e_x e_2}{V_{2y}} + \frac{e_1 e_2}{V_{12}} \right) \]

\[ V_{\Pi} = \frac{e_x e_1}{V_{1y}} + \frac{e_x e_2}{V_{2y}} + \frac{e_y e_1}{V_{1y}} \]

Which \( V \) do we use in our formula? \( T \)

\[
T(E) = \frac{1}{(E-H_0) + \frac{(H-H_0)}{E-H+i\epsilon}} (H-E_{\Pi})
\]

\[
= \frac{1}{E-H+i\epsilon} (H-E_{\Pi})
\]

It makes no difference.

On the energy shell:

\[
T_{\text{thdall}} = V_{\Pi} + V_{\Pi} \frac{1}{E_{\Pi} - H + i\epsilon} V_{\Pi}
\]

Now:

\[
T_{\text{chm}} = \langle \Pi | V_{\Pi} | \Pi \rangle \frac{1}{2} \langle \Pi | V_{\Pi} | \Pi \rangle = \langle \Pi | H - H_0 | \Pi \rangle \frac{1}{2} \langle \Pi | H - H_\Pi | \Pi \rangle
\]

Chemists
8) $K^0, \overline{K^0}$ Decay Problem

$K^0 \rightarrow \pi^+ + \pi^-$  \hspace{1cm} a_{K^0}

$\overline{K^0} \rightarrow \pi^+ + \pi^- \hspace{1cm} a_{\overline{K^0}}$

\[ i \dot{a}_{K^0} = E_0 a_{K^0} + \sum_{\pi} M_{K^0 \rightarrow \pi} b_{\pi} \]

\[ i \dot{a}_{\overline{K^0}} = E_0 a_{\overline{K^0}} + \sum_{\pi} M_{\overline{K^0} \rightarrow \pi} b_{\pi} \]

\[ i \dot{b}_{\pi} = E_{\pi} b_{\pi} + \sum_{K^0, \overline{K^0}} M^{*}_{K^0, \overline{K^0} \rightarrow \pi} a_{K^0, \overline{K^0}} \]

Write
\[ b_{\pi}(t) = \int_{0}^{t} e^{i(E_{\pi} - E_0)\tau} M^{*} \left[ a_{K^0}(\tau) + a_{\overline{K^0}}(\tau) \right] d\tau \]

Then
\[ i \dot{a}_{K^0} = \sum_{\pi} e^{i(E_{\pi} - E_0)\tau} M_{\pi} M^{*} \left[ a_{K^0}(\tau) + a_{\overline{K^0}}(\tau) \right] d\tau \]

\[ i \dot{a}_{\overline{K^0}} = (\Delta - i\frac{\pi}{2}) \left[ a_{K^0}(t) + a_{\overline{K^0}}(t) \right] \]

\[ i \dot{a}_{\overline{K^0}} = (\Delta - i\frac{\pi}{2}) \left[ a_{K^0}(t) + a_{\overline{K^0}}(t) \right] \]

Solving
\[ a_{K^0} + a_{\overline{K^0}} = c e^{-i\Delta t} e^{-\sigma t/2} \]
\[ a_{K^0} - a_{\overline{K^0}} = D \]

Any $a_{K^0} = 1$ $a_{\overline{K^0}} = 0$

\[ a_{K^0} = \frac{1}{2} \left[ 1 + e^{-\sigma t/2} e^{-i\Delta t} \right] \]
\[ a_{\overline{K^0}} = \frac{1}{2} \left[ 1 - e^{-\sigma t/2} e^{-i\Delta t} \right] \]
Thus \( |a_{\nu_0}|^2 = \frac{1}{4} \left[ 1 + 2 \cos (\Delta t) e^{-\pi t/2} + e^{-\pi t} \right] \)

\( |a_{\bar{\nu}_0}|^2 = \frac{1}{4} \left[ 1 - 2 \cos (\Delta t) e^{-\pi t/2} + e^{-\pi t} \right] \)

Thus production of \( \nu \) in a sheet

\[ \begin{array}{c}
\text{This general effect is true for any system with two states, } \nu_0, \bar{\nu}_0 \\
1|\nu_1\rangle = \frac{1}{\sqrt{2}} (|\nu_0\rangle + |\bar{\nu}_0\rangle) \\
1|\nu_2\rangle = \frac{1}{\sqrt{2}} (|\nu_0\rangle - |\bar{\nu}_0\rangle)
\end{array} \]

\[ \begin{array}{c}
a_{\nu_1} = \frac{1}{\sqrt{2}} (a_{\nu_0} + a_{\bar{\nu}_0}) \\
a_{\nu_2} = \frac{1}{\sqrt{2}} (a_{\nu_0} - a_{\bar{\nu}_0})
\end{array} \]

Thus in our problem, \( \nu_2 \) cannot decay into \( \nu_1 + \nu_1 \).
Thus \( |\nu_1\rangle \neq |\nu_2\rangle \) are best states to work with.

\( \Delta \) is mass difference between \( \nu_1 \) & \( \nu_2 \), \( \Delta = 485 \) eV

\( \sim 5-6 \) eV.

Uses this to argue against negative mass theory of antimatter.
But it is found $K_2$ does decay into $\pi^+, \pi^-$ at large times. This $\Rightarrow N_{\pi^0} \neq N_{\pi^0} \Rightarrow CP$ is not conserved. One of the best understood problems today. Must break CP.

Mentioning "fifth force" theory. Maybe universe is asymmetric. Theories explain this experiment, but predict weird things in other areas.

Thusly this is "involved for this generation."
Angular Momentum

Problem: Extend this week's work on angular momentum as far as you can. (Bendix 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 an isolated system described by a state $|\psi\rangle$.

Now rotate the apparatus which prepares $|\psi\rangle$. Then we produce a new rotated state $|R\psi\rangle$ with 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,

$$|\psi\rangle = \Lambda_{c} |l \ i\rangle$$

$$|R\psi\rangle = \Lambda_{d} |l \ j\rangle$$

But if $R$ is linear,

$$|R\psi\rangle = \Lambda_{c} |R\ i\rangle$$

Now we can also expand

$$|R\ i\rangle = \Lambda_{d} |l \ j\rangle$$

to find

$$\Lambda_{d} = \Lambda_{c} \Lambda_{d} |c \ j\rangle.$$
To every rotation there is associated a matrix $D^k$.

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.) $C(BA) = (CB)A$

This is called a "continuous group" since continuity of rotations corresponds to different angles. Actually a 3-parameter group.

Now note i.) means

$$|R_3 \Phi_i \rangle = |R_2 (R_1 \Phi_i) \rangle = \sum_j (R_2 \Phi_j) \langle D^k_{ij} \Phi_i$$

$$= \sum_{\Phi} D^R_{kj} D^R_{ij} |\Phi_k \rangle$$

Thus

$$D^R_{kj} = \sum_{\Phi} D^R_{k\Phi} D^R_{\Phi j}$$

or as a matrix product

$$D^R = D^R_2 D^R_1$$

to within a phase which can be approximately chosen.
To find how angles combine during rotations in a question of geometry, this is one way:

\[ x' = x \]
\[ y' = y \cos \alpha + z \sin \alpha \]
\[ z' = z \cos \alpha - y \sin \alpha \]

\[ \alpha' \] about \( y \) axis
\[ \alpha'' \] about \( x \) axis

Substitute in and use general transformations to do this. Also write

\[ x_i = \sum_{j} L \cdot x_j \]
\[ L R^2 = L R^2 L^R \]

an example with 3x3 matrices

2) Construction of Angular Momentum Operators (Generators)

We can now find our matrices by considering these infinitesimal rotations.

Take \( \epsilon \) about \( z \) axis. Then \( D^\epsilon \). Now for \( \alpha \) about \( z \),

we have

\[ D^\epsilon \rightarrow D^\epsilon, \quad D^\epsilon \]

Only need to know \( D \) to order \( \epsilon \)

Thus write

\[ D^\epsilon = 1 + i \left( \frac{J_z}{\hbar} \right) \epsilon \]

where \( J_z \) is an undetermined

Thus

\[ |\text{Rot}_{\alpha z} \psi \rangle = |\psi \rangle + \frac{i \xi}{\hbar} J_z |\psi \rangle \]

\( J_z \) is called the "generator of the rotation".

Now rotation of \( \alpha \) about \( z \)

\[ \alpha^z = (1 + \frac{i \xi}{\hbar} J_z)(1 + \frac{i \xi}{\hbar} J_z) \cdots (1 + \frac{i \xi}{\hbar} J_z) \]

\[ = (1 + \frac{i \xi}{\hbar} J_z)^{\alpha \hbar} \]

\[ = 1 + i\alpha J_z + \frac{(i\alpha)^2}{2!} J_z^2 + \frac{(i\alpha)^3}{3!} J_z^3 + \cdots \]

\[ = e^{i\alpha J_z} \]

Thus to find \( \alpha^z \), we only need the generator \( J_z \).

Now suppose state is unchanged by rotation

\[ |\text{Rot}_\alpha \psi \rangle = e^{i\alpha} |\psi \rangle \]

But \( \text{Rot}_z \text{Rot}_z = \text{Rot}_{\alpha_1 + \alpha_2} \)

\[ \Rightarrow \quad S(\alpha_1 + \alpha_2) = S(\alpha_1) + S(\alpha_2) \]

\[ \Rightarrow \quad S = \max \quad \text{in context of proportionality} \]

\[ \text{in angular momentum about } z \text{ axis} \]
Now suppose

\[ J_z |\psi\rangle = m |\psi\rangle \]

Then

\[ \text{Rot}_z |\psi\rangle = \delta^{\text{rot}} |\psi\rangle = e^{i\alpha J_z} |\psi\rangle = e^{i\alpha m} |\psi\rangle \]

Why is this called angular momentum? Merely convenient

since if we suppose a particle rotating in a track

\[ e^{i \alpha} \text{ after } t = e^{i \alpha \frac{p_a}{\hbar}} \]

\[ m \rightarrow \frac{p_a}{\hbar} \]

But \( p_a = \text{angular momentum} \)

Thus with corresponds to classical angular momentum

Suppose \(|\psi\rangle = \hat{f}(x, y, z)\)

\[ \text{Rot}_z |\psi\rangle = \hat{f}(x', y, z) = \hat{f}(x + \epsilon y, y - \epsilon x, z) \]

\[ = \hat{f}(x, y, z) + e \left( y \frac{\partial \hat{f}}{\partial x} - x \frac{\partial \hat{f}}{\partial y} \right) \]

Thus identity

\[ J_z = \frac{\hbar}{i} \left( \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right) = y p_x - x p_y \]
3) Restrictions on Eigenvalues of $J$

We have found

$$|K\psi\rangle = |\psi\rangle + i|J_z|\psi\rangle$$

We noted if $J_z|\psi\rangle = m|\psi\rangle$ then $e^{im\phi}$ phase change.

Also found if our state is a function then define $J_z \rightarrow L_z$

where

$$L_z = -i \left( \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

Note: we found this purely by rotations, useful correspondence with classical mechanics. Now if we have

$$L_z |\psi\rangle = m|\psi\rangle$$

then

$$L_z f(x,y,z) = m f(x,y,z) \Rightarrow L_z = \frac{1}{i} \frac{\partial}{\partial \phi}$$

$$f(r,\theta,\phi) = F(r,\theta)e^{im\phi}$$

[Note this specific example concerns spherical angular momentum i.e. any mom. due to position $(x,y,z)$]

---

What values do we have to choose? For 2-dimensional groups $m$ is arbitrary! This is so because we can put state back by properly defining our phase.

Need to go to 3-dimension.
Three dimensions

\[ \begin{align*}
1R_x\Psi &= 1\Psi + i\eta J_x \Psi \\
1R_y\Psi &= 1\Psi + i\eta J_y \Psi
\end{align*} \]

What about

\[ \begin{align*}
1R_{\text{about} V}\Psi &= 1\Psi + i\eta J_v \Psi
\end{align*} \]

Note

\[ (\eta V_x \text{about } x)(\eta V_y \text{about } y)(\eta V_z \text{about } z) = (\eta \text{ about } V) \quad \text{if } \eta \text{ is very small} \]

Thus we can write this notation as

\[ (1 + i\eta V_z J_z)(1 + i\eta V_y J_y)(1 + i\eta V_x J_x) \Psi \]

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

\[ J_v = V_x J_x + V_y J_y + V_z J_z = \vec{V} \cdot \vec{J} \]

[Note \( \vec{J} \) is both a vector and an operator]
Now we must make sure that

\[ \text{if first } R_1, \text{ second } R_2 \rightarrow R_3 \]
\[ \Rightarrow \quad D^{R_2} D^{R_1} = D^{R_3} \]

What properties must the J's have so this holds? We studied continuous groups and found if we could get

\((\ast)\) to work to second order, it will work for any order. Can we thus

\[
\left( D^{E_{V_2}} D^{E_{V_2}} D^{E_{V_2}} \ldots D^{E_{V_2}} \right) \left( D^{E_{V_1}} D^{E_{V_1}} \ldots D^{E_{V_1}} \right) = \left( D^{E_{V_3}} \ldots D^{E_{V_3}} \right)
\]
\[
\frac{\alpha^2}{\epsilon} \quad \frac{\alpha^1}{\epsilon} \quad o(\epsilon^2)
\]

Note rotations do not commute

\[
\text{(1st rotate x) (2nd } \eta \text{ about } y) \neq (\text{1st } \eta \text{ about } y) (\text{2nd rotate x})
\]

Try to undo it by applying them

\[
(\text{3rd - rotate x}) (\text{4th - } \eta \text{ about } y)
\]

This gives

\[
(1)(2)(3)(4) = (\epsilon \eta \text{ about } z)
\]

This is a fact of geometry, not of man. Ideas humans only understand 3-dimensional commutative groups. Bird and fish understand 3-dimensional
Demonstration: Imagine the disks fixed on a sphere.

1. About x
2. y about y
3. -y about x
4. -y about y

We can see that an rotation of y about z is necessary to return to the original a.

Thus we have found to second order:

\[
(1 - i\eta J_y - \frac{\eta^2}{2} J_y^2)(1 + i\eta J_y - \frac{\eta^2}{2} J_y^2)(1 + i \eta J_y - \frac{\eta^2}{2} J_y^2) = (1 + i \eta J_z)
\]
On expanding

\[ 1 + \left( i \epsilon J_x + i \eta J_y - i \epsilon J_x - \eta J_y - \epsilon^2 J_x^2 - \eta^2 J_y^2 \right) \]

\[ + \left( - \epsilon \eta J_y J_x + \epsilon^2 J_x^2 + \epsilon \eta J_x J_y + \epsilon \eta J_y J_x \\ + \eta^2 J_y^2 - \epsilon \eta J_x J_y \right) \]

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

\[ D_x^2 D_y = D_y^2 D_x \]

\[ D_x^2 D_y = D_y^2 D_x \]

[This is a much more logical derivation than the more elementary one from classical mechanics.]

We can also find

\[ J_x J_z - J_z J_x = i J_y \]

\[ J_y J_z - J_z J_y = i J_x \]
Thus \( D^R_x D^R_y = D^R_z \Rightarrow \)

\( \mathbf{J} \cdot \mathbf{J} \)

\( \mathbf{J}_x \mathbf{J}_y - \mathbf{J}_y \mathbf{J}_x = i \mathbf{J}_z \)

\( \mathbf{J}_y \mathbf{J}_z - \mathbf{J}_z \mathbf{J}_y = i \mathbf{J}_x \)

\( \mathbf{J}_z \mathbf{J}_x - \mathbf{J}_x \mathbf{J}_z = i \mathbf{J}_y \)

These handle any angles or rotations.

We now could use algebra to generate the c.o. and e.f. of the J's.

Define

\( \mathbf{J}_\pm = \mathbf{J}_x \pm i \mathbf{J}_y \)

Then using \([K, \mathbf{J}_i] = 0\) where \( K = \mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2 \)

we consider

\( \mathbf{J}_z |m\rangle = m |m\rangle \)

\( K |m\rangle = k |m\rangle \)

Our commutation rules become

\( \mathbf{J}_z \mathbf{J}_+ - \mathbf{J}_+ \mathbf{J}_z = \mathbf{J}_+ \)

\( \mathbf{J}_z \mathbf{J}_- - \mathbf{J}_- \mathbf{J}_z = -\mathbf{J}_- \)

\( \mathbf{J}_+ \mathbf{J}_- - \mathbf{J}_- \mathbf{J}_+ = K - \mathbf{J}_z (\mathbf{J}_z - 1) \)

\( \mathbf{J}_- \mathbf{J}_+ = K - \mathbf{J}_z (\mathbf{J}_z + 1) \)
Thus \( J_\pm J_\mp |m\rangle = [\hat{J}_0 - m(m+1)] |m\rangle \)

Applying
\[
J_z (J_+ |m\rangle) = J_+ |m\rangle + J_+ J_z |m\rangle
= (m+1) |J+1\rangle
\]

Thus
\[
J_+ |m\rangle = C_m |m+1\rangle
\]

Also
\[
J_- |m+1\rangle = C_m^* |m\rangle
\]

Thus
\[
J_- J_+ |m\rangle = C_m C_m^* |m\rangle
\]

\[\Rightarrow |C_m|^2 = \frac{\hbar}{2} - m(m+1)\]
\[ J_x J_y - J_y J_x = i J_z \]
\[ J_y J_z - J_z J_y = i J_x \]
\[ J_z J_x - J_x J_z = i J_y \]

\[ \tilde{J}_x \tilde{J}_y = i \tilde{J}_z \]

\[ [J_x, J_y] = i J_z \quad \text{etc.} \]

We had found \( J_z |m\rangle = m |m\rangle \) by commutative algebra.

\[ \tilde{J}_x \tilde{J}_y |m\rangle = j(j+1) |m\rangle \]

\[ m \text{ goes from } -j \text{ to } j \text{ in integer steps} \]

\[ \Rightarrow j \text{ is a half-integer} \]

Also,

\[ \langle m' | J_+ | m \rangle = \delta_{m', m} \sqrt{j(j+1) - mm'} \quad m' = m + 1 \]

\[ \langle m' | J_- | m \rangle = \delta_{m', m} \sqrt{j(j+1) - mm'} \quad m' = m - 1 \]

We can then deduce

\[ \langle m' | J_x | m \rangle = \delta_{m', m} \frac{1}{2} \sqrt{j(j+1) - mm' \pm \epsilon} \]

\[ \langle m' | J_z | m \rangle = \delta_{m', m} \]

Thus the \( |m\rangle \) states provide a representation for the group of rotations, so that

\[ \langle m' | D^R | m \rangle = D_{m' m}^R \]

(might try to work these out)
Other forms since
\[ \sqrt{j(j+1)-m(m+1)} = \sqrt{(j-m)(j+m+1)} \]

Thus
\[ \langle m | J_{\pm 1} m \rangle = \sqrt{(j+m_1)(j-m_1)} \]

5. Could study these for special \( j \)'s

\( j = 0 \):
\( m = 0 \)
\( J_{\pm 1} m \rangle = 0 \)
\( J_{x,y,z} | m \rangle = 0 \)
A rotation of any kind produces the same state \( | \psi \rangle = | \psi \rangle \)

\( j = \frac{1}{2} \):
\( m = \pm \frac{1}{2} \)
\( | + \rangle = | \alpha \rangle \)
\( | - \rangle = | \beta \rangle \)

Call \( J = \frac{1}{2} \) for this special case.

\( S_z | + \rangle = \frac{1}{2} | + \rangle \)
\( S_z | - \rangle = -\frac{1}{2} | - \rangle \)
\( S_x | + \rangle = \frac{1}{2} | - \rangle \)
\( S_x | - \rangle = \frac{1}{2} | + \rangle \)
\( S_y | + \rangle = i \frac{1}{2} | - \rangle \)
\( S_y | - \rangle = i \frac{1}{2} | + \rangle \)

Sometimes one uses Pauli matrices
\[ \sigma \]
\[ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]
\[ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]
\[ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \]

\( \sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1 \)
\( \sigma_x \sigma_y - \sigma_y \sigma_x = 2i \sigma_z \)
\( \sigma_x \sigma_y = i \sigma_z = -\sigma_y \sigma_x \)
Since these matrices and (69) can represent any
they are used quite frequently in 2-state systems.

In the beginning, only integral $j$ were allowed since if
we use $S$-equ, $j = \frac{1}{2}$ yield the negative of the
state (eigen) after rotating 360°. Thus Pauli
used his matrices to handle 2 wave fields, $\psi_+, \psi_-.$
Why can't we have spin $\frac{1}{2}$

$$|m\rangle \rightarrow e^{i\frac{1}{2}2\pi} |m\rangle = e^{i\delta} |m\rangle$$

Why must 2 rotations around 360° reverse state to
original value, while one rotation doesn't have to.

Consider restoring rotations (path of successive rotations
which restore coordinate system) = turn.

Consider 2 turns infinitesimally close to each other. We
suppose these turns are in the same class.

Let 0 turn have phase 0. Then consider class of turns
infinitesimal from 0. Assume these turn have phase 0. These
does of turns have same phase. Will show

$$720° \quad 0°$$

$$360° \quad 0° \quad \text{not possible}$$

Will show that 720° has phase 0, & 360° has
phase 1. Thus, 720° is different from 360°
from a geometrical standpoint.
To prove this, he demonstrates that a class containing both $720^\circ$ and $0^\circ$ exists.

He shows you can do this for $360^\circ$. A curious property of 3 dimensional rotations.

\[ j = 1 : \begin{array}{ccc} 1^+ & 10^- & 1^- \end{array} \]

\[ \begin{align*}
    l_+1^+ & = 0 \\
    l_+10^- & = \sqrt{2} l^+ \\
    l_+1^- & = \sqrt{2} 10^- \\
    l_-1^+ & = \sqrt{2} 10^- \\
    l_-10^- & = \sqrt{2} 1^- \\
    l_-1- & = 0 \\
\end{align*} \]

If we rotate coordinate system $1x > 1y > 1z >$

\[ 1^+ = \frac{1}{\sqrt{2}} (1x + i1y) \]

\[ 1^- = \frac{1}{\sqrt{2}} (1x - i1y) \]

\[ 10^- = 1z > \]

A particle of spin $1$ is called a vector particle in field theory since it behaves as a vector.
Problem:

i) anything you want

ii) find the quantities in letting

\[ J_z = \frac{1}{2} \left[ v_x \frac{\partial}{\partial v_x} - v_y \frac{\partial}{\partial v_y} \right] + \frac{\partial}{\partial v_z} (v_x, v_y, v_z) \]

\[ J_y = \frac{1}{2} \left[ v_x \frac{\partial}{\partial v_x} - v_y \frac{\partial}{\partial v_y} \right] + \frac{\partial}{\partial v_z} (v_x, v_y, v_z) \]

\[ J_x = \frac{1}{2} \left[ v_z \frac{\partial}{\partial v_z} - v_x \frac{\partial}{\partial v_x} \right] + \frac{\partial}{\partial v_y} (v_x, v_y, v_z) \]

Let

\[ \lambda = \lambda v_z \]

\[ \chi = -\lambda v_y \phi \]

\[ \psi = \lambda v_x \phi \]

Claim: Total angular momentum must be an integer.

iii) Consider two coupled objects (radius j electron) with

\[ J_a, J_b \]. Assume neither object is excited. Assume

\[ H = A \frac{1}{j_a} \frac{1}{j_b} + B \left( \frac{4}{j_a} \left( \frac{V}{j_a} \right) + \frac{4}{j_b} \left( \frac{V}{j_b} \right) \right) \]

a. In general, for very small B, find the energy levels of the combined system, and find formula for magnetic moment.

b. For special values of \( j_a, j_b \) find energy as \( B \) for arbitrary \( B \)
1. Introduction

Consider a system comprised of two points \( a \) and \( b \)

\[
a : \quad |\psi_a\rangle \quad \text{any } |\psi_a\rangle \\
|\psi_a\rangle \quad \text{any } |\psi_a\rangle \\
2j_a + 1 \quad \text{states}
\]

\[
\mathbf{a} = -j_a \times \mathbf{v}_a
\]

\[
b : \quad |\psi_b\rangle \quad \text{any } |\psi_b\rangle \\
|\psi_b\rangle \quad \text{any } |\psi_b\rangle \\
2j_b + 1 \quad \text{states}
\]

\[
\mathbf{b} = -j_b \times \mathbf{v}_b
\]

Now try to represent the base states of the combined system

\[
|\Psi\rangle = |\psi_a\rangle |\psi_b\rangle = |\mathbf{a}\rangle |\mathbf{b}\rangle
\]

Thus \((2j_a + 1)(2j_b + 1)\) states.

Example: \( j_a = 1 \quad j_b = \frac{1}{2} \)

\[
|+\rangle |\frac{1}{2}\rangle, \quad |0\rangle |\frac{1}{2}\rangle, \quad |-\rangle |\frac{1}{2}\rangle, \quad |+\rangle |-\frac{1}{2}\rangle, \quad |0\rangle |-\frac{1}{2}\rangle, \quad |-\rangle |-\frac{1}{2}\rangle
\]

Suppose we want to form from these states, more states of definite total angular momentum \( J, M \). What do we mean?

\[
\Delta \Psi = \mathbf{a} \otimes \mathbf{b} |\psi_a\rangle |\psi_b\rangle = (\mathbf{a} \otimes \mathbf{b}) |\psi_a\rangle |\psi_b\rangle
\]

Let \( R = e^{|\Delta \Psi|} \)

\[
|\Psi\rangle + i \in J_2 |\Psi\rangle = (1 + i e^{J_2}) |\Psi_a\rangle (1 + i e^{J_2}) |\Psi_b\rangle
\]

\[
\Rightarrow \quad J_2 |\Psi\rangle = (J_2 a^b + J_2 b^a) |\psi_a\rangle |\psi_b\rangle
\]

\[
\Rightarrow \quad J = J_2 a^b + J_2 b^a
\]
Try to find
\[ Jz \psi = M \psi = (J_z^a + J_z^b) |m_a \ge a |m_b \ge b \]
\[ = (m_a + m_b) |m_a \ge a |m_b \ge b \]

For our example, max. \( M = \frac{3}{2} \Rightarrow J = \frac{3}{2} \)
\[ \Rightarrow m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \]
\[ \Rightarrow J = \frac{3}{2}, \frac{1}{2} \text{ left over} \]
Thus don't get a definite \( J \) in general.

In general, a possible \( J = ja + jb \), also consider another possibility \( J = ja + jb - 1 \), \( J = ja - jb \). Thus
\[ |ja - jb| \le J \le ja + jb \] (borrow rule)
\[ 2J + 1 \text{ state for each } J. \]

Now what are these states, e.g. \( |J, M \rangle = (\frac{3}{2}, \frac{3}{2}) \)?

For the highest \( J \)
\[ (\frac{3}{2}, \frac{3}{2}) = 1 \langle \frac{3}{2}, \frac{3}{2} | \frac{1}{2}, \frac{1}{2} \rangle \]
But for
\[ (\frac{3}{2}, \frac{1}{2}) = a (0 \langle 0 | \frac{1}{2} \rangle _0 + b |1 \rangle _a | -\frac{1}{2} \rangle _b \]

What combination will work? Find \( a, b \). These are Chirch-Lodan 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 eigenvector, just work up or down from a known state]

\[ J_- \frac{1}{2}, \frac{3}{2} \rangle = \sqrt{3} \frac{1}{2}, \frac{1}{2} \rangle = (J_a + J_b) \frac{1+1}{1+1} \]

\[ \sqrt{3} \frac{1}{2}, \frac{1}{2} \rangle = \sqrt{2} \frac{1}{2}, \frac{1}{2} \rangle + \frac{1}{2}, -\frac{1}{2} \rangle \]

\[ \Rightarrow a = \sqrt{3}, \ b = \frac{1}{\sqrt{2}} \]

\[
\begin{align*}
J_- \{ & \frac{1}{2} > 1 \\
& -\frac{1}{2} > \frac{\sqrt{2}}{2} \\
& j = \frac{1}{2} \}
\end{align*}
\]

\[
\begin{align*}
& \frac{3}{2} > \frac{\sqrt{3}}{2} \\
& -\frac{1}{2} > \frac{\sqrt{1}}{4} \\
& j = \frac{3}{2} \}
\end{align*}
\]

\[
\begin{align*}
& 2 > \frac{\sqrt{1}}{4} \\
& 0 > \frac{\sqrt{1}}{4} \\
& j = 2 \}
\end{align*}
\]

How do we reduce J now? Try to get \( \frac{1}{2}, \frac{3}{2} \rangle 

\[ \frac{1}{2}, \frac{3}{2} \rangle = -\sqrt{3} \frac{1}{2}, \frac{1}{2} \rangle + \frac{\sqrt{3}}{2} \frac{1}{2}, -\frac{1}{2} \rangle \]

Use orthogonality

General method: 1) get \( J_{\max} \), and use \( J_- \) to get \( |J_{\min}\rangle \)

2) use orthogonality to get \( |J_{\min}\rangle \)
4) Method 3: Straight Forward Method  

The best way to generate C.G. coefficients is to play with \( J_\pm \). However, to evaluate one in the middle. Say we want

\[
|2, 1\rangle = a |2a, 1-1\rangle + b |1+1, 10\rangle + c |10, 1+1\rangle
\]

Want \( J=2, M=1 \), i.e.

\[
(J_2 + J_\theta^2) |2, 1\rangle = +1 |2, 1\rangle \quad \text{Eqn} \ (1)
\]

\[
\langle J_\theta | 2, 1 \rangle = J (J+1) |2, 1\rangle = 6 |2, 1\rangle
\]

Now

\[
\hat{J}_\theta \cdot \hat{J} = (\hat{J}_a + \hat{J}_b) \cdot (\hat{J}_a + \hat{J}_b) = \hat{J}_a \cdot \hat{J}_a + \hat{J}_b \cdot \hat{J}_b + 2 \hat{J}_a \cdot \hat{J}_b
\]

Thus

\[
\hat{J}_\theta \cdot \hat{J}_a |J, M\rangle = J_\theta (J_\theta + 1) |J, M\rangle + 2 J_\theta J_\theta |J, M\rangle + J_a + J_b + J_\theta - J_\theta |J, M\rangle
\]

or

\[
\begin{bmatrix}
8 + 2J_\theta J_\theta + J_a + J_b + J_\theta - J_\theta
\end{bmatrix}
\begin{bmatrix}
\alpha |1+2, 1-1\rangle + b |1+1, 10\rangle + c |10, 1+1\rangle
\end{bmatrix}
\]

\[
= 6 \alpha |2, 1-1\rangle + 6b |1, 10\rangle + 6c |10, 1+1\rangle
\]

\[
|1+2, 1-1\rangle : \quad 4a + 2\sqrt{2}b = 6a \Rightarrow a = 52 \quad b = 1
\]

\[
|1+1, 10\rangle : \quad 2\sqrt{2}a + \sqrt{3}b + 2\sqrt{2}c = 6b
\]

\[
|10, 1+1\rangle : \quad \sqrt{2} \sqrt{2}b + 8c = 6c \quad \Rightarrow \quad c = -\sqrt{3}
\]
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 \( \alpha \) and \( \beta \). \( \alpha, \beta \) are parameters of the group. Now still have

\[ D^6 |\psi\rangle = |\psi'\rangle \]

Again find: \( D^6 = D^2 D^4 \)

Can follow our work on angular momentum since there are six groups. Take

\[ \beta = 0 \quad \alpha = 1 \quad G_1 \]

\[ \beta = i \varepsilon \quad \alpha = 1 \quad G_4 \]

\[ \beta = \varepsilon \quad \alpha = 1 + i \varepsilon \quad G_2 \]

Again: \( D^6 = 1 + i \varepsilon M_1 \quad G_2 \).
It turns out this group is similar to groups for spin \( \frac{1}{2} \) objects. Thus we introduce isotopic spin, so we can use the words on \( \frac{1}{2} \) spin objects. Set

\[
T_\pm \quad (J^z)
\]

\[
T_+ \quad (J^+)
\quad T_+ \quad (J^-)
\]

just a matter of convenience.

3) The Eightfold Way

PROBLEM: Consider a system of 3 objects

\[
|p> = \alpha|p> + \beta|n> + \gamma|\bar{n}>
\]

\[
|n> = \alpha'|p> + \beta'|n> + \gamma'|\bar{n}>
\]

\[
|\bar{n} > = \alpha''|p> + \beta''|n> + \gamma''|\bar{n}>
\]

8 independent numbers [8 parameters]

Not analogous to rotation groups anymore, but use same procedure. Representation

1. singlet
2. triplet
3. \( j \)
4. \( \bar{j} \) etc.

This is called "8-fold way" in high energy physics.

\[
N, p, \Lambda, \Xi^+, \Xi^0, \Xi^-, \Omega^-, \Omega^0
\]
If we consider only strong interactions, they all have some energy. But nature is much more complicated with this group. This group is called $SU_6$. Think now that all particles can be represented by such groups $SU_2$, $SU_6$, $SU_{12}$.

2 states
3 states
6 states

Actually, mesons correspond to isotopic spin $T = 1$ for $T = 0$.

3/3 are like integer; $1/2$ integer in angular momentum. Have you seen any 3 yet?

People have tried to combine angular momentum with quality and found $SU_6 \times SU_2 = SU_{12}$.

Don't really know much about it yet. Some regularities appear, but may be coincidental. $SU_{12}$ has 6 states.
Special Case: spin $j = \frac{1}{2}$

Suppose we want

$\langle \frac{1}{2} | \frac{1}{2} \rangle$, $\langle \frac{1}{2} | \frac{1}{2} \rangle$, $\langle \frac{1}{2} | \frac{1}{2} \rangle$

$\langle \frac{1}{2} | \frac{1}{2} \rangle$, etc.

We are calculating matrix elements between two $\frac{1}{2}$ states that differ only by the value of $m_z$ -- $j = \frac{1}{2}$ remains fixed. Thus have internal state, differs only by $m_z$.

Recall any matrix for spin $\frac{1}{2}$ can be written with spinors

$$M = \alpha \frac{1}{2} + \alpha_x x + \alpha_y y + \alpha_z z$$

We can then write our matrix elements as

$$\langle m_2 | x | m_1 \rangle = \delta_{m_1, m_2} \quad \text{(stated on 4 values)}$$

Then

$$x = \delta_0 I + \delta_0 x + \delta_0 y + \delta_0 z$$

$$y = \gamma_0 I + \cdots$$

$$z = \gamma_0 I + \cdots$$

Now since $x, y, z$ are components of a vector, the matrix must transform (rotate) like a vector. We are saying

$$\langle m_2 | \vec{r} | m_1 \rangle \propto \langle m_2 | m_1 \rangle \begin{pmatrix} \delta_+ & \delta_- \\ \delta_- & \delta_+ \end{pmatrix}$$
\[ \langle m_2 | 1 \times 1 \m_i \rangle = \lambda \langle m_2 | 0 \times 1 \m_i \rangle \]
\[
\begin{pmatrix}
\frac{5}{2} + \frac{5}{2} \\
1 \\
\frac{5}{2} - \frac{5}{2}
\end{pmatrix}
\]

Suppose we are calculating matrix elements relating to quadrupole moments. Then we want the matrix elements to transform under rotations such that they behave as tensors, i.e., the result of the rotation must behave like a tensor.

\[ \langle m_2 | 1 \times 1 \m_i \rangle \]
\[ \langle 1 \times 1 \m_i \rangle \]

Choose new matrix elements between scalars:
\[ 1 \times 0 + 1 \times 0 + 2 \times 0 = \text{scalar} \]

E.g., new matrix formed by taking linear combination -- get symmetric tensor of zero rank:
\[
\begin{align*}
x \rho_x - \frac{1}{3} (x \rho_x + y \rho_y + z \rho_z) \\
x \rho_y + y \rho_x \\
y \rho_y - \frac{1}{3} (x \rho_x + y \rho_y + z \rho_z) \\
y \rho_z + z \rho_y \\
x \rho_z + z \rho_x
\end{align*}
\]

Take 5 so they will be independent.
When doing calculation of matrix elements like \( |x \rangle |y \rangle \), etc., follow 3 steps.

i.) Take matrix elements of a set of quantities which is a scalar.

\[
\langle m_1 | x P_x + y P_y + z P_z | m_2 \rangle = \mu \langle m_1 | I | m_2 \rangle
\]

ii.) Take matrix elements of a set of quantities which is a vector.

\[
\langle m_1 | x P_y - y P_x | m_2 \rangle = \lambda \langle m_1 | \sigma_x | m_2 \rangle
\]

iii.) Take matrix elements of a set of quantities which is a tensor.

\[
\langle m_1 | \text{tensor comp} | m_2 \rangle = \kappa \langle m_1 | \sigma_x \sigma_x - \frac{1}{3}(\sigma_x \sigma_x + \sigma_y \sigma_y + \sigma_z \sigma_z) | m_2 \rangle
\]

Tensor components are zero \((\kappa = 0)\) for spin \( \frac{1}{2} \) problem since there in the end only 2 unknowns \(
\begin{align*}
\text{tensor components are not independent, i.e.,} \\
\langle \Psi_f | T | \Psi_i \rangle \\
J = J + 1, J + 2, \ldots, J - 2 \\
\text{for } J = \frac{1}{2} \quad J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, \frac{7}{2}
\end{align*}
\)
We have been considering non-diagonal elements. Now let's try to find matrix elements for diagonal terms of angular momentum.

\[ \langle m_2 | \hat{P} \hat{l} m_1 \rangle \quad \langle m_2 | \hat{P} m_1 \rangle \]
\[ \langle m_2 | \hat{A} m_1 \rangle \quad \langle m_2 | \hat{P} m_1 \rangle \]

We have \( J_x, J_y, J_z \)

\[ \frac{4 \text{ numbers}}{2j+1} \]

Matrix is

\[ \begin{pmatrix} 2j+1 \\ 2j+1 \end{pmatrix} \]

Need \( (2j+1)^2 \) matrix elements --

numbers -- in operation we know we only have 4 numbers

But we also know \( J_x J_x, J_y J_y, J_z J_z, \ldots \)

Can't include \( J_x J_y \) because \( J_z \) which we have, so must watch out for restrictions. Still must have \( 2j+1 \) of combinations? However don't really have this many, e.g., for \( j = 1 \)

\[ (j+1) j (j-1) m \rangle = 0 \quad \text{for all} \quad m = 0 \]

\[ J_z^3 - J_z = 0 \quad \text{so can't allow} \quad J_z J_z J_z \text{ on} \quad J_x J_y J_z, \]

Can't make combination of 3, so we cannot make a vector from 2\( J \)'s

\[ \langle m_2 | \hat{P} m_1 \rangle = \lambda \langle m_2 | \hat{P} m_1 \rangle \]
Generally, for arbitrary \( i \),

\[
\langle m_1 \mid \rho_1 \rho_2 \mid m_2 \rangle = \frac{1}{J} \langle m_1 \mid J \mid m_2 \rangle
\]

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

\[
\langle J = 11 \mid J = 11 \rangle = 0
\]

because \( 0 + 0 = 0 \) so can have

\( J = 4, 3, 2 \)

Putting m.e. together, e.g.

\[
\langle m_2 \mid \rho_x \rho_x \mid m_1 \rangle = \langle m_2 \mid \rho_x - \frac{1}{3} (\rho_x^0 + \rho_y + \rho_z) \mid m_1 \rangle + \frac{1}{3} \langle m_2 \mid \rho_x + \rho_y + \rho_z \mid m_1 \rangle
\]

Important point is a traceless tensor can be written as

\[
\langle m_2 \mid \rho_x \mid m_1 \rangle = c \langle m_2 \mid J_x - \frac{1}{3} (J_x^2 + J_y^2 + J_z^2) \mid m_1 \rangle
\]

\[
+ \frac{1}{3} a \langle m_2 \mid J \mid m_1 \rangle
\]

\[
= c \langle m_2 \mid J_x J_x \mid m_1 \rangle + (\frac{5}{3} a - \frac{1}{3} c) \delta_{m_1, m_2}
\]

tracewise
Can prove that a nucleus of spin \( \frac{3}{2} \) cannot have a quadrupole moment -- no magnetic moment if spin is 0, because need

\[
\langle m_1 | j \times \mathbf{m}_1 \rangle \propto \langle m_2 | j \times \mathbf{m}_1 \rangle
\]

\[\mathbf{m}_1 \text{ vector, } \mathbf{m}_2 \text{ scalar}\]

\[\Rightarrow \text{ scalar} = 0, \text{ no mag. moment}\]

\[\text{for } j = 0 \text{ object}\]
To learn this field, one must read and to gain experience of the various phenomena. Refer to our books ideas to develop theory.

Types of crystals

molecular: sugar, cellulose etc.

covalent: diamond

ionic: NaCl

metallic:

We will be concerned with 2 topics, phonon interactions and conduction in crystalline materials.
From statistical mechanics, if a crystal is at temperature $T$ at equilibrium, the prob. of being in state $i$ is
\[ p_i \propto e^{-E_i/kT} \]
\[ = Q e^{-E_i/kT} \]

where $Q = \sum_i e^{-E_i/kT}$ is the partition function.

Can get all of thermodynamics from this.

\[ U = \text{internal energy} = \sum_i E_i p_i = \frac{\sum_i E_i e^{-E_i/kT}}{Q} \]

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

\[ Q = e^{-F/kT} \]

where $F = -kT \ln Q$ is the Helmholtz free energy.

Then find

\[ U = -T^2 \frac{\partial}{\partial T} \left( \frac{F}{T} \right) = F - T \frac{\partial F}{\partial T} \]

where $S$ is entropy.

\[ \therefore U + TS = F \]
The energy of a molecule is a function of the position of the nuclei: \( U(R, R_2, \ldots) \). Thus

\[
H \psi = \sum_i \left( -\frac{\hbar^2}{2M_i} \nabla_i^2 \right) \psi(R, R_2, \ldots) + U(R, R_2, \ldots) \psi = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \psi}
\]

**Problem:** Why is this equation right and how did we arrive at it? Assume that the correct S. E. qu is for Coulomb interactions and use mass differences of \( N \), etc. Try to separate electronic and ionic motion.

[First consider case of fixed nuclei]

\[
\sum_i \frac{\hbar^2}{2M_i} \nabla_i^2 \chi_i(R) + V(R, R_2, \ldots) \chi_i(R) = E \chi_i(R)
\]

Find contact

Note \( E = E(R, \ldots) \) and idea is for \( E = U \).

Want to show exact wave function

\[
\psi \approx \psi(R, R_2, \ldots) \chi_{R, R_2, \ldots}(R_2)
\]
PROBLEM: Find $F$ and $U$ for an harmonic oscillation of natural frequency $\omega_0$, mass $m$, temperature $T$.

We were considering

$$\left\{ -\frac{b^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + U(x_1, x_2, \ldots) \right\} \psi(x) = -\frac{d}{dt} \frac{\partial \psi}{\partial t} = \varepsilon \psi(x) \ldots \ (1)$$

One of these laws of physics which seems to reproduce itself (like Newton's law $F = ma$)

Since potential $U$ varies very rapidly, unless motion is quite small and under wave terms are pretty localized for vibration, thus we can approach solved (1) by expanding about equilibrium $x_i = 0$. Let $x_i \to x_1, x_2 \ldots$ from equilibrium

$$\left\{ -\frac{b^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + U(x_1, x_2, \ldots) \right\} \psi = 0 \ldots \ (2)$$

Expand $U(0, 0, \ldots) + x_1 \left( \frac{\partial U}{\partial x_1} \right)_0 + \frac{1}{2} \sum \left( \frac{\partial^2 U}{\partial x_i \partial x_j} \right)_0 + \ldots$

Redefine energy at $U(0, 0, \ldots)$, Note $v_0$ is zero.

Thus we have

$$\left\{ -\frac{b^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} \sum \left( \frac{\partial^2 U}{\partial x_i \partial x_j} \right) \right\} \psi_{ij} = H$$

Redefine $\psi_i = \sqrt{m_i} \psi_i$, let $\hbar = 1$

$$\left\{ -\frac{b^2}{2} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} \sum \left( \frac{\partial^2 U}{\partial x_i \partial x_j} \right) \right\} \chi_{ij} = H$$

where

$$\chi_{ij} = \frac{1}{\sqrt{m_i m_j}} \left( \frac{\partial U}{\partial x_i x_j} \right)_0$$
This is just a set of coupled harmonic oscillators. First look at the classical analogue:

\[ \frac{d^2 x_i}{dt^2} + \frac{1}{\lambda} \frac{\partial}{\partial q_i} \left[ \sum_{j} C_{ij} q_i \right] = \frac{1}{\lambda} \frac{\partial H}{\partial q_i} \]

to find

\[ \dot{q}_i = -\frac{1}{\lambda} \frac{\partial H}{\partial q_i} = -\frac{1}{\lambda} C_{ij} q_j \]

Use \( q_i = a_i e^{i\omega t} \)

\[ -\lambda^2 a_i = \sum_j C_{ij} a_j \]

\[ \Rightarrow \lambda \left( C_{ij} - \omega^2 \delta_{ij} \right) = 0 \]

Find \( \omega \) roots yielding three \( \omega^{(1)} \) eigenvalues also

\[ \sum_i a_i^{(2)} a_i^{(1)} = 5 \lambda^2 \] since \( C_{ij} \) is symmetric.

Apply to \( \text{CO}_2 \) molecule

9 modes:

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
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\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
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\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]

\[ \begin{array}{ccc}
\sigma_v & \sigma_v & \sigma_v \\
\sigma_v & \sigma_v & \sigma_v \\
\pi & \pi & \pi
\end{array} \]

\[ \omega = 0 \quad \omega \neq 0 \]
We can express $q_i = \sum_q a_i^{(\alpha)} Q_\alpha$, i.e. $q_i$ is a sum of the eigenmodes. Can show

$$Q_\alpha = \sum_q a_i^{(\alpha)} q_i$$

This separates the harmonic oscillators. Can also do this in Q.M.
We were considering

\[ H = \frac{1}{2} \sum_i p_i^2 + \frac{1}{2} \sum_{i<j} C_{ij} q_i q_j \]

and found

\[ \omega^2 a_i^{(v)} = \sum_j C_{ij} a_j^{(v)} \]

\[ \sum_i a_i^{(v)} = 0 \]

\[ \sum_i a_i^{(w)} = 0 \]

To simplify, we substitute the normal coordinates

\[ Q^x = \sum_i a_i^{(x)} q_i \]

as new variables \( q_i = \sum_x a_i^{(x)} Q^x \), to find

\[ H = \frac{1}{2} \sum_i p_i^2 + \frac{1}{2} \sum_x \omega^2 Q^x \]

\[ = \sum_x h x \]

where \( h x = \frac{1}{2} p_i^2 + \frac{1}{2} \omega^2 Q^x \)

**Example:**

\[ \text{Example} = E_{mc} + E_{mc} + \cdots = \sum_{x} E_{c} \]

\[ = h \omega_1 (n_1 + \frac{1}{2}) + h \omega_2 (n_2 + \frac{1}{2}) + \cdots \]

\[ = \sum_{x} h \omega_{x} (n_{x} + \frac{1}{2}) \]
ii) Write wave functions as $\phi_n(x)$ (Hermite polynomials)

$$\Psi = \phi_{n_1}(q_1) \phi_{n_2}(q_2) \cdots$$

$$\Psi = \prod_n \phi_n(q_a)$$

iii) Ground state of system: $n_a = 0$, $E_g = \frac{\xi^2}{2} h \omega Q_a + U(0,0,0)$

wave function

$$\Psi_g = \prod_a e^{-\frac{i}{2} \omega_a Q_a^2} = e^{-\frac{i}{2} \xi \omega_a Q_a^2}$$

$$\Psi_g = e^{-\frac{i}{2} \xi \omega_a Q_a^2}$$

Might try to express $\Psi_{ij} = e^{i \omega_a Q_a^2}$ as a sum of $\Psi$

$$\Psi_{ij} = C \left[ e^{i \omega_a Q_a^2} = C_{ij} \right]$$

iv) $\bar{n} = \frac{1}{e^{h \omega_a/(kT)} - 1}$

Thus internal energy

$$U = \frac{\xi^2}{2} h \omega_a (n_a + \frac{1}{2}) = \frac{\xi^2 h \omega_a}{2} + \frac{\xi^2}{2} e^{h \omega_a/(kT)}$$

To show $\bar{n}$, consider probability occupation of states by $1/\Omega$

$$P_n = \frac{1}{\Omega} e^{-h \omega_a (n_a + \frac{1}{2})}$$

But

$$\frac{\xi P_n}{n} = 1 = \frac{1}{n} \frac{1}{\Omega} e^{-h \omega_a (n_a + \frac{1}{2})}$$

$$\bar{n} = \sum_n n P_n \sim (1-x) \frac{\xi}{n} n e^{-\xi \omega_a/(kT)} = \frac{x}{1-x}$$
Example:

Neutron scattering of a nucleus in a solid, which is heavy, results in no energy loss. Neutron-nucleus potential $V(R-q_k)$ is so space limited, we use Born approx.

Interaction $V(R-q_k) \approx a\delta(R-q_k)$

Initial state $e^{iP_n\cdot R} \psi_i(q,\ldots) = \psi(R, q)$

Final state $e^{iP_f\cdot R} \psi_f(q,\ldots)$

Prob of transition $= \ldots 1 |M_{fi}|^2$

$M_{fi} = \int \psi_f^* e^{iP_f\cdot R} S(R-q_k) e^{iP_i\cdot R} \psi_i \, d^3R \, dq$

Define $K = P_f - P_i = $ momentum transfer

$\int \psi_f^* \left( q \right) e^{iK \cdot q} \psi_i \left( q \right) \, dq$

[i.e., sudden approximation of $\psi_i$, $\psi_f = e^{iK\cdot R \text{final} \psi_i}$.]

Or for $\omega$

$\int \psi_0 e^{i\tilde{K} \cdot \tilde{q}} \tilde{q} \, d\tilde{q} = \int_{\text{all states}} e^{-\frac{1}{2} \omega \delta \Omega_s} e^{iK \cdot \delta \Omega_s} \, dq \, dq_s \ldots$
\[ \Pi \left( \int e^{-\omega \sum_{a} (\mathbf{q}_a^2 + i \mathbf{v}_a \cdot \mathbf{q}_a \cdot \mathbf{a}_0)} \, d\mathbf{q}_a \right) = \xi \left( \frac{k^2}{4\omega} \right) \]

Thus

\[ \text{proof} = e^{-\kappa^2 S} \]

\[ S = \frac{\left( \frac{\alpha k}{2} \right)^2}{\alpha} \]

\[ \text{PROBLEM: One can find} \quad \langle \mathbf{q}_k^2 \rangle = \int \psi_0 \mathbf{q}_k \psi_0 \, d\mathbf{q} = S \]

Thus

\[ \text{proof} = e^{-\kappa^2 \langle \mathbf{q}_k^2 \rangle / \hbar^2} \]

\[ \text{PROBLEM: Prove the same formula for the system at temperature } T \quad [\text{i.e. that probability no energy is transferred to system is}] \]

\[ \text{proof} = e^{-\kappa^2 \langle \mathbf{q}_k^2 \rangle / \hbar^2} \]

where \( \langle \mathbf{q}_k^2 \rangle \) is the variance of \( \mathbf{q}_k \) at temp. \( T \).
We found

\[ \text{Prob. to remain in ground state} = e^{-p^2/2\hbar^2} \]

Note we cannot scatter from zero-w wave modes (translational).
Always define elastic scattering in center of mass system so as to view each translational mode.

**PROBLEM:** Suppose system in ground state. Show:

\[ \langle \text{energy lost by neutron if Pb induced} \rangle = \frac{p^2}{2m_k} \]

\[ \text{mean energy gained by crystal} \]
\[ \text{As wave function is } \psi = e^{ipx} = \frac{p^2}{2m_k} \text{ (conical result)} \]

1.) **prove for ground state**
2.) **... any state**
3.) **...** system

\[ \text{Prove for ground state} \]

\[ \text{Caused a difference (only if we cannot distinguish which atom was hit). When is this true? When} \]

\[ \text{Proton} \to \text{P zero point energy} \]
**PROBLEM:** Show that elastic scattering gives a diffraction. Show that inelastic scattering does not give a diffraction pattern.

Nucleus inside a crystal lattice at $t$. Expect a recoil (classically)

$$E_r = E_0 - \frac{p^2}{2m}$$

They could absorb this $t_i$ in a similar nucleus (resonance absorption).

Mössbauer discovered recoilless emission and absorption. Analogue to elastic neutron scattering. Very precise effect.
Back to Harmonic Oscillator

\[ H = \frac{1}{2} p^2 + \frac{1}{2} \xi^2 \]

\[ p = \frac{1}{i} \frac{\partial}{\partial \xi} \]

Recall

\[ H \phi_n = E_n \phi_n \]

\[ E_n = (n + \frac{1}{2}) \]

\[ \phi_n(\xi) = \frac{1}{\sqrt{\pi n!}} H_n(\xi) e^{-\frac{1}{2} \xi^2} \]

\[ n = 0 \quad e^{-\frac{1}{2} \xi^2} \]

\[ n = 1 \quad \xi e^{-\frac{1}{2} \xi^2} \]

\[ n = 2 \quad (2\xi^2 - 1) e^{-\frac{1}{2} \xi^2} \]

Interesting that we can get a generating function

\[ e^{-\xi^2 + 2\xi s} = \sum_n \frac{H_n(\xi) s^n}{n!} \]

Also have

\[ \sum_n \frac{\phi_n(\xi) s^n}{\sqrt{n! 2^n}} = \frac{1}{\sqrt{4\pi}} e^{-\frac{1}{2} (\xi - s)^2} e^{s^2/4} \]
Example:

\[ \sum_{m} = \int \Phi_m(\xi) e^{ips} \Phi_n(\xi) \, d\xi \]

Calculate

\[ \sum_{m} \frac{e^{itn}}{\sqrt{2\pi n!}} \frac{1}{\sqrt{2\pi m!}} = \delta(m, n) \]

\[ = \frac{\langle \Phi_m | \Phi_n \rangle}{\sqrt{2\pi m!} \sqrt{2\pi n!}} \]

\[ = \frac{\int \Phi_m(\xi) e^{ips} \Phi_n(\xi) \, d\xi}{\sqrt{2\pi m!} \sqrt{2\pi n!}} \]

\[ = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{1}{2} (\xi - s)^2} e^{ips} \, ds \]

\[ = \frac{1}{\sqrt{\pi}} \int e^{-\frac{1}{2} (s + \xi + ip)^2} e^{-\frac{1}{2} (s + ip)^2} \, ds \]

\[ = \frac{1}{\sqrt{\pi}} \int e^{-\frac{1}{2} (s - \frac{s + ip}{2})^2} \, ds \]

\[ = e^{-\frac{ip^2}{4}} \frac{s + ip}{2} \]

Now, just expand in \( \sum_{m} \frac{e^{itn}}{\sqrt{2\pi n!}} \)

\[ = e^{itn} \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \frac{(s + ip)^k}{k!} \]

\[ = e^{-\frac{ip^2}{4}} \frac{s + ip}{2} \]

\[ = \frac{2^{mn}}{\sqrt{2\pi m!} \sqrt{2\pi n!}} = e^{-\frac{ip^2}{4}} \frac{(ip)^{m+n-2k}}{k!} \frac{2 - k}{k! (w-k)! (n-k)!} \]
Problem: A crystal at temp $T$. Find $\Delta E$ for scattering waves (for given $\Gamma$) elastically.

Hint: If single oscillator, $P_{\text{scat}} = \langle n|e^{i\Gamma}|n\rangle$

$$\xi \equiv \frac{e^{-\Delta E/kT}}{\Delta} \langle n|e^{i\Gamma}|n\rangle^2$$

Then show $P_{\text{scat}} = e^{-\rho^2\langle q^2 \rangle}$

Problem: Show:

$$\sum_n \Phi_n(x)\Phi^*_n(x) e^{i\Gamma n} = \left(\frac{\mu \omega}{2\pi \sin \omega t}\right)^{1/2} e^{i\frac{\mu \omega}{2\pi \sin \omega t} \left[ (\cos \omega t) (5^2 \xi^2) - 2 \xi \right]}$$

Problem: Consider:

$$\frac{\partial}{\partial t} \psi(x,t) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \psi(x,t) + \frac{1}{2}\xi^2 \psi(x,t)$$

Suppose $\psi(x,0) = \delta(x-x_0)$. Try to solve the time-dependent eqn:

Hint: $\psi(x,t) = e^{\alpha t}x^2\frac{\partial}{\partial x} + b(t)\delta(x) + c(t)$
\[ H = \frac{1}{2} \frac{d^2}{d\xi^2} + \frac{1}{2} \xi^2 \]

\[ p = \frac{1}{i} \frac{d}{d\xi} \]

\[ \phi_0 (\xi) = e^{-\xi^2/2} \]

\[ \phi_n (\xi) \]

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

\[ \Psi_n (p) = i^n \phi_n (p) \]

\[ \phi \text{ phase from } \Psi (p) = \int e^{ip \xi} \phi(\xi) d\xi \]

Recall we had given

\[ \lambda_{mn} = \int \phi_m^*(\xi) e^{ip \xi} \phi_n (\xi) d\xi = \int \phi_m^*(p) \phi_n (p + \xi) dp \]

\[ -\frac{1}{r} \frac{d}{dr} \left[ r \psi \right] + \frac{\xi}{r} \left[ r \psi \right] = rE \left[ r \psi \right] \]

\[ -\hbar \frac{1}{i} \frac{d}{dp} \left( \frac{\hbar^2}{2m} \phi (p) \right) + \phi (p) = -E \frac{\hbar^2}{2m} \frac{d^2}{dp} \]

Thus

Now return to

\[ H = \frac{1}{2} \frac{p^2}{m} + \frac{\hbar^2}{2m} \phi^2 \]

\[ \frac{11/16/67 \text{Lecture}}{} \]
Now define
\[ a = \sqrt{\frac{m}{2\omega}} (\omega q + i p/m) \quad [\frac{1}{i\hbar} (\xi + \frac{1}{\xi})] \]
\[ a^+ = \sqrt{\frac{m}{2\omega}} (\omega q - i p/m) \quad [\frac{1}{i\hbar} (\xi - \frac{1}{\xi})] \]

Then
\[ q = \sqrt{\frac{1}{2m\omega}} (a + a^+) \]
\[ p = (\frac{1}{i\hbar}) (a - a^+) \]

Note \[ pq - qp = -i \] for all the in a's

\[ a^+a = \frac{1}{\omega} H - \frac{1}{2} \]
\[ aa^+ = \frac{1}{\omega} H + \frac{1}{2} \]

Thus \[ aa^+ - a^+a = 1 \]

Also
\[ H = \omega a^+a + \frac{\omega}{2} \]

Excitation energy for harmonic oscillator
Can figure out eigenvalues and matrix elements

Sometimes define \[ N = a^+a \]
If \( |n\rangle = n|n\rangle \), then
\[
a^+|n\rangle = \sqrt{n+1}|n+1\rangle
\]
\[
a|n\rangle = \sqrt{n}|n-1\rangle
\]

Thus, \( a^+ \) creation operator, \( a \) annihilation operator.

\[
\langle m|a^+|n\rangle = \delta_{m,n+1}\sqrt{n+1}
\]
\[
\langle m|a|n\rangle = \delta_{m,n-1}\sqrt{n}
\]

**Conclude**

\[
(a^+)^n|0\rangle = \frac{1}{\sqrt{n!}}|n\rangle
\]

where we define \( |0\rangle \) by

\[
a|0\rangle = 0
\]

**Example:**

\[
\delta_{mn} = \langle m|(a+a^+)|n\rangle
\]

\[
= \langle 0|a^m(a+a^+)(a^+_n)|0\rangle \sqrt{n!} \frac{1}{\sqrt{n!}}
\]

Use \( \langle 0|a^+_n = 0 \), \( \langle 0|0\rangle = 0 \) to work out.

\[
\delta_{mn} = \langle 0|a^m \frac{e^{i\rho(a^+_n)}}{\sqrt{m!n!}} (a^+_n)^n|0\rangle
\]
There are \( N \) independent oscillators, define
\[
a^+_\alpha = \left( M \omega_\alpha Q_\alpha + i \frac{P_\alpha}{\hbar} \right) \sqrt{\frac{M \omega_\alpha}{2\mu}}
\]

Now show
\[
a^+_\alpha a_\beta - a_\beta a^+_\alpha = 2 \delta_{\alpha\beta}
\]
\[
a_\beta a_\alpha = a^+_\alpha a_\beta
\]

Thus
\[
H = \frac{\hbar \omega_\alpha}{2} + \sum \omega_\alpha a^+_\alpha a_\alpha
\]

Can arbitrarily assign oscillator to any state it has \( \gamma \) "excitations." Thus \( a^+_\alpha \) a create and annihilate vibrations.

This is very convenient for more complicated problems.

\[ E \text{ in cavity: photons} \]
\[ \text{crystal: phonons} \]

"Calling a state of motion by a name," like "vortex." ["Can't step in same river twice." "Eating + anti-process"]

Human as a pattern of motion.
Now return to our discussion of a polyatomic molecule

\[ H = \frac{1}{2} \sum \frac{p_{i}^{2}}{m_{i}} + \frac{1}{2} \sum \varepsilon_{ij} q_{i} q_{j} \]

and try to extend it to a crystal.

Select location in a crystal

\[ \mathbf{N} \] cell

\[ \mathbf{r} \] atom in cell

If \( n \) atoms/with cell, \( \mathbf{r} \) has 3 \( n \) values

\( \mathbf{a}, \mathbf{b}, \mathbf{c} \) are directions which reproduce the crystal

Then to find \( \mathbf{N} \)

\[ \mathbf{N} = n_{a} \mathbf{a} + n_{b} \mathbf{b} + n_{c} \mathbf{c} \]

Now \( H \) for the crystal becomes

\[ H = \sum_{N} \frac{p_{N}^{2}}{2m_{N}} + \frac{1}{2} \sum_{N_{1},N_{2}} \varepsilon_{N_{1},N_{2}} q_{N_{1},N_{2}} q_{N_{1},N_{2}} \]
Now \[ C_{n, r, M, s} = \Gamma_{r, s} (M-N) \]

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

\[ \omega^2 \cdot b_{m, r} = \sum_{M, s} (M-N) \cdot b_{m, s} \]
\[ H = \sum_{N,r} \frac{P_{n;r}^2}{2} + \frac{1}{2} \sum_{N,r;M,s} \Gamma_{r,s}(N-M) P_{n;r} P_{m;M,s} \]

Now consider

\[ \omega_n^2 \psi_{n,r} = \sum_{M,s} \Gamma_{r,s}(N-M) \psi_{m;M,s} \]

**Example:**

\[ \begin{array}{c}
\text{Choose a potential} \\
\frac{A}{2} (q_n - q_{n+1})^2 + \frac{B}{2} (q_n - q_{n+2})^2 + \ldots
\end{array} \]

At first take \( B \); longer range terms vanish. Then

\[ H = \sum_{N} \frac{P_n^2}{2} + \frac{1}{2} \sum_{N} A (q_n - q_{n+1})^2 \]

\[ \sum_{N} A q_n^2 - \sum_{N} A q_n q_{n+1} \]

\[ \sum_{n,m} (n-m) q_n q_m \]

Thus \( \Psi(0) = 2A, \Psi(1) = A, \Psi(-1) = -A \)

Our e.o. problem becomes

\[ \omega_n^2 q_n = A(q_n - q_{n+1}) - A(q_n - q_{n-1}) \]

Let

\[ \begin{pmatrix} 2A - \omega^2 & -A \\
-A & 2A - \omega^2 & -A \\
0 & -A & 2A - \omega^2 & -A \end{pmatrix} \]

a band matrix

and as b.c. use \( \psi_{m;n} = 0 \)
Rather than solve det \( \Lambda \), we merely solve eqn by letting \( q_n = e^{i\alpha} \).

to find
\[
c^2 e^{i\alpha} = A[e^{i\alpha} - e^{i(n+1)\alpha}] - A[e^{i\alpha} - e^{i(n-1)\alpha}]
\]
\[
c^2 = A[1 - e^{i\alpha} - e^{-i\alpha} + 1] = 2A(1 - \cos \delta)
\]

We also require \( q_{n+n} = q_n \)
\[
e^{iN\alpha} = 1 \Rightarrow \delta = \frac{2\pi l}{N} \quad l = 0, \ldots, N-1
\]
\[
\text{or} \quad l = \frac{N - 1}{2}\frac{n}{2}
\]

Then we find our \( c^2 \) 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 $x$ to $s$ to $k$, suggestive of a wave motion.

$$k = \frac{s}{a}$$

Phase difference $s = 2\pi$.

Then,

$$\omega^2_k = 2\pi \left(1 - \cos ka\right)$$

$$k = -\frac{\pi}{a} \text{ to } \frac{\pi}{a}$$

Spacing of $k = \frac{2\pi}{N^2} = \frac{2\pi}{L}$

For long wavelength,

$$\omega_k^2 \sim Aa^2 k^2$$

$$\Rightarrow \omega \sim k.$$  [This is what it is anyway]

$$\Rightarrow c_s = \sqrt{Aa^2}$$

Now for the normal modes,

$$Q_k = \sum \alpha_i q_i = \sum \frac{e^{i k m a}}{\sqrt{N}}$$

and $H$ becomes

$$H = \sum \frac{p_{k_i}^2}{2} + \sum \frac{\omega_k^2}{2} Q_k^2$$

Now have "phonons" of wavelength $k$. Thus sound has a maximum $\omega$ at min. wavelength [corresponding to $a$].
Now returning to our general problem

\[ \Theta_{\text{MS}} = g_s^1 e^{iM \cdot \mathbf{K}} \]

Thus we take into account the phase difference between cells and between atoms. Thus

\[ \omega^2 g^1_s e^{iM \cdot \mathbf{K}} = \sum_{\mathbf{M}, \mathbf{S}} \Gamma_{\text{KS}}(M-N-M) e^{iK \cdot (\mathbf{K}-\mathbf{M})} g^1_s \]

Now define

\[ \sum_{M, \mathbf{K}} \Gamma^*(M) e^{-iK \cdot \mathbf{K}} = \gamma_{\text{KS}}(\mathbf{K}) \]

(Kind of a Fourier transform)

Thus letting \( \omega g_s^1 \rightarrow \omega^2 g_s^1(\mathbf{K}) \)

\[ \omega^2 g_s^1(\mathbf{K}) \Theta^1_{\text{MS}} = \sum_{\mathbf{M}, \mathbf{S}} \Gamma_{\text{KS}}(\mathbf{K}) g_s^1_s \]

Now this problem is just for atoms in cell and we can revert to our analysis of polyatomic molecules [we have the infinite periodic unit cell by the \( \mathbf{K} \)]

\( B \) has \( 3p \) value for each \( \mathbf{K} \). Now spacing of \( \mathbf{K} = \frac{2\pi}{\text{Vol}} \).

\[ \sum_{\mathbf{K}} \rightarrow \sqrt{\frac{3! K}{(2\pi)^3}} \text{ Vol} \]

Where are repetition boundaries of \( \mathbf{K} \) space? We'll return to these in a moment.
Consider a one dimensional $k_z = \omega^2$ plane where each unit cell has 1 atom - 3 modes per $k$.

Thus 3 types of sound waves - longitudinal and 2 transverse. [Not actually either]

In other directions waves are different. Thus $c_s$ are different in different directions.

Acoustical / optical branches

$\bullet \bullet$ 2 atoms/unit cell (NaCl)
Problems:

1) One-dimensional line of atoms spanning a limit case $k \ll 1$ to develop the q.m. of a continuous material (long waves). $\hat{q}_n = q(x)$. This is quantum field theory.

2) Find the frequency spectrum for some crystal, specific heat. Like cubic crystal.

Recall

$$C_{N,r,M,s} = \Gamma_{rs}(N-M)$$

$$\sum_{N} \Gamma_{rs}(N)e^{i\mathbf{K}\cdot\mathbf{r}} = \chi_{rs}(\mathbf{K})$$

Then solved

$$\Omega_{p}^{2}(\mathbf{K}) q_{r}^{'} = \sum_{s} \chi_{rs}(\mathbf{K}) q_{s}^{'}$$

and

$$Q_{r}^{'}(\mathbf{K}) = \sum_{r} Q_{r}(\mathbf{K}) q_{r}^{'}$$

$$Q_{r}(\mathbf{K}) = \sum_{N} Q_{r,N}(\mathbf{K}) e^{-i\mathbf{K}\cdot\mathbf{r}}$$
Continues discussing polyatomic crystals.

Because of dipole moment, one can excite modes in optical bands with infrared light. Thus near low energy absorption of class III frequencies or \( k_z \to 0 \). Radiative frequency, thus reflects non-radiative beam. Would be an intense dye – if only not infrared. Laser would 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 monodimincystal).
Determination of \( \omega_p \): 

For every \( k \), \( \omega_p \) frequency \( \sqrt{k^2 + \omega_p^2} \) 

Not hard to show that if you bounce waves from crystals

\[
\begin{align*}
\text{Pin} - \text{Port} &= \text{P} \\
\text{Excite a mode of } k \text{ if} \\
\text{Can plot energy of motion}
\end{align*}
\]

By looking at peaks, we can get \( \omega_p \) directly.

Now in \( k \)-space

\[
\frac{\varepsilon}{k^2} \rightarrow \int \frac{d^3 k}{(2\pi)^3 \text{vol}}
\]

Now \( N = n_a a + n_b b + n_c c \)

We can try to find \( \varepsilon \), and that

\[
k'' = k + \varepsilon
\]

gives same answer.
$e^{iH\cdot \mathbf{N}} = e^{i\mathbf{N} \cdot \mathbf{I}}$

$\Rightarrow e^{i\mathbf{I} \cdot \mathbf{N}} = 1$

Thus

$(\mathbf{I} \cdot \mathbf{a}) = 2\pi$ (integer)

$(\mathbf{I} \cdot \mathbf{b}) = 2\pi$ (integer)

$(\mathbf{I} \cdot \mathbf{c}) = 2\pi$ (integer)

---

So we know $(\mathbf{I} \cdot \mathbf{a}) = L_a$  $(\mathbf{I} \cdot \mathbf{b}) = L_b$  $(\mathbf{I} \cdot \mathbf{c}) = L_c$

Then one can show we can write the vector $\mathbf{I}$ as

$\mathbf{I} = L_a \frac{\mathbf{a} \times \mathbf{c}}{|\mathbf{a} \times \mathbf{c}|} + L_b \frac{\mathbf{c} \times \mathbf{b}}{|\mathbf{c} \times \mathbf{b}|} + L_c \frac{\mathbf{a} \times \mathbf{b}}{|\mathbf{a} \times \mathbf{b}|}$

---

Here $L_a, L_b, L_c = 2\pi$ integers. This forms a lattice of points in $K$-space analogous to the reciprocal of the original cubic crystal called the reciprocal lattice. Very important in diffraction waves (which is elastic).

In $K$-space, can separate regions $\mathbb{R}$ which respect new reciprocal lattice. These is first Brillouin zone in $K$-space.
Solid-state physicists (frequently chemists) characterize crystals. True physicists always work with cubic crystals.

Specific Heats:

These nuclear vibrations are main contribution to specific heat in most problems,

\[ U(N) = \sum_{\mathbf{k}} \frac{\hbar^2 c^2 k^2}{8 \pi^2} \frac{\cosh(\hbar c k / k_B T)}{\cosh(\hbar c k / k_B T) - 1} \]

\[ = \sum_{\mathbf{k}} \frac{\hbar^2 c^2 k^2}{8 \pi^2} \frac{d^3 k}{(2\pi)^3} \frac{d^3 k}{(2\pi)^3} \cdot \frac{1}{\sqrt{\cosh(\hbar c k / k_B T) - 1}} \]

Can find

\[ C_V = \frac{\partial U}{\partial T} , \text{ etc.} \]
\[ \omega_n(k) = \text{mode frequencies} \]

\[ U = \text{internal energy (derivation)} = \sum_{k} \frac{3^{1/3} k \text{Vol}}{(2\pi)^{3/2}} \frac{\hbar \omega_n(k)}{e^{\hbar \omega_n(k)/k T} - 1} \]

\[ C_v = \frac{\partial U}{\partial T} = k \text{Vol} \sum_{k} \frac{3^{1/3} k \text{Vol}}{(2\pi)^{3/2}} \frac{\left(\frac{\hbar \omega_n(k)}{k T}\right)^2}{e^{\hbar \omega_n(k)/k T} - 1} \]

Phonon description is quite good for many crystals (soft metals, magnets, etc., however). We can discuss \( C_v \) at high temperatures:

If \( \hbar \omega_n \gg k T \) (usually at room temp),

\[ \frac{\hbar \omega_n}{e^{\hbar \omega_n/k T} - 1} \rightarrow k T \]

\[ U = k T \sum_{k} \frac{3^{1/3} k \text{Vol}}{(2\pi)^{3/2}} = 3NkT \]

\[ C_v = 3Nk = 3R \text{ per } \circ C, \text{ per mole} \]

\( \sim 6 \text{ cal per } \circ C \text{ per mole} \)

Pretty good at high T.
Low Temperatures:

$kT < \text{any frequency} \implies \text{get } e^{-\frac{kT}{\hbar}} - \text{essential singularity}$

But no lowest frequency

Thus assume 3 values of $\omega_i$ summing and

$\omega_{e\omega} (\text{HC}) = C_{\omega_i} |K|$}

\[
U = kT \sum_i \left[ \frac{\hbar^2 k_i^2}{2m} \cdot \frac{\hbar k_{\omega_i} K}{e^{\hbar k_{\omega_i} K/k_B T} - 1} \right]
\]

\[
= kT \sum_i \int \frac{d\omega_i}{4\pi} \left( \frac{\hbar k_i}{\hbar c_{\omega_i}} \right)^3 \frac{1}{2\pi} \int_0^{\infty} \frac{x^2 e^x}{e^x - 1} dx \pi^4 \ Vol
\]

\[
= \frac{(kT)^4 \pi^2}{10} \int \frac{d\omega_i}{4\pi} \left( \frac{\hbar k_i}{\hbar c_{\omega_i}} \right)^3 \frac{1}{3} \int_0^{\infty} \frac{x^2 e^x}{e^x - 1} dx \pi^4 \ Vol
\]

\[
= \frac{(kT)^4 \pi^2 \ Vol}{10 c_0^3} \text{ are speed-dependent } \frac{kT}{c_i} = \frac{1}{c_i^3} \ Vol
\]

\[
CV \sim T^3
\]
The number of modes at low $T$ is given by $N \sim \frac{1}{T^3}$.

However, as we approach $0^\circ$ (10^-6 degrees), we find $C_v \propto T^3$. Why? Because $k \rightarrow 0$ for very small crystals which are used at very low $T$. Then there is a lowest frequency, then essential singularity

$$U = 3kT \sqrt{\frac{\alpha^3 h}{(2\pi)^3}} \frac{\hbar \omega_{0}(k)}{e^{\frac{\hbar \omega_{0}(k)}{kT}} - 1}$$

$$= \frac{(kT)^{\frac{3}{2}}}{\hbar} \frac{\pi^2}{10} \left(\frac{\Theta}{T}\right)^{\frac{3}{2}}$$

where $\Theta = \frac{K \omega_0}{k}$

Debye temperature is a useful way to characterize a crystal.

$C_v$ vs $T$ does not show a peak, unfortunately. Always plot $\Theta D$ vs $T$. 
Neutron Scattering

\[ \langle \Psi | \psi \rangle \]

Actually this is gotten from

\[ \langle e^{-i\mathbf{kr}_i} | \mathbf{V} (\mathbf{r}_i - \mathbf{r}_f) | e^{i\mathbf{kr}_f} \rangle \]

where we assume Fermi pseudopotential \( V_0 \approx \alpha_0 (r) = \text{const.} \).

Now suppose elastic scattering \( i = f \)

\[ \text{Prob}_{f \rightarrow i} = | \langle i | \Psi | \Psi \rangle |^2 \]

Put \( \mathbf{R}_i = \mathbf{R}_0 + \mathbf{q}_i \)

\[ \text{Prob}_{f \rightarrow i} = | \langle i | e^{i\mathbf{p}_0 \cdot \mathbf{R}_0} e^{i\mathbf{p}_i \cdot \mathbf{q}_i} | \Psi \rangle |^2 \]

\( \text{If we take } e^{i\mathbf{p}_i \cdot \mathbf{q}_i} \approx 1, \quad \text{Prob}_{f \rightarrow i} = \text{Prob}_{i \rightarrow i} \)

However, carry \( e^{i\mathbf{p}_i \cdot \mathbf{q}_i} \) along

\[ \sum e^{i\mathbf{p}_0 \cdot \mathbf{q}_i} \langle i | e^{i\mathbf{p}_i \cdot \mathbf{q}_i} | \Psi \rangle \]

\[ e^{-\frac{p^2 q_i^2}{2}} \]
Now for inelastic

\[ \langle \Psi | e^{i \mathbf{P} \cdot \mathbf{R}_0} | \psi \rangle \]

For some reason we don't get any interference from inelastic scattering since we can always identify the excited atom.

Maybe a tiny bit of interference due to coupling between modes in crystal.

Try to work out for linear.

Now \[ \Psi_{\text{after}} = e^{i \mathbf{P} \cdot \mathbf{x}} \Psi_{\text{before}} \]

\[ \langle \Psi_{\text{after}} | H | \Psi_{\text{after}} \rangle \]

\[ \langle \Psi_{\text{after}} | e^{-i \mathbf{P} \cdot \mathbf{x}} \frac{\partial}{\partial \mathbf{x}} e^{i \mathbf{P} \cdot \mathbf{x}} - H | \Psi_{\text{after}} \rangle \]

Now use \[ \frac{\partial}{\partial \mathbf{x}} (e^{a \mathbf{x}} f) = e^{a \mathbf{x}} \left( \frac{\partial}{\partial \mathbf{x}} + a \right) f \]

to find

\[ \langle \Psi_{\text{after}} | \left( \frac{\partial^2}{\partial \mathbf{x}^2} + \cdots \right) | \Psi_{\text{after}} \rangle \]

\[ = \frac{\partial^2}{\partial \mathbf{x}^2} \langle \Psi_{\text{after}} | \Psi_{\text{after}} \rangle + \mathbf{P} \cdot \mathbf{P} \langle \Psi_{\text{after}} | \Psi_{\text{after}} \rangle \]

when \[ \langle \Psi_{\text{after}} | \frac{\partial}{\partial \mathbf{x}} \Psi_{\text{after}} \rangle = 0 \], get classical result.
The $| \langle \phi, \phi \rangle \rangle$ is kind of a Doppler correction.

---

**Prob. No excitation from $e^{ipQ}$.** Initially state is $|n\rangle$.

**Prob of no excitation is** $| \langle n | 1 - e^{ipQ} | n \rangle |^2$. At thermal equilibrium,

**Prob of excitation** $= \frac{\langle n | e^{-E_n/kT} | n \rangle}{\langle n | 1 - e^{ipQ} | n \rangle |^2}

= \frac{e^{-E_n/kT}(1 - e^{-E_n/kT})}{\langle n | e^{ipQ} | n \rangle |^2}$

First find $\langle n | e^{ipQ} | n \rangle = \langle 0 | \frac{a^+ e^{ip(a+a^*)}}{n!} \frac{a^*}{n} | 0 \rangle$

$= \sum_{n} \frac{e^{ip}\frac{1}{2^n}}{n!} \langle 0 | a^n(a+a^*) \frac{a^*}{n} | 0 \rangle$

Use $a^*a = a^*a + na^{n-1}$.
\[ \mu^- \text{ to stimulate } p + p \rightarrow d + e^+ + \nu. \]

\[ \text{Hence, for your keen learning. Each } \mu^- \text{ only lives } T = 2.2 \times 10^{-6} \text{ sec.} \]

\[ \text{So, the } \mu^- \text{ would survive too long. But maybe another} \]

\[ \text{longer-lived heavy quark changed particle.} \]

\[ \text{At high } T, \text{ can get breaking treatment for} \]

\[ p + p \rightarrow d + e^+ + \nu. \]

---

**Problem**: Changing limit of atoms to a continuum

\[ H = \frac{p^2}{2} + \frac{\alpha}{2} (\xi_n - \xi_{n+1})^2 \]

\[ \xi_n = \frac{\xi_n}{N} e^{\frac{i k x_n}{N}} \]

Set \( \xi_n = \alpha n \). Thus \( g(x) \) replaces \( \xi_n \). Recall we found

\[ \omega^2 = 2\alpha (1 - \cos k) \]

For large \( k \), \( g(x) \) continuous.

\[ \omega^2 = 2\alpha \frac{k^2}{a^2} \]

\[ Q_n = \int g(x) e^{i k x} \frac{dx}{\alpha N} \]

\[ Q'_n = \int g(x) e^{i k x} dx \]

\[ \xi_n = \sqrt{Q_n} \frac{dx}{2\pi} \]

\[ \xi'_n = \frac{Q_n}{\alpha N} \]
\[ H = \mathcal{F}\left(\frac{\pi^2}{2a}\right)^2 + \frac{1}{2a} \alpha a^2 \left(\frac{\partial}{\partial x}\right)^2 \right] dx \]

\[ \text{P.E.} \]

\[ \text{K.E.} \]

\[ \Pi(x) = P_0 \quad a \]

\[ \phi_0 + P_0 \cdot \phi_n = -i \delta m \]

\[ \phi(x) \Pi(x) - \Pi(x) \phi(x) = i \delta(x-x') \]

\[ H = \int \left[ \frac{-\hbar^2}{2} \Pi^2(x) + \frac{\hbar^2}{2} \left(\frac{\partial}{\partial x}\right)^2 \right] dx \]

**Thus we have defined a field** — a q.m. field — of two conjugate variables \( \phi(x), \Pi(x) \) [corresponds to vibrating string]. **Note we can “diagonalize” \( H \) using**

\[ \phi(x) = \int e^{ikx} Q(k) \frac{dk}{2\pi} \]

\[ \Pi(x) = \int e^{-ikx} P(k) \frac{dk}{2\pi} \]

\[ \Rightarrow \quad P(k) Q(k') - Q(k') P(k) = -2\pi i \delta(k-k') \]

\[ H = \frac{1}{2} \int \left[ (P(k))^2 + k^2 \right] \frac{dk}{2\pi} \quad 1 \left(\frac{\partial}{\partial x}\right)^2 \right] \frac{dx}{2\pi} \]

\[ \therefore \quad \omega^2(x) = c k \]
We could have applied this to electrodynamics.

QED field theory in 3-d

\[ Q(x) : Q_x(x), Q_y(x), Q_z(x) \]

\[ \text{K.E.} = \frac{1}{2} \int \frac{\partial Q}{\partial t} \cdot \frac{\partial Q}{\partial t} \, d\text{Vol} \]

\[ \text{P.E.} = \frac{1}{2} \int C_{ij,k\ell} C_{ij} C_{\ell \kappa} \, d^3x \]
PROBLEM: Diffusion of phonons (finite mfp) 1/31/67 Lectures

This is local diffusion. Needed higher order
perturbation theory. \((q_i - q_j, r_j) + \cdots\) so
a perturbation theory. \((\text{Use } a \cdot a \cdot \epsilon)\)

Phonon-phonon scattering

Undeformed processes: \(HK + HK' = HK'' + L\) because propagation

is local. One needs a local Boltzmann theory. Here we need a

failed diffusivity, i.e., second order. \((\text{linear dispersion}

relation is } m \propto v)\). At low T not many phonons

exist.\(\) Thermal phonons exist.\(\)

Hence the scattering is

impossible. The scattering by phonons can be treated as a free

phonon crystal.\(\)

\(HK = 0\)

\(HK + HL = L\)

PROBLEM: Some density of imperfections. Phonons of different

energy can be treated separately. Phonons will scatter

off of these.

For small \(T\) how does

thermal conductivity depend on \(T\) and \(n\)?
Continuum Approximation

\[ \psi(x), \Phi(x) \rightarrow \Phi(x) \psi(x) - \psi(x) \Phi(x) = -i \delta(x-x') \]

K.E. = \( \frac{1}{2} \int \left( \frac{\partial \Phi}{\partial x} \right)^2 dx = \frac{1}{2} \int [\Phi''(x)]^2 dx \)

P.E. = \( \frac{c^2}{2} \int \left( \frac{\partial \psi}{\partial x} \right)^2 dx \)

Thus

\[ H = \frac{1}{2} \int [\Phi'(x)]^2 dx + \frac{c^2}{2} \int [\nabla \psi]^2 dx \]

Can find

\[ \psi(x) = \sum_n \frac{1}{\sqrt{2\omega_n}} \left[ (\alpha_n^* + \alpha_n) e^{-ikx} \right] \]

\[ \Phi(x) = \sum_n \frac{i\sqrt{\omega_n}}{\sqrt{2}} \left[ (\alpha_n^* - \alpha_n) e^{ikx} \right] \]

\( \omega_n = c^2 \frac{\Delta^2}{2} \)

\[ a_{n+1}^* - a_n^* a_n = (2\pi)^3 \delta^3(\mathbf{k} - \mathbf{k'}) \]

\( \sum_n \rightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3} \)
He demonstrates

\[
[T(x), \phi(x)] = -i \xi_x e^{i H \cdot (x-x')} = -i \delta^3(x-x')
\]

The representation is very convenient for most physical problems. Can find

\[
H = \int d^3k \left[ a_k^* a_k + \frac{1}{2} \right] + \hbar \omega_k
\]

We can rewrite this with \( a \). Note

\[
\langle \psi| A^* \phi \rangle = \frac{1}{\hbar} \langle \psi| A \phi \rangle
\]

provided \( \psi, \phi \) solve S. eqns

\[
= \langle \psi| A \phi \rangle - i \langle \psi| A \phi \rangle + i \langle \psi| A \phi \rangle
\]

\[\Rightarrow A = a \phi + i [H, \phi]\]

Thus

\[
\dot{\phi}(y) = i \left[ H, \phi(y) \right]
\]

\[= i \left[ \frac{1}{2} \left( \frac{\text{d}}{\text{d}x} \phi(x)^2 \phi(y) - \phi(y) \phi(x)^2 \frac{\text{d}}{\text{d}x} \right) \right] d^3x \]

\[\pi(x) \left[ \frac{\text{d}}{\text{d}x} \phi(x) \phi(y) - \phi(y) \phi(x) \frac{\text{d}}{\text{d}x} \right] + \left[ \frac{\text{d}}{\text{d}x} \phi(x) \phi(y) - \phi(y) \phi(x) \frac{\text{d}}{\text{d}x} \right] \pi(x) \]

\[= \int \pi(x) \delta(x-y) d^3x = \pi(y)\]

\[\therefore \dot{\phi}(x) = \pi(x)\]
\[ \Pi(y) = \pm [H, \pi] = i \int d^3x \left\{ (\nabla \varphi(x))^2 \pi(y) - \pi(y) (\nabla \varphi(x))^2 \right\} \]
\[ \nabla \varphi(x) \left\{ \nabla \varphi(x) \pi(y) - \pi(y) \nabla \varphi(x) \right\} \]
\[ \nabla_x \left[ i \delta(x-y) \right] \]

to find
\[ \Pi(x) = + c^2 \nabla^2 \varphi(x) \]

Thus we find from (3) \& (4)
\[ \frac{\partial \varphi}{\partial t^2} = c^2 \frac{\partial^2}{\partial x^2} \varphi(x) \]

This is called quantum field theory. [variables at every point in space].

Example:

In elastic theory we need a vector field
\[ \varphi_i(x), \quad \Pi_i(x) \]

Now,
\[ \Pi_i(x) \varphi_i(y) - \varphi_i(y) \Pi_i(x) = -i \delta_{ij} \delta(x-y) \]

\[ \left[ \varphi_i(x), \varphi_j(y) \right] = 0 = \left[ \Pi_i(x), \Pi_j(y) \right] \]
\[
\text{K.E.} = \frac{1}{2} \int \left( \frac{\partial \mathbf{x}}{\partial t} \cdot \frac{\partial \mathbf{x}}{\partial t} \right) \, dt = \frac{1}{2} \int \mathbf{n} \cdot \mathbf{n} \, dt
\]

\[
\text{P.E.} = \frac{1}{2} \int \sum_{i,j,k} C_{ij,kl} \left( \frac{1}{2} \left( \frac{\partial \mathbf{y}}{\partial x_i} + \frac{\partial \mathbf{y}}{\partial x_k} \right) \right) \, dt
\]

\[
= \frac{1}{2} \int \sum_{i,j,k} \frac{\partial}{\partial x_i} \left( \frac{\partial \mathbf{y}_i}{\partial x_j} \right) \, dt
\]

\text{using symmetry}

One can find the function

\[
\mathbf{u}(\mathbf{x}) = \sum_{i,j,k} C_{ij,kl} \frac{\partial}{\partial x_j} \left( \frac{\partial \mathbf{y}_i}{\partial x_k} \right)
\]

\text{[wave equation in anisotropic media]}

\text{Anisotropic media}

\[
\dot{\mathbf{a}} = \lambda_1 \nabla^2 \mathbf{a} + \lambda_2 \nabla (\nabla \cdot \mathbf{a})
\]
For free fields

\[ L = \frac{1}{2} \int \left[ (\mathbf{E} \cdot \mathbf{E} - \mathbf{B} \cdot \mathbf{B}) d^3x + \int \mathbf{J} \cdot \mathbf{A} + \rho \mathbf{E} \right] d^3x \]

\[ = \frac{1}{2} \int \left[ -(\nabla \varphi)^2 - \frac{\mathbf{A}^2}{\mathbf{g}} \right] d^3x \]

\[ = \frac{1}{2} \int \left[ (\nabla \varphi)^2 - 2 \nabla \varphi \cdot \mathbf{A} + \mathbf{A}^2 \right] d^3x \]

State that \( \nabla^2 \varphi = 0 \) and identify \( \mathbf{A} \) as an operator. Define a

\[ \mathbf{T} \mathbf{T} (\mathbf{x}) = \frac{\partial \mathbf{A}}{\partial \mathbf{t}} \]

\[ \mathbf{T}_i (\mathbf{x}) \mathbf{A}_j (\mathbf{x}') - \mathbf{A}_j (\mathbf{x}) \mathbf{T}_i (\mathbf{x}) = -i \varepsilon^{ij} (\mathbf{x} - \mathbf{x}') \delta_{ij} \]

\[ \mathbf{H} = \frac{1}{2} \int \mathbf{T} \mathbf{T} (\mathbf{x}) \cdot \mathbf{B} \mathbf{x} + \frac{1}{2} \int (\nabla \mathbf{A})^2 d^3x \]
In classical mechanics we use
\[ \sqrt{L(q, \dot{q})} \, dt = S \]
and Euler equations (principle of least action). For classical mechanics we use
\[
S = \frac{1}{2} \int \left[ -\nabla \phi - \frac{\partial A}{\partial t} \right]^2 - (\nabla \times A)^2 \, d^3x \, dt
\]
\[ + \int \mathcal{J}_V \, (x) \, A_\mu \, (x, t) \, d^3x \, dt \]
Our variables corresponding to \( q \) and \( \dot{q} \) are \( \phi \) and \( A_\mu \).

We make our quantum theory in analogy, only take out the classical-motion term \( \nabla \cdot A = 0 \). Then we can determine \( \phi \) from
\[ \nabla^2 \phi = \rho \]
via instantaneous Coulomb interactions. We just use \( q = m \) in the classical-motion term \( \mathcal{J}_V \) appears. Thus we can determine \( \phi \) from.

\[ \nabla^2 \phi = \rho \]

via instantaneous Coulomb interactions. Using quantum mechanics, we get variables
\[ A(x) \quad R(x) \]
and
\[ H = \frac{1}{2} \sqrt{(R \cdot R)} \, d^3x + \frac{1}{2} (\nabla \times A)^2 \, d^3x + \int \mathcal{J} \cdot A \, d^3x + \text{Matter} \]
free field
\[ [\Pi_i(x), A_j(y)] = -i \delta^3(x-y) \delta_{ij} \]

**Problem:** Derive Maxwell equations as operator equations.

\[ \Pi = i[H, A - \Phi H] \quad A = i(HA - AH) \]

**Problem:** Find

\[ [A_i(x, t), A_j(x', t)] \]

for free fields

One can write \( A \) as a superposition of plane waves (photon)

\[ A(x) = \sum_{k, \alpha = 1, 2} \frac{1}{\sqrt{2\omega_{k\alpha}}} \left[ e_{k\alpha} a_{k\alpha} e^{-i k \cdot x} + e^*_{k\alpha} a_{-k\alpha} e^{i k \cdot x} \right] \]

\[ \Pi(x) = \ldots \]

**Comments:**

1. Many more assumptions are needed in B.E.D. than in our crystal theory (2nd quantization).
2. The form of operators,
3. Very similar to static quantization
4. Except for curv. terms.
5. Which will reproduce \( \Pi = iH \), \( \Pi \) -- now with proper \( C_{ij} \), \( \delta \).
This term is all the difference. In 19th century people didn't realize this, and since then we've all been about... taking waves, trying to study "issues" of KE wave propagation, and into trouble. Nothing works, who god right idea, but more listens to him. We now listen to people like this (Einstein), learn from past mistakes. When we get stuck it is not because we haven't tried all of what was done before. Need new ideas in strange parts. Every generation must reinvent its own methods.

PROBLEM: Surface interactions

Consider 2-dimensions "gas". Can get two dimensions condensation.

For 3-dimensions, 3 phases. In 2-D, 2-phases are claimed: condensate or expanded phase. Why? Is the condensed phase a solid or liquid?

Might be suddenly metastable. If we get a deep diffraction pattern?

Friedel sums $c_2 = 00$ in $p^2/\hbar^2$. If so, we solved?

Try shear effects (no symmetry breaking). treatment...
ELECTRON THEORY OF METALS

Degenerate Electron Gas

Disregard ionic potential, Coulomb interaction. Assume they are free.

Consider a box of volume $V$ with $N$ electrons. What is behavior at 0 K? Finite T? 0 means lowest temp.

In k-space. Only discrete values for states fill up a certain energy level.

$k_{\text{max}} = \frac{V}{V_{\text{sph}}} = \frac{V_{\text{sph}}}{V}

$V_{\text{sph}} = \frac{4\pi}{3} r^3$

$V = \frac{4}{3} \pi r^3$

Now, No. of states filled is

$\frac{V_{\text{sph}}}{V} = \frac{4}{3} \pi r^3 = \frac{4}{3} \pi \frac{V}{\text{Vol}}

= \text{Vol} \cdot 2 \frac{4\pi}{3} \frac{k_{\text{sph}}^3}{V_{\text{sph}}^3}

\therefore n = 2 \frac{4\pi}{3} \frac{k_{\text{sph}}^3}{V_{\text{sph}}^3}

Energy of electron

$E = 2 \sqrt{\frac{V_{\text{sph}}}{(2\pi)^3}} \text{Vol} \frac{k_{\text{sph}}^2}{2m} = \frac{3}{8} \frac{k_{\text{sph}}^2}{2m} N$

Energy/particle

$\varepsilon = \frac{3}{8} \varepsilon_{\text{F}}$

$\varepsilon_{\text{F}} = \frac{k_{\text{sph}}^2}{2m}$

Pressure $= \rho \frac{k_{\text{sph}}^2}{2m}$ (Density $= \rho$)

Crazy, but it works.
PROBLEMS: Determine the size of stars from your axis by balancing Fermi-Dirac repulsion against gravitational attraction. Find critical mass (gravitational collapse). They find out what happens above critical mass (good luck). Take $T = 0^\circ$.

$p \propto \rho$. Use electrons as fermions (forget about Coulomb potential). $p = \rho^{5/3}$ - modify relativistically. \[ \frac{dp}{dr} = \frac{GM(p)}{r^2} - \xi(p) \]

$M(r) = \int_0^r \rho(r') r'^2 dr'$

$\xi (r) = \sqrt{\int \rho(r') r'^2 dr'}$

PROBLEMS: Find magnetic effect of spin (Pauli's paramagnetism).

Disregard magnetic effect of spin in strong B. Consider Larmor precession - find energy levels using fermions and plot $\chi = \frac{\alpha}{\omega}$.

$U = \int \epsilon(k) \frac{d^3 k}{(2\pi)^3} \text{Vol} \quad \epsilon(k) = \sqrt{m^2 + k^2} - M$

$p \propto \rho^{4/3}$ high density. Neglect mass of protons (don't correct $M(p)$ due to $U$). Ignore general relativity.
What are characteristic wave functions.

What is

$$\Psi(R, R_2, \ldots, R_i, \ldots)$$?

Use independent nature of electrons and consider only spin. Use exclusion principle (antisymmetric $$\Psi$$)

$$\Psi(R, \ldots) = e^{iK_{a_1} \cdot R} e^{iK_{a_2} \cdot R_2} \ldots$$

$$= e^{iK_{a_2} \cdot R_1} e^{iK_{a_2} \cdot R_2} \ldots$$

$$\vdots$$

$$= \frac{1}{\sqrt{N!}} \sum_{P} (-1)^{P} \prod_{i} e^{iK_{a_{P_i}} \cdot R_i}$$

$$= \frac{1}{\sqrt{N!}} \det \left( \begin{array}{c}
\phi_1(R_1) & \phi_2(R_1) & \cdots \\
\phi_1(R_2) & \phi_2(R_2) & \cdots \\
\vdots & \vdots & \ddots 
\end{array} \right)$$

where $$\phi_d(R) = e^{iK_d \cdot R}$$

Note that this also means $$K_{a_1} \neq K_{a_2}$$ or $$\Psi \equiv 0$$.

Say we find electron at $$R_a$$. What is prob. finding

$$P(r)$$

density of gas

$$.\frac{\text{density of gas}}{r}$$
Calculate instead prob. of finding e at \( R_a \) or \( R_b \).
Indeed calculate average values
\[
\langle \psi \mid \hat{S}(R_a-R_b) \mid \psi \rangle
\]
\[
= \langle \psi \mid \hat{S}(R_a-R_b) \hat{S}(R_b-R_a) \mid \psi \rangle
\]
\[
= \sum_{\text{all } k_1 \text{ occupied}} \sum_{\text{all } k_2 \text{ unoccupied}} e^{i(k_1-k_2) \cdot (R_a-R_b)}
\]
\[
\text{direct term} \quad \text{exchange term}
\]
\[
= \sum_{k_1} \sum_{k_2} -|\langle k_1, k_2 | \psi \rangle|^2
\]
\[
\text{or pass from} \quad \sum_\Sigma \rightarrow \int_{\Sigma}
\]
\[
= 1 - \left\{ \frac{3}{\lambda^2} \left[ \sin x - x \cos x \right] \right\}^2
\]
\[
\quad x = \frac{\lambda}{\sqrt{\pi}} \rho
\]
At high temp., the prob. of occupation of an electron state is

\[ \psi = e^{-E/\alpha T} \]

\[ \alpha = \text{Fermi energy or chemical potential} \]

Can find at low temp., \( U = T^2 \), \( C = T \). At zero temp we fill up the momentum sphere of radius \( k \).

Electrons are excited with energy \( kT \). How many can be excited? Only ones on surface of sphere.

No. of electron in region within \( kT \) of surfaces of Fermisphere

\[ \sim k^3 t \]

Thus \( U \sim k^4 T^2 \)

For phonons, \( u \sim kT \)

\[ \sim u \sim T^3 \sim u \sim T^4 \]

Since working with \( g \) and need entire volume of sphere.

We can plot

Graph of \( g \) vs. \( T^2 \), electrons vs. \( T \)
PERIODIC POTENTIALS

We now try to solve the Schrödinger equation for this potential [need Hartree-Fock to get correct potential]

We consider bringing two potentials to get

First degeneracy is destroyed. For many atoms

Now \[-\frac{h^2}{2m} \nabla^2 \psi + V(R) \psi = E \psi\]

But \[V(R) = V(R+a)\]
Using "phony-scary" periodicity
\[ \psi(R + n\alpha) = \psi(R) e^{i kna} \]

Can find
\[ E \]

\[ E_0 \]

\[ -\pi/a \]
\[ \pi/a \]
\[ \kappa \]

[Remember can only define to within]

Frequently people use
\[ \psi(R) = e^{i kr} U_k(R) \]
and
\[ U_k(R + a) = U_k(R) \]

Mention all of this as it applies to group theory

\[ T [S-eqn] = [S-eqn] \]

\[ \Rightarrow T \psi(R) = \psi(R) \]
But this does not describe free propagation. We neglected higher states. Thus $\gamma \rightarrow 0$ is not free particle behavior.
Weak Potentials
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x) \psi = \varepsilon \psi \]

\[ V(x) = \sum V_n e^{i(k_n x)} \]

\[ \psi(x) = e^{ik_n x} u_{k_n}(x) \]

\[ = \sum A_n e^{i(k_n + L) x} \]

Hence
\[ \left[ \frac{\hbar^2}{2m} (k_n + L)^2 - \varepsilon \right] A_n = -\sum V_{nL} A_{nL} \]

Choose \( V_0 = 0 \), all other \( V \)'s small. First approximation
\( A_0 = 1 \), other \( A_i \) very small. Then (1) for \( L = 0 \) gives
\[ \varepsilon \sim \frac{\hbar^2}{2m} k^2 \quad \text{if } L = 0 \]
\[ A_0 = \frac{-V_0}{\frac{\hbar^2}{2m} (k+n)^2 - \frac{1}{2} \hbar^2 k^2} \quad \text{if } L \neq 0 \]

[Can solve for \( \varepsilon \) analytically for \( \sum \) or \( \prod \).
Otherwise use a computer approximation solution]

For second order, use
\[ \left( \frac{\hbar^2}{2m} k^2 - \varepsilon \right) A_0 = \sum V_{nL} A_{nL} = \sum \frac{|V_{nL}|^2}{\frac{\hbar^2}{2m} [(k_n + L)^2 - k^2]} \]

... \( \varepsilon \approx \frac{1}{2m} k^2 - \sum \frac{|V_{nL}|^2}{\frac{1}{2m} [(k_n + L)^2 - k^2]} \)
This is OK except when $K \not\in (K + L)^2 - 4K^2$. Consider at $K'$

$$K^2 = (K + L)^2$$

get a gap now at edge of Brillouin zone.

If $K \not\in (K + L)^2 - K^2 \sim V$
we can start from by considering $A_0$ and $A_1$ not small -- all.
other $A_i$ small. Then (1) gives

$$L = 0 \quad \left( \frac{-h^2}{2m} K^2 - e \right) A_0 = -V_L A_L$$

$$L = 1 \quad \left( \frac{-h^2}{2m} (K + L)^2 - e \right) A_1 = -V_{+L} A_0$$

$$\Rightarrow \left[ \frac{1}{2m} (K + L)^2 - e \right] = \left[ \frac{1}{2m} K^2 - e \right] = |V_L|^2$$

Can find

$$e = \frac{w(K + L) + w(K)}{2} \pm \sqrt{\left( \frac{w(K + L) - w(K)}{2} \right)^2 + |V_L|^2}$$

$$V_L << \frac{w(K + L) - w(K)}{2}$$

$$= \frac{w(K) - |V_L|^2}{w(K + L) - w(K)}$$

Thus a discontinuity at $K'$.
Strong Potentials:

\[ \psi_N = \sum_{n} e^{i k \cdot \mathbf{r}} f(n - \mathbf{r}) \]

where \( f(n) \) is solvable in one of these potentials:

\[ -\frac{1}{2m} \nabla^2 \psi + V_H \psi = E \psi \]

where \( V = \frac{\mathbf{r}}{\mathbf{r}^2} \)

Can find:

\[ \varepsilon = \frac{\int \psi^* \mathbf{H} \psi \, dV}{\int \psi^* \psi \, dV} = \frac{N}{D} \]

where \( \psi \) is trial function.
Now
\[ D = \sum_{\text{M}} e^{ik \cdot (\mathbf{n} - \mathbf{n}')} \sqrt{f^*(\mathbf{n} - \mathbf{n})} f(\mathbf{r} - \mathbf{n}) d^3r \]
\[ = 1 + \sum_{\text{M}} e^{ik \cdot \mathbf{M}} I(\mathbf{M}) \]
\[ I(\mathbf{M}) = \int f^*(\mathbf{r} - \mathbf{M}) f(\mathbf{r}) d^3r \]
\[ N = \sum_{\text{M}} e^{ik \cdot (\mathbf{n} - \mathbf{n}')} \int f^*(\mathbf{r} - \mathbf{n}')( - \frac{\hbar^2}{2m^2} \nabla + \frac{\pi}{\hbar^2} V(\mathbf{r} - \mathbf{n}')) f(\mathbf{r} - \mathbf{n}) d^3r \]
\[ E_0 - \nu(\mathbf{r} - \mathbf{n}) \]
\[ J(\mathbf{M}) = \sqrt{f(\mathbf{r} - \mathbf{M})} \left[ V(\mathbf{r}) - \nu(\mathbf{r}) \right] f(\mathbf{r}) d^3r \]
\[ G = E_0 + \frac{J_0 + \sum_{\text{M} \neq 0} J(\mathbf{M}) e^{ik \cdot \mathbf{M}}}{1 + \sum_{\text{M} \neq 0} I(\mathbf{M}) e^{ik \cdot \mathbf{M}}} \]

Note if \( M = 0 \)
\[ J(0) = \int |f(\mathbf{r})|^2 \left[ V(\mathbf{r}) - \nu(\mathbf{r}) \right] d^3r \]

\( J(\mathbf{M}) \) falls off rapidly with \( M \).

average of all potentials except \( V(\mathbf{r}) \)
Thus for say a cubic lattice

$$E = E_0 + \frac{J_0 + 2 J_{100} (\cos Ka + \cos Kb + \cos K a)}{1 + 2 J_{100} (\cos Ka + \cos Kb + \cos K a)}$$
We had found
\[ \varepsilon = E_0 + \frac{J_0 + 2J_{100}(\cos k_x a + \cos k_y a + \cos k_z a)}{1 + 2J_{100}(\cos k_x a + \cos k_y a + \cos k_z a)} \]

really don't use this, but books rarely mention this.

Can get a "submodel" using s-states of helium as basis

\[ i \dot{a}_n = \gamma_0 a_n + A[a_{n+1} + a_{n-1} + a_{n+1_y} + \ldots] \]

\[ = \gamma_0 a_n + \sum_{M_l} A_M a_{n+M} \]

This model tells us all we need to know about bands. Could also set it up for \( s \leq p \) states.

\[ i \dot{a}_n = \gamma_{00} a_n + \sum_{M_l} A_{M_l} a_{n+M_l} \]

\[ i \dot{b}_n = \gamma_{00} b_n + \sum_{M_l} B_{M_l} b_{n+M_l} \]

HeLiBeBCNOF
NeN,MgAlSiPSCl
Comments again on point view of band theory. Must consider electron interactions. Feynman 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 generally called) little problem: understand and properties of materials at high pressures, lots of experimental data.

**Problem:** How apply constant field

\[
\frac{d (k_x)}{dt} = e \left( \frac{E}{m} + V_x E \right)
\]

\[V_x = \frac{2 E}{\hbar k_x}
\]

Prove these.

Band theory works quite well for semi-conductors however.
Coulomb Interaction in a Fermi Gas

Energy per electron
\[
\frac{\text{Energy per electron}}{\text{Vol}} = \frac{2.22}{r_s^2} - \frac{0.916}{r_s} + \varepsilon_c
\]

where \( r_s = \frac{\rho_0}{\text{charge}} \) - Bohr radius

\[
\frac{4\pi r_s^3}{3} = \text{Vol per electron}
\]

We use a uniform positive charge to neutralize electrons. The \( \frac{0.916}{r_s} \) term is due to Coulomb interaction between electrons.

\( \varepsilon_c = \text{"correlation energy"} = \) all other junk

(\text{Bad physics to call it this})
Problem: Find the speed of sound in an ideal gas for long wavelengths. Now include effect of the Coulomb potential on "r(r)"

Conductivity of Metals:

Two origins of resistance due to collisions:

1) Imperfections in crystal

\[ H = -\frac{\hbar^2 a^2}{2m} + \frac{1}{2} N \left( V(r - \mathbf{r}) + \frac{1}{2} \left[ U(r - \mathbf{r}) - V(r - \mathbf{r}) \right] \right) \]

Here is to find scattering cross-sections and then to solve Boltzmann equation:

\[ \langle \mathbf{r}', H \mathbf{r}, \mathbf{r} \rangle = \sqrt{U_{\mathbf{r}'} (\mathbf{r}) U_{\mathbf{r}'} (\mathbf{r})} \int \mathbf{r} \mathbf{e}^{i \mathbf{r} (\mathbf{r} - \mathbf{r}')} \]

Must include charge shielding effects however. Very few have been able to do this correctly. The nightmare of the inner shell. Van Kleeck's formula does work to distinguish 2s from 1s in Li, for instance.
11) Phonon scattering from atomic interaction

\[ \rho \leftrightarrow \nabla V(\mathbf{k} \cdot \mathbf{N} - q) = \frac{e^{i \mathbf{q} \cdot \mathbf{N}}}{H_0} \sum_{n} \langle \text{phonon} | \sum \nabla V(\mathbf{k} \cdot \mathbf{N}) | \text{phonon} \rangle \]

\[ = \sum_{n} \langle \text{phonon} | \nabla V(\mathbf{k} \cdot \mathbf{N}) | \text{phonon} \rangle \int \psi_{n}^{*}(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{r}} \nabla V(\mathbf{k} \cdot \mathbf{N}) \psi_{n}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} d\mathbf{r} \]

\[ = \sum_{n} e^{i\mathbf{k} \cdot \mathbf{N}} \sum_{n'} e^{i(\mathbf{k} - \mathbf{k'}) \cdot \mathbf{N}} \psi_{n}^{*}(\mathbf{k}) \nabla V(\mathbf{k} \cdot \mathbf{N}) \psi_{n'}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} d\mathbf{r} \]

Use

\[ \sum_{n} e^{i\mathbf{k} \cdot \mathbf{N}} e^{i(\mathbf{k} - \mathbf{k'}) \cdot \mathbf{N}} \rightarrow \delta(\mathbf{k} - \mathbf{k} + \mathbf{k'} + \mathbf{N}) \]

This vaguely relates conservation of momentum mod \( \mathbf{N} \).
Can have electron-electron scattering using virtual phonon.

This is very important in superconductivity since it leads to bound electrons in pairs (BCS).
Creation Operators for Electrons

Recall we had defined for photons and phonons

\[ a_{i, p}^* a_{j, p} \rightarrow a_{i, p}^* a_{j, p} = 6_{i, j} \]

\[ a_{i, p}^* c_{i, p}^* = a_{i, p}^* a_{i, p} = 0 \]

\[ a_{i, p} a_{j, p} - a_{j, p} a_{i, p} = 0 \]

Similar operators are used for electrons. We define

\[ \begin{align*}
    c_{k, p} & \quad \text{annihilates electron of momentum } k, \\
    c_{k, p}^* & \quad \text{creates } c_{k, p}
\end{align*} \]

Now in \( H \) we include an interaction term to describe this

\[ H_{\text{int}} = \sum_{k, k', \sigma} \begin{array}{c}
    g_{k, k', \sigma} \text{ photon } c_{k, \sigma}^* c_{k', \sigma} \\
    \text{ (assumes } c_{k', \sigma} \text{ makes } k')
\end{array} \]

This is just formal mathematics for now.
Actually to make $H$ hermitian, use

$$
1 + \sum_{k_k,k_{k'},k_{k''}} a_{k_k} c_{k_{k'}}^{*} c_{k_{k''}}^{*} \\
+ \sum_{k_k,k_{k'},k_{k''}} a_{k_{k'}} c_{k_{k''}}^{*} c_{k_k}^{*}
$$

Now consider the $c_{k_k}^{*}$'s in general

$c_{k_k}^{*}$ creates an electron in state $i$

Very useful since it is a way out for many problems without inventing new operators.

Exclusion principle allows only two states:

- No electron in $i$ \( \rightarrow 10 \)
- One electron in $i$ \( \rightarrow 11 \)

Thus

$$
c_{k_k}^{*}10 = 11
$$

$$
c_{k_k}^{*}11 = 0
$$

$$
<11> = <10>
$$

$$
<10> = 0 \quad \text{as properties of operator}$$
Now for correct adjoints
\[ <\text{n}'\text{l}'\text{c}'\text{ln}>' = <\text{n}'\text{lc}\text{ln}> \]

Applying this yields
\[ <\text{1}'\text{l}'\text{c}'\text{10}> = 1 \]
\[ <\text{0}'\text{l}'\text{c}\text{11}> = 1 \]

so phases of states are properly fixed.

Now
\[ \text{C}'\text{C} = 0 \]

since
\[ \text{C}'\text{C}'\text{10} = 0, \text{C}'\text{C}'\text{11} = 0 \]

Also
\[ \text{CC} = 0 \]

Now
\[ \text{CC}'\text{10} = 10 > \]
\[ \text{CC}'\text{11} = 0 \]
\[ \text{C}'\text{C}\text{10} = 0 \]
\[ \text{C}'\text{C}\text{11} = 11 > \]

Thus we write
\[ \text{C}'\text{C}_i = N_i \]

Ms. Flanders in
Now
\[(c^*c + cc^*) |0\rangle = |0\rangle \]
\[(c^*c + cc^*) |1\rangle = |1\rangle \]

Thus
\[c^*c + cc^* = 1\]
\[c^*c = 0\]
\[cc = 0\]

One could now work backwards and find the representations for these operators (eigenvalues and eigenstates) only from these equations.

Now consider different states

\[
\begin{array}{c|c}
| & \\
\hline
\text{a} & \text{b} \\
\text{c} & \text{c}^* \\
\text{d} & \text{c}_b \\
\end{array}
\]

\[
\begin{align*}
\text{Ca}^*\text{Ca} + \text{Ca}\text{Ca}^* &= 1 \\
\text{C}_b^*\text{C}_b + \text{C}_b\text{C}_b^* &= 1 \\
\text{Ca}^*\text{Ca} &= 0 = \text{Ca} \text{Ca} \\
\text{C}_b^*\text{C}_b &= 0 = \text{C}_b \text{C}_b
\end{align*}
\]

How do we conclude these?

\[c^*c^* = -c_b^*c_a^*
\]

since we are developing Fermi statistics.
Can also show

\[ C_0^*C_a + C_a C_0^* = 0 \]

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

\[ C_i^* C_i + C_i C_i^* = 0 \]

\[ C_d^* C_d + C_d C_d^* = 0 \]

Can build

\[ C_c^* = \frac{1}{\sqrt{2}} (C_a^* + C_b^*) \]

Then use

\[ C_c^* C_c + C_c C_c^* = 0 \]

\[ l = (\alpha C_a^* + \beta C_b^*) (\alpha^* C_a + \beta^* C_b) + (\alpha C_a + \beta^* C_b^*) (\alpha^* C_a^* + \beta C_b^*) \]

\[ = \alpha \alpha^* (C_a C_a^* + C_a C_a^*) + \beta \beta^* (C_b^* C_b + C_b C_b^*) \]

\[ + \alpha \beta^* (C_a C_b + C_b C_a^*) + \beta \alpha^* (C_b^* C_a^* + C_b C_b^*) \]

Now normalized state \( |l\rangle \) reduces to:

\[ |l\rangle \Rightarrow |d\rangle \]

\[ \Rightarrow C_a^* C_b + C_b C_a^* = 0 \]

\[ C_a^* C_b^* + C_b^* C_a = 0 \] in some way.
For bosons

\[ a_i^* \text{ creates particle in state } i \]
\[ a_i a_j^* - a_j^* a_i = \delta_{ij} \quad (= \langle i | i \rangle) \]
\[ a_i^* a_j^* - a_j a_i^* = 0 \]
\[ a_i a_j - a_j a_i = 0 \]

For fermions

\[ c_i^* \text{ creates particle in state } i \]
\[ c_i c_j^* + c_j^* c_i = \delta_{ij} \]
\[ c_i^* c_j^* + c_j c_i^* = 0 \]
\[ c_i^* c_i^* = 0 \]
\[ c_i^* c_i = N_i = \text{no. of fermions in } i \]

Example: Consider \[ c_\mathbf{p}^* \text{ creates electron with momentum } \mathbf{p} \text{ (without spin)} \]
\[ c_\mathbf{p}^* \text{ vacuum} = \text{state of electron } e^{i \mathbf{p} \cdot \mathbf{x}} \]

Now create one electron which has amplitude \( \alpha_1 \) to have \( \mathbf{p}_1 \)
and \( \alpha_2 \) to have \( \mathbf{p}_2 \)

\[ c_\mathbf{p}_1^* \text{ vacuum} = \text{state of one electron of } \alpha_1 e^{i \mathbf{p}_1 \cdot \mathbf{x}} + \alpha_2 e^{i \mathbf{p}_2 \cdot \mathbf{x}} \]

\[ \Rightarrow \quad c_\mathbf{p}^* = \alpha_1 c_\mathbf{p}_1^* + \alpha_2 c_\mathbf{p}_2^* \]
$C_{\Psi}^*$ creates one electron which has amplitude $\Psi(p)$ to be in momentum state $|p\rangle$, i.e.,

$$C_{\Psi}^* |\text{vac}\rangle = \text{state one electron which has wave for }$$

$$\Phi(p) e^{i p \cdot x} = |p\rangle$$

where $\Phi(p) = \int d^3x e^{-i p \cdot x}$.  

Thus

$$C_{\Psi}^* = \int \Phi^*(p) \Phi(p)$$

$$= \langle \Psi | p \rangle \langle p | \Psi \rangle$$

$$= \langle \Psi | \Psi \rangle$$

Now operator which creates electron at $x_0 = 44^\dagger(x_0)$

$$44^\dagger(x_0) |\text{vac}\rangle = \text{state one electron with wave from } 8(x-x_0)$$

$$= \int \frac{d^3p}{(2\pi)^3} e^{-i p \cdot x_0} \Phi(p)$$

Thus

$$44^\dagger(x_0) = \int \frac{d^3p}{(2\pi)^3} e^{-i p \cdot x_0} \Phi^*(p)$$

Similarly

$$44 (x) = \sqrt{\frac{2 \sqrt{2} \pi^3}{3}} \Phi(p) C_p$$

Note also

$$C_{\Psi}^* = \sqrt{44^\dagger(x) \Phi(x) dx}$$
We expect then
\[ \hat{\gamma}^*(x) \hat{\gamma}(y) + \hat{\gamma}(y) \hat{\gamma}^*(x) = \delta^2(x-y) \]
\[ \hat{\gamma}^*(x) \hat{\gamma}^*(y) + \hat{\gamma}(y) \hat{\gamma}(x) = 0 \]
\[ \hat{\gamma}(x) \hat{\gamma}(y) + \hat{\gamma}(y) \hat{\gamma}(x) = 0 \]
\[ \hat{\gamma}^*(x) \hat{\gamma}(x) = \text{"no of electrons at } x \text{" = density of electrons at } x \]

**EXAMPLE:** We return to bound theory. Recall we had for a single electron
\[ \frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(\mathbf{r}) \psi \]
We found solutions \( \psi = e^{ik \cdot \mathbf{r}} \) \( N_k(m) = f_{ik}(m) \)
Then
\[ n f_{ik}(m) = e_{ik} f_{ik}(m) \]
Now to use our new notation, let
\[ \phi_{ik} = \text{create electron of propagation vector } k \text{ with } f_{ik}(m) \]
\[ = \sqrt{\frac{m}{2\pi \hbar}} f_{ik}(m) d^3 \mathbf{r} \]
Now this is the **creation** of an individual electron.

Hamiltonian
\[ H_{\text{total}} = \sum_{k} \hbar \omega_k N_k = \sum_{k} \hbar \omega_k \phi_{ik}^* \phi_{ik} \]

[Note how similar this formulation is to phonon work]
Note

\[ H_{\text{final}} = \sum_{k} \xi_{ik} C_{ik}^* C_{ik} = \int \psi^*_k(x) \psi_k(x) \, dx \] 

For admittances we

\[ \psi^*_k(x) = \sum_{k'} \xi_{k'k} \psi^*_{k'}(x), \quad C_{ik}^* \]

\[ \psi_{ik}(x) = \sum_{k'} \psi_{ik'}(x) C_{ik'} = \sum_{k'} \xi_{ik'} \psi_{ik'}(x) \]

We multiply by \( \psi_{ik}(x) \) and integrate, and use orthogonality to find (*)

We had

\[ \text{amp} \Gamma_{\text{el},kk'} = \text{amp \ electron} \quad \text{Heck} \to \text{Heck}' \quad \text{decays}\] 

We can then write \( H \) for a system of electrons and phonons as

\[ H = \sum_{k} \xi_{ik} C_{ik}^* C_{ik} + \sum \omega_{\alpha \beta} a^\dagger_{\beta} a_{\alpha} + \sum \Gamma_{\text{el},kk'} C_{ik}^* C_{ik} a_{\alpha} a^\dagger_{\beta} \]

\[ + \sum \Gamma_{\text{el},kk'} \psi_{ik}^* \psi_{ik'} \alpha^\dagger_\beta \]

\[ \text{[need to make } H \text{ hermitian] } \]

Note

\[ \text{amp} \Gamma_{\text{ph},kk'} = \text{amp \ direct \ Heck} \to \text{Heck}' \text{ emitting \ phonon \ of \ mode \ } k \]
This is the basis of the theory of conductivity and superconductivity.

[Note the above and its comments.]
We now discuss electron-electron interactions, say by $e^2/r_{ij}$. Ordinarily we would write

\[ H = -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_i U(x_i) + \frac{1}{2} \sum_{i,j} V(x_i - x_j) \]

Consider first-order scattering of electrons for $\mathbf{P}_1 + \mathbf{P}_2 = \mathbf{P}_3 + \mathbf{P}_4$

\[ \begin{array}{c}
\mathbf{P}_1 \\
\mathbf{Q} \\
\mathbf{P}_2 \\
\mathbf{P}_3 \\
\mathbf{P}_4
\end{array} \]

with

\[ \psi = \psi_0 e^{-i\mathbf{Q} \cdot \mathbf{P}_1} \]

where $\mathbf{Q} = \mathbf{P}_3 - \mathbf{P}_1$

\[ \psi(\mathbf{Q}) \equiv \sum_{\mathbf{P}_1, \mathbf{P}_2} \psi_0 e^{-i\mathbf{Q} \cdot \mathbf{P}_1} \]

Then for $U = 0$,

\[ H = \sum_{\mathbf{P}_1, \mathbf{P}_2} \left( \frac{\hbar^2}{2m} \right) \mathbf{C}_p^* \mathbf{C}_p + \sum_{\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3, \mathbf{P}_4} \mathbf{C}_p^* \mathbf{C}_q \mathbf{C}_r^* \mathbf{C}_s \]

(6)

Now $H$ is quadratic in $C$. Thus we can represent these interactions using the $C_p$ operators.

We can try to represent this in terms of $\mathbf{C}_p^* U(\mathbf{x})$ where

\[ \mathbf{C}_p^* = \int e^{i\mathbf{P} \cdot \mathbf{x}} U^*(\mathbf{x}) d^3x \]

The first term in (6) yields

\[ \int U^*(\mathbf{x}) \left[ -\frac{\hbar^2}{2m} \nabla^2 \right] U(\mathbf{x}) d^3x \]
\[ H_{\text{ext}} = \sqrt{\frac{\left( \frac{p_x^2 + p_y^2 + p_z^2}{2m} \right)}{(2\pi \hbar)^3}} e^{-i \mathbf{p} \cdot \mathbf{x}} = \int \frac{d^3x}{(2\pi \hbar)^3} \frac{1}{\sqrt{p_x^2 + p_y^2 + p_z^2}} e^{-i \mathbf{p} \cdot \mathbf{x}} \]

\[ = \int d^3x \, Q(x) \, \delta^3(x-x_0) \, \psi^* \psi \]

\[ = \int d^3x \, \psi^* \psi \, \psi^* \psi \, \delta^3(x-x_0) \, d^3x + \int d^3x \, \psi^* \psi \, V(x) \, d^3x \]  \hspace{1cm} (2)


Suppose we invert the order of

\[ \psi^* \psi \, \psi^* \psi = -\psi^* \psi \, \psi^* \psi + \delta^3(x-x_0) \]

Then

\[ H_{\text{int}} = -\int \frac{d^3x}{(2\pi \hbar)^3} \frac{1}{\sqrt{p_x^2 + p_y^2 + p_z^2}} \]

\[ + \int \frac{d^3x}{(2\pi \hbar)^3} \frac{1}{\sqrt{p_x^2 + p_y^2 + p_z^2}} V(x) \, d^3x \, d^3x \]  \hspace{1cm} (3)

Classically we expect

\[ \text{Energy} = \frac{1}{2} \int \rho(x) \, V(x-x) \, \rho(x) \, d^3x \]  \hspace{1cm} (4)

Three remarks:

1. factor \( \frac{1}{2} \)
2. any
3. extra term
The last term is a self-energy term (energy of particle
interacting with itself). This is true in classical but since
\((4)\) also includes self-energy.

If we don't want self-energy, go back to \((2)\)
(base with Coulomb interaction where \(\nu(C) = \infty\))

\[ \frac{1}{2} \text{ comes from a mistake in original sum} \]

\[ \sum \nu(C) \, \text{C}_p \text{C}_q \text{C}_2 \text{C}_p \]

Hence

\[ H_{\text{ext}} = -\frac{1}{2} \int \psi^*(x) \psi^*(y) \, V(x-y) \psi(x) \psi(y) \, d^3x \, d^3y \]  \hspace{1cm} (5)

and

\[ H_{\text{ext}} = \frac{1}{2} \int \psi^*(x) \psi^*(y) \, V(x-y) \psi(x) \psi(y) \, d^3x \, d^3y \]

\[ -\frac{1}{2} \int \psi^*(x) \psi^*(y) \, V(0) \, d^3x \]

The sign comes in also from initial ordering in \(E\). Need

\[ \frac{1}{2} \lesssim \psi (x) \text{C}_p \text{C}_q \text{C}_p \text{C}_q \]

Have a negative self-energy term. Do you want it not (otherwise not)?
Thus neglecting self-energy, our $H$ for a system of electrons is

$$H = \int 4 \psi(x) \left[ -\frac{1}{2m} \left( \frac{\partial}{\partial x} \right)^2 + \frac{i}{\hbar} A(x^i) \right] \psi(x) \ d^3x$$

$$+ \frac{1}{2} \int 4 \psi(x) \overline{\psi(y)} \frac{e^2}{|x-y|} 4 \psi(y) \overline{\psi(x)} \ d^3x \ d^3y$$

Note because of the double annihilation, this contains no self-energy terms [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.

---

How can we use (7) to the S-eqn

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = H \psi$$

Now

$$N = \int 4 \psi(x) \overline{\psi(x)} \ d^3x$$

Can show $[H, N] = 0$. Then can show

$$N \psi = n \psi$$

where $n$ is an integer.
How do we deal with "holes" in our formal theory? Again use

\[ C_i^* \text{ creates electron in state } i \quad \phi_i(x) \]

Then \[ H = \sum_i C_i^* C_i + \sum_{i,i'} \lambda_{i,i'} C_i^* C_{i'} \]

where \[ \lambda_{i,i'} = \int \phi_i^*(x) \lambda(x) \phi_{i'}(x) dx \]

is our perturbing potential.

Suppose some empty levels above ground state. Try to imagine perturbation operating on holes in ground state. Define new indices as shown. Recall

\[ C_i^* C_i + C_i C_i^* = \delta_{i,i'} \]

If \( i = j \) write \( C_i = C_j \)

If \( i = k \) write \( C_i = b_k^* \Rightarrow b_k = C_i^* \)

Ex: \[ C_i^* C_i + C_ic_i^* = 1 \rightarrow b_k^* b_k^* + b_k^* b_k = 1 \quad \text{for } i \in S_b \]

\[ C_i C_i = 0 \rightarrow b_k^* b_k^* = 0 \]

\[ C_i^* C_i^* = 0 \rightarrow b_k b_k = 0 \]
We now regard $b^*$ as "creating a hole".

$G^*_i$ creates an electron in state $i$.

$b^*_k$ creates a hole in state $k$.

Then if we neglect perturbation

$$H = \sum_i \epsilon_i G^*_i G_i + \sum_k \epsilon_k b^*_k b_k$$

$$- \sum_k \frac{\epsilon_k - \Theta_k}{\hbar^2} b^*_k b_k$$

$\sum_k b_k b_k = 0$

Our perturbation becomes

$$\sum_{i,j} \lambda_{ij} G_i^* G_j + \sum_{k,j} \lambda_{kj} b^*_k b_j$$

$$\sum_{i,j} \lambda_{ij} G_i^* b^*_j + \sum_{k,j} \lambda_{kj} b^*_k b_j$$

$$- \sum_{k,j} \lambda_{kj} b^*_k b_j + \sum_k \sum_{k'} b^*_k b_{k'}$$

We now examine conditions.
Use arrows to mark different types of particles.

\[ \sum_{i} = \int \phi_{i}(x) \chi(x) \phi_{i}(x) \, d^3x \]

These arrows tell where to put states in matrix elements. Enter and leave types. Don't use initial and final states in time as a concept or you'll get confused.

Can play now with more complicated interactions like

\[ G_{i} G_{i}^{*} G_{i}^{*} G_{i} \]

let things like

Can just picture this as bending the diagrams (arrows) around.
These schemes are used very frequently in perturbation theory.

Consider now usual 2nd order perturbation theory in this formalism.

\[ \text{amp} = \int \Phi^+(x_b, t_0) \chi(x_b, t_0) K_0(x_0, t_0; x_0, t_0) \chi^*(x_0, t_0) \Phi(x_0, t_0) \, dt_0 \, dt_0 \]

where the propagator is

\[
K_0(b, a) = \int e^{-iE(t_b - t_a)} U_i(x_b) U_i^*(x_a) H(t_b - t_a) \cdot U_i(x_a) U_i^*(x_b) H(t_b - t_a)
\]

where \( H_{ii} = \epsilon_i U_i \).

Now let \( \phi_2 = U_i(x_a) e^{-i\epsilon_2 t_a} \) and \( \chi_2(x_a, t_a) = e^{-i\epsilon_2 t_a} \).

We then find

\[
\text{amp} = \int e^{i\epsilon_2 t_b} e^{i\epsilon_2 t_0} e^{-i\epsilon_1(t_b - t_a)} e^{-i\epsilon_1 t_0} e^{-i\epsilon_1 t_a} \, dt_a \, dt_b
\]

\[ = 0 \quad \text{unless} \quad \epsilon_2 + \epsilon_2 = \epsilon_1 + \epsilon_1 \quad \text{as expected}
\]

\[ = \int_{-a}^{t_b} e^{-i\epsilon_1(t_b - t_a)} e^{-i(\epsilon_1 + \epsilon_2)(t_a - t_b)} \, dt_b \cdot \chi_{2i}(t_a) \chi_{i1}
\]
\[ \text{Amp} = \sum \frac{(2)}{\lambda_{2i}} \frac{-i}{(\varepsilon_i - (\varepsilon + \omega) - i\eta)} \lambda_{1i} \]

Now, can we write this allowing holes? We guess by drawing pictures.

\[ \sum \frac{(2)}{\lambda_{2i}} \frac{-i}{(\varepsilon_i - (\varepsilon + \omega) - i\eta)} \lambda_{1i} \]

"Virtual pair production"

\[ \sum \frac{(2)}{\lambda_{2k}} \frac{-i}{(\varepsilon_{k1} + \varepsilon_{2} + \omega - i\eta)} \lambda_{2k} \]

This is correct.
Can we combine these into (1) terms and return to our general perturbation theory? Write second term as

\[ + \sum_{\ell} \frac{\Lambda}{\ell} \frac{-1}{\ell - (\zeta + \alpha) - i\epsilon} \]

Thus just let i range over both j, k.
\[ H = \sum_{i} C_i^* C_i + \sum_{i,k} b_i^* b_k + H_{\text{int}} \]

where \( H_{\text{int}} = \sum_{i} \lambda_i \cdot C_i^* C_i + \sum_{i,k} \lambda_{ik} \cdot b_i^* C_i + \sum \lambda_{ik} C_i^* b_k^* - \sum \lambda_{ik} b_i^* b_k \).

Perturbation gives

\[ \lambda_1 = \frac{1}{\gamma_1 - \omega_i - \lambda_{12}} \quad \lambda_{12} = \frac{\gamma_1 + \lambda_{12}}{\gamma_1 + \gamma_2 + \omega_i} \]

This can also be written

\[ \int (x_0, t_0) \chi(x_0, t_0) \kappa_1(\gamma_1, 2, t_1, t_2) \chi(x_1, t_1) \kappa_2(\gamma_2, 2, t_1, t_2) dx_0 dt_0 dx_1 dt_1 dt_2 \]

\[
\begin{cases}
K_1(2, 1) = \sum \left( e^{-i \epsilon_i (t_2 - t_1)} \phi_i(x_1) \phi_i^*(x_1) \right)_{t_2 > t_1} \\
K_2(2, 1) = -\sum \left( e^{-i \epsilon_k (t_1 - t_2)} \phi_k(x_2) \phi_k^*(x_2) \right)_{t_1 > t_2}
\end{cases}
\]

[No violation of commutativity]
IV. RELATIVISTIC QUANTUM MECHANICS

A. Introduction

Some of the achievements of QM are:

i.) Prediction of antiparticles (CPT theorem)

ii.) Conservation of spin ½ obey Fermi statistics

iii.) Wave function of H-atom

There seems to be three ways to present this subject.

1.) One way is easier to understand since it works from
\[
\frac{\partial}{\partial t} \psi = -i \frac{\hbar}{2m} \nabla^2 \psi
\]

in form of Dirac eqn. However we lose the manifest covariance.

2.) Relativistic invariance is obvious, but notation is

harder to understand (Ehrenfest, Schrödinger, etc.)

3.) Abstract formulation -- immediately implies position,

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)

\[ \text{Action} = \int \left[ \left( \nabla \Phi - \frac{\partial A}{\partial t} \right)^2 - (\nabla \times A)^2 \right] \, d\text{Vol} \, dt + \int (\partial A_x - j \cdot A) \, d\text{Vol} \, dt \]

Equivalent to (imagine \( \nabla \cdot A = 0 \) -- makes QED no longer manifestly covariant)

1.) Instantaneous Coupling: \( \varepsilon \frac{\partial}{\partial t} \)

2.) \( H = \sum_i \omega_n a_i^* a_i + \text{coupling} \)

\[ H_{1,2} \]

where \( \omega_n = n \omega \)

\( \text{coupling} \rightarrow \int \chi(\omega) \cdot A(\omega) \, d^3 x \)

and

\[ A(x) = \sum_{k,i} \sqrt{\frac{2 \delta}{\omega_k}} \left[ e^{i \omega_k t} a_{k,i} + e^{-i \omega_k t} a_{k,i}^* \right] \]
Recall in classical theory,

\[ E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \text{and} \quad P = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}} \]

so that

\[ E^2 - P^2 = m_0^2 \quad \text{c}^2 = 1, \quad \hbar = 1 \]

or \[ E^2 - (P^2)P = m_0^2 \]

Hereafter we denote 4-vectors by

\[ A^\mu = (A^0, A^1, A^2, A^3) \]

Also use summation convention

\[ A^\mu B_\mu = A_1 B_1 - A_2 B_2 - A_3 B_3 - A_0 B_0 = \text{invariant} \]

We use also

\[ \delta_{\mu \nu} = 1 \quad \text{if} \quad \mu = \nu = \tau \]
\[ \delta_{\mu \nu} = -1 \quad \text{if} \quad \mu = \nu = x, y, z \]
\[ \delta_{\mu \nu} = 0 \quad \mu \neq \nu \]

and note \[ \delta_{\mu \nu} A_\nu = A_\mu \]

Finally

\[ \Delta \mu = \left( \delta_1 - \frac{2}{\hbar^2} - \frac{2}{\hbar^2}, - \frac{2}{\hbar^2} - \frac{2}{\hbar^2} - \frac{2}{\hbar^2} \right) \]
\[ \mathbf{p}_\mu = (E, p_x, p_y, p_z) \]
\[ k_\mu = (\omega, k_x, k_y, k_z) \]

De Broglie \( \mathbf{p}_\mu = \hbar k_\mu \) \( \text{wave goes as } e^{-i \mathbf{k} \cdot \mathbf{x}} \)

Also \( \mathbf{p}_\mu \cdot \mathbf{p}_\mu = m^2 \)

Note \( \omega = \sqrt{k^2 + m^2} \)

\[ V_{qr} = \frac{\partial \omega}{\partial k} = \frac{\partial E}{\partial p} = V_{ql} \]

since \( V_{qr} = \frac{\partial \omega}{\partial k} = \frac{k}{\sqrt{k^2 + m^2}} = \frac{\mathbf{k}}{\omega} = \frac{\mathbf{p}}{E} \)

A free particle of momentum \( p \) has

\[ e^{-i (\mathbf{p}_\mu \cdot \mathbf{x})} \]

Also

\[ \mathbf{p}_\mu \cdot \mathbf{p}_\mu = m^2 \]

These contain all of classical special relativity (A. De Broglie)
Now to formulate q.m. we need some math to generate $e^{-i\hbar \omega \mu}$ in n.q.m.

Now

$$-\frac{\hbar}{i} \frac{\partial}{\partial \mu} = \left( \frac{\hbar}{m}, \frac{\hbar}{m} \right) \psi$$

held in n.r.q.m.

Thus we seek a linear eqn. The fool begins with

$$-\frac{\hbar}{i} \frac{\partial}{\partial \mu} = \sqrt{m^2 + \left( \frac{\hbar^2}{2m} \right)} \psi$$

But trouble with $\sqrt{\cdot}$. If we include vector potential this gets foiled up.

---

Start over again with goal

$$E^2 - P \cdot P = m^2 \quad \text{leads to}$$

$$\left( -\frac{\hbar}{m} \right)^2 \psi - \frac{\hbar}{m} \left( \frac{\hbar}{m} \right) \psi = m^2 \psi$$

or

$$-\Box \psi = m^2 \psi$$

or

$$-\Box \psi = m^2 \psi$$

Now we must pick in an interaction, guess

$$\left( -\frac{\hbar}{m} - A \right)^2 \psi - \left( \frac{\hbar}{m} - A \right) \cdot \left( \frac{\hbar}{m} - A \right) \psi = m^2 \psi$$

or

$$\left( i \gamma_\mu - e A_\mu \right) \left( i \gamma_\nu - e A_\nu \right) \psi = m^2 \psi$$
Is this even OK? Must test it

i.) cons. prob

ii.) reduce to S-eqns

iii.) H-atom

iv.) causality

PROBLEM: Try all of these to see if it works? iii.) is most serious.

[Doesn't include spin]
\((i\nabla_x - eA_x)(i\nabla_y - eA_y)\psi = m^2\psi\)

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.

\[ H\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial t^2} \]

He then guessed only first-order derivatives in space appear.

\[ H = \left( \alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z} + \beta m \right) \]

He also knew Pauli matrices. Thus he proposed \(\beta\)'s for a free particle. For a potential

\[ (-\frac{\hbar^2}{2m} - eV)\psi = [\alpha_x (\frac{\partial}{\partial x} - eA_x) + \alpha_y (\frac{\partial}{\partial y} - eA_y) + \alpha_z (\frac{\partial}{\partial z} - eA_z) + \beta m] \psi \]

\[ \textit{Dirac Equation} \]

\[ \psi = u e^{-i(\xi t - P\cdot x)} \]

\(u\) and \(P\) are operators only.
We substitute this in and we find

$$Eu = [(a \cdot p) + \rho m] u$$

From this we get

$$E^2u = [(a \cdot p) + \rho m]^2u$$

But we know $E^2 = P^2 + m^2$. Multiply out operators:

$$E^2u = \alpha^2 E_x^2 + (\alpha_x d_y + \alpha_y d_x) P_x P_y +$$

$$+ (\alpha_x \beta + \beta \alpha_x) P_y m + \beta^2 m$$

Thus we choose $\alpha, \beta$ so

$$\alpha_x^2 = 1 = \alpha_y^2 = \alpha_z^2$$

\[
\begin{align*}
\alpha_x d_y + \alpha_y d_x &= 0 \\
\alpha_y d_z + \alpha_z d_y &= 0 \\
\alpha_z d_x + \alpha_x d_z &= 0 \\
\beta \alpha_x + \alpha_x \beta &= 0 \\
\beta^2 &= 1
\end{align*}
\]

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 4x4 matrices. We set it up for a spin 1/2 object (neutrons, muons, etc.)
\[ \alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \]

\[ \alpha_y = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & -i & 0 & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \]

Of course the \( \alpha \)'s are 4-component, for matrix representation consider splitting up into spinors

\[ u = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} u_0 \\ u_\alpha \end{pmatrix} \]

Then

\[ \beta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]

Thus for a free particle

\[ E^2 u = (\beta \beta + m^2) u \]
We can rewrite the Dirac equation in various ways:

\[ (-\frac{i}{\hbar}\gamma^\mu - e\gamma^0) \psi = \alpha \cdot \left[ -\frac{i}{\hbar} \gamma^\mu - A^\mu \right] \psi + \beta m \psi \]

Still another way is:

\[ \begin{cases} \beta \left( -\frac{i}{\hbar} \gamma^\mu - e\gamma^0 \right) - \beta \alpha \cdot \left[ -\frac{i}{\hbar} \gamma^\mu - A^\mu \right] \end{cases} \psi = m \psi \]

We can define other matrices:

\[ \gamma_t = \beta \]
\[ \gamma_x = \beta d_x \]
\[ \gamma_y = \beta d_y \]
\[ \gamma_z = \beta d_z \]

Then the Dirac equation becomes:

\[ \gamma_t (i \gamma^0 - eA^0) \psi = m \psi \]

where

\[ \gamma_t \gamma_x + \gamma_x \gamma_t = 2 \gamma_x \]
\[ \gamma_t^2 = 1 \quad \gamma_x^2 = -1 \quad \gamma_y^2 = -1 \quad \gamma_z^2 = -1 \]

This can looks relativistically invariant. But support makes a calculation with:

\[ \gamma = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} \]
But suppose someone measures $w.r.t$ to the very different $\bar{\delta}$s. Do we still have invariance? Yes! Commutation properties are invariant.

We can write the equation in spinor form

$$\Psi = \left( \begin{array}{c} \psi_a(x,t) \\ \psi_b(x,t) \end{array} \right)$$

and we have

$$\alpha \Psi = \left( \begin{array}{c} 0 \\ 0 \end{array} \right) \left( \begin{array}{c} \psi_a \\ \psi_b \end{array} \right) = \left( \begin{array}{c} 0 \\ 0 \end{array} \right)$$

we can find

$$(-\frac{i}{\hbar} D_t - eV) \psi_a = \nabla(-\frac{i}{\hbar} A - eA) \psi_b + m \psi_a$$

$$(-\frac{i}{\hbar} D_t - eV) \psi_b = \nabla(-\frac{i}{\hbar} A - eA) \psi_a - m \psi_b$$

The argument that relativity + spin $\Rightarrow$ spin is circular. Rests upon assumption that a spin $\Rightarrow$ force

$$-\frac{i}{\hbar} D_t \Psi = H \Psi$$

Only for spin $\frac{1}{2}$ particles. For neutrinos

$$-\frac{i}{\hbar} D_t \psi_b = 0 \Rightarrow (-\frac{i}{\hbar} A)^\psi_b$$

$$-\frac{i}{\hbar} D_t \psi_a = 0 \Rightarrow (-\frac{i}{\hbar} A)^\psi_a$$

(Not true good for neutrinos, photons, etc. May fail for for leptons.)
Suppose Klein–Gordon was right. Write

\( (i \frac{\partial}{\partial t} - eV) \psi = \chi \)

\( (i \frac{\partial}{\partial t} - eV) \chi = (-\frac{i}{\hbar} \nabla - eA)^2 \psi - m^2 \psi \)

We can then convert this into \( \psi = \left( \frac{i}{\hbar} \right) \chi \)

\( H = eV + p + m (-\frac{i}{\hbar} \nabla - A)^2 \)

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.

Idea: Frequently bad logic leads to good answer.
Dirac Equation (Cont.)

\[-\frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = H \Psi\]

\[H = \gamma m + eV + \alpha \cdot (p - \frac{e}{c} A)\]

\[p = \frac{\hbar}{i} \nabla\]

\(\alpha\)'s, \(\gamma\) 4x4 matrices which anticommute squares = 1

Eq:

\[\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \Psi = \begin{pmatrix} \Psi_a \\ \Psi_b \end{pmatrix}\]

\[\left(-\frac{\hbar}{i} \frac{\partial}{\partial t} - eV\right) \Psi_a = \gamma^0 \cdot (\gamma^0 - \frac{e}{c} A) \Psi_b + m \Psi_a\]

\[\left(-\frac{\hbar}{i} \frac{\partial}{\partial t} - eV\right) \Psi_b = \gamma^0 \cdot (\gamma^0 - \frac{e}{c} A) \Psi_a - m \Psi_b\]

To learn more about this equation, we will play with things.

Now His derivation. Because we also have

\[\frac{2}{\hbar} \int \Psi^* \Psi \, d\text{vol} = 0\]

Thus can normalize

\[\int \Psi^* \Psi \, d\text{vol} = 1\]
What does this mean? Write

\[ \Psi^* = \frac{\Psi_1^* \Psi_2^* \Psi_3^* \Psi_4^*}{ } \]

to find inner product. Can take matrix elements in usual manner

\[ \langle \Psi_1 | \Psi \rangle = \int \Psi_1^* \Psi \, d\vec{r} \]

Now

\[ \langle 5 | \alpha | 1 \rangle = \int \Psi_1^* \alpha^* \Psi_1 \, d\vec{r} \]

\[ \alpha_* = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \]

\[ \alpha \Psi = \begin{pmatrix} \Psi_4 \\ \Psi_3 \\ \Psi_2 \\ \Psi_1 \end{pmatrix} \]

\[ \langle 5 | 0 | 1 \rangle = \int \Psi_1^* \Psi_1 \, d\vec{r} \left[ \Psi_5^* \Psi_1^* + \Psi_2^* \Psi_1^* + \Psi_3^* \Psi_1^* + \Psi_4^* \Psi_1^* \right] \]

Thus all of q.m. goes through in some way.

We can set up a probability density \( j \) current \( J \in \nabla \cdot j \)
\[ p(x,t) = \psi^*(x,t) \psi(x,t) \]
\[ = \psi_1^* \psi_1 + \psi_2^* \psi_2 + \psi_3^* \psi_3 + \psi_4^* \psi_4 \]
\[ j^\circ = \psi^*(x,t) \otimes \psi(x,t) \]

\( \alpha_x^1 = S^{-1} \alpha_x \leq \beta \) here \( \text{Polarization} \quad \psi^* = S \psi \)

---

4 components of Dirac wave function \underline{multiply} with a 4-vector.

Example: for 3-D, we get 2-component spinor. Again no connection.

However, the matrices do form a 4-vector \([\xi, \eta] \]

We use \( \psi_0 = \psi_\alpha + \psi_\beta \), \( \psi_1 = \psi_\alpha - \psi_\beta \) and find

\[ [ (E- \mathbf{e} \cdot \mathbf{v})^2 - (\mathbf{p} - \mathbf{e} \mathbf{A})^2 + \text{const} (B+iE)] \psi_\alpha = m^2 \psi_\alpha \]

Two-component wave functions are necessary.

Solutions are difficult to calculate electrically coupling in 3-direction.
What do 4 components mean? Can we get S-eqn?

First Shade S-eqn. Assume A, U time-independent,

\[ E = m + U \quad W, V \ll \ll \ll m \]

\[ \frac{P}{m} \sim V \quad \frac{(\ell)^2}{c^2} \ll 1 \]

Writing out eoms:

\[ (m + U - eV) \psi_a = \sigma_0 (\mathbf{P} - e \mathbf{A}) \psi_a + m \psi_a \]

\[ (m + U - eV) \psi_b = \sigma_0 (\mathbf{P} - e \mathbf{A}) \psi_a - m \psi_b \]

\[ \psi_b \sim \frac{1}{2m} \sigma_0 (\mathbf{P} - e \mathbf{A}) \psi_a \]

Renewing in:

\[ (U - eV) \psi_a = \frac{[\sigma_0 (\mathbf{P} - e \mathbf{A})] [\sigma_0 (\mathbf{P} - e \mathbf{A})]}{2m} \psi_a \]

Now \( (\sigma \cdot a)(\sigma \cdot a) \neq a \otimes a \)

But \( (\sigma \cdot A)(\sigma \cdot B) = A \cdot B + i \epsilon \cdot (A \times B) \)

\[ \frac{[\sigma_0 (\mathbf{P} - e \mathbf{A})] [\sigma_0 (\mathbf{P} - e \mathbf{A})]}{2m} = \frac{1}{2m} \left[ (\mathbf{P} - e \mathbf{A}) \otimes (\mathbf{P} - e \mathbf{A}) \right] \]

\[ + \frac{e \hbar}{2mc} \sigma_0 (\mathbf{v} \times \mathbf{A}) \]
Thus we find non-relativistic limit

\[ H \Psi_0 = \left[ eV + \frac{1}{2m} \left( p - \frac{e}{c} A \right)^2 + \frac{eB}{2mc} (\sigma \cdot B) \right] \Psi_0 \]

\[ \Rightarrow \mu = \frac{eB}{2mc} \]

They we have deduced numerical value for magnetic moment of electron. One of great triumphs of Dirac equation.

Thus we get a spin connection to S-wave.

---

Consider free particle at rest \( \psi \approx 1 \) assume

\[ \Psi = u e^{-i(Et - p \cdot x)} \] and substitute into Dirac equation.

\[ H = \beta m \]

\[ \Rightarrow Eu = m \beta u \]

or \( E u_1 = m u_1 \quad E u_2 = m u_2 \)

\( E u_3 = -m u_3 \quad E u_4 = -m u_4 \)

\( \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \) spin up, \( E = +m \)

\( \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \) spin down, \( E = +m \)
spin up $E = -\frac{1}{2}m$

spin down $E = -\frac{3}{2}m$

Both $\pm$ energy.

Hence proposed our world has filled band of electrons with $E < 0$. Can get holes however $\Rightarrow$ positrons.
Recall the Dirac equation in the form

\[ -\frac{i}{2} \frac{\partial \Psi}{\partial t} = H \Psi \]

where

\[ H = Bm + eV + \beta_0 (\vec{p} - \frac{e}{c} \vec{A}) \]

\[ \beta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \dot{\vec{a}} = \begin{pmatrix} \vec{a}_0 \\ 0 \end{pmatrix} \]

If we multiply (1) by $\beta$, and note $\beta \cdot \beta = 1$

\[ -\frac{i}{2} \beta \frac{\partial \beta \Psi}{\partial t} = \left[ m + e\beta v + \beta_0 \cdot \left( \vec{p} - \frac{e}{c} \vec{A} \right) \right] \Psi \]

On reorganizing

\[ \left\{ \beta \left[ -\frac{i}{2} \frac{\partial^2}{\partial t^2} - eV \right] - \beta_0 \cdot (\vec{p} - \frac{e}{c} \vec{A}) \right\} \Psi = m \Psi \]

\[ \frac{\partial^2}{\partial t^2} \text{ term dependent} \quad \beta \text{ term independent} \]

Define the $\xi$ matrices which are conventionally used to make non-relativistic part obvious:

\[ \xi_0 = \beta \quad \xi = \beta \vec{a} = \begin{pmatrix} 0 & \vec{a} \\ -\vec{a} & 0 \end{pmatrix} \]

Also define

\[ \vec{d} = \xi_0 \vec{B}_0 - \vec{B}. \vec{B} \]
The Dirac equation then becomes

\[ [\not p - \not \epsilon \not X - m] \psi = 0 \]

**Case I:** \( \hat{A} = 0, \ \hat{p} = 0 \) (free particle at rest)

\[ [\not p \psi_0 - m] \psi = 0 \quad \text{where} \quad \psi = (\psi_1, \psi_2) \]

or

\[ \left\{ -\frac{i}{\hbar} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - m \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0 \]

This yields

\[ (E-m) \phi = 0 \]

\[ (-E-m) \chi = 0 \]

Thus

\[ \phi = (a) e^{-i\hbar m t} \]

\[ \chi = (c) e^{i\hbar m t} \]

Note the two 2-component spinors are decoupled.
Case II: \( \dot{A} = 0, \dot{\vec{P}} \neq 0 \) (moving free particle)

Then

\[
[\gamma \sigma - m] \psi = 0
\]

or

\[
[E \psi_0 - \dot{\vec{P}} \cdot \sigma - m] \psi = 0
\]

or

\[
\{ E \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 0 & \dot{\vec{P}} \cdot \sigma \\ -\dot{\vec{P}} \cdot \sigma & 0 \end{pmatrix} - m \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \} \psi = 0
\]

or

\[
\begin{bmatrix} E-m & -\dot{\vec{P}} \cdot \sigma \\ \dot{\vec{P}} \cdot \sigma & -(E+m) \end{bmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = 0
\]

or

\[
(E-m)\phi - \dot{\vec{P}} \cdot \sigma \chi = 0
\]

\[
\dot{\vec{P}} \cdot \sigma \phi - (E+m)\chi = 0
\]

Now \( \phi \) and \( \chi \) are coupled. Solve for

\[
\chi = \begin{pmatrix} \dot{\vec{P}} \cdot \sigma \\ E+m \end{pmatrix} \phi
\]

and then

\[
(E-m)\phi = \begin{pmatrix} \dot{\vec{P}} \cdot \sigma & (\dot{\vec{P}} \cdot \sigma)(\dot{\vec{P}} \cdot \sigma) \end{pmatrix} \phi
\]

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 the I solution as $p \to 0$, we need the negative sign from the square root. Then

$$\psi = \begin{pmatrix} -\frac{\bar{\psi} \chi}{\sqrt{p^2 + m^2}} \\ \chi \end{pmatrix} e^{i\sqrt{p^2 + m^2}t + i\vec{p} \cdot \vec{x}}$$

(1)

The + sign gives

$$\psi_+ = \begin{pmatrix} \phi \\ \sqrt{\frac{\vec{p} \cdot \vec{\sigma} \phi}{E + m}} \end{pmatrix} e^{-i\sqrt{p^2 + m^2}t + i\vec{p} \cdot \vec{x}}$$

(2)

Since (1) involves negative energies, we try to understand by rewriting solving $\psi_-$ to try $\psi_+$ and get it to look like (2). Define

$$\vec{p}^\prime = -\vec{p} \quad E^\prime = +\sqrt{p^2 + m^2}$$

Then

$$\psi_- = \begin{pmatrix} \frac{\bar{\psi} \chi}{\sqrt{E + m}} \\ \chi \end{pmatrix} e^{-iE^\prime t + i\vec{p}^\prime \cdot \vec{x}}$$

This now looks like $\psi_+$ except with momentum reversed.
Drac Equation Including Electromagnetic Interactions

We first try to get the non-relativistic limit. Don't try to normalize \( \Psi \)

\[
\left[ \frac{\mathbf{p} - \frac{e}{c} \mathbf{A}}{\mu} - m \right] \Psi = 0
\]

Our writing it out

\[
\begin{bmatrix}
E - m - \frac{eV}{c} & (\mathbf{p} - \frac{e}{c} \mathbf{A}) \cdot \mathbf{\hat{r}} \\
-\mathbf{\hat{r}} \cdot (\mathbf{p} - \frac{e}{c} \mathbf{A}) & -(E + m - \frac{eV}{c})
\end{bmatrix}
\begin{pmatrix}
\phi \\
\chi
\end{pmatrix} = 0
\]

We can solve, taking \( \chi \) as the smallest component, to find

\[
\chi = \frac{-1}{(E+m-\frac{eV}{c})} \mathbf{\hat{r}} \cdot (\mathbf{p} - \frac{e}{c} \mathbf{A}) \phi
\]

Then plugging back in

\[
\begin{bmatrix}
E - m - \frac{eV}{c} \\
\phi
\end{bmatrix} = \mathbf{\hat{r}} \cdot (\mathbf{p} - \frac{e}{c} \mathbf{A}) \left( \frac{1}{(E+m-\frac{eV}{c})} \mathbf{\hat{r}} \cdot (\mathbf{p} - \frac{e}{c} \mathbf{A}) \phi \right)
\]

\[
E = m + W \\
\mathbf{\pi} = \mathbf{p} - \frac{e}{c} \mathbf{A}
\]

To get the non-relativistic limit, assume potential energy small and expand

\[
\frac{1}{2m+W-\frac{eV}{c}} \sim \frac{1}{2m} - \frac{(W-\frac{eV}{c})}{(2m)^2}
\]

Plug this in to get

\[
(W-\frac{eV}{c}) \phi = \mathbf{\hat{r}} \cdot \mathbf{\pi} \frac{1}{2m} \mathbf{\hat{r}} \cdot \mathbf{\pi} \phi
\]
as follows: Let \( \psi' = \frac{1}{2} \psi \)

\[
\left[ 1 + \left( \frac{\nabla \cdot n}{2m} \right)^2 \right] (w-v) \left[ 1 + \left( \frac{\nabla \cdot n}{2m} \right)^2 \right] \phi = \frac{1}{2m} (\nabla \cdot n) \phi 
+ \frac{1}{8m^2} \left[ (\nabla \cdot n)^2 (w-v) - 2\nabla \cdot n (w-v) \nabla \cdot n + (w-v) (\nabla \cdot n)^2 \right] \phi 
\]

Let

\[
\Box = \left[ 1 - \left( \frac{\nabla \cdot n}{2m} \right)^2 \right] \phi 
\]

since to first order,

\[
\psi + \psi = \phi + \phi + \chi + \chi \sim \phi + \phi \left[ 1 + \left( \frac{\nabla \cdot n}{2m} \right)^2 \right] 
\]

and to first order

\[
\phi \sim \Box - \left( \frac{\nabla \cdot n}{2m} \right) \phi 
\Rightarrow \psi + \psi \sim \Box 
\]

Using this in (3) and using

\[
\left[ 1 + \left( \frac{\nabla \cdot n}{2m} \right)^2 \right]^{-1} \sim \left[ 1 - \left( \frac{\nabla \cdot n}{2m} \right)^2 \right] 
\]

we find

\[
(w-v) \Box = \frac{1}{2m} (\nabla \cdot n)^2 \Box - \frac{\nabla \cdot n}{8m^2} \Box 
\]

\[
+ \frac{1}{8m^2} \left\{ (\nabla \cdot n)^2 (w-v) - 2\nabla \cdot n (w-v) \nabla \cdot n + (w-v) (\nabla \cdot n)^2 \right\} \Box 
\]
To rewrite the \( \{ \} \) expression, use the commutation relation
\[
\]
and let
\[
A = \hat{\tau}, \quad B = \hat{N} - \hat{V}.
\]
Now, since \( \hat{E} \rightarrow \hat{N} \), if \( \hat{A} \) is time dependent it would commute with \( \hat{E} \). Assume
\[
\frac{\partial \hat{A}}{\partial t} = 0
\]
so that \( \hat{A} \) commutes with \( \hat{E}, \hat{m}, \hat{V} \). Now worry about \( \hat{\tau}, \hat{\rho} \) which commutes with \( \hat{E} \). Thus
\[
\left[ \hat{\tau}, (\hat{\rho} - \hat{\sigma} \hat{A}), \hat{E} - \hat{m} - \hat{V} \right] = \left[ \hat{\tau}, \hat{\rho}, -\hat{V} \right] = -i e \hat{\sigma} \cdot \hat{E}
\]
Then in (4)
\[
\{ \} = \kappa \left[ \hat{\tau}, \hat{\rho}, -\hat{E} \right]
\]
Now use
\[
(\hat{\tau}, \hat{E})(\hat{\tau}, \hat{\pi}) = -(\hat{\tau}, \hat{\pi})(\hat{\tau}, \hat{E})
\]
and
\[
(\hat{\tau}, \hat{a})(\hat{\tau}, \hat{b}) = \hat{a} \cdot \hat{b} + i \hat{\sigma} \cdot (\hat{a} \times \hat{b})
\]
to find
\[
\hat{E} \cdot \hat{\tau} + i \hat{\sigma} \cdot (\hat{E} \times \hat{\pi}) = \hat{\pi} \cdot \hat{E} - i \hat{\sigma} \cdot (\hat{\pi} \times \hat{E})
\]
\[
\hat{p} \times \hat{E} = -\hat{E} \times \hat{p}
\]
Hence
\[
\{ \} = -e \left[ \nabla \cdot \mathbf{E} - 2 \mathbf{\hat{a}} \cdot (\mathbf{\hat{p}} \times \mathbf{E}) \right]
\]

and (4) becomes
\[
W \mathbf{\hat{x}} = V' \mathbf{\hat{x}} + \frac{1}{2m} (\mathbf{\hat{p}} \cdot \mathbf{\hat{p}})^2 \mathbf{\hat{x}} - \frac{(\mathbf{\hat{a}} \cdot \mathbf{\hat{p}})^2}{8m^3} \mathbf{\hat{x}}
\]
\[
- \frac{e}{8m^2} \left[ \nabla^2 E + 2 \mathbf{\hat{a}} \cdot (\mathbf{\hat{p}} \times \mathbf{E}) \right] \mathbf{\hat{x}}
\]

Use
\[
(\mathbf{\hat{a}} \cdot \mathbf{\hat{p}})(\mathbf{\hat{a}} \cdot \mathbf{\hat{p}}) = \mathbf{\hat{p}} \cdot \mathbf{\hat{p}} - e \mathbf{\hat{a}} \cdot \mathbf{B}
\]

Then
\[
W \mathbf{\hat{x}} = \sqrt{V' \mathbf{\hat{x}}} + \frac{1}{2m} \left[ \mathbf{\hat{p}} \cdot \mathbf{\hat{p}} - e \mathbf{\hat{a}} \cdot \mathbf{B} \right] \mathbf{\hat{x}}
\]

\[
- \frac{(\mathbf{\hat{a}} \cdot \mathbf{\hat{p}})^2}{8m^2} \mathbf{\hat{x}} - \frac{e}{8m^2} \left[ \nabla^2 E + 2 \mathbf{\hat{a}} \cdot (\mathbf{\hat{p}} \times \mathbf{E}) \right] \mathbf{\hat{x}}
\]

1st order
Relativistic correction
to K.E.

Spin-orbit coupling
\[ W\chi = \left\{ V + \frac{1}{2m} (P - \frac{e}{c} A)^2 - \frac{1}{8m^3} (P - \frac{e}{c} A)^4 \right\} \chi \]

\[ + \frac{e}{2m} \sigma \cdot B + \frac{e}{2m} \left[ \frac{1}{2} \sigma \cdot \left( \frac{e}{m} A \times E \right) + \frac{i}{2m} \nabla \cdot E \right] \chi \]

**Significance of terms:**

\[ \frac{1}{8m^3} (P - \frac{e}{c} A)^4 \]

**Consider**

\[ E = \sqrt{m^2 + p^2} = m + \frac{p^2}{2m} = \frac{p^4}{8m^3} \]

We can identify the terms directly.

\[ \frac{e}{2m} \left[ \frac{1}{2} \sigma \cdot \left( \frac{e}{m} A \times E \right) + \frac{i}{2m} \nabla \cdot E \right] \]

Can understand \( i \cdot (W\chi E) \) as magnetic field seen by moving object. [But doesn't account for \( \frac{1}{2} \) term.]

Note: \( E = \frac{Z e^2 R}{4m \hbar^3} \), thus get a \( \frac{1}{18} \) term --

"spin-orbit coupling" (Does not apply)

\[ \text{In an H-atom} \quad \mathbf{P} \cdot \mathbf{E} \rightarrow 4 \pi z e S^3 (1R) \]
Pauli's Correction for the Proton (Anomalous moment)

The electron has a moment \( \frac{\hbar}{2m} \). But the proton has \( \frac{2.17}{2} \) (c.m. magnetic moment). Pauli suggested an alternate equation by adding terms to Dirac equation

\[
\left[ i \gamma_\mu (\gamma_\mu - e A) - m \right] \psi = \frac{i}{\hbar c} \gamma_\mu \gamma_\nu F_{\mu \nu} \psi + \gamma_0 \partial^2 A_\mu \psi
\]

where \( F_{\mu \nu} \) is field tensor

\[
F_{\mu \nu} = \frac{2}{\hbar c} \partial_\mu A_\nu - \frac{2}{\hbar c} \partial_\nu A_\mu
\]

Multiply by \( \beta \) to find

\[
i \frac{\partial \psi}{\partial t} = \left[ \mathcal{H} + V + \alpha (\mathbf{p} - \frac{e}{c} \mathbf{A}) \right] \psi + \beta \mathbf{B} \left[ \mathbf{D} \cdot \mathbf{B} - \alpha \cdot \mathbf{E} \right] \psi
\]

In the non-relativistic limit this leads to

\[
\mathcal{H} \chi = \left\{ V + \frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 - \frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 \right\} \chi
\]

\[
+ (\mathbf{p} + \frac{e}{2m}) \mathcal{C} \cdot \mathbf{B} + (\mathbf{p} + \frac{e}{4m}) \left[ \mathbf{D} \cdot (\mathbf{p} - \frac{e}{2c} \mathbf{A}) \mathbf{E} + \frac{\hbar}{2m} \right] \chi
\]

where

\[
\mathbf{C} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{spin operator for Dirac equation}
\]

\[
\mathbf{r} = i \alpha_x \alpha_y
\]
Note the \((\mu + \frac{e}{4m}) = (\mu + \frac{e}{2m} - \frac{e}{4m})\) term.

The extra \(-\frac{1}{2}\) term comes from Thomas precession.

Thomas Precession

Must account for fact that electron real system is accelerating. Thus going systems of electron precesses slowly.

\[
\begin{array}{c}
\rightarrow \\
\ \ \ \ \\
\ \ \ \ \\
\ \ \ \ \\
\rightarrow
\end{array}
\]

\[
\begin{array}{c}
-17 \\
-9 \\
5' \\
17
\end{array}
\]

\[
\begin{array}{c}
S' \\
S
\end{array}
\]


depend on daily transformation said

commute. Their commutator involves restrained operator.

At present we don't know what makes the \(\mu\) comes from guts of proton (maybe means quark). Maybe "ideal proton" satisfies Dirac eqn which means about it satisfy Klein Gordon eqn. (Glashow's idea).

Doesn't appear electron has guts, although if Dirac eqn predicts 100% agreement gives 1.001147. But we can handle this just consider e.g. for interaction potential (use Q.E.D.), some thing would for universal.

Thus contrary and common predict satisfy the Dirac eqn -- at least to within experimental evidence.
We also have an "ideal" electron which satisfies
\[ \tau \psi (i\gamma^\mu - \frac{e}{c} A^\mu) \psi = m \psi \]

and an ideal photon which satisfies Maxwell's equations. However, there is an interaction which gives rise to angular electron moment. The radiation resistance term in classical EM
\[ m \frac{d^2 \psi}{dt^2} = \tau \nu \frac{d\psi}{dt} = \psi (F_{\text{self}} + F_{\text{system}}) \]

No experiment has produced any failure in these equations. Any disagreement can be attributed to lack of knowledge about strong interaction.

- Force of motion of electron
- Dirac equation
- Maxwell's equations
- Strongly interacted particles (Call-Mann eqn 1970)

**Problem:** Explain physical interpretation of $\frac{1}{m} \partial^2 \psi / \partial t^2$.

**Problem:** Can write Dirac $\psi$

\[ H_0 = \psi_0 \left( \alpha \left( P - \frac{e}{c} A \right) + m \right) \]

But from g.m.
\[ \dot{\psi} = i (H_0 \psi - \psi H_0) \]
An s. can we find \( \dot{x} = \frac{P - iA}{\hbar} \) \( \dot{P} = -\nabla V + \cdots \)

Try this game with Dirac case.

**Problem:** Given \( \alpha \), \( \beta \), \( \alpha_x \), \( \alpha_y \), \( \alpha_z \), \( \beta_x \), \( \beta_y \), \( \beta_z \), find how many are really different (to get used to commutation laws).

---

Now we want to study free pointwise Dirac solutions to try to interpret components of Dirac spinor.

\[ \Psi = \begin{pmatrix} \Psi_0 \\ \Psi_b \end{pmatrix} \text{ and } \psi = e^{-i(E+P_x)x} \Psi_{a,b} \]

\[ (E + m) \Psi_0 = (\mathbf{P} \cdot \mathbf{P}) \Psi_a \]

\[ (E - m) \Psi_a = (\mathbf{P} \cdot \mathbf{P}) \Psi_0 \]

\( P, E \) are numbers

Combined

\[ (E^2 - m^2) \Psi_0 = (\mathbf{P} \cdot \mathbf{P}) (E + m) \Psi_0 = (\mathbf{P} \cdot \mathbf{P}) (\mathbf{P} \cdot \mathbf{P}) \Psi_a = (P^2 + P \cdot P) \Psi_a \]

\( \Rightarrow \)

\[ E^2 - m^2 = P \cdot P \]

\[ E = E_0 = \sqrt{m^2 + P \cdot P} \]

\[ = -E_0 \]
Suppose $E = E_0$ and solve

$$\Psi_0 = \frac{1}{\sqrt{E_0 + m}} \left( \begin{array}{c} 0 \\ -1 \end{array} \right) \Psi_0$$

Consider case where $p \cdot n = m \cdot \hat{z}$ direction.

Also

$$\sigma_z \Psi_0 = + \Psi_0 \quad (\Psi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix})$$

Then

$$\Psi_0 = \frac{1}{\sqrt{m + E_0}} \sigma_z \hat{P} \Psi_0 = \frac{\hat{P}}{E + m} \Psi_0$$

$$\sigma_z \Psi_0 = +1 \Psi_0$$

Spin is in up direction

But you really want to normalize $\Psi_b$, $\Psi_b \Psi_b + \Psi_0 \Psi_0 = 1$

Then find

$$\Psi = \frac{1}{\sqrt{2E_0}} \left( \begin{array}{c} \sqrt{E_0 + m} \\ 0 \\ \sqrt{E_0 - m} \\ 0 \end{array} \right)$$

Particle in $z$ direction, up spin since $\sigma_z \Psi = +1 \Psi$

Now for spin down:

$$\Psi = \frac{1}{\sqrt{2E_0}} \left( \begin{array}{c} 0 \\ \sqrt{E_0 + m} \\ 0 \\ -\sqrt{E_0 - m} \end{array} \right)$$

Particle in $z$ direction, down spin.
Now for spin in x-direction, recall we have:

\[ \sigma_x X = X \]

Thus we expect:

\[ \psi = \frac{1}{\sqrt{2E_0}} \left( \begin{array}{c} \sqrt{E_0 + m} \\ \sqrt{E_0 + m} \\ \sqrt{E_0 - m} \\ -\sqrt{E_0 - m} \end{array} \right) \]

\[ \text{p in z-direction: spin in x-direction (?)} \]

But \[ \sigma_x \psi \neq \psi \]

What is the matter? \( \psi \) is certainly a solution of the eigenvalues, but \( \sigma_x \) does not commute with \( H \). Mentioned right? left definite concept.
We have seen that \([\sigma_x, H_0] \neq 0\), thus no definite angular mom in \(x\)-direction.

Now say \(P\) not in \(z\)-direction.

For case of positive helicity we require

\[
\left(\sigma^0 \cdot P\right) \psi = +\psi
\]

Now

\[
\sigma^0 \psi_a = +\psi_a \quad \text{where} \quad \psi_a = \begin{pmatrix} \cos \theta/2 e^{i\phi_1/2} \\ \sin \theta/2 e^{-i\phi_1/2} \end{pmatrix}
\]

from n.r.g.m.

Thus in n.g.m.

\[
\psi = \sqrt{\frac{1}{2E_0}} \begin{pmatrix} \sqrt{E_0 + m} \cos \theta/2 e^{i\phi_1/2} \\ \sqrt{E_0 - m} \sin \theta/2 e^{-i\phi_1/2} \end{pmatrix}
\]

for positive helicity \(\sigma^0 = +1\)
Now consider $E = -E_0$

- In $z$-direction, $\sigma_2 = +1$
  \[ \frac{1}{\sqrt{2E_0}} \begin{pmatrix} \sqrt{E_0 - m} \\ 0 \\ + \sqrt{E_0 + m} \end{pmatrix} \]

- $\sigma_2 = -1$
  \[ \frac{1}{\sqrt{2E_0}} \begin{pmatrix} 0 \\ + \sqrt{E_0 - m} \\ 0 \end{pmatrix} \]

Note 4: in this spinors for free particle (4 base states).

These components cannot be easily interpreted.

Equation (3) has no simple meaning.

From proposed all negative states in vacuum are full. A "hole" is a positive.
**Example:** Scattering cross-section of an electron from a nucleus of $\frac{Z}{e}$. Use Born approx.

\[ H_0 = c_0p + Pm + V_{\text{int}} \]

\[ Rate = \sigma U_m = \frac{2\pi \delta(E_f - E_i) \frac{d^3p_2}{(2\pi)^3} |W_2|^2}{r} \]

**Note:** Relativity only enters into $H_0$, not into state density.

\[ M_{f_i} = \int \psi_i^+(x) H_{\text{int}} \psi_f(x) d^3x \]

Now use free wave-funs

\[ \psi(x) = e^{iP \cdot X} u \]

where $u$ is \( \leftrightarrow \) a number (spinor)

\[ M_{f_i} = \int u_2^+ e^{-iP \cdot X} \frac{Z e^2}{r} e^{iP \cdot X} u_1 d^3x \]

\[ = (u_2^+ \cdot u_1) \int e^{i(P_1 - P_2) \cdot X} \frac{Z e^2}{r} d^3x \]

\[ = \frac{4\pi Z e^2}{Q^2} \]
Note that except for \((y_2 + 1 \mu)\), everything is the same as in n.r.q.m. However, actually we have differences as for

\[ 0 - v_1 = 2\pi \left( \sqrt{m_2^2 + p_2^2} - \sqrt{m_1^2 + p_1^2} \right) \frac{P_2^2 dP_2 d\Omega_2}{12\pi^3} \left( \frac{4\pi Z^2}{Q^2} \right)^2 \left| (u_2 + 1\mu) \right|^2 \]

\[ = \frac{1}{(2\pi)^2} \sqrt{\frac{m_2^2 + p_2^2}{p_2}} P_2^2 d\Omega_2 \left( \frac{E_2}{P_2} \right)^2 \]

\[ \frac{E_2}{P_2} \]

\[ \frac{E_2 dP_2}{dP_2} \]

\[ \frac{E_2}{P} \]

\[ \frac{E_2}{P} \]

Note

\[ S(E_2 - E_1) P_2^2 dP_2 = S(E_2 - E_1) P_2 \frac{P_2^2 dP_2}{P} \]

Now

\[ \frac{E_2}{E_1} \]

\[ |P_2| = |P_1| \]

\[ Q = 2P \sin \theta_1 \]

Now to calculate \((y_2 + 1 \mu)\). We need more information about initial and final spins.
in state 1
+ helicity
\[ u_1 = \frac{1}{\sqrt{2E}} \begin{pmatrix} \frac{E_1 + u_1}{\sqrt{E_1 - u_1}} \\ \frac{E_1 - u_1}{\sqrt{E_1 - u_1}} \\ 0 \end{pmatrix} \]
- helicity
\[ u_1 = \frac{1}{\sqrt{2E}} \begin{pmatrix} 0 \\ \frac{E_1 - u_1}{\sqrt{E_1 - u_1}} \\ -\frac{E_1 + u_1}{\sqrt{E_1 - u_1}} \end{pmatrix} \]

and state 2
+ helicity
\[ u_2 = \frac{1}{\sqrt{2E}} \begin{pmatrix} E_2 \cos \theta_2 \\ E_2 \sin \theta_2 \\ 0 \end{pmatrix} \]
- helicity
\[ u_2 = \frac{1}{\sqrt{2E}} \begin{pmatrix} -E_2 \sin \theta_2 \\ E_2 \cos \theta_2 \\ 0 \end{pmatrix} \]

\[(+ \rightarrow +) = \frac{1}{\sqrt{2E}} \left[ \sqrt{E_1 + \mu} \cos \theta_2^2 + O + \sqrt{E_1 - \mu} \cos \theta_2^2 + O \right] \]
\[ = \cos \theta_2 \quad \text{(mass flip)} \]

\[(+ \rightarrow -) = \frac{1}{\sqrt{2E}} \left[ \sqrt{E_1 + \mu} \sin \theta_2^2 + \sqrt{E_1 - \mu} \sin \theta_2^2 \right] \]
\[ = -\frac{\mu}{E} \sin \theta_2 \quad \text{(spin flip)} \]

\[ (+ \rightarrow \text{unknown helicity}) \]
\[ \sigma_T = \frac{4Z^2 e^4}{Q^4} \hat{E}_p \hat{d}S \left( \hat{u}^2 \hat{\theta}^2 + \frac{\mu^2}{E^2} \sin^2 \hat{\theta}^2 \right) \]
\[ \text{relativistic modification} \]
Note as \( m/E \to 1 \) we get usual Coulomb scattering, i.e.

\[
\cos^2 \theta / 2 + \frac{m^2}{E^2} \sin^2 \theta / 2 = 1 - \frac{m^2}{E^2} \sin^2 \theta / 2
\]

To get \((- \to \text{anything})\) must use parity invariance of EM interactions to get correct sign.
"Quantum Mechanics + Relativity = Cosmology"

R.P. Feynman

Consequences

1) Independence
2) Spin + Statistics added
3) CPT invariance (in definite way)
4) No arbitrary functions
5) Divergence problems

**Theorem:** In general we can expand \( f(t) \) in \( \omega > 0 \)

\[
f(t) = \int \phi(\omega) e^{-i\omega t} d\omega
\]

uniquely from \( f(0) \equiv 0 \) over a finite \( t \).

(Identity theorem)

We want to include causality in QM. What we dream of is that future cannot affect the past. We imagine the state of a certain time \( |\psi\rangle \), consider second order scattering in a potential.

\[
\langle x'|\psi\rangle = \sum_{\phi} \langle x'|\phi\rangle \langle \phi|A|\psi\rangle
\]

\[
\Delta A + i\hbar \partial_t
\]
If \( \Psi \) is a particle only and scattering is local

\[
E_3 = \sqrt{\mu^2 + \mathbf{P}_3 \cdot \mathbf{P}_3}
\]

\[
\text{scat} = \frac{\mathcal{E} \beta d}{\mathcal{P}_3} e^{i [\mathbf{E}_3 (\mathbf{b} - \mathbf{b}_a) \cdot \mathbf{X}_a]} e^{-i [\mathbf{E}_3 (\mathbf{b} - \mathbf{b}_a) \cdot \mathbf{X}_b - \mathbf{E}_3 \mathbf{X}_b \cdot \mathbf{X}_a]} e^{i [\mathbf{E}_3 (\mathbf{a} - \mathbf{b}) \cdot \mathbf{X}_a]}
\]

\[
\text{for}\ \text{invariance}, \ \alpha, \beta = \text{const.}
\]

\[
\mathcal{E} \rightarrow \sqrt{\frac{d^3 \mathcal{P}_3}{(2\pi)^3 2E_3}}
\]

\[
\text{scat} = \mathcal{P}_3 e^{i \mathbf{P}_3 \cdot \mathbf{b}} e^{-i \mathbf{P}_3 \cdot \mathbf{b}_a} N(b - a) \text{ for } t_b > t_a
\]

\[
N(Xt_1) = \sqrt{\frac{d^3 \mathcal{P}}{(2\pi)^3 \sqrt{2 + \mathcal{P}}} e^{-i [\mathbf{X}_a \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{X}_a]}}
\]
Causality can't mean $N \to 0$ across time line because a guy in another causal system wouldn't.

$t_0 < t_a$ -- hub doesn't help matters.

Neither are invariant because $t_0 \geq t_a$.  

Outside light cone:

$N(x_1, t_1) \neq 0, \textup{But} \, t_1 \\
N(x, 0) = 0$ \\
$N = N^*$

$e^{-R}$

$e^{-R}$

$e^{-R}$

$e^{-R}$
Consider emission from a pt. We expect velocity of particle \( \leq c \)
\( \text{i.e. no influence outside light cone. But if we try to} \)

\[
\mathcal{E}(\alpha) = \int e^{i \mathbf{P} \cdot \mathbf{X}} d^3 \mathbf{p} e^{-\sqrt{\mathbf{p}^2 + m^2}}
\]

But by our theorem, events cannot be zeroing a finite range, and localicity is not compatible with velocity

(antimatter)

Only one way out, and that is to take \( t < t_a \)

\[
\int d \mathbf{p} e^{i \mathbf{P} \cdot \mathbf{b}} e^{-i \left[ E (\mathbf{p} t_a + \mathbf{P} \cdot \mathbf{X_b} - \mathbf{X_a}) \right]} e^{-i \mathbf{P} \cdot \mathbf{a}}
\]

\[
= \int d \mathbf{P} e^{i \mathbf{P} \cdot \mathbf{b}} e^{-i \left[ E (\mathbf{P} t_a + \mathbf{P} \cdot \mathbf{X_b} - \mathbf{X_a}) \right]} e^{-i \mathbf{P} \cdot \mathbf{a}}
\]

\( \mathbf{b} \) is outside lightcone of \( \alpha \)

we find from \( t_a \) to \( \mathbf{b} \)

\( \text{second from } t_a \) to \( \mathbf{b} \)

\( \text{to get invariant result & causality} \)
In vacuo, assume for pair products in vacuum:

\[ \text{pair product + pair product added} \]
\[ \text{amp} = \frac{1}{2} (X + \frac{1}{2} X^2) \lambda a^2 \]
\[ \text{prob} = 1 - X |a|^2 \]

\[ \text{pair product + pair product added} \]
\[ \text{amp} = \frac{1}{2} (X + \frac{1}{2} X^2) \lambda a^2 \]
\[ \text{prob} = 1 - X |a|^2 \]

\[ \text{pair product + pair product added} \]
\[ \text{amp} = \frac{1}{2} (X + \frac{1}{2} X^2) \lambda a^2 \]
\[ \text{prob} = 1 - X |a|^2 \]

Note: It doesn't add up... unless we assume amp for pair prod in vacuum is less than in presence of pair product.

\[ \Rightarrow \text{prob something happens} \quad c |a|^2 + x |a|^2 + d |a|^2 \]

\[ \Rightarrow \text{base statistics} \quad \text{(since we assumed no spin)} \]
"One man's particle is another man's 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 statistics. Basic idea is unitarity ($\Xi = (\text{amp})^2 = 1$). Consider first

\[ \text{amp at} \quad \text{prob at} = C |a|^2 \]

\[ \text{amp without} \quad \text{prob without} \quad 1 - \frac{1}{2} C |a|^2 \]

\[ \Xi(\text{prob}) = 1 \quad \text{iff} \quad C = C. \]
Spin $\frac{1}{2}$: For particle standing still

\[ |+\rangle_\uparrow, |0\rangle_\downarrow \]

For particle moving, he uses Lorentz transformations.

\( (\text{lost me here}) \Rightarrow \text{shows spin } \frac{1}{2} \Rightarrow \text{pseudoscalar} \)

Now:

\[ p^2 \text{something} \]

\[ 1 - c^2 - v^2 \text{something} \]

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 looks OK so far.
In order to get rid of negative energy states, we must introduce antiparticles. Consider again 2nd order scattering and sum over intermediate states.

$$e^{i\lambda_{a}}, e^{-i\lambda_{b}} \Rightarrow e^{i\lambda_{a}}, e^{-i\lambda_{b}}$$

This amplitude should remain, but the condition $t_b > t_a$ is not invariant. One way to avoid this is to replace 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 $E = E_1 - E_3 + E_2$ may be negative. But we cannot have $x < 0$ since then vacuum would be unstable. Thus we must try something else.
Thus, one cannot extend the formula \((\ast)\) for negative times directly.

The correct way out is to notice in the sum \((\ast)\) that

\[
N(x,t) = \sqrt{\frac{2\pi}{(2\pi)^3}} \int \frac{dp}{\sqrt{2p^2 + m^2}} e^{-i(\sqrt{x^2 + p^2} + m \cdot x)}
\]

\(\therefore \quad R = \sqrt{x^2 + p^2} > t, \quad N \text{ real,} \)

Thus, we can propose for \(t_0 < t_a\) to use the same formula as for \(t_0 > t_a\)

\[
(\ast) = -e^{-i(E_{3t_0} - P \cdot X_0)} e^{i(E_{3t_a} - P \cdot X_a)}
\]

except

\[
(\ast) = \alpha \neq e^{-i(E_{3t_0} - P \cdot X_0)} e^{i(E_{3t_a} - P \cdot X_a)},
\]

Then the diagram is

\[
\begin{array}{c}
\text{Now causality requires us to continue to allow "backward scat" --- pair production --- for all situations (doesn't matter what constant when pair is produced), but the formula \((\ast)\) is relativistically invariant for } t_0 < t_a, \\
\text{because } N(x,t) \text{ is real in space-like region.}
\end{array}
\]

\[
\text{The new diagram gives us new physics ---}
\]

\[
\text{antisymmetric.}
\]
Problem: Do Compton effect

\[ \begin{array}{c}
K_1, e_1 \\
\uparrow \quad \downarrow \\
K_2, e_2 \\
\end{array} \]

Note we can write:

\[ N = \quad \begin{array}{c}
+ \\
\text{pair production} \quad \text{pair annihilation} \\
\end{array} \]

Actually we must integrate:

\[
\sqrt{a} \int d^3x_0 d^3x_1 d^3x_2 \left[ \sum_{\mathbf{p}_3} e^{i\mathbf{p}_3 \cdot \mathbf{x}_3} e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_0 - \mathbf{x}_1)} e^{-i\mathbf{p}_2 \cdot \mathbf{x}_2} \right] \chi(x_{b, t_0}) \chi(x_{a, t_0})
\]

\[
\left[ \sum_{\mathbf{p}_0} e^{i\mathbf{p}_0 \cdot \mathbf{x}_0} e^{i\mathbf{p}_1 \cdot (\mathbf{x}_b - \mathbf{x}_0)} e^{-i\mathbf{p}_2 \cdot \mathbf{x}_2} \right] \chi(x_{b, t_0}) \chi(x_{a, t_0})
\]

\[ t_0 < t_a \]

\[ t_0 > t_a \]
To describe spin-\(\frac{1}{2}\) particles without hypothesizing the Dirac equation (which presumes antiparticles), we have:

\[
[J_x, J_y] = i J_z
\]

Also Lorentz generators \(1 + i \sigma \in \mathbb{N}_2\) found:

\[
[J_x, N_3] = 0
\]

\[
[N_x, N_y] = -i J_z
\]

\[
[N_x, J_y] = i N_z
\]

Also a momentum operator \(P\):

\[
[J_z, P_x] = i P_y
\]

\[
[J_x, P_x] = 0 = [J_z, P_z]
\]

\[
[N_z, P_z] = i P_x
\]

\[
[N_x, P_x] = i P_z \quad \text{etc.}
\]

Can try to find representation for these groups.

However, consider a particular case.

State \(10, i\)
Consider uniform motion
\[ e^{i v r} |0; i\> \equiv |p_z; i\> \]
creates state of uniform motion
\[
\tan \theta = \frac{p}{E} \\
\sinh \theta = \frac{p}{E} \\
\cosh \theta = \frac{E}{P_z}
\]
Can prove
\[ P_z |p_z r p_z; i\> = |p_z r p_z; i\> \]
and
\[ P_z e^{iN_z \theta} = e^{iN_z \theta} \left[ P_z \cosh \theta + P_z \sinh \theta \right] \]
The indices i give the spin in the rest system only.
A rotation
\[ J_z = i \left[ P_x \frac{\partial}{\partial y} - P_y \frac{\partial}{\partial x} \right] + J_z \]
and
\[ N_z = i \left[ P_z \frac{\partial}{\partial z} - P_z \frac{\partial}{\partial z} \right] + \left( \frac{i \times \mathbf{P}}{E + m} \right)_z \quad P_z = \sqrt{m^2 + P^2} = E \]
He then used these to set up a system of states for spin \( \frac{1}{2} \) particle.
Now we want to apply this to scattering problems

\[ |\Psi\rangle = \sum_{p} \alpha_{p} |p, p\rangle + \alpha_{p} |p, -p\rangle \]

For elastic scattering

\[ |p\rangle \rightarrow |p\rangle \]

Use interaction \( V(p, p') \), which includes the matrices.

We now consider scattering from a scalar potential

\[ V(p, p') = 0 \]

This is enough to determine 2 solutions:

\[
\frac{(E_{1} + i\eta)(E_{2} + i\eta) - E_{1}E_{2} - i\eta}{\sqrt{2\eta(E_{1} + i\eta)2\eta(E_{2} + i\eta)}} \quad \text{scalar}
\]

and

\[
\frac{(E_{1} + i\eta)(i\sigma_{p} - i\sigma_{p}) - (i\sigma_{p} - i\sigma_{p})}{\sqrt{2\eta(E_{1} + i\eta)2\eta(E_{2} + i\eta)}} \quad \text{pseudoscalar}
\]
Now considered 2nd order scattering.

Turns out amp. for creation is

\[
\frac{(E_2 + \lambda)(\sigma_0 \rho_3) - (E_2 + \lambda)(\rho_0 \sigma_3)}{\sqrt{2\epsilon(E_2 + \lambda)^2 \rho_2(E_2 + \lambda)}}
\]

annihilation

\[
\frac{(E_1 + \lambda)(\sigma_0 \rho_3) - (E_1 + \lambda)(\rho_0 \sigma_3)}{\sqrt{2\epsilon(E_1 + \lambda)^2 \rho_2(E_1 + \lambda)}}
\]

But turns out they are not "fermionic." Then this carries fermi statistics. Note also these formulas look general even though potential was scalar. Means proton has negative parity from enron.

He died for general; he is even all p's are even. Even mystery, off i odd all powers of E's are odd. No fermionic, Fermi statistics.
A simpler kind of argument suggests that for every state \( I \), a time reversed state, and phase un-defined, e.g.

\[ I \rightarrow \quad T| I \rangle = e^{i\theta} | I \rangle \]

However, this argument breaks if \( \frac{\hbar}{2} \) causes

\[ T \left\{ \alpha | a \rangle + \beta | b \rangle \right\} = \alpha^* T | a \rangle + \beta^* T | b \rangle \]

Also

\[ T | - \rangle = \eta | + \rangle \]

Actually, one fixes either \( \eta = \frac{1}{\sqrt{2}} \) or \( \eta = \frac{i}{\sqrt{2}} \). Fix \( \eta = \frac{1}{\sqrt{2}} \)

\[ T | + \rangle = | - \rangle \]

\[ T | - \rangle = \frac{1}{\sqrt{2}} ( | + \rangle - | - \rangle ) \]

Note

\[ T | + \rangle = e^{i\theta} \left\{ | + \rangle - i | - \rangle \right\} \]

\[ \frac{1}{\sqrt{2}} T \{ | + \rangle + | - \rangle \} = \frac{e^{i\theta}}{\sqrt{2}} \{ | + \rangle - | - \rangle \}
\]

\[ | + \rangle + \frac{\sqrt{2}}{2} e^{i\theta} | - \rangle = e^{i\theta} \left\{ | + \rangle - | - \rangle \right\} \]

\[ \Rightarrow \]

\[ T | + \rangle = | - \rangle \]

\[ T | - \rangle = - | + \rangle \]

(\text{T ime \text{\text{\text{\textit{Reversed}}}} \text{\text{\text{\textit{Charged}}}} \text{\text{\text{\textit{Spin}}}}) \frac{1}{2} \]
Double time reversal throws in a phase for spin $\frac{1}{2}$

$T(T|1+\rangle) = T|1-\rangle = -|1+\rangle$

$T(T|1-\rangle) = T(-|1+\rangle) = -|1-\rangle$

Ospin

$T|0\rangle = e^{i\phi}|0\rangle$

$T(T|0\rangle) = T(e^{i\phi}|0\rangle) = e^{-i\phi}T|0\rangle = |0\rangle$

$\Rightarrow$ + phase for integral spin
Compton Scattering

This first calculation will be rather lengthy. 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

\[ p_1' = (m, 0, 0, 0) \]
\[ k_1 = \omega_1 (1, 0, 0, 1) \]
\[ k_2 = \omega_2 (1, \sin \theta, 0, \cos \theta) \]
\[ p_2 = (E_2, p_2 \sin \phi, 0, p_2 \cos \phi) \]

Note

\[ p_2 = p_1' + k_1 - k_2 \]

Squaring

\[ m^2 = m^2 + 0 + 0 + 2 \mathbf{p}_1 \cdot \mathbf{p}_2 - 2 \mathbf{k}_1 \cdot \mathbf{k}_2 - 2 \mathbf{k}_1 \cdot \mathbf{k}_2 \]
or using our 4-vectors

\[ 0 = m \omega_1 - m \omega_2 - \frac{\omega_1 \omega_2}{c^2} (1 - \cos \theta) \]

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.

Also add in polarizations

\[ e_1 = (0, 0, 1, 0) \quad \text{plane} \]
\[ e_1 = (0, 1, 0, 0) \quad \text{in plane} \]

\[ e_2 = (0, \cos \theta, 0, -\sin \theta) \quad \text{in plane} \]
\[ e_2 = (0, 0, 1, 0) \quad \text{plane} \]

[To get recoil momentum, square

\[ \mathbf{p}' = \mathbf{p} + \mathbf{k}_1 - \mathbf{k}_2 \]

to get \( 0 = \cdots \). Etc.]
Now we develop Klein-Nishina formula for $\sigma$,

$$\sigma_{\text{total}} = 2\pi S (E_{\text{cm}} - E_{\text{in}}) \frac{k^2}{(2\pi)^3} \frac{1}{M^2}$$

Now recall

$$H = \beta m + \alpha^2 (p - \frac{e}{c} A) = H_0 + H_{\text{int}}$$

where

$$H_0 = \beta m + \alpha^2 p$$

$$H_{\text{int}} = \frac{e}{c} \alpha^2 A$$

Now recall

$$\langle A \rangle = \frac{1}{\sqrt{2\omega}} \left[ \Phi^r_{\text{in}} e^{i\mathbf{k} \cdot \mathbf{x}} + \Phi^l_{\text{in}} e^{-i\mathbf{k} \cdot \mathbf{x}} \right]$$

Then

$$M = \left\langle \frac{\langle i H_{\text{int}} \rangle}{E - E_{\text{ex}}} \right\rangle$$

Write upide

$$\sigma_{\text{total}} = \pi S \left( \frac{\sqrt{\omega^2 + (k_1^2 + k_2^2)^2} + \omega_2 - m - \omega_1}{\omega^2} \right) \frac{k_2^2}{k_1^2} \frac{d\omega_1}{d\omega_2} \frac{1}{M^2}$$

$$\left( \frac{1}{\sqrt{\omega_1^2 + k_1^2 + k_2^2 - 2i\kappa_1 \cos \theta + k_2 - m - \omega_1} \right)$$

We use

$$\int f(x) \, dx = \frac{1}{f(0)}$$
\[
\frac{d}{dN_2} = \frac{\nu_2 - \nu_1 \cos \theta}{\sqrt{\frac{E_2}{E_2}}} + 1 = \frac{\nu_2 - \nu_1 \cos \theta + E_2}{E_2} = \frac{E_1 + \omega_1 - \omega_1 \cos \theta}{E_2} = \frac{m c^2}{E_2 \omega_2}
\]

and using conservation of energy

or

Compton formula

Thus integrating over \( N_2 \)

\[
\text{Pred} = \sigma_{\nu} = \sigma_c = \omega_2^2 \frac{\omega_2 E_2}{m c^2} \frac{1}{(2\pi)^2} |M|^2
\]

Now for matrix element, we consider possible intermediate states

\[
\langle \text{photon 2 emitted} | \text{photon 1 emitted} \rangle \text{ A}
\]

\[
\langle \text{photon 1 emitted} | \text{photon 2 emitted} \rangle \text{ B}
\]
Then

\[ A = \frac{\langle 2 | e^{i k_1} | i \rangle \langle i | e^{-i k_2} | 1 \rangle}{E_1 + \omega_1 - E_1} \]

\[ B = \frac{\langle 2 | e^{i k_1} | j \rangle \langle j | e^{-i k_2} | 1 \rangle}{E_1 - \omega_2 - E_3} \]

Can associated pictures with these:

\[ \text{A} \]
\[ \text{B} \]

[Have actually calculated

\[ M_{\text{2} \rightarrow \text{1} \rightarrow \text{2}} (\frac{\hbar}{2})^2 = A + B \]

For more elaborate problems we need \( i \) for resonances.

Note we have made these calculations in a conventional non-relativistic way -- but they contain hints relativistically plane wave states...\]
Can write using Dirac plane waves

\[ A = \sum_{E_i} \frac{\langle u_{2}^* | \alpha_{1} | u_{1} \rangle \langle u_{1}^* | \alpha_{1} | u_{1} \rangle}{E_i + \omega_{1} - |E_{i}|} \]

\[ P_j = P_i - \hbar k_2 \]

\[ B = \sum_{E_i} \frac{\langle u_{2}^* | \alpha_{1} | u_{1} \rangle \langle u_{1}^* | \alpha_{1} | u_{1} \rangle}{E_i - \omega_{2} - |E_{i}|} \]

\[ \text{But all negative } E \text{ states are full. Need 2 new possibilities} \]
$$C = -\frac{\lambda}{2} \left\langle \frac{2 |d_1 e^{ik_1 x} | k \rangle \langle k | d_2 e^{-ik_2 x} | \rangle}{E_1 + \omega_1 - (E_1 + E_2 + 1E_k)} \right\rangle$$

Fluid: \( F_1 = P_2 - 1N_1 = P_1 - 1N_2 = P \) before

Can also show demon = \( \omega_2 - E_1 - 1E_k \)
\[ \text{Rate} = \sigma \omega = 2 \pi \hbar \left( E_{\text{in}} - E_m \right) \frac{1}{(2\pi)^3} |M|^2 \]

\[ \sqrt{2\omega_1 \omega_2} \frac{1}{e^2} M = A + B \]

\[ A = \sum_{\text{spin}} \frac{(u_2^* d_2 u_1) (u_3^* d_1 u_1)}{E_1 + \omega_1 - |E_2| + i\epsilon} \]
\[ B = \sum_{\text{spin}} \frac{(u_2^* d_2 u_1) (u_3^* d_1 u_1)}{E_1 + \omega_1 + |E_1| - i\epsilon} \]

\[ B = 2 \iff 1 \]

\[ \omega_1, \omega_2 \iff -\omega_2, -\omega_1 \]

Technically the main difference in the last line is in the ±i\epsilon. Only important for resonances, but since resonances can't vanish in Compton scattering, we disregard this.

Now we can pick polarization of electron & photon, and calculate after some algebra. We will go on to the shortest cuts however.
\[ (u_2^2, u_2 u_1) (u_1^* u_1) \]

or

\[ (u_2^* u_1^*) (u_1^* u_1) \]

or

\[ \sum_{b \neq a} \lambda_{ab} u_a u_b^* \]

\[ \lambda_{ab} = \sum_{b \neq a} \frac{u_a u_b^*}{|u_a|^2} \]

This is the form \( u \) into which we now want to get. We will work out backwards to the initial form

\[ E = \sqrt{\not{u}_2^2 + \not{u}_1^2} \]

\[ u = \frac{1}{\sqrt{2E}} \begin{pmatrix} 1 \\ \not{u}_2 \\ \not{u}_1 \end{pmatrix} \]

\[ u a u_b^* = \frac{1}{2E} \begin{pmatrix} 1 \\ \not{u}_2 \\ \not{u}_1 \end{pmatrix} = \frac{1}{2E} \begin{pmatrix} E + \not{u}_1^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

\[ u = \frac{1}{\sqrt{2E}} \begin{pmatrix} E + \not{u}_1^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

Some idea

\[ = \frac{1}{2E} \begin{pmatrix} E + \not{u}_1^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]
\[ \lambda = \frac{1}{2E} \begin{pmatrix} E+\mu & 0 & 0 & 0 \\ 0 & E+\mu & 0 & -\rho \\ -\rho & 0 & E-\mu & 0 \\ 0 & 0 & 0 & E-\mu \end{pmatrix} \]

\[ = \frac{1}{2E} (E1 + \mu \beta + \alpha^2 \rho) \]

in general,

\[ \lambda = \frac{1}{2E} (E1 + \mu \beta + \alpha \cdot 0 \cdot 1 \rho) \]

then

\[ A = \frac{u_2^* \alpha_2 (|E_i| + \mu \beta + \alpha \cdot 0 \cdot 1 \rho_i) \alpha_i U_i}{2 |E_i| (E_i + \omega_i - |E_i|)} \]

\[ + \frac{u_2^* \alpha_2 (E_i - \mu \beta - \alpha \cdot 0 \cdot 1 \rho_i) \alpha_i U_i}{2 |E_i| (E_i + \omega_i + |E_i|)} \]

\[ E_i = \sqrt{\mu^2 + (\rho + 1 \omega_i)^2} \]
Note we might have deduced this by using
\[ \langle 21A_1i \rangle \langle i | B_1i \rangle = \langle 21AB1i \rangle \]

But note also
\[ \langle u_2^* N (H_{ip} + L_{ij}) u_i \rangle = \frac{1}{2E_{ij}} \]

\[ = \langle \sum_{pm} (u_2^* Nu_{pm}) (u_i^* Nu_{mi}) \rangle \]

\[ = \frac{u_2^* N (1E1+H) Nu_i}{2E_{1j}} \]

This is what we could have done to get \( \tilde{A} \), used the concept of projection operator \( 1E_{1j} + H \). (Verify!)

Next add terms to find
\[ A = \frac{u_2^* \alpha_2 (E_{1j} + \omega, -\mu \beta - \alpha^0 \cdot \mathbf{r}_i) \alpha_1 u_i}{(E_{1j} + \omega)^2 - 1E_{1j}^2} \]

We now find a way to write this directly.
\[ A = \frac{\alpha_2^2 \left( E_1 + \omega_1 + \sigma (p_1 + ik_1) + i\beta \right) \alpha_4 \alpha_4}{(E_1 + \omega_1)^2 - (p_1 + ik_1)^2 - \mu^2} \]

Note how this appears rel. invariant. How can we make the invariance obvious by cleaning up Dirac notation.

Recall we had:

\[ \gamma_+ = \beta \]
\[ \gamma_x = \beta \gamma_0 \alpha_x \quad \gamma_y = \beta \gamma_0 \alpha_y \quad \gamma_z = \beta \gamma_0 \alpha_z \]

so we can rewrite Dirac equation

\[ (E_0 \beta - \beta \alpha_0 \alpha_0) \mu = m \mu \]

\[ P_\mu \gamma_+ \mu = m \mu \]

Thus put \( A \) in terms of \( \gamma_+ \)
\[ A = \frac{\left( u_2 \varphi_2 \left( \mu_1 + \lambda \mu \right) \left( \varphi_1 + \mu \right) \right) \varphi_1 u_1}{\left( \mu_1 + \lambda \mu \right) \left( \mu_1 + \lambda \mu \right) - \mu^2} \]

Can imagine \( \varphi \cdot e_i = \varphi \mu \varepsilon_i \) where \( \varepsilon_i = (0, \ldots, 0) \)

Define \( u^* \beta = \bar{u} \) \hspace{1cm} \text{relativistic conjugate} \]

\[ u^* = u_1^* u_2^* u_3^* u_4^* \]

\[ \bar{u} = u_1^* \ u_2^* - u_3^* - u_4^* \]

and

\[ \gamma \mu \varepsilon_i = \varphi \]

Then

\[ A = \frac{\bar{u}_2 \varphi_2 \left( \mu_1 + \lambda \mu \right) \varphi_1 u_1}{\left( \mu_1 + \lambda \mu \right)^2 - \mu^2} \]

Note: "strength of intermediate state depends on"

\[ 1 \]

\[ \left( \lambda \mu + \mu \right)^2 - \mu^2 \]
Problem:
Positron annihilation: \( e^+ + e^- \rightarrow 2\gamma \) (dissipative model)

Estimate lifetime of positronium
Decay polarization character of photons

Compton Effect (continued)

Note: \( B \) is topologically different from \( A \). Now write amplitudes in new notation

\[
A = \frac{(\bar{u}_2 \gamma_2 (p_1 + k_1 - m) \gamma_1 u_1)}{(p_1 + k_1)^2 - m^2}
\]

\[
B = \frac{(\bar{u}_2 \gamma_2 (p_1 - k_2 + m) \gamma_1 u_1)}{(p_1 - k_2)^2 - m^2}
\]

Can we figure out a way to write these directly? Recall notation

\( a \cdot b = a_x b_x + a_y b_y + a_z b_z \)

\( \gamma_a = (\gamma_i, -\beta \gamma_i, -\beta \gamma_i) \)

\( \chi_a = (\beta, \beta \gamma_1, \beta \gamma_2, \beta \gamma_3) \)

\( a \cdot \chi_a = \beta (a_+ - \beta \cdot a) \)
\[ \mathcal{A} = \nabla \psi = \frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial y} + \frac{\partial \psi}{\partial z} + \frac{\partial \psi}{\partial t} \]

\[ = \beta \left[ \frac{\partial \psi}{\partial t} + \omega \cdot \mathbf{A} \right] \]

Now
\[ \beta^2 = g_{\mu} \cdot g_{\mu} \]
\[ \beta = \beta \Rightarrow g_{\mu} = b_{\mu} \]

Sometimes he uses \( \gamma \) for 4-vectors also \((\gamma, \beta)\)

\[ \alpha \psi = 2(a \cdot b) - b \cdot a \] \([\text{express commutation laws of } \alpha \text{'s}]\)

\[ \phi x u + v u d = 2a u \]
\[ \gamma u x u + v u y u = 2 \phi u d \]

The Dirac equation now becomes

\[ (i \mathcal{A} - \frac{\gamma}{2} \mathcal{A} - m) \psi = 0 \]

\[ \text{Ex: } \phi = -\gamma x, \quad \psi = m \phi + \text{etc.} \]

Current Density
\[ j_{\mu} = \overline{\psi} \gamma_{\mu} \psi \]

\[ \overline{\psi} = \left( \psi^* \psi_2^* - \psi_2^* \psi^* \right) \]

\[ \psi \times \phi \text{ density} \]

\[ \psi \times \psi \text{ current} \]
Now our matrix element looks relativistic invariant.

1) But $u_1$ & $u_2$ are not strictly invariant because of normalization.

2) Formula for prob/see: please space density $\rho$

3) Rel. mass of $e$

---

1) Normalization: we have been looking

$$u^*u = 1 = \bar{u}e^u = \alpha \xi u$$

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 $\frac{1}{2E}$ factor in front of operator]

$$\bar{u}e^u = 2E = u^*u$$

Also change $M$ as

$$M = M \sqrt{2E} \sqrt{Z_e} \sqrt{Z_w} \sqrt{\frac{1}{2}} \text{ energy of every free particle}$$
2. Our old formula was

\[ \text{Rate} = 2\pi \delta(E_f - E_i) \frac{d^3 k_z}{(2\pi)^3} \frac{1}{2E_2 \omega_2 \omega_2} |M|^2 \]

\[ = \frac{(2\pi)^4 \delta(E_f - E_i) \delta^3(p_z - p_i) d^3 k_z}{2E_2 \omega_2} \frac{d^3 p_z}{(2\pi)^3 \omega_2} \frac{d^3 p_i}{(2\pi)^3 \omega_2} |M|^2 \]

\[ \text{d}p_z \neq \text{d}p_z \text{ limit } \frac{d}{E} = \frac{d}{E} \text{ for } \text{invariant} \]

Actually rate isn't invariant due to \( \frac{1}{E_2 \omega_2} \)

Structured people use

\[ 2\pi \delta(p_z - p_i^2) \frac{d^3 p_z}{(2\pi)^3} \text{ as invariant differential.} \]

This in general

\[ \text{Rate} = (2\pi)^4 \delta^4(4\text{momentum out} - 4\text{momentum in}) \]

\[ \frac{1}{2E \text{ in} \text{ out}} \frac{d^3 \text{Pos}}{(2\pi)^3 2E \text{ in} \text{ out}} |M_{fi}|^2 \]

\[ \text{End. manipulation} \]
\[
\text{Rate} = \left( \frac{1}{2E_m} \right) \left( \frac{1}{2E_\text{out}} \right) \cdot \text{density of initial states}/\text{unit energy range} \cdot 2\pi \cdot |M|^2 \\
\]

\[
= \left( \frac{1}{2E_m} \right) (2\pi)^4 \cdot S^4 \left( \frac{\Delta P_m - \Delta P_\text{out}}{\Delta P_\text{out}} \right) \prod_{\text{out}} 2\pi \cdot S(p^2-m^2) \cdot \frac{d^4P}{(2\pi)^4} \cdot |M|^2 \\
\]

where

\[
2\pi \cdot S(p^2-m^2) \cdot \frac{d^4P}{(2\pi)^4} = \frac{d^3P}{(2E_1)(2\pi)^3}
\]

Compton scattering yields

\[
M = \frac{\bar{u}_2 \gamma_2 (p + \frac{k}{E_1} + m) \gamma_1 \kappa_1}{(p + \frac{k}{E_1} + m)^2 - m^2} + \frac{\bar{u}_2 \gamma_1 (p - \frac{k}{E_2} + m) \gamma_2 \kappa_2}{(p - \frac{k}{E_2} + m)^2 - m^2}
\]

The main idea was to write the rate in a manner in which the relativistic invariance is obvious. Note for 2 particles in

\[
\text{Rate} = 0 \quad \text{if} \quad |\mathbf{v}_1 - \mathbf{v}_2| \\
\]

The cross-section should be invariant. Note from earlier this means \(|v_1 - v_2|\) is invariant since the rate transforms as \(v_1, v_2\). Can try to demonstrate this.

For only one particle in,

\[
\text{Rate} = \frac{1}{\tau}, \quad \tau = \text{lifetime}
\]
In our expression for $M$, \[ \frac{p + k + m}{(p + k + m)^2 - m^2} \] is called the propagator of a virtual photon. In general for an electron propagator

\[ \frac{p + m}{p^2 - m^2 + i \epsilon} \]

For interaction with a photon of polarization $\epsilon$,

\[ \omega_{\text{ph}} = \sqrt{4\pi} e \epsilon \]

The amplitude for a free electron to enter is $\psi$ and leave $\psi$.

Thus we can construct the matrix element directly

\[ \langle \text{amp for electron beeline to } \overline{U}_2 \rangle \langle \text{amp. to interact with photon} \rangle \langle \text{propagator from entry point } \rangle \langle \text{amp to photon} \rangle \langle \text{beeline to } \overline{U}_1 \rangle \]

\[ \overline{U}_2 \quad \overline{U}_1 \]

\[ \frac{(p + k_1 + m_1)}{(p + k_1 + m_1)^2 - m_1^2} \]

\[ \frac{(p + k_2 + m_2)}{(p + k_2 + m_2)^2 - m_2^2} \]
Note the propagator is usually written as
\[ \frac{1}{\not{p} - m} \]
on the reciprocal of a number.

Must solve \((\not{p} - m) \chi = 1\)

\[ \frac{(\not{p} - m)(\not{p} + m)}{p^2 - m^2} = \frac{p^2 - m^2}{p^2 - m^2} = 1 \]

\[ \Rightarrow \frac{1}{\not{p} - m} = \frac{\not{p} + m}{p^2 - m^2 + i \epsilon} \]

Thus the propagator is in general the reciprocal of a Dirac operator. Consider

\[ (\not{p} - m) \psi = S \]
as Dirac eqn for free particle

Take F.T.

\[ (\not{p} - m) \psi = S \]
or \[ \psi = \frac{1}{\not{p} - m + i \epsilon} S \]

Thus a mnemonic is to regard each interaction as a source of waves.

\[ \overline{u}_2 \phi_2 \frac{1}{\not{p} + \not{k}_2 - m} \phi_1 u_1 \]
Consider

\[(i \nabla - \kappa - m) \psi = 0\]

or

\[(i \nabla - m) \psi = \kappa \psi\]

Solve by Neumann series

\[\psi_0 = \phi, \quad \text{with } (i \nabla - m) \phi = 0\]

Next solve

\[(i \nabla - m) \psi_1 = \kappa \psi_0\]

\[\psi = \phi + \frac{1}{i \nabla - m} \kappa \phi + \frac{1}{i \nabla - m} \kappa \psi + \cdots\]

This is just a perturbation expression.

Thus it is important to learn these kinds because they make the calculations so much simpler.

Also idea of representing a scattering as a 2nd order process
In general, for $\nabla A = 0 \quad \phi = 0$

\[ A_{\mu} = e_\mu e^{-i k \cdot x} = e_\mu e^{-i (\omega t - k \cdot x)} \]

\[ \nabla A = 0 \Rightarrow \phi X = 0 \quad \phi = 0 \Rightarrow e_t = 0 \quad e \cdot e = 1 \]

But note:

\[ e_\mu k_\mu = e_\omega = e_1 k_1 = 0 \]

\[ e_\mu e_\mu = -1 \]

But expect that we could possibly transform to a 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 case.

\[ (\nabla - \gamma \cdot A - m) \psi = 0 \]

\[ (\nabla - \gamma \cdot A - \kappa X - m) \psi'' = 0 \]

Hence, \[ \psi'' = e^{i \chi} \psi \] we get same physics. Thus gauge invariance introduces a phase.
Substituting in
\[ \xi_{\mu} \left( i \gamma_{\mu} - A^{\prime}_{\mu} \right) e^{i x} \psi - m e^{i x} \psi = 0 \]

\[ e^{-i x} \left[ \gamma_{\mu} \left( -i \partial_{\mu} + \bar{A}_{\mu} \right) \right] \psi = m e^{i x} \psi \]

or
\[ \xi_{\mu} \left[ i \partial_{\mu} - (A^{\prime}_{\mu} - \bar{A}_{\mu}) \right] \psi = m \psi \]

\[ \xi_{\mu} \]

Q.E.D.

Thus rule is to use
\[ A^{\prime\prime}_{\mu} = A_{\mu} + \partial_{\mu} x \]
\[ \psi^{\prime\prime} = e^{i x} \psi \]

Thus support we have phase won

\[ A_{\mu} = e_{\mu} e^{-i k_{\mu} x} \]
\[ A^{\prime\prime}_{\mu} = e_{\mu} e^{-i k_{\mu} x} = A_{\mu} + \partial_{\mu} x \]
\[ = e_{\mu} e^{-i k_{\mu} x} + b_{\mu} e^{-i k_{\mu} x} \]

Thus \[ e_{\mu} = e_{\mu} + b_{\mu} \] without changing physics.

Can always use the gauge invariance to get rid of the time component \[ e_{\mu} \]. Thus can always wipe out of the scalar potential.

Klein demonstrated this on Compton wave demand.
\[ M_{\text{new}} = M_{\text{old}} + \alpha \overline{u}_2 \overline{f}_2 \frac{1}{\beta + K_1 - m} u_1 + \overline{u}_2 \overline{f}_1 \frac{1}{\beta - K_1} \frac{1}{\beta - K_1 - m} u_1 \]

\[ \overline{u}_2 \overline{f}_2 \frac{1}{\beta + K_1 - m} (\beta + K_1 - m) u_1 - \overline{u}_2 \overline{f}_1 \frac{1}{\beta - K_1} \frac{1}{\beta - K_1 - m} \alpha u_1 \]

\[ \overline{u}_2 \overline{f}_2 u_1 - \overline{u}_2 \overline{f}_2 u_1 = 0 \]

\[ \Rightarrow M_{\text{new}} = M_{\text{old}} \Rightarrow \text{formula is gauge invariant} \]

Note: Both terms in the matrix elements are of equal significance in determining gauge invariance. Thus, it requires that our diagram is "larger" than another one involving

\[ \Rightarrow \Rightarrow \]

In general, a simple diagram is relativistic invariant but not gauge invariant.

Need all diagram for gauge invariance.
We now double the arithmetic of the Complex formula

\[ \vec{k}_1 \]

\[ \vec{k}_2 \]

\[ \vec{p}_1 = \vec{u}(1,0,0,0) \]

\[ \vec{p}_2 = \vec{k}_1 = \omega_x (1,0,0,1) \]

\[ \vec{k}_2 = \omega_z (1,0,0,0,0) \]

Recall\[ \frac{1}{\omega_2} - \frac{1}{\omega_1} = \frac{1}{u_4} (1 - \cos \theta) \]

Also used\[ \vec{p}_2 + \vec{k}_2 = \vec{p}_1 + \vec{k}_1 \]

\[ \text{yields} \quad \omega_2 = \omega_1 (E_2 - P_2) \]

Now recall\[ M = \frac{-\vec{u}_2 \cdot \vec{p}_2 (P + k + u)}{(P_1 + k_1)^2 - u_1^2} + \frac{-\vec{u}_1 \cdot \vec{p}_1 (P_1 - k_1 + u)}{(P_1 - k_1)^2 - u_1^2} \]

\[ \text{But} \quad \vec{M} = \frac{-\vec{u}_2 \cdot \vec{p}_2 (P + k_1 + u)}{\omega_1} - \frac{\vec{u}_1 \cdot \vec{p}_1 (P_1 - k_1 + u)}{\omega_2} \]

Possible cases:\[ \vec{u}_{1+} = \left( \begin{array}{c} 1 \\ 0 \\ 0 \\ 0 \end{array} \right) \text{ pos z-spin} \quad \vec{u}_{1-} = \left( \begin{array}{c} 0 \\ 0 \\ 0 \\ 1 \end{array} \right) \text{ neg z-spin} \]

\[ \vec{u}_{2+} = \left( \begin{array}{c} \sqrt{\frac{E_x + E_y}{2}} \cos \frac{\alpha_2}{2} \\ \sqrt{\frac{E_x - E_y}{2}} \sin \frac{\alpha_2}{2} \\ \sqrt{\frac{E_x + E_y}{2}} \cos \frac{\alpha_2}{2} \\ \sqrt{\frac{E_x - E_y}{2}} \sin \frac{\alpha_2}{2} \end{array} \right) \text{ p and y spin} \quad \vec{u}_{2-} = \left( \begin{array}{c} \sqrt{\frac{E_x - E_y}{2}} \sin \frac{\alpha_2}{2} \\ -\sqrt{\frac{E_x - E_y}{2}} \cos \frac{\alpha_2}{2} \\ -\sqrt{\frac{E_x - E_y}{2}} \sin \frac{\alpha_2}{2} \\ \sqrt{\frac{E_x - E_y}{2}} \cos \frac{\alpha_2}{2} \end{array} \right) \text{ p and y spin} \]

\[ \alpha_1 = \theta_x \quad \text{or} \quad \alpha_{1b} = \theta_y \]

\[ \alpha_2 = \theta_x \cos \theta_2 + \theta_2 \sin \theta_2 \quad \text{or} \quad \alpha_{2b} = \theta_y \]

\[ \text{plane pol} \]

\[ \text{plane pol} \]
Thus unwind work on \( M \) for 16 different cases. We do 1 case

\[ u_{1t}, u_{2t}, e_{1a}, e_{2a} \]

\[ \mathbf{A} = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

\[ \mathbf{A} = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

Prepare:

\[ \sigma_X = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \sigma_Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad 1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]

\[ \gamma_Y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \gamma_X = \begin{pmatrix} 0 & \sigma_Y \\ \sigma_X & 0 \end{pmatrix} \]

\[ \gamma_X \gamma_Y = \begin{pmatrix} 0 & \sigma_Y \\ \sigma_X & 0 \end{pmatrix} \quad \gamma_X \gamma_Y = -i \begin{pmatrix} 0 & \sigma_Y \\ \sigma_X & 0 \end{pmatrix} \quad i \gamma_X \gamma_Y = \sigma_Z \]

\[ \gamma_X \gamma_Y \gamma_Z = \gamma_X \gamma_Y = -i \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

\[ \gamma_X \gamma_Y \gamma_Z = \gamma_X \gamma_Y = -i \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

\[ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

where \( \gamma_Z = \gamma_X \gamma_Y \gamma_Z \gamma_X = i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \)

\[ A = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

\[ \mathbf{A} = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

\[ = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

\[ = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

\[ = \frac{U_{2t}}{U_{1t}} \left( \sigma_X \cos \theta - \sigma_Z \sin \theta \right) \left( u_{1t} + m + \omega_1 \phi_1 + \omega_2 \phi_2 \right) \mathbf{u}_{1t} \]

\[ = \left( \frac{U_{E1} \cos \theta}{1 + \frac{U_{E1}}{U_{1t}}} \right) \cos \left( \omega_2 \frac{m}{2} \right) \cos \left( \omega_1 \phi_1 \right) \cos \left( \omega_2 \phi_2 \right) \]

\[ = \left( \frac{U_{E1} \cos \theta}{1 + \frac{U_{E1}}{U_{1t}}} \right) \cos \left( \omega_2 \frac{m}{2} \right) \cos \left( \omega_1 \phi_1 \right) \cos \left( \omega_2 \phi_2 \right) \]

\[ = \left( \frac{U_{E1} \cos \theta}{1 + \frac{U_{E1}}{U_{1t}}} \right) \cos \left( \omega_2 \frac{m}{2} \right) \cos \left( \omega_1 \phi_1 \right) \cos \left( \omega_2 \phi_2 \right) \]

\[ = \left( \frac{U_{E1} \cos \theta}{1 + \frac{U_{E1}}{U_{1t}}} \right) \cos \left( \omega_2 \frac{m}{2} \right) \cos \left( \omega_1 \phi_1 \right) \cos \left( \omega_2 \phi_2 \right) \]
Hamiltonian Form of Q.E.D. (many electron systems) 4/23/67 Lecture

\[ H = \frac{1}{2 \hbar} \int (E^2 + B^2) \, dV + \int \Phi^*(x) \left[ \beta m + e \phi(x) + \alpha \cdot \left( \frac{\hbar}{i \hbar} \nabla - e A \right) \right] \Phi(x) \, d^3x \]

\[ = \frac{1}{2 \hbar} \int (E^2 + B^2) \, dV + \int \Phi^*(x) \left[ \beta m + \alpha \cdot \left( \frac{\hbar}{i \hbar} \nabla - e A \right) \right] \Phi(x) \, d^3x \]

\[ + e \int \Phi^*(x) \left[ \Phi(x) - \alpha \cdot A \right] \Phi(x) \, d^3x \]

Hint of decay of field with \( \Phi \).

Now choose \( \nabla \cdot A = 0 \quad \left[ \nabla^2 \phi = \frac{e}{\hbar^2} \phi \right] \)

Then write

\[ A(x) = \frac{\hbar}{2 \alpha m} (e_i a_{ik} e^{ik \cdot x} + e^* a^*_{ik} e^{-ik \cdot x}) \]

\( e_{k,i} \) = polarization vector of photon of momentum \( k \)

\( i \) = index of photon pol. (2 values)

\( a_{k,i} \) = annihilation op. for photon
\[ H = \sum_{k,i} \hbar \omega_{k,i} a_{k,i}^\dagger a_{k,i} + \int \Psi^* \left[ \left( \omega_{m+i} \right)^2 - 1 \right] \Psi \, d^3x \]

\[ = -\frac{e^2}{2} \int \frac{\Psi^* \Psi \Psi^* \Psi}{R_{xy}} \, d^3x \]

Now write

\[ \Psi(x) = \sum_{p,q} C_{p,q} U_{p,q} e^{-ip \cdot x} \]

\[ \Psi^*(x) = \sum_{p,q} C^*_{p,q} U^*_{p,q} e^{-ip \cdot x} \]

where \( \left( \omega_{m+i \cdot p} \right) U_{p,1} = \xi U_{p,1} \)

where \( \xi = \pm E_p \)

Use indeed

\[ U_{p,q} = \text{solution for (energy solution)} \]

\[ \Psi_{p,q} = \text{(- energy solution)} \]

\[ \Psi_{p,q} = | \Psi_{p,q} |^2 \]
Then
\[ H_{\text{rel, pos}} = \sum_{P_k} E_{P_k} C_{P_k} \]
\[ = \sum_{P_k} E_{P_k} C_{P_k} - \sum_{P_j} E_{P_j} C_{P_j} \]

Define
\[ C_{P_k} = \text{means annih. diatron of mean } P \text{, spin } k \]
\[ C_{P_j} = \frac{1}{Z_{P_j}} \text{ positron of mean } P \text{, spin } j \]

\[ H_{\text{rel, pos}} = \sum_{P_k} E_{P_k} C_{P_k} + \sum_{P_j} E_{P_j} C_{P_j} - \sum_{P_j} E_{P_j} C_{P_j} \]

Now
\[ H_{\text{int, prop, photons}} = -e \sum_{P_k, P'_k, P''_k, \eta, \eta'} \sqrt{\frac{4 \pi e^2}{2 m c}} \left[ u_{P_k} (\bar{c} \cdot \eta \phi_{P_k}) u_{P'_k} \right] \bar{C}_{P_k} \bar{C}_{P'_k} \alpha_{P_k} \cdot \bar{S}(P_k P'_k \eta) \]
\[ \sum_{P_j, P'_j, P''_j} \left[ u_{P_j} (\bar{c} \cdot \eta \phi_{P_k}) u_{P'_j} \right] \bar{C}_{P_j} \bar{C}_{P'_j} \alpha_{P_j} \cdot \bar{S}(P_j P'_j \eta) \]

3. more terms before this. Very Summary. Diagramatically.
Now have 16 terms from Hamilton with diagrams like
Pair Production

Our diagrams are:

\[ \sqrt{4\pi e^2} (\bar{u}_2 u_1) \frac{1}{q^2} (\bar{u}_2 \gamma^\mu (p_1 + K - \mu) u_1) \]

For considering grids of proton, replace \((\bar{u}_2 u_1)\) by:

\[ \bar{p}_2 (\gamma_\mu F_1(q) + \frac{i}{4\pi} (\gamma_\mu \gamma_5 - \gamma_5 \gamma_\mu) F_2(q)) u_1 \] where \(i\) is current operator

Bremsstrahlung

Assume fixed potential \(\hat{V}(R) = \frac{Ze^2}{R}\) usually since most amp comes from small \(q^2\) implies not affected

Also a diagram:

\[ a \rightarrow p_1 + p_2 + K \]

\[ 0 \rightarrow p_1 + p_2 \]
\[
(\frac{1}{2} \lambda^2 e^{w_1}) \left( \frac{1}{(\lambda^2 + N)^2} \right) \left( \frac{1}{(\lambda^2 + N - P^2)^2} \right) \left( \frac{1}{(\pi e^2)^2} \right)
\]

Note: same as beam scattering.
and so on,

\[ \frac{4 \pi e^2}{(p_3 \cdot p_4)} \frac{(v_3 \cdot v_4)}{(p_2 - p_1)^2} \]

As position now, expect same in final order. If potential

Prov mod
Bremsstrahlung (from potential scattering, $a_{\mu}(q)$)

$q = p_2 + k_z - p_1$

\[
\begin{align*}
\text{Scattering with no emission} & \quad \text{Rate} = 2\pi \delta(E_2 - E_1) \frac{d^3P_2}{(2\pi)^3 2E_2 2E_1} \left| \left( \bar{u}_2 a_{\mu} u_1 \right) \right|^2 \\
\text{For both processes above} & \quad \text{Rate} = 2\pi \delta(E_2 + \omega - E_1) \frac{d^3P_2}{(2\pi)^3 2E_2 2E_1} \frac{d^3k}{2\omega} \frac{1}{(2\pi)^3} \left| M \right|^2 \\
M & = \frac{u_2}{p_2 + k - \omega} \frac{d\sigma}{d\Omega} u_1 + \frac{u_2}{p_1 + k - \omega} \frac{d\sigma}{d\Omega} u_1 \sqrt{4\pi} e^2 \\
& = \frac{u_2}{2p_2 \cdot k} (p_2 + k + \omega) d\sigma u_1 + \frac{\bar{u}_2}{-2p_1 \cdot k} (p_1 - k + \omega) d\sigma u_1 \\
\text{We want to consider low $\omega$ behavior (neglect $k \ll p_2 + \omega$)}
\end{align*}
\]
Using commutation law: \( \phi \cdot A = -\hbar \phi - 2(A, b) \)

\[
W = \frac{\bar{u} \left( -m^2 + \frac{2m_0 c + \phi \cdot A}{\sqrt{m^2 + \phi \cdot A}} \right) \phi \cdot A}{2m_0 c} + \frac{\bar{u} \cdot A}{2m_0 c^2} \phi \cdot A
\]

\[
= \left( \frac{\bar{u} \cdot A}{2m_0 c} \right) \left\{ \frac{P \cdot e}{P_0 \cdot k} - \frac{P \cdot e}{P_0 \cdot k} \right\} \sqrt{4\pi e^2}
\]

\[\text{w.m} \quad \text{momentum for scattering without emission of photons}\]

\[\text{amp. that if scattered}\]

\[\text{outside in photon}\]

Thus

\[
\text{Rate} = 2\pi S (E_2 - E_1) \frac{\frac{1}{2} \bar{u} \cdot A (\phi \cdot A)^2}{(2\pi)^3 2E_2 E_1} \left\{ \frac{\omega \left( \frac{P \cdot e}{P_0 \cdot k} \right)^2}{\frac{\omega \left( \frac{P \cdot e}{P_0 \cdot k} \right)^2}{1 + \frac{\omega^2}{\beta^2 k^2}} \frac{1}{2\pi^2} \right\}
\]

\[\text{Treat with no photon emitted}\]

\[\text{prob. that if}\]

\[\text{scattering\ is\ just\ a\ small}\]

\[\text{plastic}\]

\( \frac{d\phi}{d\phi} \) independent of process
To analyze in more detail, consider coordinates:

\[ p_1 \cdot k = E_1 \omega - p_1 \omega \cos \theta = \omega E_1 (1 - v_1 \cos \theta) \]

where \( v_1 = \frac{p}{E} \)

\[ p_1 \cdot e = - p_1 \cdot e = -E v_1 e \]

Given:

\[ \left\{ \begin{array}{c}
\frac{v_1 \cdot e}{1 - v_1 \cos \theta_1} = \frac{v_2 \cdot e}{1 - v_2 \cos \theta_2}
\end{array} \right. \]

\[ = \frac{v_1 \sin \theta_1}{1 - v_1 \cos \theta_1} = \frac{v_2 \sin \theta_2}{1 - v_2 \cos \theta_2} \quad \text{part in plane of collision} \]

Can get same result from classical physics.

**Problem:** Emission of two independent photons.
Classical Bremsstrahlung:

Instead of using Fermi-Dirac potentials, do a different way. Consider a path in 4-space. Now to write current density:

\[ J_\mu(x) = e^{\int Z_\mu(y) \delta^4(x - z(y)) dy} \]

Now we have:

\[ \Box^2 A_\mu = j_\mu \]

Also define F.T.:

\[ A_\mu(k) = \sqrt{A_k(x) e^{-ik \cdot x} d^4 x} \]

Now take F.T. of \( j_\mu \),

\[ k^2 A_\mu(k) = \int e^{-ik \cdot x} j_\mu(x) dx \]

\[ = \sqrt{\int e^{-ik \cdot x} \int Z_\mu(y) \delta^4(x - z(y)) dy dx d^4 x} \]

\[ = \sqrt{\int Z_\mu(y) e^{-ik \cdot z(y)} dy} = J_\mu(k) \]

For \( \alpha < 0 \), \( Z_\mu(\alpha) = P_{\mu} \alpha \)

For \( \alpha > 0 \), \( Z_\mu(\alpha) = P_{\mu} \alpha \)

Thus:

\[ J_\mu(k) = \int_{-\infty}^{0} P_{\mu} e^{-ik \cdot P_{\mu} x} dx + \int_{0}^{\infty} P_{\mu} e^{-ik \cdot P_{\mu} x} dx \]
\[ j(x)(k) = i \left( \frac{P_{1n}}{P_{1n} \cdot k} - \frac{P_{2m}}{P_{2m} \cdot k} \right) \]

which agrees with what we found from QED.

Classical expected energy in dx = \( \hat{E} C(x) dx \). But mean energy liberated is \( \hat{E}^2 C(x) dx \). Then no. of photons is \( \hat{E}^2 C(x) dx \). Like Poisson distribution:

\[
\frac{(\bar{n})^n}{n!} e^{-\bar{n}}
\]
Group

\[ u(x,y) = \xi(x,y) \frac{\partial f}{\partial x} + \eta(x,y) \frac{\partial f}{\partial y} \]

Once-extended group

\[ u'(x,y,y') = \xi(x,y) \frac{\partial f}{\partial x} + \eta(x,y) \frac{\partial f}{\partial y} + \eta'(x,y,y') \frac{\partial f}{\partial y'} \]

where

\[ \eta'(x,y,y') = \frac{D}{Dx} \eta(x,y) - y' \frac{D}{Dx} \xi(x,y) = \frac{\partial}{\partial x} + \left( \frac{\partial y'}{\partial y} - \frac{\partial \xi}{\partial y} \right) y' - \frac{\partial \xi}{\partial y} y'^2 \]

The general form of the ODE is

\[ \xi(x,y,y') = 0 \quad \text{-- a surface} \]

We want \( u \cdot b = 0 \) for invariance

\[ = \xi \frac{\partial f}{\partial x} + \eta \frac{\partial f}{\partial y} + \eta' \frac{\partial f}{\partial y'} = 0 \quad (\text{x}) \]

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 \( W(v,w) = v - w(u) = 0 \)
We are free to choose

\[ u(x, y, y') = u(x, y) \quad \Rightarrow \quad \xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} = 0 \]

\[ \Rightarrow \quad \frac{dx}{\xi} = \frac{dy}{\eta(\xi y')} \Rightarrow \quad u(x, y) = \text{const.} = c \]

\[ \Rightarrow \quad y = y(x, c) \]

Suppose path curves \( u(x, y) = \text{const.} \) are common. Then can solve

\[ \frac{dx}{\xi(x, y(x,c))} = \frac{dy'}{\eta(x, y(x,c))y' + (\eta y' - \xi)y'^2} \Rightarrow \quad v(x, y', c) = c \]

\[ \frac{dy'}{dx} = \frac{1}{\xi} \frac{dx}{dy'} + \frac{1}{\xi} (\eta y' - \alpha) y' - \frac{\xi}{\eta} y'^2 \]

\[ = F(x; c) + F_1(x; c) y' + F_2(x; c) y'^2 \]

\[ F(x; c) + F_1(x; c) y' + F_2(x; c) y'^2 \]

\[ \text{General form of Ricatti equation} \]

Then can write \( y'(x) = y_0(x) + y(x) \)

\[ y_0(x) = \frac{\eta}{\xi} \quad \text{is particular solution} \]

\[ \int (\xi y' - \eta) = 0 \]

\[ (\xi + \frac{y'\xi}{\eta}) y' + \xi \frac{dy'}{dx} - (\eta + y' y_x) = 0 \]
Now if we substitute \((x)\) into \((x, x)\) we get a linear equation for \(g(x)\):

\[
\frac{dg}{dx} = -F(x, c)g(x) - 2\gamma \beta F_2(x, c)g(x) - F_2(x, c)
\]

This can be integrated by quadratures to find \(g(x)\).

---

An alternative method is to introduce canonical coordinates: \(v(x, y), s(x, y)\) so \(\Delta = \varphi = \psi = 0\).

Now ODE is \(W(v, s, \frac{ds}{dr}) = 0\). To admit translation group we require

\[
\frac{ds}{dr} - F(s) = 0
\]

Now substitute \((x, y)\), we have

\[
\frac{s_x + s_y y'}{r_x + r_y y'} - W(s, x, y) = 0
\]
Example: Similarity Transformation \[ \nabla f = x \frac{\partial f}{\partial x} + y \frac{\partial f}{\partial y} \]

Then \[ \nabla (x f) = x \frac{\partial (x f)}{\partial x} + y \frac{\partial (x f)}{\partial y} = \nabla f \]

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.

\[ \Rightarrow \quad y' = \frac{dy}{dx} = F \left( \frac{y}{x} \right) \]

is general form of ODE admitting \( \nabla f \).

Example: Rotation Group \[ \nabla f = -y \frac{\partial f}{\partial x} + x \frac{\partial f}{\partial y} \]

\[ \nabla f = -y \frac{\partial f}{\partial x} + x \frac{\partial f}{\partial y} + (1+y^2) \frac{\partial f}{\partial y} \]

To find invariants \[ \frac{dx}{x} = \frac{dy}{y} = \frac{dy'}{1+y'^2} \]

and \( u(x, y) = x^2 + y^2 \)

take \( \\tan^{-1}(y') - \sin^{-1} \left( \frac{y}{x} \right) = \tan^{-1} v \)
\[ v = \tan\left(\frac{\tan^{-1} y - \tan^{-1} y}{x}\right) = \frac{y - y' x}{1 + y' y x} = \frac{xy' - y}{x + yy'} = f(x + y) \]

In this way you can use different groups to generate a table of 1st order ODE which limits these groups.
Second Order ODE's

Now this parameter family of curves
(2 initial conditions or b.c.)

\( \omega(x, y, a, b) = 0 \)

where \( a, b \) are essentially independent

Invariance under point transformations

\[ \begin{align*}
    x_1 &= \Phi(x, y) \\
    y_1 &= \Psi(x, y)
\end{align*} \]

\[ T[\omega] = \omega(x_1, y_1, a, b_1) = 0 \]

Example: all st. lines in plane

\[ \omega(x, y, a, b) = y - ax - b = 0 \]

Should be invariant under rotation:

\[ \begin{align*}
    x &= x_1 \cos \theta + y_1 \sin \theta \\
    y &= y_1 \cos \theta - x_1 \sin \theta
\end{align*} \]

Can verify this by direct calculation
Now consider $\omega(x_1, y; a, b) = 0$

\[ \frac{\partial}{\partial x} \omega = \omega_x + a \frac{\partial}{\partial y} y' = 0 \]

\[ \frac{\partial^2}{\partial y^2} \omega = \omega_{yy} y'' = 0 \]

Can eliminate $a/b$ from these to obtain some 2nd order ODE

\[ \Omega(x_1, y, y', y'') = 0 \]

Cannot talk about invariance of this ODE \( \Theta \)

\[ \Omega(x_1, y, y', y'') = 0 \]

[\( \Theta \) is some function in \( \text{invar} (***)) \]

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

\[ y_1'' = \frac{\partial y_1'}{\partial x} = \frac{\partial \chi}{\partial y'} = \frac{\chi_x + \chi_y y' + \chi_y y''}{\Phi_x + \Phi_y y'} \]
Need to construct twice extended infinitesimal transformation

$$U'' f(x, y, y', y'')$$

$$U'' f = \frac{\partial f}{\partial x} \frac{\partial y''}{\partial x} + \frac{\partial f}{\partial y} \frac{\partial y''}{\partial y} + \frac{\partial f}{\partial y'} \frac{\partial y''}{\partial y'} + \frac{\partial f}{\partial y''} \frac{\partial y''}{\partial y''}$$

Now

$$y' = \frac{D}{Dx} y - y' \frac{Dy}{Dx}$$

Can also

$$y'' = \frac{D}{Dx} y' - y'' \frac{Dy}{Dx}$$
Example - $eN$ scattering

\[ P_2 = (m, 0, 0, 0) \]
\[ P_1 = (E, p, 0, 0) \]
\[ P_4 + P_3 = P_1 + P_2 \]
\[ P_1^2 = m^2 \]
\[ P_2^2 = m^2 \]
\[ P_3^2 = m^2 \]
\[ P_4^2 = m^2 \]
\[ P_4 (N, p, \theta, \bar{\theta}, 0) \]  \rightarrow all kinematic formulas.

Then

\[ R_{NN} = \frac{1}{2m} \frac{1}{2m} \frac{1}{2m} \]

\[ \frac{1}{(2\pi)^4} \delta^4 (\vec{p}_m - \vec{p}_in) \delta (p_4^2 - m^2) \delta (p_3^2 - m^2) \delta (p_2^2 - m^2) \delta (p_1^2 - m^2) \]

\[ \frac{1}{(2\pi)^4} \frac{1}{(2\pi)^4} \frac{1}{(2\pi)^4} \]

\[ \frac{1}{(2\pi)^4} \frac{1}{(2\pi)^4} \frac{1}{(2\pi)^4} \]
The role for emission of one soft photon

\[ \text{Rate} = \frac{2 \pi^2}{(2\pi)^3} \frac{(k_2, g_2 m_2)^2}{c \Delta \omega \Delta \omega' \phi} \left\{ \frac{\hat{p}_1 \hat{e}_1}{\hat{p}_1 \cdot \hat{e}_1} \right\} \left\{ \frac{\hat{p}_2 \hat{e}_2}{\hat{p}_2 \cdot \hat{e}_2} \right\} \]

Rate depending
radiative coupling

A more elaborate calculation gives

\[ \sigma_{\text{radiation}} = \sigma_{\text{hard}} \cdot C \]

\[ \sigma_{\text{radiation}} = \sigma_{\text{hard}} \cdot \left( \frac{d \sigma}{d \tilde{\omega}} \right)^{(\theta_1, \theta_2)} \cdot C \]

\[ \sigma_{\text{radiation}} = \sigma_{\text{hard}} \cdot \frac{1}{2} \int \frac{d \sigma}{d \tilde{\omega}} \cdot d \tilde{\omega} \cdot f(\tilde{\omega}) \cdot d\tilde{\omega} \cdot C \]

\[ \text{Total interaction cross} = \sigma_{\text{hard}} \cdot C \cdot E \]

Now will find
\[ C = e^{-\int d \tilde{\omega} f(\tilde{\omega}) d\tilde{\omega}} \]

for soft photons

As \( \omega \to 0 \), integral diverges.

However for \( \alpha_E \) experienced with finite parameter, find

\[ \sigma_{\text{radiation}} = \sigma_{\text{hard}} \cdot e^{-\alpha E} \]

\( \alpha \approx \frac{1}{137} \)

This was originally called the "infrared catastrophe!"
c is merely the result of a dumb question.

**BACK TO DIAGRAMS**

Consider e-e scattering

\[ M = \frac{\sqrt{4\pi \alpha^2} \left( \frac{v_4}{v_3} \bar{v}_4 \bar{v}_3 \right) \left( \frac{v_1}{v_2} \bar{v}_1 \bar{v}_2 \right)}{(p_1 - p_3)^2} \]

But there is an exchange possibility. Must also consider

\[ -\sqrt{4\pi \alpha^2} \frac{\left( \frac{v_3}{v_4} \bar{v}_3 \bar{v}_4 \right) \left( \frac{v_1}{v_2} \bar{v}_1 \bar{v}_2 \right)}{(p_1 - p_4)^2} \]

Note: consider something cute, e+e- scattering

\[ M = \sqrt{4\pi \alpha^2} \frac{\left( \frac{v_4}{v_3} \bar{v}_4 \bar{v}_3 \right) \left( \frac{v_1}{v_2} \bar{v}_1 \bar{v}_2 \right)}{i(p_1 - p_3)^2} \]
But also can have annihilation + pair production

\[ W = - \sqrt{4m_1^2 - (p_2 \cdot U_2)(U_2 \cdot U_4)} \]

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**

Suppose we don't want to measure exit spin. Then use

\[ \Xi \left( \bar{u}_2 N u_1 \right)^2 = \Xi \left( \bar{u}_2 N u_1 \right)^\ast \left( \bar{u}_2 N u_1 \right) \]

Now define \( \bar{N} = (\bar{g} N f)^\ast = (\bar{f} N g)^\ast \) (relativistic def.)

Then

\[ \Xi \left( \bar{u}_1 \bar{N} u_2 \right) \left( \bar{u}_2 N u_1 \right) \]|_{\text{limit}} \left( \beta + m \right)
\[ |\bar{u}_2 N u_1|^2 = (\bar{u}_1 \bar{N} (\phi + \mu) \bar{N} u_1) \]

and also
\[ |\bar{u}_2 N u_1|^2 \leq TV [ (\phi + \mu) \bar{N} (\phi + \mu) \bar{N}] \]

To find \( N \) where
\[ N = \lambda B \phi \]
\[ \bar{N} = \bar{\phi}^{*} \phi^{*} \]
Recall
\[ H_0 = \beta m + \alpha \cdot (p - A) + V \]

Now calculate velocity operator
\[ \dot{x} = i \left( H_0 \cdot \alpha - \alpha \cdot H_0 \right) = \alpha x \]

But \[ \alpha x \alpha = 1 \] \( \Rightarrow \) e.v. are \( \pm 1 \). Thus if you measure velocity in \( x \)-direction, you get \( \pm c \)? Zunis Dirac's explanation using simultaneous measurements and ones

\[ \left\langle \frac{X + T - X - T}{T} \right\rangle^2 \sim \frac{P}{\sqrt{P + \hbar^2}} \quad \text{if} \quad T > \frac{\hbar}{mc^2} \]

Whole idea is that Dirac eqn. does not describe motion of a single electron, but rather a combination of electron

No one has been able to interpret \( \alpha_x \alpha_x = 1 \)

Directly. Other interpretations trouble with
\[ \frac{\hbar}{T} (\alpha_x \alpha_y \alpha_z) \quad \text{etc.} \]

Only one interpretable is \( p = E + \alpha \times B \)

No one has ever made a detailed study of how to
interpret the Dirac eqn. Not just a one electron eqn.

\[ \rightsquigarrow \]
How do we know Dirac eqn is relativistically invariant.

\[ \nabla \cdot (\vec{D} - \vec{A} - \vec{m}) \psi = 0 \]

\[ \begin{align*}
\dot{x}' &= dx \\
\dot{y}' &= dy \\
\dot{z}' &= dz \\
\dot{t}' &= dt
\end{align*} \]

these all measurements will be OK.

Suppose Mot's prefers uses

\[ \begin{align*}
\dot{x}' &= x' \\
\dot{y}' &= y' \\
\dot{z}' &= z' \\
\dot{t}' &= t'
\end{align*} \]

Must show Mot's prof. gets same answer as Woe. This is challenge. How unique one quantities \( \gamma \).

Let \( \begin{align*}
\dot{x}' &= x' \\
\dot{y}' &= y' \\
\dot{z}' &= z' \\
\dot{t}' &= t'
\end{align*} \) and ask question to whether physics can be maintained.

Note have some problem in notation.
Problem: mass corrections to electron in from higher order self-interaction

\[ 2m \Delta m = \left( \frac{e^2}{\pi} \right) \int \frac{(\bar{u} \gamma_k (\not{p} - \not{k} + \not{u}) \gamma_m u)}{(p - k)^2 - m^2} \frac{dk^2}{k^2 (2\pi)^4} \]

Try to derive this from non-relativistic thinking

\[ \Delta E = \sum_n \frac{\text{H}_n \text{H}_m}{E_n - E_i} \]

[Easy to do in relativistic notation]

---

Bakets our examination of \( \Psi \) matrices. Consider

\[ [\gamma_\mu (i\gamma_\nu \mu - A_\nu) + m] \Psi = 0 \]

Consider \( \Psi'' = S\Psi \quad S = S(\Psi') \)

Then

\[ [\gamma_\mu (i\gamma_\nu \mu - A_\nu) + m] \Psi'' = 0 \]

\[ = [\gamma_\mu (i\gamma_\nu \mu - A_\nu) + m] S\Psi = 0 \]

\[ \Rightarrow \quad S^{-1} \psi'' S(\gamma_\mu (i\gamma_\nu \mu - A_\nu) + m) \Psi = 0 \]

\[ \Rightarrow \quad \text{physics are same if} \]

\[ \psi'' = S \psi' S^{-1} \]
That is, all F's related by equivalent transformations will give some physics. All commutation relations hold if

\[ S = S^{-1} \quad \text{"relativistically unitary"} \]

where \( S \) defined by

\[ (\tilde{\mathbf{f}} \mathbf{Mg})^* = (\tilde{\mathbf{g}} \mathbf{Mf}) \quad \text{relative adjoint} \]

\[ \Rightarrow \quad \tilde{\mathbf{M}} = \mathbf{S} \mathbf{M}^T \mathbf{S} \]

In the standard representation of Dirac and

\[ \mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \tilde{\mathbf{M}} = \begin{pmatrix} a^+ & -c^+ \\ -b^+ & d^+ \end{pmatrix} \]

Note that means

\[ \tilde{x}_\mu = x_\mu \]

\[ \begin{pmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad \text{as matrices are self-adjoint relativistically.} \]

Demonstrates with

\[ \begin{align*}
\tilde{x}_1^+ &= (\cosh \omega) x_1 - (\sinh \omega) x_2 \\
\tilde{x}_1 &= x_1 \\
\tilde{x}_2 &= x_2 \\
\tilde{x}_2 &= (\cosh \omega) x_1 - (\sinh \omega) x_2
\end{align*} \]

where

\[ \frac{y}{c} = \tanh \omega \]

\[ \cosh \omega = \frac{1}{1 - y^2} \quad \sinh \omega = \frac{y}{\sqrt{1 - y^2}} \]
Fluid \[ S = e^{\frac{1}{2} \Delta z} \]

Recall in rotation,

\[ x' = x \]
\[ y' = y \cos \theta + \frac{1}{2} z \sin \theta \]
\[ y' = -y \sin \theta + \frac{1}{2} z \cos \theta \]
\[ z' = z \]

Cay fluid

\[ J_z = (p x v)_z + \frac{1}{2} \frac{x v}{L_z} \cdot \frac{1}{2} \frac{x v}{L_z} = L_z + \frac{1}{2} \sigma_z \]
Techniques

If we have to sum

$$
\sum_{\text{Spin} \ u_3} (\bar{u}_3 A u_1) (\bar{u}_1 B u_2)
$$

Note: if we had to sum over

$$
\sum_{\text{Spin} \ u_3} (\bar{u}_3 A u_1) (\bar{u}_1 B u_2) = (\bar{u}_3 A B u_2)
$$

$$
\sum_{\text{Spin} \ u_3} (\bar{u}_3 A u_1) (\bar{u}_1 B u_2) = \bar{u}_3 \left(A (\mathbf{p}_1 + \mathbf{m}) B\right) u_2
$$

$$
\sum_{\text{Spin} \ u_3} (\bar{u}_2 u_1) |^2 = \sum_{\text{Spin} \ u_1, u_2} (\bar{u}_2 M (\mathbf{p}_1 + \mathbf{m}) M (\mathbf{p}_2 + \mathbf{m}) u_2

\sum_{\text{Spin} \ u_1, u_2}

= 8p \left[M (\mathbf{p}_1 + \mathbf{m}) M (\mathbf{p}_2 + \mathbf{m})\right]
$$

Now

$$
M : \quad \text{reverse order of all } u
$$

Change applied: i to -i

Useful information:

$$
8p 1 = 4 \quad \text{and} \quad 8p \partial = 0 \quad \text{and} \quad x^2 y = 0
$$
\[ Sp[AB] = Sp[BA] \]

\[ 8p[ABC] = 8p[CAB] + 8p[CBA] \quad \text{[must maintain cyclic order]} \]

\[ 8p[a] = 0 \]

\[ 8p[a.b] = 4(a.b) \]

\[ 8p[a.b.c] = 0 \]

\[ 8p[a.b.c.d] = 4 \frac{1}{2} (a.b)(c.d) + (b.c)(a.d) - (a.c)(b.d) \]

\[ \sum \text{summing over possible polynomials } \phi, \]

\[ \sum_{\text{pol}} \phi \left[ \begin{array}{cccc} \phi & \phi & \phi & \phi \\ \phi & \phi & \phi & \phi \\ \phi & \phi & \phi & \phi \\ \phi & \phi & \phi & \phi \end{array} \right] \]

\[ \text{from gauge invariance} \]
SUMMARY OF RULES FOR PERTURBATION CALCULATIONS

\[ \text{Product transitions} = 2\pi \rho(E) \frac{\Gamma}{m} \frac{\Gamma}{m} \frac{m^2}{m} \]

\[ = (2\pi)^4 \delta^4(p_0) \delta^4(p) \frac{\Gamma}{m} \frac{\Gamma}{m} \left( 2\pi \right) S(p^2 - m^2) \frac{d^4 p}{(2\pi)^4} \]

Now for calculation of matrix element \( M \)

\[ \epsilon \mu \mu = -1 \]

\[ A \mu = 2m \]

Sum over states because for one electron incident

\[ 2p \left[ (p + m) M (p + m) M \right] \]

Electron propagator \[ \frac{1}{p - m + i\epsilon} \]

Photon propagator \[ \frac{1}{p^2 + i\epsilon} \]

Meson propagator (scalar, pseudoscalar) \[ \frac{1}{p^2 - m^2 + i\epsilon} \]
Compliments

Real photon \( \phi \)

Potential \( A(x) = \sqrt{e^{i\theta x}} A(x) \mathrm{d}^4 x \)

Closed loop (fermion) \( -g \phi \)

Virtual photon: \( \Gamma^\mu \rightarrow \Gamma^\mu \)

\( \sqrt{4\pi e^2} \) for each photon coupling

\( \sqrt{4\pi g_\sigma^2} \) for each meson coupling

Pseudoscalar meson \( \chi_0 \rightarrow \chi_0 \)

Scalar meson \( I = 1 \)

Sum each indeterminate momentum by \( \sqrt{\frac{dp}{2\pi^2}} \)

To get phases right,

\( +i \) each electron propagator

\( -i \) each photon

\( +i \) " spin zero meson"

\( -i \) " photon coupling"

Energy \( 2E = \) expectation values of \( i \) \( M \)
In normal form: M_i = \sum \frac{H_i(H_i)}{E_i - E_n}

Also,

\[ \Delta E_i = M_i = \sum \frac{H_i H_i}{E_i - E_n} \]

Thus if we adopt rate formulas to calculate diagonal elements, then

\[ \Delta \text{Energy} = 2E \text{ at values of } i M \]
Self-Energy of Electron

Understanding energy deviation due to interaction with E-H field.

Note momentum $\mathbf{p'}$ is not determinable.

\[
2E \Delta E = \sqrt{\frac{2\hbar^2}{(2\pi)^4}} \left( \frac{\mathbf{U} \cdot \mathbf{U}}{\mathbf{p} - \mathbf{p'} - m^2 + i\epsilon} - \frac{\mathbf{U} \cdot \mathbf{U}}{\mathbf{p}^2 + i\epsilon} \right) - \frac{4\hbar^2 e^2}{\mathbf{p}^2 + i\epsilon}
\]
PROBLEM: $\beta$-decay

Example: $\mu \rightarrow e + \bar{\nu}_e + \nu_e$

Suppose a 4 pt. interaction

Suppose $\nu$ satisfies Dirac eqn with $\mu = 0$

\[ W = \frac{(\bar{d}u\gamma^\mu u_c)(\bar{e}u\gamma^\mu u_a)}{(\bar{c}c)(\bar{d}d)} \sqrt{E} \]  

\[ \alpha = \frac{1 + i85}{2} \]

From experiment

\[ \frac{G_{\mu e}^2}{\tau c} = 1.01 \times 10^{-3} \]

For our example  

\[ (\bar{e}\nu_e)(\bar{\mu}\mu) = (\bar{e}\nu_e)(\bar{\mu}\nu_e)(\bar{\nu}_e\nu_e)(\mu\mu) \]

But this leads to $\mu + \bar{\nu}_e \rightarrow e + \nu_e$. However, using anti-particle we get right result.

\[ \mu \rightarrow e + \bar{\nu}_e + \nu_e \]
Find spectrum of $\mu$-decay, and also demonstrate non-conservation of parity.

Notice that this is lowest order contribution from process -- no propagators, etc. Actually, if we do not assume a complete interaction, get a intermediate interaction.

Suppose we can represent this by current operators

$$M = G_F Q J^*_\mu J^\mu$$

where

$$J^\mu = (\bar{\nu}_\mu \gamma_\mu u_e) + (\bar{u}_e \gamma_\mu d_\mu) + J_{\mu \text{ strong}}$$

$$J^{*\mu} = (\bar{u}_\mu \gamma_\mu u_e) + (\bar{e}_\mu \gamma_\mu d_e) + J^{*\mu \text{ strong}}$$

Note these introduce a number of other processes like

$$e + \nu_e \rightarrow e + \nu_e, \quad e + \bar{\nu}_e \rightarrow e + \bar{\nu}_e, \quad e + \bar{e} \rightarrow \nu_e + \bar{\nu}_e$$
We need the strong force \( N \rightarrow p + e^- + \bar{\nu}_e \). Use things like

\[
\langle \text{proton} | \sum_i J_i | \text{medium} \rangle = (\bar{u}_p \left[ \frac{\gamma_{\mu} + i \gamma_5 \gamma_{\mu} \gamma_{126 \ldots}}{2} \right] u_n) \tag{1.97}
\]

Also, the v_e contribution is \( O(1\%) \).
\[ \Delta (m^2) = -4\pi e^2 i \int \left( \frac{1}{p - k - m + i\epsilon} \cdot \frac{1}{m} \cdot \frac{1}{k^4} \right) \frac{d^4k}{(2\pi)^4 k^2 + i\epsilon} \]

\[ = -\frac{4\pi e^2 i}{m} \int \frac{2m^2 + 2\lambda k}{k^2 - 2\lambda k} \frac{d^4k}{k^2 (2\pi)^4} \]

\[ \sim \frac{2m^2}{\lambda k} + \frac{4(e\lambda)^2}{k^2 k^4} \]

\[ \sim \int \frac{3m^2}{k^4} \log \text{Logarithmic integral} \]

Thus could cut this integration off at \( \Lambda \)

\[ \sim \frac{3\pi^2}{11} \ln \frac{\Lambda}{m} \]

Indicate connection to QED. End of theory.

How can we keep trying for calculation? Any problem with fixed indeterminate momentum gives us a hint. Another way to stop integration.

Multiply integrand by \( C(k^2) \). \( C \rightarrow 0 \) for \( k > \Lambda \).

E.g.,

\[ C(k^2) = \frac{-\Lambda^2}{k^2 - \Lambda^2} \]
Find that all physically measurable processes do not depend on \( \hbar \), thus can take \( \hbar \to 0 \) and get invariant predictions of QED.

This is to use

\[ m^2 = m^2 + \frac{3e^2 \mu^2}{\pi} \ln \frac{\Lambda}{\mu} + \ldots \]

to cancel odd logs before taking limit \( \Lambda \to \infty \).

[Mass renormalization]: Current state of research.
Scattering in a potential to $O(e^2)$

\[ \phi(q) \quad q^2 = p^2 - p_1^2 \]

\[ I = \sqrt{\left( \frac{\bar{u}_2}{p_2 - k - m} \right) \left( \frac{\bar{u}_1}{p_1 - k - m} \right) \frac{1}{k^2} \frac{d^4 k}{(2\pi)^4}} \]

Complication arising for any free particle problem

\[ II = \bar{u}_2 \left( \frac{4\pi e^2}{p_1 - m} \right) \sqrt{\frac{\bar{u}_1}{p_1 - k - m}} \frac{1}{k^2} \frac{C(k^2)}{12\pi^4} u_1 \]

\[ \frac{p_1 + m}{(m^2 - m_1^2)} \quad (m^2 - m_1^2) \quad \text{mass correction} \]

\[ = \bar{u}_2 \bar{u}_1 u_1 u_2 \]
\[ 4 \pi e^2 \left( \frac{u_2}{q^2} \right) \int d^4p \left[ \frac{1}{p-m} \frac{1}{p+q-m} \phi^2 \right] \frac{d^4p}{(2\pi)^4} \]

Need a new type of cutoff (charge renormalization)
Subtract 3 terms

\[ 2p \left[ \frac{1}{p-M} \frac{1}{p+q-M} \phi^2 \right] - 2p \left[ M_2 \right] - 8p \left[ M_3 \right] \]

As before, this is

\[ \begin{array}{c}
  + \\
  + \\
  + \\
\end{array} \]

Use

\[ e_{\text{ep}} = \frac{e^2}{1 - (\ln \frac{A}{m}) e^2 \nu} \]
as charge renormalization

See many books.
We were calculating
\[ r = \frac{4\pi e^2}{(2\pi)^2} \sqrt{\frac{\zeta}{\zeta - \frac{1}{P - m \omega}}} \frac{P^2}{m} - \frac{1}{P - m \omega} \frac{\alpha^2 k^2}{\omega^2} \left\{ h \right\} \left| \frac{\pi}{h} = m \right. \]

Consider the probability of the virtual process for long-time propagation
\[ \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \ldots \]

\[ \frac{1}{P - m_0} + \frac{1}{P - m_0} (a \phi + b) \frac{1}{P - m_0} + \ldots = \frac{1}{P - m_0 - (a \phi + b)} \]

Want to examine this near pole
\[ = (1 + r) \frac{1}{P - M} \text{ new} \frac{P^2}{M^2} \]

Examine
\[ \frac{1}{\left[ 1 - a(p^2) \right]} \frac{1}{\left[ P - f(p^2) \right]} \]

where \( f = \frac{m_0 + b(p^2)}{1 - a(p^2)} \)
\[ = \frac{1}{1 - a} \left[ \frac{p + f(p^2)}{p^2 - f(p^2)^2} \right] \]

Suppose \( M \) satisfies \( M = f(M^2) \), for \( a \), be small
\[ M = m_0 + b(m_0^2) + m_0 a(m_0^2) = m_0 + [m_0 a(m_0^2) + 6(m_0^2)] \]

just old formula for mass correction
Use \( f(p^2) = M^2 + 2M(p - M)\delta'(M^2) + \ldots \)

\[
\frac{1}{1 - \frac{p^2}{(p^2 - M^2)[1 - 2M\frac{\delta'(M^2)}{\delta p^2}]]} = (1 + r) \frac{1}{p - M}
\]

where

\[1 + r = \frac{1}{[1 - \frac{p}{M}][1 - 2M\frac{\delta'(M^2)}{\delta p^2}]} \sim \frac{1}{1 - \frac{p}{M}}
\]

\[r \sim \frac{1}{M} \sqrt{1 - \frac{p}{M}}
\]

\[
v \sim a + 2M(b + Ma^2)
\]

\[
= \left. \frac{\partial}{\partial p^2} [a(p^2)\delta^2 + b(p^3)] \right|_{p = M}
\]

To differentiate \( \sqrt{A} \), use

\[
\frac{1}{A + \Delta A} = \frac{1}{A} - \frac{1}{A} \Delta A + \ldots
\]

Rather than using a new propagator, easier to include \((1 + r)\) in coupling as

\[
\frac{\sqrt{\mu^2}}{\mu} (1 + r)
\]

Thus shift in pole ⇒ shift in vertex

Change in strength of pole ⇒ change in coupling

\( \frac{1}{Z} \) unfortunately is divergent
\[ A \pi^2 \int \frac{\nu}{\vec{p}^2 - \vec{k}^2 - m^2} \frac{1}{\vec{p}^2 - \vec{k}^2 - m^2} \frac{1}{\vec{p}^2 - \vec{k}^2} \frac{\nu}{\vec{p}^2 - \vec{k}^2} \cdot \vec{C}(k^2) \]

\[
= 4 \pi^2 \int \frac{\nu m (\vec{p}^2 - \vec{k}^2 + m^2) - \vec{p} (\vec{p}^2 - \vec{k}^2 + m^2) \nu}{(\vec{p}^2 - 2 \vec{p} \cdot \vec{k}) (\vec{p}^2 - 2 \vec{p} \cdot k) (\vec{p}^2 - \vec{k}^2 - m^2) (\vec{p}^2 - \vec{k}^2)} \frac{\nu}{\vec{p}^2} \cdot \vec{C}(k^2) \]

---

Returns Pauli correction of Dirac eqn

\[
\left[ i \frac{\hbar}{m} \not{\psi} + e A \not{\psi} - \frac{\hbar c}{\not{m}} \left( \not{p} + \frac{i}{\not{\hbar}} \not{A} \right) \right] \psi = \mu \psi
\]

\[
i \frac{\hbar c}{m} (\not{A} \not{A} - \not{A} \not{A}) = \frac{1}{2} \left( \not{A} \not{A} - \not{A} \not{A} \right)
\]

After adding all above diagrams we get an expansion in powers of \( \frac{1}{\hbar^2} \)

\[
\left[ x \not{\phi} + y \left( \not{\phi} - \not{\phi} \right) + z \left( \not{\phi} \not{\phi} - \not{\phi} \not{\phi} \right) + \cdots \right] \psi
\]
First, find me, we need only calculate integral to first order. Thus we examine a technique for doing integrals:

\[
\int \frac{1}{(k^2 - L^2)^3} \frac{d^4 k}{(2\pi)^4} = \frac{1}{32\pi^2 L}
\]

\[
\int \frac{1}{(k^2 - 2p \cdot k + \Delta)^3} \frac{d^4 k}{(2\pi)^4} = \int \frac{1}{[k^2 - (p + \Delta)^2]_3} \frac{d^4 k}{(2\pi)^4} = \frac{1}{32\pi^2} \frac{1}{(p^2 + \Delta)}
\]

\[
\int \frac{k \cdot k}{(k^2 - L^2)^3} \frac{d^4 k}{(2\pi)^4} = 0
\]

\[
\int \frac{k \cdot k}{(k^2 - 2p \cdot k + \Delta)^3} \frac{d^4 k}{(2\pi)^4} = \frac{1}{32\pi^2} \frac{P_1}{p^2 + \Delta}
\]

\[
\int \frac{1}{(k^2 - 2p \cdot k + \Delta)(k^2 - 2p^2 \cdot k + \Delta)} \frac{d^4 k}{(2\pi)^4}
\]

\[
\frac{1}{\sqrt{(k^2 - 1P_x^2 - k^2 - \Delta)^2}} \quad P_x = xP_1 + (1-x)P_2 \quad \Delta_x = x\Delta_1 + (1-x)\Delta_2
\]

Using

\[
\frac{1}{a \cdot b} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2}
\]

very useful
\[ III = \left( \bar{u}_2 \gamma_5 u_1 \right) \frac{4 \pi e^2}{g^2} \int \frac{d^4p}{(2\pi)^4} \left( \frac{1}{p-m} \gamma^\mu \frac{1}{p+\not{q}-m} \right) \right) \operatorname{det} \left[ \gamma^0 \right] (-1) \frac{k^4}{(2\pi)^4} \]

**Vacuum Polarization Term**

\[ \gamma^\mu = 4\pi e^2 \int \frac{d^4k}{(2\pi)^4} \frac{1}{p-k-m} \frac{1}{p-k-m} \gamma^\mu \frac{1}{k^2} C(k^2) \]

Roughly:

\[ \rho_i = \rho_0 + \Delta \rho \]

\[ \gamma_{\mu} = \frac{1}{\rho_0 + \not{p} - m} \gamma_{\mu} = \gamma_{\mu} \frac{1}{\rho_0 - k - m} \gamma_{\mu} + \gamma_{\mu} \frac{1}{p - k - m} \Delta \rho + \frac{1}{\rho - k - m} + \ldots \]

\[ \left[ \frac{1}{\lambda^4} = \frac{1}{A} - \frac{1}{A} \frac{1}{B} \frac{1}{A} + \frac{1}{A} \frac{1}{B} \frac{1}{A} \frac{1}{B} \frac{1}{A} + \ldots \right] \]
add virtual photons $e^2$

write
Problem: Neutral K decay

Background: a K meson is a bodon 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 \( \pi^\pm p \rightarrow \Lambda^0 K^0 \).

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.

\[
S(\Lambda^0) = S(\Xi^+) = S(\Xi^-) = -1
\]

\[
S(K^+) = S(K^-) = +1, \quad S(\bar{K}^0) = S(\bar{\Xi}^0) = 0
\]

If we postulate that strangeness be conserved in strong (i.e. fast) reactions, we predict

\[
\pi^- p \not\rightarrow \Xi^+ K^- \quad \pi^- p \rightarrow \Xi^- K^+
\]

To date predictions of this sort have always worked. However, the theory is rather peculiar in that it predicts two 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 constituents - 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:**

\[ K^0 \rightarrow \pi^+ \pi^- \quad \bar{K}^0 \rightarrow \pi^+ \pi^- \]

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 $\kappa^0$ all alone in a box at $t=0$, what is the probability as a function of time of finding a $\kappa^0$ in the box for $t > 0$?

For people who worry about infinities:

There are some reactions which distinguish between $\kappa^0$ and $\overline{\kappa}^0$ although they have small probability.

$$
\kappa^0 \rightarrow \pi^- + \left( \frac{\mu^+}{e^+} \right) + \nu \\
\overline{\kappa}^0 \rightarrow \pi^+ + \left( \frac{\mu^-}{e^-} \right) + \overline{\nu}
$$

MORE ON THE THEORY OF LINE WIDTHS

Suppose $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I$

Consider the following model:

$\mathcal{H}_0$ has as its eigenstates both

1) a collection of discrete states $\kappa^0, \kappa^+ \kappa^-$ with energies $E^i$

2) a continuum. Each state in the continuum consists of one $\kappa^i$ state, and $n$ particles of a different type called $b$. Each $b$ particle has an energy $E^{bi}$. The $\kappa^i$ state or particle is assumed to always have energy $E^i$ (i.e. it never gets kinetic energy in this model).

**Spectrum of $\mathcal{H}_0$**

$$
\begin{array}{c}
E_{\kappa^0} \\
E^{\text{corrections}} \\
E_{\kappa^+ \kappa^-} \\
E_{\kappa^0 + 2\lambda_0} \\
E_{\kappa^i} \\
E^{\text{corrections}} \\
E_{\kappa^0 + 2\lambda_0} \\
\text{etc}
\end{array}
$$

$\mathcal{H}_I$, as usual, induces transitions between the states of $\mathcal{H}_0$

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 $a_{mn}$; those of the continuum states by $b_k$

$$
i \dot{a}_m(t) = \sum_{m} u_{mm}(t) a_m(t) + \sum_{k} v_{mk}(t) b_k(t)
$$
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 $b_{\nu}$ are small compared to the $a_{\sigma}$; the feeding of continuum states may be assumed to comm mostly from the discrete ones. Hence we arrive at

$$i \dot{a}_m(t) = \sum_n u_{nm}(t) a_m(t) + \sum_{\nu} M_{mn} b_{\nu}(t) e^{-i(E_m-E_\nu)t}$$

$$i \dot{b}_{\nu}(t) = \sum_{m} M_{mn}^* e^{i(E_m-E_\nu)t} a_m(t)$$

Integration gives

$$\dot{a}_m = -i \sum_n u_{nm}(t) a_m(t) - \int_0^t \sum_{\nu} |M_{mn}|^2 e^{-i(E_m-E_\nu)(t-t')} a_m(t') dt'$$

$$\dot{b}_{\nu} = \sum_{m} M_{mn}^* e^{i(E_m-E_\nu)t} a_m(t)$$

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 $\Delta + \Pi$ such that

$$\dot{a}_m = -i \sum_n u_{nm}(t) + \Delta a \sum_n \bar{u}_{nm} a_m(t) - \frac{\Pi_m}{a} a_m(t)$$

$$\Pi = 2 \sum_n \sum_{\nu} |M_{mn}|^2 (E_m - E_{\nu})$$

Define $u_{nm}(t) + \Delta s_{nm} = u_{nm}^{\prime}(t) = u_{nm}(t) e^{-i(E_m-E_\nu)t}$

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 $\nu$

then

$$P_m = \left| \langle a_m(t) | \right|^2 = \left[ \frac{e^{-P_m t} - e^{-P_m t} - 2e^{-\left(\frac{P_m + P_n}{2}\right)t} \cos (E_m - E_\nu)t} {(E_m - E_\nu)^2 + \left( \frac{P_m - P_n}{2} \right)^2} \right]$$

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 $\nu$ which came from this transition. This is

$$P_m + \text{probability that this took place and then the atom in state b decayed}$$
As \( t \) goes to infinity, this total probability approaches \( P_{\text{decayed}} \)

Rate of decay = \( \frac{d}{dt} \left[ \text{Probability that the state has decayed} \right] \)

\[ \phi = \Pi_b P_{m}(t) \]

\[ P_{\text{decay}} = \Pi_b \int_0^\infty P_m(t) \, dt \]

Assuming \( V_{mn}(t) = V(t) \), we find \( V_{mn} = V_{mm}, \ m \neq m \)

\[ P_{\nu}(\omega) = \left| V_{mm} \right|^2 \frac{\Pi_b}{\left[ \gamma^2 + \left( \frac{3a + 3b}{a} \right)^2 \right]^\frac{1}{2}} \left[ \frac{1}{\gamma a} + \frac{1}{\gamma b} = \frac{1}{\gamma a} \left( \frac{\gamma a + \gamma b}{\gamma^2 + \left( \frac{3a + 3b}{a} \right)^2} \right) \right] \]

\[ = \left| V_{mm} \right|^2 \frac{\Pi_b}{\gamma a} \left[ \frac{1}{\gamma a} \left( \frac{\gamma a + \gamma b}{\gamma^2 + \left( \frac{3a + 3b}{a} \right)^2} \right) \right] \]

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

\[ \frac{\gamma a + \gamma b}{\gamma^2 + \left( \frac{3a + 3b}{a} \right)^2} \to 2\pi \delta(\nu) \]

thus

\[ P_{\nu}(\omega) = \left| V_{mm} \right|^2 \frac{2\pi}{\gamma a} \delta(\nu) \]

and the total probability of emitting some photon is

\[ \int P_{\nu}(\omega) \, dnu \, d\Omega = \frac{2\pi}{\gamma a} \left| V_{mm} \right|^2 \rho(\epsilon_a - \epsilon_b) \]

This looks different from what we had before, because of the \( \frac{1}{\gamma a} \)

However, it is easily explained:

Rate = \( 2\pi \left| V \right|^2 \delta(\Delta \epsilon) \times \text{Probability to be in upper state} \)

\[ = 2\pi \left| V \right|^2 \delta(\Delta \epsilon) e^{-P_{at}} \]

Total probability of emission = \( \int \text{Rate} \, dt = 2\pi \left| V_{mm} \right|^2 \frac{P}{\gamma a} \rho(\epsilon_a - \epsilon_b) \)

= \( \frac{P_{at} \times \text{mean life time}}{\gamma a} \)

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 \( \frac{1}{E_c - E_d + \omega} \).

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.

\[
\tilde{a}_q(t) = -i \sum_j V_{jq} a_j(t) e^{-i (E_j - E_q) t},
\]

\[
\tilde{a}_e(t) = -\frac{N_e}{2} \sum_m V_{em} a_m(t) e^{-i (E_m - E_e) t},
\]

\[
\tilde{a}_q(t') - i \int_0^t V_{jq} a_j(t) e^{-i (E_q - E_j) t} dt',
\]

Assume we start with \( a_q = 1 \), all other states unpopulated.

\[
\tilde{a}_e(t) \quad \text{the amplitude to reach some excited state is, to a first approximation}
\]

\[
\tilde{a}_e = -\frac{N_e}{2} \sum_j V_{eq} e^{-i (E_q - E_j) t} f,
\]

\[
f = -i \int_0^t e^{i t'} V_{eq} e^{-i (E_q - E_e) t'} dt',
\]

\[
\tilde{a}_e = \frac{V_{eq}}{E_q - E_e + i \gamma_e/2} \left[ e^{-i (E_q - E_e) t} - e^{-N_e t/2} \right]
\]

Then the transitions to another stable state are given by

\[
a_j(t) = -i \int_0^t \sum_k V_{jk} V_{kq} a_k(t') e^{-i (E_k - E_j) t'} dt'.
\]

\[
= -i \int_0^t \sum_{k' j' q} V_{jk} V_{k' q} \frac{1}{E_q - E_k + i \gamma_k/2} \left[ e^{-i (E_q - E_k) t} - e^{-N_e t/2} \right] dt'.
\]

For light scattering \( V_{ji}, V_{ij} \) are second order, \( a_j \) is first order; \( a_q = 1 + f \).

Hence keeping only second order terms gives

\[
a_j(t) \rightarrow -i \left[ V_{j} j + \sum_{k' j' q} \frac{V_{jk} V_{k' q}}{E_q - E_k + i \gamma_k/2} \right] \int_0^t e^{-i (E_q - E_j) t'} dt' + i \int_0^t \sum_{k' j' q} \frac{V_{jk} V_{k' q}}{E_q - E_k + i \gamma_k/2} \left[ e^{-i (E_q - E_k) t} - e^{-N_e t/2} \right] dt'.
\]

Explicit calculation shows that the last terms can be neglected compared to the other terms at long \( t \).

Hence if \( M_{ji} = V_{j} j + \sum_k \frac{V_{jk} V_{k i}}{E_q - E_k + i \gamma_k/2} \), we find
\[
\text{Probability} = |M_{ji}|^2 \frac{\sin^2 (E_j - E_i) \tau/2}{(E_j - E_i)^2}
\]

\[
\text{Rate} = 2\pi \delta (E_i - E_j) |M_{ji}|^2
\]

Near the resonance the scattering amplitude looks like

\[
\frac{1}{E_i - E_k + i \Gamma/2}
\]

a Breit-Wigner form

(this method of treating widths is sometimes called the Wigner-Weisskopf method)
Last week we obtained:

\[
\mathcal{R}_{nm} = z \prod_{\Delta} \delta \left( \frac{E_m - E_n}{\epsilon} \right) \left| T_{nm} \right|^2
\]

where \( T_{nm} = V_{nm} + \sum_k V_{nmk} \frac{1}{(E_m - E_k + i\epsilon)} \frac{1}{V_{km}} + \sum_{k,f} V_{nmk} \frac{1}{(E_m - E_k + i\epsilon)} \frac{1}{E_m - E_f + i\epsilon} \).\]

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 \( |\psi\rangle \) of the unperturbed system. At \( l \) it gets bumped into state \( |\phi\rangle \) by the perturbation. It moves from \( l \) to \( k \) in state \( |\phi\rangle \), then it is bumped into state \( |\eta\rangle \), etc.

Associate a time with each corner. Along a given straight line:

 state \( |\eta\rangle \) at \( t_0 \), \( n \) becomes state \( |\phi\rangle \) at \( t_1 \).

Hence the graph, which might be written:

\[
(-z)^2 \langle \overrightarrow{n,m} | \psi_{l_{\Delta}} | \overrightarrow{1} \rangle \langle \overrightarrow{1} | \phi_{l_{\Delta}} | \overrightarrow{2} \rangle \langle \overrightarrow{2} | \eta_{l_{\Delta}} | \overrightarrow{3} \rangle \langle \overrightarrow{3} | \gamma_{l_{\Delta}} | \overrightarrow{0} \rangle
\]

takes on the form:

\[
(-z)^2 V_{nl} V_{lm} e^{-i(E_k - E_m)(t_2 - t_1)} e^{-i(E_f - E_l)(t_2 - t_1)} e^{-i(t_1) \frac{E_{\Delta}}{2} (E_m - E_n)}
\]

Since \( t_0 \) is just a constant, set it equal to 0 (this won't influence the rate):

\[
(-z)^2 V_{nl} V_{lm} e^{-i(E_k - E_m)(t_2 - t_1)} e^{-i(E_f - E_l)(t_2 - t_1)} e^{-i(t_1) \frac{E_{\Delta}}{2} (E_m - E_n)}
\]

The perturbation could act at any points \( t_{12}, t_{23} > t_{12}, t_{23}, t_{1} > t_{2} > t_{0} \).

To sum the contributions, integrate over \( t_{12} + t_{23} \).

Change of variables gives:

\[
(-z)^2 \int_{t_1}^{t_3 - t_2} \int_{x=0}^{x=t_1} V_{nl}(x + t_1) V_{lm}(t_1) e^{-i(E_k - E_m)x} e^{-i(t_1) \frac{E_{\Delta}}{2} (E_m - E_n)} dxdt_1
\]

Consider first:

\[
\int_{t_1}^{t_3 - t_2} V_{nl}(x + t_1) e^{-i(E_k - E_m)x} dx
\]
In most cases \( \sqrt{ } \) and \( \sqrt{ } \) vary very slowly with time compared to the exponential. Thus we have
\[
V_{m_2}(t_1) \int_0^\infty e^{-i(E_m - E_{m_2} - i\varepsilon)x} dx
\]
\[
V_{m_2}(t_1) \left[ \frac{e^{-i(E_\varepsilon - E_{m_2} - i\varepsilon)(t_3 - t_1)} - 1}{-i(E_\varepsilon - E_{m_2} - i\varepsilon)} \right]
\]
It is reasonable to replace \( t_3 \) by \( \infty \) in most situations. Then the final result is
\[
\left(-i\frac{V_{m_2}}{E_m - E_{m_2} + i\varepsilon}\right) \int_0^\infty e^{-iE_\varepsilon(t_1^\prime)} dt_1
\]
Notice that all terms in the expansion of \( T \) have the same number of \( \varepsilon \)s
\[
(\varepsilon_\varepsilon^\prime)^m \varepsilon_\varepsilon^{m-1} = -i^m \varepsilon_\varepsilon^{m-1}
\]
The factor \( \frac{1}{E_m - E_{m_2} + i\varepsilon} \) is just the propagator in energy space (\( E_m \) is the energy variable)
obtained by Fourier transforming \( e^{-iE_\varepsilon^\prime} \) (\( t \) is a time difference). In the representation
where \( \hat{H}_0 \) is diagonal,
\[
\hat{e}^{-iE_\varepsilon^\prime} \hat{e} = \hat{e}^{-i\hat{H}_0 t}
\]
Thus we may write
\[
\int_0^\infty \hat{e}^{-iE_\varepsilon^\prime} \hat{e}^{-i\hat{H}_0 t} dt = \frac{1}{E - \hat{H}_0 + i\varepsilon}
\]
Pursuing this leads to the formal expression
\[
\hat{T}(E) = \hat{V} + \hat{V}^* \frac{1}{E - \hat{H}_0 + i\varepsilon} + \hat{V} + \ldots
\]
In interpreting operator inverses like the above, keep in mind that
\[
\frac{1}{A + B} = G(oTch) \left( A + B \right) (oTch) = (oTch)^{-1} (A + B)^{-1}
\]
where \( A, B, 1 + \hat{G}oTch \) are all operators,
\[
G/oTch = \frac{1}{A} - \frac{1}{A^2} B + \frac{1}{A^3} B A^2 - \ldots
\]
works here. Thus we set it equal to
\[
\frac{1}{A + B}
\]
By use of this trick,
\[
\hat{T} = \hat{V} + \hat{V}^* \hat{W}(E)^{\prime} \hat{V}
\]
with
\[
\hat{W}(E) = \frac{1}{E - \hat{H}_0 + i\varepsilon} + \frac{1}{E - \hat{H}_0 + i\varepsilon} + \ldots
\]
may be written
\[
\hat{W}(E) = \frac{1}{E - \hat{H}_0 + i\varepsilon} + \frac{1}{E - \hat{H}_0 + i\varepsilon} + \ldots
\]
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 \( \hat{H}_0 \).
The evaluation of
\[
\langle \psi_n \mid \frac{1}{E - \hat{H}_0 + i\varepsilon} \mid \psi_k \rangle
\]
is non-trivial.
Hence one is forced to try approximation schemes.
Example 1
\[ \langle \Omega_m | T | \Omega_n \rangle = \langle \Omega_m | V | \Omega_m \rangle + \sum_k \frac{\langle \Omega_m | V | \Psi_k \rangle}{E_k - E_m + i\varepsilon} \langle \Psi_k | V | \Omega_m \rangle \]

Here \( |\Psi_k\rangle \) is an eigenstate of \( H_{\text{ion}} \). 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 \( \frac{H_e}{e^+} + \frac{H}{e^-} \rightarrow \frac{p}{p} + \frac{e^-}{e^-} \)

It is only reasonable to split up the Hamiltonian in a different way in the initial state than in the final one

\[ H_{101} = K + (A_{muc}) + k_2 (A_{elec}) + k_3 (B_{muc}) + k_4 (B_{elec}) \]
\[ + C_1 (A_{muc} - B_{muc}) + C_2 (A_{elec} - B_{muc}) + C_3 (A_{muc} - A_{elec}) \]
\[ + C_4 (B_{muc} - B_{elec}) + C_5 (B_{elec} - A_{elec}) + C_6 (B_{elec} - A_{muc}) \]

where \( K \) is kinetic energy; \( C \) is Coulomb energy

\[ V^{\text{I}} = C_1 + C_2 + C_5 + C_6 \]
\[ V^{\text{II}} = C_1 + C_2 + C_4 + C_5 + C_6 \]

The \( V \)'s contain those pieces not in the individual Hamiltonians of the ions and atoms.

Then the formula for \( T \) becomes

\[ \left( H - E_I \right) + \left( H - E_{II} \right) \left( \frac{1}{E_I - H + i\varepsilon} \right) \left( H - E_I \right) \]

\[ \left( V^{\text{I}} \right) + \left( V^{\text{II}} \right) \left( \frac{1}{E_I - H + i\varepsilon} \right) V^{\text{I}} \]

To apply this, one must still approximate \( H \).

Notice that

\[ \langle N_{II} | V^{\text{I}} | N^{\text{I}} \rangle = \langle N_{II} | H - E_1 | N^{\text{I}} \rangle \]

\[ \langle N_{II} | V^{\text{II}} | N^{\text{I}} \rangle = \langle N_{II} | H - E_2 | N^{\text{I}} \rangle \]

These matrix elements are the same because the \( T \) matrix is multiplied by

\[ \delta \left( E_1 - E_2 \right) \]
\( \kappa^0 \) decay problem

\[
\begin{align*}
\hat{\mathcal{L}}_{\kappa^0} &= E_1 a_{\kappa^0} + \sum \frac{1}{n} M_{\kappa^0, \pi^0} b_{\pi^0} \\
\hat{\mathcal{L}}_{\kappa^0} &= E_2 a_{\kappa^0} + \sum \frac{1}{n} M_{\kappa^0, \pi^0} b_{\pi^0} = E_1 a_{\bar{\kappa}^0} + \sum \frac{1}{n} M_{\kappa^0, \pi^0} b_{\pi^0} \\
\hat{\mathcal{L}}_{\pi^0} &= \mathcal{E}_{\pi^0} b_{\pi^0}(t) + M_{\kappa^0, \pi^0} a_{\kappa^0}(t) + M_{\kappa^0, \pi^0} a_{\bar{\kappa}^0}(t)
\end{align*}
\]

set the energy scale such that \( \mathcal{E}_1 = 0 \)

\[
\begin{align*}
b_{\pi^0} &= e^{-i(\mathcal{E}_{\pi^0} - E_1)t} \int_0^t e^{i(\mathcal{E}_{\pi^0} - E_1)\tau} e^{i E_1 \tau} M_{\kappa^0, \pi^0} [a_{\kappa^0}(\tau) + a_{\bar{\kappa}^0}(\tau)] d\tau \\
\end{align*}
\]

and

\[
\begin{align*}
e^{-i(\mathcal{E}_{\pi^0} - E_1)t} \int_0^t e^{i(\mathcal{E}_{\pi^0} - E_1)\tau} e^{i E_1 \tau} M_{\kappa^0, \pi^0} [a_{\kappa^0}(\tau) + a_{\bar{\kappa}^0}(\tau)] d\tau \\
&= \left[ \Delta - i \frac{\mathcal{E}_{\pi^0}}{2} \right] [a_{\kappa^0}(t) + a_{\bar{\kappa}^0}(t)]
\end{align*}
\]

\[
\begin{align*}
\hat{\mathcal{L}}_{\kappa^0} &= \left( \Delta - i \frac{\mathcal{E}_{\pi^0}}{2} \right) [a_{\kappa^0} + a_{\bar{\kappa}^0}]
\end{align*}
\]

Solving gives

\[
\begin{align*}
a_{\kappa^0} + a_{\bar{\kappa}^0} &= e^{-2i\Delta t - \pi t} \\
a_{\kappa^0} = a_{\bar{\kappa}^0} &= \frac{1}{2}
\end{align*}
\]

\[
\begin{align*}
|a_{\kappa^0}|^2 &= \frac{1}{4} \left[ 1 + e^{-2\pi t} + 2 \cos(2\Delta t) e^{-\pi t} \right] \\
|a_{\bar{\kappa}^0}|^2 &= \frac{1}{4} \left[ 1 + e^{-2\pi t} - 2 \cos(2\Delta t) e^{-\pi t} \right]
\end{align*}
\]

It is clear that \( 2\Delta \) represents a mass difference between the states \( a_{\kappa^0} \) and \( a_{\bar{\kappa}^0} \). The relatives size of \( \Delta < \pi \) determines whether it is possible to detect the wiggles. The wiggles can be seen and \( \Delta \) comes out to be \( \sim 4.5 \pi \).

For \( \gamma < 4.5 \pi \), this gives an energy difference of \( \Delta \mu e \gamma \).

This mass split is of interest because:

1) 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.)
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 \( \pm 2 \times 10^4 \text{ MeV} \).

Thus we can dispose of speculations that antiparticles have negative masses.

\[ a_{K^0} - d_{\bar{K}^0} \text{ are eigenstates of the operator CP (which takes an antiparticle into its particle and vice versa). Our result showed that one CP eigenstate decays into two } \pi^1 \text{ s (also an eigenstate of CP), whereas the other doesn't.} \]

For some time after its discovery, the long lived eigenstate \( \bar{K}^0 \) was observed to go only into \( \pi^0 \) and lepton pairs (lepton pairs aren't CP eigenstates, so the \( \bar{K}^0 \) go into them as well). Hence it was believed that CP was conserved in all interactions.

It is now known that \( \bar{K}^0 \) does go into two \( \pi^0 \) s, but with 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 \( \bar{K}^0 \) 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 inviected state as a plane wave. This is not quite correct, however. Due to the range of the Coulomb potential, we must actually use the Coulomb wave function [confined hypergeometric function].
**Problem:** Consider neutrons in $\text{He}$ and that the energy as a function of momentum is

$$E(p) = E_0 + \frac{1}{2m} (p - p_0)^2$$

where $E_0$ and $p_0$ are constants. Suppose also

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

What is the probability of emitting a photon of momentum $k$ in terms of $n_0, \Delta_0, d,$ and $c_s$?

Consider the $\text{He}$ contained in a box of volume $V$. Near the density in the box, the wave equation

$$\nabla^2 \rho - \frac{\partial^2 \rho}{\partial t^2} = 0$$

classically.

We wish to quantize this fluid field. First if we imagine harmonic b.c., we can represent $\rho$ as the sum of plane waves

$$\rho(r, t) = \sum_{k} Q_k(t) e^{-ikr}$$

Then plug this into (3) we find

$$-\hbar^2 \frac{\partial^2}{\partial r^2} Q_k - \frac{\partial^2}{\partial t^2} Q_k = 0$$

From this we find

$$-\hbar^2 \frac{\partial^2}{\partial r^2} Q_k - \frac{\partial^2}{\partial t^2} Q_k = 0$$

Just sho. of $\omega = \frac{\hbar \omega_0}{m}$.
Due to pass to q.m, we find the energy
\[ E = \int (p \cdot p) \, dV. \]

Now we can write the interaction by noting
\[ E(p) = \frac{1}{2m} (p \cdot p)^2 + \Delta_0 + (p - q_0) \cdot p \]
interaction term

Thus
\[ H_{\text{int}} = \frac{1}{2m} (\hat{p} - \hat{q}_0)^2 + \Delta_0 - \hat{p} \cdot \hat{q}_0 + \sum \frac{e^2 d}{4\pi \varepsilon_0 |r_i|} \]
where \[ H_{\text{int}} = \frac{1}{2} \mu + \mu \frac{e^2 \tilde{q}_0}{2\varepsilon_0} \]
\[ \mu = \frac{Q_0 m_0}{2} \]

Now our unperturbed Hamiltonian is
\[ \hat{H}_{\text{int}} = \frac{1}{2m} (\hat{p} - \hat{q}_0)^2 + \Delta_0 - \hat{p} \cdot \hat{q}_0 \]

Note these will give states corresponding to that of a free particle given \( \Delta_0 - \hat{p} \cdot \hat{q}_0 = \text{const} \), e.g. \( V = \text{const} \) in the S.eq. With these
\[ \langle \hat{p} | \hat{p} \rangle = \frac{e^{iK_0 r} + e^{-iK_0 r}}{1 + k_0^2} \]
\[ \text{From our formula:} \]
\[ \frac{P_{\text{max}}}{P} = 2n^{3}(\frac{\alpha^{2}}{2m} - \frac{P^{2}}{2m} - \frac{\hbar}{2m}) \left| \langle p | \tilde{Y}_{\ell} | p \rangle \right|^{2} \frac{1}{2m^{1/2} \hbar} \]

The remainder of the analysis should be shown. Note the \( P_0 \) means that the ion will eventually decay to a ground state energy of \( \frac{\alpha^{2}}{2m} + \Delta \). One should be able to say something about the behavior of He \( \text{II} \) from this.
3. Our problem is now to consider

\[ I_{\text{2 photon emission}} \]

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

\[ \frac{e^2}{2\hbar c} \tilde{A}(\vec{r}_1) \cdot \tilde{A}(\vec{r}_2) \]

term for the field interaction. The field, therefore, is

\[ H = \frac{1}{2} \sum_{\vec{k}} \left[ \frac{p_{\vec{k}}^2}{2\hbar^2} + m \left( \frac{\hbar c k}{2} \right)^2 \right] \]

\[ H_{\text{interaction}} = \sum_{\vec{k}, \vec{k}'} \frac{\hbar^2}{2\varepsilon_0^0} \hat{Q}_{\vec{k}} \hat{Q}_{\vec{k}'} + \sum_{\vec{k}, \vec{k}', \vec{k}''} \frac{\hbar^2 c^2}{2\varepsilon_0^0} e^i(\vec{k}'' + \vec{k}) \cdot \hat{Q}_{\vec{k}'} \hat{Q}_{\vec{k}''} \]

where \( \hat{Q}_{\vec{k}} \) is the first order operator on p. (34).

Now since the first order bremsstrahlung is forbidden, we can conclude

\[ \langle \psi_1 | \mathcal{P} | \psi_2 \rangle = 0 \] [parity violated]

What we now need is a nice handy dandy formula like

\[ R_{\text{2-photon}} = \frac{2\pi}{\hbar c} \left( \varepsilon_0 - \varepsilon_0 - \varepsilon_R \right) \left\langle \phi \left| \phi' \right| \right\rangle^2 \frac{N_{\text{2-photon}}}{2\hbar^2 c^2} \]

for 2nd order theory. I'll wait for E to derive it... if not, I'll do it myself.
We wish to solve
\[ -\frac{i}{\hbar} \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle \]

Write
\[ H(t) = H_0 + U(t) \]

and expand
\[ |\Psi(t)\rangle = \sum_n C_n(t) |\Phi_n\rangle \]

Plug into (1)
\[ \sum_n -\frac{i}{\hbar} \dot{C}_n(t) |\Phi_n\rangle = \sum_n C_n(t) E_n |\Phi_n\rangle + \sum_n C_n(t) U(t) |\Phi_n\rangle \]

Take a scalar product with \(<\Phi_m|\)
\[ -\frac{i}{\hbar} \dot{C}_m(t) = E_m C_m(t) + \sum_n C_n(t) <\Phi_m|U(t)|\Phi_n> \]

This suggests we try
\[ C_n(t) = e^{-iE_n t} \chi_n(t) \]

Then (2) becomes
\[ \dot{\chi}_n(t) = -i \sum_m \chi_m(t) e^{-iE_m t} <\Phi_m|U(t)|\Phi_n> e^{iE_n t} \chi_n(t) \]

\[ = -i \sum_m \chi_m(t) \chi_n(t) \]

(What relationship does \(\chi_m\) have to \(\chi_n\)?) Now we want
\[ \chi_m(t_f) = \sum_n \chi_{mn}(t_f, t_i) \chi_n(t_i) \]

Thus
\(\chi_{mn}\) is some integral of \(\chi_n(t)\).
To evaluate the num complicate fact, we take a specific case of \( \psi_n(t) \) and compute \( \chi_m(t) \) by integrating (3) and iterating

\[
\chi_m(t) = S_{mn} + (-i) \int_{-i}^{t_1} \psi_{mn}(t) dt_1 + (-i)^2 \int_{-i}^{t_1} \psi_{mn}(t_1) dt_1 \frac{1}{t_2} \int_{-i}^{t_1} \psi_{mn}(t_2) dt_2
\]

and then identifying

\[
\chi_m(t_f) = \chi_{mn}(t_i, t_f)
\]

such that

\[
\chi_{mn}(t_i, t_f) = S_{mn} + (-i) \int_{-i}^{t_f} \psi_{mn}(t) dt + (-i)^2 \int_{-i}^{t_f} \psi_{mn}(t) dt \frac{1}{t} \int_{-i}^{t} \psi_{mn}(t_1) dt_1
\]

If we consider a constant perturbation \( V \) applied at time \( t_i \), we find

\[
\chi_{mn}(t_i, t_f) = \chi_{mn}(t_i-t_f) = S_{mn} + (-i) \int_{-i}^{t-f} \psi_{mn} e^{it_f V t} dt + \ldots
\]

\[
= S_{mn} + e^{i(\widetilde{E}_n - \widetilde{E}_m) t_f} \frac{1}{(E_n - E_m)} + \ldots
\]

The idea here is that if we can represent the state at \( t_i \) as a pure state \( |\phi_i\rangle \) of the unperturbed Hamiltonian \( H_0 \), then the probability the state will be in an unperturbed state \( |\phi_n\rangle \) at \( t_f \) is \( |\langle \phi_n | \phi_i \rangle|^2 \). Note that since \( |\langle \phi_n | \phi_i \rangle|^2 \) is in general the perturbation \( V \) mixes the pure state \( |\phi_n\rangle \) and requires us to regard \( |\phi_i\rangle \) as a superposition of the \( |\phi_n\rangle \) and \( |\phi_m\rangle \). Of course this merely requires \( |\phi_i\rangle \) is not a C.O.M. for the perturbed system.
Now we can define the $S$-matrix as

$$ S_{mn} = \lim_{\alpha \to \pm \infty} S_{mn}(-\alpha, +\alpha) $$

Then

$$ S_{mn} = S_{mn} + (-i) \int_{-\infty}^{0} e^{i(E_n - E_m)t} V_{nm}(t) dt + (-i) \int_{0}^{\infty} e^{-i(E_n - E_m)t} V_{mn}(t) dt + \cdots $$

$$ + \int_{0}^{\infty} \int_{-\infty}^{\infty} e^{i(E_n - E_m)t_2} V_{ml}(t_2) V_{lm}(t_1) dt_1 dt_2 + \cdots $$

$$ = S_{mn} + (-i) \sum_{\ell} V_{mn}^{F,T}(E_n - E_\ell) + (-i)^2 \sum_{\ell} V_{ml}^{F,T}(E_n - E_\ell) V_{lm}^{F,T}(E_\ell - E_m) + \cdots $$

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 $t = t_i$, $|\psi(0)\rangle = |\phi_{in}\rangle e^{-iE_n t_i}$. Then we require by conservation of probability,

$$ \sum_{\ell} |C_{\ell n}(t_i)|^2 \leq N $$

or since $C_{\ell n} = e^{-iE_{\ell} t_i} k_{\ell n}$,

$$ \sum_{\ell} \left| D_{\ell n}(t_i, t_f) \right|^2 = 1 \leq N $$

Thus

$$ \left| S_{mn} + (-i) \int_{t_i}^{t_f} V_{mn}(t) dt + (-i)^2 \int_{t_i}^{t_f} \int_{t_i}^{t_2} \sum_{\ell} D_{\ell n}(t_2) V_{ml}(t_2) \sum_{\ell} D_{\ell m}(t_1) V_{lm}(t_1) \cdots \right|^2 = 1 $$

This seems pretty strong.
Instead of a differential test, consider the first term as an integral equation

\[ \chi_m(t) = \chi_m(t_i) + (-i) \int_{t_i}^{t} \sum_n \gamma_{nm}(t_i) \chi_n(t_i) \, dt. \]  \hspace{1cm} (10)

Define the integral operator

\[ \mathcal{L}(t, t_i) = (-i) \int_{t_i}^{t} \sum_n \gamma_{nm}(t_i) \, dt, \]  \hspace{1cm} (11)

so that (10) becomes

\[ \chi_m(t) = \chi_m(t_i) + \mathcal{L} \{ \chi_m(t_i) \} \]

or

\[ \chi_m(t) = \left[ 1 - \mathcal{L}(t, t_i) \right]^{-1} \chi_m(t_i) \]  \hspace{1cm} (12)

Thus we can identify an "evolution operator" \( U_m(t, t_i) \)

\[ U_m(t, t_i) \equiv \left[ 1 - \mathcal{L}(t, t_i) \right]^{-1} \]  \hspace{1cm} (13)

such that

\[ \chi_m(t) = U_m(t, t_i) \chi_m(t_i) \]

It would even be better to define a \( U(t, t_i) \) such that

\[ |\psi(t_i)\rangle = U(t, t_i) |\psi(t_i)\rangle \]  \hspace{1cm} (14)
Central Potential Scattering:

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

Thus we have plane waves from

\[ H\Phi_n = \hbar^2 k^2 \Phi_n \]

Thus \( \Phi_n = \hat{k} \Phi_n \), \( \Phi_n = \hat{k} \Phi_n \)

Thus we expand

\[ \Psi(k) = \sum \frac{\langle \Phi_n | \Phi_r \rangle}{k} \]

Actually we usually consider scattering from one continuum \( k \) to another continuum \( k' \). Using our work on first Born approx.

\[ \text{Rate} \frac{d^2{\sigma}}{dE dK} = 2\pi S(k^2 - k'^2) \left| V_{kk'} \right|^2 \]

Note the \( S(k^2 - k'^2) \) merely ensures conservation of energy

where \( V_{kk'} = \langle \Phi_r | V(r) | \Phi_n \rangle \)

\[ = \int d^3r e^{i\vec{q}\cdot\vec{r}} \frac{d^2\sigma}{dE dK} = V(q) \]

where \( q = k - k' \)
We want

\[
\frac{dX}{d\tau} = \frac{\text{well defined at overdamped about 25 kHz}}{\text{infinite}}
\]

\[
\frac{b\psi^2 V}{k} \frac{1}{\tau^2}
\]

\[
k \psi^2 \phi V
\]
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

\[ \hat{J}_x = \frac{\hbar}{\gamma} \left[ \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \right] + \gamma \hat{V}_z \]
\[ \hat{J}_y = \frac{\hbar}{\gamma} \left[ \frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial x^2} \right] - \gamma \hat{V}_y \phi \]
\[ \hat{J}_z = \frac{\hbar}{\gamma} \left[ \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right] + \gamma \hat{V}_x \phi \]

\[ \phi = \arccos \frac{\hat{V}_x}{\hat{V}_y} \]

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 are combined, with a Hamiltonian of the form

\[ H = A \hat{J}_x \cdot \hat{J}_b + B \left[ \frac{\mu_a}{j_a} \left( \hat{J}_a \right)_z + \frac{\mu_b}{j_b} \left( \hat{J}_b \right)_z \right] \]

where \( B \) is a fixed field.

1) 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

\[ J_a = \gamma, \quad J_b = \gamma \]

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
\[ R |14_i\rangle \equiv R |14_i\rangle = D_j \left( R \right) |14_i\rangle \]
\[ R |14_2\rangle \equiv D_{12} \left( R \right) |14_2\rangle \]
where \( D_j \) is a matrix which acts on the spin indices of the wave functions.

Thus we presumably have some matrix \( D \) such that
\[ R |14\rangle = D \left( R \right) |14\rangle \]
To see what size \( D \) should have:

\[ |14_1\rangle \text{ has } (2j_1+1) \text{ components} \]
\[ |14_2\rangle \text{ has } (2j_2+1) \text{ components} \]
\[ |14\rangle \text{ has } (2j_1+1)(2j_2+1) \text{ components} \]

However, \( D \) is not necessarily one of the fundamental ("irreducible") representations of rotations - i.e. it does not necessarily correspond to one particular spin.

Because it is a representation, it can be broken up into a direct sum of these irreducible representations.

This means that \( |14\rangle \) can be written as \( \sum_i \alpha_i |\psi_i\rangle \) where the \( |\psi_i\rangle \) correspond to each to a particular spin, and the \( \alpha_i \) are completely determined by \( |14_1\rangle \) and \( |14_2\rangle \)
\[ |\psi_1^{3i}\rangle \mid |\psi_2^{3i}\rangle = \sum_i \alpha_i |\psi_i^{3i}\rangle \]

The problem is to determine:

a) Which \( j_i \) will appear

b) What are the \( \alpha_i \)

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 \( \alpha_i \) (Clebsch-Gordan 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!

1) Apply an infinitesimal rotation about the z axis \( (1+i \varepsilon \mathcal{J}_z) |\psi_1^{3i}\rangle \mid (1+i \varepsilon \mathcal{J}_z) |\psi_2^{3i}\rangle \)
\[ = (1+i \varepsilon m_1) (1+i \varepsilon m_2) |\psi_1^{3i}\rangle \mid |\psi_2^{3i}\rangle \]
Here \( \mathcal{J}_z \) is just the appropriate operator in \( \mathcal{D} \)
\[ \Rightarrow \mathcal{J}_z |\psi\rangle = m |\psi\rangle \]
\( m = m_1 + m_2 \)
Rule 1) The magnetic quantum numbers always add

II) To find which \( j \) appear

As \( m_1 \) ranges over its \( 2j_1 + 1 \) values

\[
M_2 = \ldots = 2j_2 + 1
\]

Max\( (m_1, m_2) = j_1 + j_2 \)

Hence this is the maximum value of \( J \) allowed in the decomposition

\[
|\psi\rangle = a_{J_{\text{conf}}}|\psi_{J_{\text{conf}}}\rangle
\]
is then a new thing whose possible \( \text{max } J \) 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:

\[
(2j_1 + 1)(2j_2 + 1) = \sum_{n=0}^{M} \left[ 2(j_1 + j_2 - n) + 1 \right]
\]

\[
= 2(j_1 + j_2)(M + 1) - M^2 + 1
\]

\(
\Rightarrow M = 2j_1 \text{ or } 2j_2
\)

\[
j_1 + j_2 - 2j_1 = j_2 - j_1
\]

\[
j_1 + j_2 - 2j_2 = j_1 - j_2
\]

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 \( j_2 - j_1 \) to \( j_1 - j_2 \)

(the steps are 1 because \( m \) steps necessarily come in ones)

III) To determine the \( a_{j_1} \)

Clearly it makes no difference whether we begin with a basis \( |\bar{J} M\rangle \)

and expand it as \( \sum b_{j_1, j_2} |j_1 m_1\rangle |j_2 m_2\rangle \)

or start with \( |j_1 m_1\rangle |j_2 m_2\rangle = \sum a_{j_1} |\bar{J} M\rangle \)

It is most convenient to find the \( b_{j_1, j_2} \)

\[
|\bar{J} M\rangle = \sum b_{j_1, j_2} |j_1 m_1\rangle |j_2 m_2\rangle
\]

Clearly \( |\bar{J} M\rangle = |j_1 j_2\rangle |j_2 j_2\rangle \quad j_1 + j_2 \quad \bar{J} = j_1 \pm j_2 \)

We then just apply \( \bar{J}_- \) to both sides. Use of the relations derived last

week \( \bar{J}_- |\bar{J} M\rangle = C_M |\bar{J}_{M-1}\rangle \) will then completely specify the \( b_{j_1, j_2} \)

A word of caution is in order here:

\[
|\bar{J} M - \bar{J} m\rangle
\]

In the most general case it is quite possible that beginning at \( \Lambda \) and applying

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-Gordan tables use the same phase convention. Thus, unless you generate all your own Clebsch-Gordan 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 $|J^M,J_M\rangle$ have been determined by this method. We next must find $|J^M_{-1}, J_M\rangle$. To do this, notice that $|J^M_{-1}, J_M\rangle$ is orthogonal to $|J^M_{-1}, J_M\rangle$ and that there are only two possible states with $J^M_{-1}$ made up of $|j_1,m_1\rangle$ and $|j_2,m_2\rangle$.

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:

$$|J^M\rangle = \sum b_{m_1,m_2} |j_1,m_1\rangle |j_2,m_2\rangle$$

$$\frac{1}{\sqrt{J(J+1)}} |J^M\rangle = (\frac{\sqrt{a}}{\sqrt{a} + \sqrt{b}}) (\frac{\sqrt{a}}{\sqrt{a} + \sqrt{b}}) \sum b_{m_1,m_2} |j_1,m_1\rangle |j_2,m_2\rangle$$

$$\begin{align*}
J_a^2 &\rightarrow J_1(J_1+1) \\
J_b^2 &\rightarrow J_2(J_2+1)
\end{align*}$$

Comparison of the equations

$$|J^M\rangle = \sum b_{m_1,m_2} |j_1,m_1\rangle |j_2,m_2\rangle$$

$$|J^M\rangle = \frac{1}{\sqrt{J(J+1)}} \sum c_{m_1,m_2}$$

will often allow you to determine the b's

Suppose you start out with n objects of spin $\frac{1}{2}$, all spinning up $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$ 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 $J=m/2$ is obtained from a symmetric combination of $n$ spinors
**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

\[
|\rho\rangle \Rightarrow \alpha|\rho\rangle + \beta|m\rangle \\
|m\rangle \Rightarrow -\beta^*|\rho\rangle + \alpha^*|m\rangle 
\]

\[\Rightarrow (\alpha^2 + \beta^2) = 1\]

without changing any of the forces.

The pair \(\alpha, \beta\) determines an element of this group of transformations.

The matrix \(\begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}\) acts on the pair \(|\rho, m\rangle\) in exactly the same way as an element of the rotation group acts on an object of spin \(\frac{1}{2}\). Hence the set \(|\rho, m\rangle\) is called an isotopic spinor; and all the Clebsch-Gordanry 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** \(\Lambda\)
- **spin \(\frac{1}{2}\) representations** 
  \[\begin{pmatrix} m & \rho \\ \bar{m} & \bar{\rho} \end{pmatrix}\]
- **spin 1 representations:** 
  \[\begin{pmatrix} k^+ & k^0 \\ \bar{k}^0 & \bar{k}^- \end{pmatrix}\]
- **spin 3/2 representation:** 
  \[\begin{pmatrix} \Sigma^+ & \Sigma^0 & \Sigma^- \\ \Xi^+ & \Xi^0 & \Xi^- \end{pmatrix}\]

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 \(\Lambda\) particle as a bound state of 2 particles, we must use a \(\Sigma^+\) combination - a \(\Lambda^+\) one will not work (\(T=0 + T=1\) cannot couple to \(T=0\)).

The fact that \(\Delta\) has \(T=3/2\) makes its decay into \(\Pi^+ N^0\) easily classified

\[T=1, \quad \frac{1}{2} = \frac{1}{2}\]
Both isotopic spin and rotations can be built up from a group of transformations on spinors, where the matrices acting on the spinors have the form
\[
\begin{pmatrix}
\alpha & \beta \\
-\beta^* & \alpha^*
\end{pmatrix}
\]

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 \( \frac{3}{2} \otimes \frac{3}{2} \) (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 +

\[
\begin{array}{c}
\Sigma^+ \\
\Sigma^0 \\
\Sigma^- \\
\Xi^0 \\
\Xi^- \\
\Xi^{*0} \\
\Xi^{*-} \\
\Lambda^0 \\
\end{array}
\]

Decuplet Spin \( \frac{3}{2} \) Parity +

\[
\begin{array}{c}
\Omega^- \\
\Omega^+ \\
\Xi^{++} \\
\Xi^{*0} \\
\Xi^{*+} \\
\Delta^0 \\
\Delta^+ \\
\Delta^{++} \\
\end{array}
\]

**Mesons**

Octet Spin 0 Parity -

\[
\begin{array}{c}
\pi^- \\
\pi^0 \\
\eta^0 \\
\eta^+ \\
\kappa^- \\
\kappa^0 \\
\kappa^+ \\
\end{array}
\]
Octet Spin 1 Parity: \( K^+ \quad K^0 \quad \bar{K}^0 \quad \bar{K}^+ \quad \rho^- \quad \rho^0 \quad \omega \quad \rho^+ \quad \phi \quad \phi^* \)

No one has yet found members of the \( \frac{3}{2} \) or \( \frac{1}{2} \) 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, \( T = \frac{3}{2} \), 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: \( \vec{X}, \vec{\rho} \) and other dot products
- Vectors: \( \vec{X}, \vec{\rho}, \vec{X} \times \vec{\rho} \), etc.
- Tensors: \( \vec{X} \vec{\rho} \)

2) Re-express these so that they are separated into things with exact spin transformation properties:

- \( \vec{X} \vec{\rho} \) is an exact scalar which transforms like spin 0
- \( \vec{\rho} \) is an exact vector with transforms like spin 1

What do we mean "transforms like spin 1/2"?

The spherical harmonics \( Y^m_s \) are eigenfunctions of total angular momentum with z projection M. Under a rotation of the coordinates, the \( Y^m_s \) for a given J transform among themselves according to the appropriate \( D^J_s \).

\[
Y_{j_1}^{m_1} (\Theta_2) = \sum_{m} D^J_M (\Theta_2, \Theta_1) Y_{j_2}^{m_2} (\Theta_1)
\]
Any wave function with these properties transforms like Spin $J$.

Now look at operators of the type shown above.

The components $\gamma_i^m$ can be made to correspond to certain combination of $a^i$ for a vector $\sqrt{\hbar} = \sum a^i \hat{e}^i$

$$\gamma_i^1 \leftrightarrow -\hbar/2 (\hat{e}_x + i \hat{e}_y) \quad \gamma_i^{-} \leftrightarrow \hbar/2 (\hat{e}_x - i \hat{e}_y)$$

$$\gamma^0 \leftrightarrow \hat{e}_z$$

But $\gamma^m$ has only 5 components, whereas the spatial tensor $\epsilon_i^j \hat{e}_i \hat{e}_j$ has 9. Hence $\beta^m$ cannot transform exactly like spin 2.

To figure out the proper spin decomposition of something like $\chi \rho$, notice the following:

a) a generalization of the arguments $\delta \times r$ spinor representations made above shows that every integral spin $n$ representation can be formed from a symmetric combination of $n$ spin 1 objects.

Hence if we have two spin 1 objects ($\chi \rho$), the spin two piece (highest spin formed) must not contain any antisymmetric combinations.

**Symmetric piece**

\[
\begin{array}{c c c}
\hat{e}_x \hat{e}_x & \hat{e}_y \hat{e}_x + \hat{e}_x \hat{e}_y & \hat{e}_z \hat{e}_x + \hat{e}_x \hat{e}_z \\
\hat{e}_x \hat{e}_y + \hat{e}_y \hat{e}_x & \hat{e}_y \hat{e}_y & \hat{e}_y \hat{e}_z + \hat{e}_z \hat{e}_y \\
\hat{e}_x \hat{e}_z + \hat{e}_z \hat{e}_x & \hat{e}_y \hat{e}_z + \hat{e}_z \hat{e}_y & \hat{e}_z \hat{e}_z \\
\end{array}
\]

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**

\[
\begin{array}{c c c}
\hat{e}_x \hat{e}_y - \hat{e}_y \hat{e}_x & 0 & \hat{e}_z \hat{e}_x - \hat{e}_x \hat{e}_z \\
\hat{e}_x \hat{e}_y - \hat{e}_y \hat{e}_x & 0 & \hat{e}_z \hat{e}_x - \hat{e}_x \hat{e}_z \\
\end{array}
\]

There are three independent elements here.

We recognize this as $\chi \rho$ a vector and thus a spin 1 object.

$\chi \rho$ can contain only spins 2, 1, 0 because $\chi$ and $\rho$ are spin 1. The only remaining problem is to separate the spin 0 from the spin 2.

spin 0 looks like $\hat{e}_x, \hat{e}_y$ 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

\[
\hat{c}_x \hat{c}_y \left[ a - \frac{1}{3} (a+b+c) \right] + \hat{c}_y \hat{c}_z \left[ b - \frac{1}{3} (a+b+c) \right] + \hat{c}_z \hat{c}_x \left[ c - \frac{1}{3} (a+b+c) \right] + \frac{(a+b+c)}{3} \left[ \hat{c}_x \hat{c}_y + \hat{c}_y \hat{c}_z + \hat{c}_z \hat{c}_x \right]
\]

Spin decomposition of

- spin 0 \( \frac{1}{\sqrt{3}} \vec{x} \cdot \hat{c}_z \)
- spin 1 \( \vec{x} \times \hat{c}_z \)
- spin 2 \( x \hat{c}_x - \frac{1}{3} \vec{x} \cdot \hat{c}_z \)
  \( y \hat{c}_y + x \hat{c}_y \)
  \( z \hat{c}_z + x \hat{c}_z \)
  \( x \hat{c}_y + y \hat{c}_z \)
  \( y \hat{c}_z + x \hat{c}_z \)
  \( z \hat{c}_z - \frac{1}{3} \vec{x} \cdot \hat{c}_z \)

Having explicitly constructed all 5 independent elements of the spin 2 tensor, we put them in one-to-one correspondence with the \( \frac{1}{2} \) \( M \) \( s \)

Define

\[
X_i^1 = -\frac{1}{\sqrt{2}} (x + iy)
\]

\[
X_i^{-1} = \frac{1}{\sqrt{2}} (x - iy)
\]

\[
X_i^0 = \frac{1}{\sqrt{2}}
\]

Solving backwards gives

\[
X_i^1 P_i^1 = \frac{1}{\sqrt{2}} \left[ \frac{i}{2} (y \hat{c}_x + x \hat{c}_y) + x \hat{c}_x - y \hat{c}_y \right]
\]

\[
X_i^{-1} P_i^{-1} = \frac{1}{\sqrt{2}} \left[ -\frac{i}{2} (y \hat{c}_x + x \hat{c}_y) + x \hat{c}_x + y \hat{c}_y \right]
\]

\[
X_i^0 P_i^0 = \frac{1}{\sqrt{2}} \left[ \frac{i}{2} (y \hat{c}_x + x \hat{c}_y) + x \hat{c}_x - y \hat{c}_y \right]
\]

\[
X_i^1 P_i^{-1} + X_i^{-1} P_i^1 + 2X_i^0 P_i^0 = -\frac{1}{\sqrt{2}} \left[ x \hat{c}_y + y \hat{c}_z \right] + \frac{1}{\sqrt{2}} \left[ x \hat{c}_y - y \hat{c}_z \right]
\]

\[
X_i^0 P_i^1 + X_i^1 P_i^0 = -\frac{1}{\sqrt{2}} \left[ -i (z \hat{c}_x + x \hat{c}_z) + z \hat{c}_y + y \hat{c}_z \right]
\]

\[
X_i^0 P_i^1 + X_i^1 P_i^0 = -\frac{1}{\sqrt{2}} \left[ -i (z \hat{c}_x + x \hat{c}_z) + z \hat{c}_y - y \hat{c}_z \right]
\]

Now refer to a table of Clebsch-Gordan coefficients and construct spin 2 from two spin 1 objects

(1 1 1 1 2 2) = 1
(1 1 1 1 2 0) = \frac{1}{\sqrt{6}}
(1 1 1 1 1 0) = \frac{1}{\sqrt{6}}
(1 1 1 0 1 2) = \frac{1}{\sqrt{6}}
(1 1 0 1 1 2) = \frac{1}{\sqrt{6}}
(1 0 1 1 2 1) = \frac{1}{\sqrt{6}}

Hence

\[
\gamma_2^1 = X_i^1 P_i^1
\]

\[
\gamma_2^{-1} = X_i^{-1} P_i^{-1}
\]

\[
\gamma_2^0 = \frac{1}{\sqrt{6}} (X_i^0 P_i^1 + P_i^0 X_i^1)
\]

\[
\gamma_2^{-2} = \frac{1}{\sqrt{6}} (X_i^{-1} P_i^1 + P_i^{-1} X_i^1 - 2X_i^0 P_i^0)
\]

Thus certain linear combinations of the \( X_i^s P_j \) 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

\[ \mathbf{Y}_j^m \]

Then the rule for matrix elements is simple.

\[
\langle \alpha, j_1, m_1 | \mathbf{Y}_j^m | \alpha', j_2, m_2 \rangle = C_{\alpha j_2} \langle j_2 \mathbf{J} m_2, M | j_1, m_1 \rangle
\]

where \( \alpha \) specifies additional quantum numbers of the system.

Here \( C_{\alpha j_2} \) is a number that cannot be obtained by angular momentum arguments.

To prove this:

\[
\mathbf{Y}_j^m | \alpha, j_2, m_2 \rangle \text{ transforms under rotation like } \overline{\mathbf{J}} \overline{\alpha} \langle j_1, m_1 | \mathbf{Y}_j^m \rangle
\]

\[
| j_2 - \mathbf{J} \rangle \leq \mathbf{J}_z \leq j_2 + \mathbf{J}
\]

where the \( \alpha_i \) are the Clebsch-Gordon coefficients

\[
\langle j_2 - \mathbf{J} | \mathbf{J} m_2, \mathbf{M} \rangle \mathbf{J}_z \mathbf{v}
\]

A matrix element is just a number; hence it must be a rotational scalar. We can form this only if

\[
\langle j_1, m_1 | = \langle j_2 - \mathbf{J} | \mathbf{J} m_2, \mathbf{M} \rangle \text{ same } \mathbf{J}_z, \mathbf{v}
\]

As far as the rotational character of the states and operators is concerned, \( \alpha_i \) 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 \( \mathbf{J} \) operator, as follows:

\[ [\mathbf{J}^x, \mathbf{J}^y, \mathbf{J}^z] = 0 \]

an operator’s angular momentum properties are determined completely by its commutation relations with \( \mathbf{J} \). Because \( \mathbf{J}^x \mathbf{J}^y \) commutes with \( \mathbf{J} \) in the same way as

the unit operator, we know

\[
\langle m_1, j_1 | \mathbf{J}^x, \mathbf{J}^y | m_2, j_2 \rangle = \alpha \langle m_1, j_1 | \mathbf{J}^x | m_2, j_2 \rangle = \alpha \delta_{m_1, m_2} \delta_{j_1 j_2}
\]

where \( \alpha \) has no dependence

\[ [\mathbf{J}_z, \mathbf{J}_z] = \alpha_i^{j_1, j_2} \mathbf{J}_z
\]

where the \( \alpha_i^{j_1, j_2} \) are the same as in

\[ [\mathbf{J}_z, \mathbf{J}_z] = \alpha_i^{j_1, j_2} \mathbf{J}_z
\]

Hence

\[
\langle m_1, j_1, \alpha | \mathbf{J}^x, \mathbf{J}^y | m_2, j_2 \rangle = \alpha \langle m_1, j_1, \alpha | \mathbf{J}^x | m_2, j_2 \rangle
\]

The operator \( \mathbf{J}^x \mathbf{J}^y \) as one would expect from the above discussion, does not have exactly the same commutation relations as the most simple tensor of the form \( \mathbf{J}^x \mathbf{J}^y \)

Exercise (for fun) do the operator decomposition of \( \mathbf{J} \) 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
\[ (\mathcal{S}_2^+ \cdot \mathcal{S}_2^-) \mathcal{S}_2^\circ \mathcal{S}_2^- \cdot \mathcal{S}_2^\circ \cap \mathcal{S}_2^\circ \cap \mathcal{S}_2^- \geq 0 \]

allows you to reexpress products \( \mathcal{S}_2^3 \) in terms of \( \mathcal{S}_2^2 + \mathcal{S}_2^- \)

Similar things can be done for \( \mathcal{S}_x + \mathcal{S}_y \)

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 \( \left\langle j_1, m_1 | H | j_2, m_2 \right\rangle \propto \delta_{j_1,j_2} \delta_{m_1,m_2} \)

Hence it cannot alter the \( \mathcal{J} \) of \( \mathcal{M} \) of a system \( \left\langle j_1, m_1 | \mathcal{H} | j_2, m_2 \right\rangle \propto \mathcal{J}_1 \cdot \mathcal{J}_2 \cdot m_1, m_2 \)

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 \( \mathcal{H} \) is invariant under rotations in isotopic spin space, then it cannot connect states of different isotopic spin and z component of isospin, \( \mathcal{T}_z \) 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
\[ \left\langle a \mathcal{T}_z | H | a \mathcal{T}_z \right\rangle = \mathcal{C}_a \left( \mathcal{T} \cdot 0 \mathcal{T}_z \cdot 0 \mathcal{T}_z \right) \]

which is independent of \( \mathcal{T}_z \). Thus states which differ only in \( \mathcal{T}_z \) 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 $\mathcal{K} (I \cdot \mathbf{\hat{S}}_Z)$, but $\mathcal{K} \propto \mathbf{\hat{S}}_Z$. 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

$$\mathcal{H} = \sum \mathbf{S} \cdot \mathbf{\hat{S}}$$

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 $\mathcal{H} \mathbf{\hat{S}}_Z$ electromagnetic term; but so far the explanations of "octet dominance" are not as simple to understand as is the presence of electric charge sums.

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.
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 (e.g., 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


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:

$$p_i = \frac{1}{\mathcal{Z}} e^{-E_i/\kappa T}$$

Normalization: $p_i = \frac{1}{\mathcal{Z}} e^{-E_i/\kappa T}$

$$\sum_i p_i = 1 \Rightarrow \mathcal{Z} = \sum_i e^{-E_i/\kappa T}$$

Then the average energy of the crystal is

$$U = \frac{1}{\mathcal{Z}} \sum_i p_i E_i = \frac{1}{\mathcal{Z}} \sum_i E_i e^{-E_i/\kappa T}$$
There are common mathematical tricks that are useful in calculations at temperature \( T \):

1. If you've found \( \mathcal{Q} = \sum_i e^{-E_i/kT} \)

Then \( \frac{\partial \mathcal{Q}}{\partial T} = \frac{1}{kT^2} \sum_i E_i e^{-E_i/kT} = \frac{U \mathcal{Q}}{kT^2} \)

so that \( U = \frac{kT^2 \partial \mathcal{Q}}{\mathcal{Q}} \). \( \mathcal{Q} \) is called the Partition Function.

2. Let \( \mathcal{Q} = e^{-F/kT} \)

then \( F = -kT \log \mathcal{Q} \). \( F \) is called the Free Energy (a note of caution: there are several different kinds of "free energy" in use).

\[
U = -T^2 \frac{\partial}{\partial T} \left( \frac{F}{T} \right)
\]

\[
= F - T \frac{\partial F}{\partial T} \quad \text{entropy}
\]

1) Vibrations of Nuclei in a Crystal (or Polyatomic Molecule)

Problem: The Schrödinger Equation for the whole system (nuclei + electrons) is

\[
\left[ \sum_j -\frac{\hbar^2}{2m_j} \nabla_j^2 + V(R_1, R_2, \ldots, \mathbf{r}_i, \mathbf{r}_j, \ldots) \right] \psi = -\frac{\hbar^2}{2m} \frac{\partial \psi}{\partial t}
\]

Where \( \mathbf{R}_k \) is the position vector of the \( k \)-th nucleus

and \( V = \sum_{i,j=1}^{N} \frac{Z_i Z_j e^2}{R_{ij}} \)

\( R_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \) or \( |\mathbf{r}_i - \mathbf{r}_j| \), etc.
The problem is to show that the following equation is a good approximation for the state of lowest energy:

\[ \sum_{i \text{ (electrons only)}} \frac{-\hbar^2}{2m^e} \nabla_i^2 \chi(i) + V(R_i, \beta) \chi(i) = \frac{-\hbar}{i} \frac{\partial \chi}{\partial t} = \mathcal{E} \chi \]

Where the \( R_i \) are fixed so in such a way that

\[ E = E(R_i) \]

is a minimum.

Show that to an excellent approximation

\[ \psi = \psi(R_i) \chi \left( \frac{x_1, x_2, \cdots}{R_i} \right) \]

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 \( \mathcal{U} \) for a harmonic oscillator with natural frequency \( \omega \) 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 \( H_1 \):

\[ H = \sum_i \frac{-\hbar^2}{2m^e} \nabla_i^2 + U(x_i) \]

where \( (x_1, x_2, x_3) = \) displacement vector 1st nucleus

\( (x_4, x_5, x_6) = \) displacement vector 2nd nucleus

Then \( \psi(x) = U(0) \rightleftharpoons \chi \left( \frac{x_1, x_2, \cdots}{x_0} \right) + \frac{1}{2} \sum_i \frac{x_i}{i} \frac{\partial U}{\partial x_i} \left|_{x_i = 0} \right. + \frac{1}{2} \sum_{i < j} \frac{x_i x_j}{i j} \frac{\partial^2 U}{\partial x_i \partial x_j} \left|_{x_i = 0} \right. \cdots \)
Choose the zero of energy so that $U(0) = 0$ for convenience.

At the equilibrium configuration, $\frac{\partial U}{\partial x_i} \bigg|_0 = 0$.

Consider the displacements to be small (valid for many applications).

Then 

$$ H = \sum \frac{-\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} \sum x_i x_j V_{ij} $$

where $V_{ij} = \frac{\partial^2 U}{\partial x_i \partial x_j} \bigg|_0$.

Let $q_i = \sqrt{m_i} x_i$ and $C_{ij} = \frac{1}{\sqrt{m_i m_j}} \left( \frac{\partial^2 U}{\partial x_i \partial x_j} \right)$. Then

$$ H = \sum \frac{1}{2} p_i^2 + \frac{1}{2} \sum q_i q_j C_{ij}, $$

where $p_i = \frac{1}{\hbar} \frac{\partial}{\partial q_i}$.

This problem can be analyzed classically and this is worthwhile because the results are rather similar to the quantum-mechanical case.

Classically, $\ddot{q}_i = -\frac{\partial V}{\partial q_i} = -\sum C_{ij} q_j$.

A possible solution (periodic motion, really constant) is

$$ q_i = a_i e^{i\omega t} $$

Then we obtain the equation

$$ \omega^2 q_i = \sum C_{ij} q_j. $$

This is an eigenvalue equation and has solutions in $\omega^2$ where

$$ \det (\mathbf{C} - \omega^2 \mathbf{I}) = 0. $$
This equation is of the $n$th degree in $W^2$, and has $n$ real solutions (real because $c_{ij}$ real and $c_{ij} = c_{ji}$).

Label these solutions $W_n^x$, $x = 1, \ldots, n$.

\[ (n = \text{number of coordinates}) \]
\[ = 3N, \ N = \text{no. of nuclei} \]

Let the corresponding eigenvectors be designated $a_i^{(x)}$.

i.e.,
\[ W_n^x a_i^{(x)} = \sum_j c_{ij} a_j^{(x)} \]
\[ x \text{ is known as the mode number.} \]

We can choose normalization of the $a_i$'s so that
\[ \sum_i a_i^{(x)} a_i^{(p)} = \delta_{xp} \]

Then it is also true that
\[ \sum_x a_i^{(x)} a_i^{(p)} = \delta_{ij} \]

(corresponding to different eigenvalues)

(That the $a_i$'s are orthogonal is a well known property of the eigenvectors of hermitian matrices).

Example: $\text{CO}_2$ molecule.

\[ \text{O} \quad \text{C} \quad \text{O} \]

If you push one of the atoms, the other two atoms will respond and a complex motion will ensue.

Guess at the normal modes:

\[ \text{O} \rightarrow \text{O} \rightarrow \text{O} \rightarrow \text{(Arrows indicate initial displacement)} \]

$\chi_1 = \chi_2 = \chi_3 = \frac{1}{\sqrt{3}}$

3 modes of frequency 0 (no restoring force)

(same in $y, z$ directions for other 2 modes)
The same in the other 2 directions yields 3 modes of this type. All three frequencies are the same.

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.

\[ x^{(i)} = -x^{(3)} = - \frac{1}{\sqrt{2}}, \quad x^{(2)} = 0 \]
\[ \text{other displacements 0.} \]

\[ \frac{1}{\sqrt{6}}, \quad -\frac{2}{\sqrt{6}} = \frac{1}{\sqrt{6}} \]

The same in other directions.
\[ 3 \text{ modes of same frequency.} \]

(The numbers were chosen so as to ensure orthogonality and normalization to unity.)

Let us make a linear transformation of coordinates, using the \( a^{(i)} \) we found classically,

\[ q_i = \sum_k a^{(i)}(q) \]

Then
\[ Q_k = \sum_i a^{(i)} q_i \]

The modes separate when we use these coordinates.

Let
\[ P_k = \frac{1}{i} \frac{\partial}{\partial Q_k} \]
Then \( \frac{\partial}{\partial q^i} = \sum_x \frac{\partial x^i}{\partial q^x} \), \( \frac{\partial}{\partial p^i} = \sum_x \frac{\partial x^i}{\partial p^x} \),

\[ p_i = \sum_x a_i^{(x)} p_x \quad \text{(and, incidentally, } p_i = \sum_x a_i^{(x)} p_x) \]

\[ \frac{1}{2} \sum_i p_i^2 = \frac{1}{2} \sum_x \sum_{\beta} a_i^{(x)} p_x \sum_{\beta} a_i^{(x)} p_{\beta} \]

\[ = \frac{1}{2} \sum_{\beta} \delta_{\beta} p_\beta p_\beta \quad \text{= } \frac{1}{2} \sum_x p_x^2 \]

And \( \frac{1}{2} \sum_{ij} c_{ij} q_i q_j = \frac{1}{2} \sum_i \sum_\beta c_{ij} a_i^{(x)} a_{\beta}^{(x)} a_i q_{\beta} q_\beta \)

\[ = \frac{1}{2} \sum_i \sum_\beta \omega_i^2 a_i^{(x)} a_i q_{\beta} q_\beta \]

\[ = \frac{1}{2} \sum_\beta \omega_\beta^2 q_\beta^2 \]

So that \( H = \sum_x (H_x)_{osc} \), where \( (H_x)_{osc} = \frac{p_x^2}{2} + \frac{1}{2} \omega_x^2 q_x^2 \).

First, what does a particular energy level look like? \( E = \sum_x (\eta_x + \frac{1}{2}) \hbar \omega_x \quad \eta_x \text{ are nonnegative integers} \).

Each choice of the set of \( \eta_x \) corresponds to a possible state of the system.

Wavefunctions \( \Psi = \prod_x \phi_{\eta_x} (x) \)

where \( \phi_{\eta_x} (x) \) is the wavefunction for the \( \eta_x \)-excited state of a harmonic oscillator.

\( \phi_0 (x) \propto e^{-\frac{1}{2} \omega x^2} \), \( = e^{-\frac{1}{2} \omega E / k_B} \text{ is a harmonic for remembering} \).
Ground state: All \( n_x = 0 \)

\[
E_{\text{ground state}} = \sum \frac{1}{2} \hbar \omega x^2 + U(0)
\]

\[v_0 \text{ (zero energy)}\]

And wavefunction \( \psi = \frac{-i}{\sqrt{2\pi}} \partial \psi = e^{-\frac{1}{2} \phi \partial \psi} \)

\[
e^{-\frac{i}{2} \phi \partial \psi} \chi \phi \psi
\]

where \( \chi \chi = \sum \omega x^2 \partial \partial \psi = \text{function of matrix} \psi
\]

Exercise: Show \( \chi = C \).

At temperature \( T \), the average excitation of a harmonic oscillator is

\[
\bar{n} = \frac{1}{1 - e^{-\frac{\hbar \omega}{kT}}}
\]

At temperature \( T \), internal energy of vibration

\[
U = \frac{\sum \hbar \omega x^2 (\bar{n} + \frac{1}{2})}{2} + \frac{\sum \hbar \omega x^2}{1 - e^{-\frac{\hbar \omega}{kT}}}
\]

And to obtain the specific heat, merely calculate \( \frac{dU}{dT} \).

Theorem: Average degree of excitation of an oscillator at temp \( T \)

\[
\bar{n} = \frac{1}{1 - e^{-\frac{\hbar \omega}{kT}}}
\]

Proof:

\[
p_n = e^{-\frac{\hbar \omega x^2}{kT}} e^{-\frac{\hbar \omega x^2}{kT}} \quad \text{But} \quad \sum \bar{n} = 1 \Rightarrow \bar{A} = e^{-\frac{1}{2} \hbar \omega x^2}{kT} \frac{1}{1 - e^{-\frac{\hbar \omega}{kT}}}
So that \( \tilde{\mathbf{N}} = \sum n \mathbf{n} \mathbf{n} \)
\[
= (1 - e^{-\frac{k_B T}{N}}) \sum n \mathbf{n} \mathbf{n} = e^{-\frac{k_B T}{N}} \]
\[
= (1 - x) \frac{d}{dx} \left( \frac{1}{1-x} \right) \]
\[
= \frac{1}{1-e^{-\frac{k_B T}{N}}} \]

Comment: \( U = \frac{\frac{1}{N} \mathbf{W} e^{\frac{k_B T}{N}}} {e^{\frac{k_B T}{N}} - 1} \)

This gives a specific heat curve as a function of temperature like

\[
\text{Specific Heat (One Mode)} \]

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 the ground state before the collision. What is the probability that after the collision the molecule remains in the ground state?

As an interaction, take \( V(R) = a \delta(R - R_{\text{eq}}) \)

Initial state \( \psi_i(R, q) = e^{i \mathbf{p}_i \cdot \mathbf{R}} \psi_i(R_{\text{eq}}, q_{\text{eq}}) \)

Final state \( \psi_f(R, q) = e^{i \mathbf{p}_f \cdot \mathbf{R}} \psi_f(q) \)
Probability \propto |\mathcal{M}|^2

Make Born approximation for \( M \):

\[
M \propto \int \psi_\mathcal{f}^* \, e^{i (\mathbf{p}_\mathcal{f} \cdot \mathbf{P} - \mathbf{p}_\mathcal{f} \cdot \mathbf{R} - \mathbf{q}_\mathcal{f} \cdot \mathbf{R})} \, \mathcal{R} \, \psi_\mathcal{f} \, d^3 R \, dq
\]

\[
\propto \int \int \int \ldots e^{-\frac{\xi}{2} \mathbf{q}^2} \, e^{\frac{i}{\xi} \mathbf{k} \cdot \mathbf{q}} \, dq \, dk \, dk
\]

\[
\propto \frac{\pi}{\sqrt{\hbar \xi}} \, e^{-\frac{\xi}{2} \mathbf{q}^2} \propto e^{-\xi s} \quad \text{where} \quad s = \langle q^2 \rangle.
\]

Office hours, second term:

L. Jones     Friday 12-1.
G. Luxton    Monday 11-12.
MORP ON INTERACTIONS OF MULTIAOTOMIC 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

$$e^{-\mu^2 < q_k^2 >}$$

where $< q_k^2 >$ is the average square displacement of the oscillator.

$\mu$ 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 $\frac{\mu^2}{2m_{osc}}$, for a disturbance with matrix element

$$< q_f | e^{ipx} | q_i >$$

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 $e^{-|p|^2 / \hbar |q|}$.

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.
B1: Construct a theory of inelastic scattering from a crystal or a polyatomic molecule.

B2: The probability \( e^{-\beta q^2} \) 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 nucleus in a crystal undergoes some transition and emits a gamma ray of momentum \( \vec{p} \). Classically you would expect that

\[
E_f = \text{change of nuclear energy} = (\Delta E)^\text{Transition} - \frac{\vec{p}^2}{2M_{\text{nucleon}}}
\]

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

\[
\begin{align*}
E_f &\rightarrow \vec{p} \\
\end{align*}
\]

one is forced to shift the effective \( \Delta E_{\text{II}} \) 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 \(1\text{mm/sec}\) 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 mechanics and 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 \(m=\frac{1}{2}, \omega=1\)

\[
H = \frac{1}{2} p^2 + \frac{1}{2} \dot{x}^2 \quad \text{and} \quad p = \frac{1}{i} \frac{\partial}{\partial \dot{x}}
\]

\[
H \phi_n = E_n \phi_n
\]

The eigenvalues \(E_n = n + \frac{1}{2}\) are given by

\[
\phi_n = \frac{1}{n!} \frac{H_n(\frac{\dot{x}}{m})}{\sqrt{2}^m m!} e^{-\frac{1}{2} \dot{x}^2}
\]

Examples:

\[
H_0 = 1 \quad H_1 = 2 \dot{x} \quad H_2 = 4 \dot{x}^2 - 2
\]

They can all be written compactly in terms of a generating function

\[
e^{-\dot{x}^2/2 + 2 \dot{x} \cdot \frac{\dot{x}}{m}} = \sum_{m} \frac{H_m(\frac{\dot{x}}{m})}{m!} \dot{x}^m
\]

Hence

\[
\sum_{m} \frac{H_m(\frac{\dot{x}}{m})}{m!} \frac{\dot{x}^m}{\sqrt{2}^m m!} = \frac{e^{-\frac{1}{2} \dot{x}^2}}{n!^{1/4}} \sum_{m} \frac{H_m(\frac{\dot{x}}{m})}{m!} \left(\frac{\dot{x}}{2}\right)^m = \frac{e^{-\frac{1}{2} (3 - \dot{x})^2 + \dot{x}^4/4}}{n!^{1/4}}
\]

Sometimes you can make up other generating functions, for fun and profit.

**Example:** to compute the general matrix element

\[
\lambda_{mn} = \int \phi_m^{*}(\dot{x}) e^{i \rho \dot{x}} \phi_n(\dot{x}) \, d\dot{x}
\]
Define \( f(s, t) \) as

\[
\sum_{m} \frac{a_{m n} s^m t^n}{\sqrt{2^m 2^m m! n!}}
\]

It happens to be simpler to compute \( f \) and expand in \( s \) and \( t \) to get \( \lambda_{m n} \) than to do the explicit integral every time.

\[
f = \sum_{m n} \int_{-\infty}^{\infty} \frac{e^{i \rho \beta_{m n} s^m t^n}}{\sqrt{2^m 2^m m! n!}} \, d\beta
\]

\[
= \int \frac{e^{i \rho \beta_{m n} s^m t^n}}{\pi^{n/2}} e^{\frac{1}{4} (s-t)^2 + \frac{i}{4} s^2 + \frac{i}{4} t^2} \, d\beta
\]

\[
= e^{-\frac{\rho}{4}} \frac{i^{n/2} e^{i \rho \beta_{m n} s^m t^n}}{\pi^{n/2}}
\]

Thus,

\[
\lambda_{m n} \frac{(s, t)}{\sqrt{2^m \beta_{m n}}} = e^{-\frac{\rho}{4}} \sum_{m n} \frac{(\beta_{m n})^{l+j-2m}}{(l-m)!(j-m)! m!}
\]

**EXERCISE C:** For a crystal at temperature \( T \), find the probability for elastic scattering with a given \( \rho \).

Hint: If we had just a single oscillator, the answer would look like

\[
\left\langle m | e^{i \beta \xi} | n \right\rangle \propto e^{-\frac{\beta}{4}} \exp(-\frac{\xi^2}{4})
\]

because \( e^{-\frac{\beta}{4}} \) is the probability to be in the \( n \)th state.

One should find that the probability distribution for the energy lost again looks like

\[
e^{-\frac{\rho}{4}} \propto \exp(-\frac{q^2}{4} T)
\]

**EXERCISE D:**

Prove

\[
\sum_{m} \beta_{m n} (s, s') e^{i \beta \xi} = \sqrt{m / \beta \xi} e^{i \beta \xi / 2 \omega}
\]

**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:

\[
\frac{\partial}{\partial t} \psi(s, t) = -\frac{1}{2} \frac{\partial^2}{\partial s^2} \psi(s, t) + \frac{1}{2} \beta^2 \psi(3, t)
\]

for some set of initial conditions - e.g.

\[
t = 0 \quad \psi = f(3 - 3_0)
\]

Hint: Try \( \psi(3, t) = e^{a(t) 3^2 + b(t) 3 + c(t)} \).
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. 

\[ \psi(p) = \int e^{ip \cdot \phi(x)} \, dx \]

(Feynman's guess is that \( \psi(p) = e^{ip} \phi(x) \). What do you get?)

It may on occasion be more convenient to use the momentum space wave functions

\[ \phi_{m}(p) = \int \psi^{*}(x) \phi(x) \, dx \]

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 harmonic oscillator problem can be used to advantage elsewhere. Consider the hydrogen atom:

\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{l(l+1)}{r^2} R + \frac{2m}{\hbar^2} \left[ E - \frac{e^2}{4r} \right] R = 0 \]

For simplicity take \( l = 0 \)

\[ 2m\alpha^2 = 1 \]

\[ \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2m}{\hbar^2} \left[ E - \frac{e^2}{4r} \right] R = 0 \]

This can be easily transformed to momentum space

\[ \frac{-i}{\hbar} \frac{d}{dp} \left( \frac{p^2}{2} \phi(p) \right) + \phi(p) = -\frac{E\hbar}{\alpha} \frac{d\phi}{dp} \]

Now it is a first order differential equation, which is presumably easier to solve than the previous second order differential equation.

This equation (with \( \phi \) left in) can also be factorized into "creation" and "annihilation" operators in a manner not too unlike the one used below for the harmonic oscillator. 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**

\[ \Pi = \frac{i}{2} P^2 + \frac{m\omega^2 q^2}{2} \]

\[ a = \sqrt{\frac{m}{2\omega}} \left( \omega q + \frac{\lambda^2}{m} \right) = \frac{1}{\sqrt{2}} \left( \Phi + \frac{1}{\alpha^2} \right) \]

\[ a^* = \sqrt{\frac{m}{2\omega}} \left( \omega q - \frac{\lambda^2}{m} \right) = \frac{1}{\sqrt{2}} \left( \Phi - \frac{1}{\alpha^2} \right) \]
\( a^\dagger \) is called a creation operator and \( a \) an annihilation operator
\[
[a, a^\dagger] = i = \Rightarrow \quad a a^\dagger - a^\dagger a = 1
\]
\( a a^\dagger = \frac{1}{\sqrt{2}} \hat{H}^{+\frac{1}{2}} \)
\( a^\dagger a = \frac{1}{\sqrt{2}} \hat{H}^{-\frac{1}{2}} \)

The most useful form is \( \hat{H} = \omega a^\dagger a + \frac{\omega}{2} \), following a general rule of thumb wherein all the annihilation operators are written to the right of all the creation operators
(normal ordering)
\[
a |0\rangle = 0 \Rightarrow \quad \hat{H} |0\rangle = \omega^{\frac{1}{2}} |0\rangle
\]
and \( \omega^{\frac{1}{2}} \) can thus be interpreted as the energy of the ground state; \( \omega a^\dagger a \) as the energy above the ground state
\( n = a^\dagger a \) has integer eigenvalues \( n |m\rangle = m |m\rangle \)
on which the creation and annihilation operators act like
\[
a^m |m\rangle = \sqrt{m+1} |m+1\rangle \quad a |m\rangle = \sqrt{m} |m-1\rangle
\]

Hence
\[
\frac{(a^\dagger)^n |0\rangle}{\sqrt{m!}} = |m\rangle
\]
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)
\[
q_{nm} = \langle m | \frac{a^\dagger a}{\sqrt{2}} | m \rangle = \langle 0 | \frac{a^m}{\sqrt{m!}} \left( a + a^\dagger \right) \frac{a^\dagger}{\sqrt{2}} | 0 \rangle
\]
This can then be calculated explicitly by commuting until all operator products are in
normal order form
\[
q_{01} = \langle 0 | \left( \frac{a^\dagger a^\dagger}{\sqrt{2}} \right) a^\dagger | 0 \rangle = \langle 0 | \frac{a^\dagger a^\dagger}{\sqrt{2}} + \frac{1}{\sqrt{2}} \left( 1 + a a^\dagger \right) | 0 \rangle = \langle 0 | \frac{a^\dagger a^\dagger}{\sqrt{2}} e^{i c} | 0 \rangle
\]
Thus
\[
\lambda_{nm} = \langle 0 | \frac{a^m}{\sqrt{m!}} \left( e^{i \phi} \right)^{\frac{a^\dagger a^\dagger}{\sqrt{2}}} \frac{a^\dagger}{\sqrt{2}} | 0 \rangle
\]
If several independent oscillators are involved
\[
a^\dagger = \sqrt{\frac{\omega}{2}} \left( \omega_d Q_a + i \frac{P_a}{m_a} \right)
\]
\[a_{\beta} a_{\dagger} - a_{\alpha} a_{\dagger} a_{\beta} = \delta_{\alpha \beta}\]
\[
[a_{\beta}, a_{\alpha}^\dagger] = 0 \quad [a_{\beta}^\dagger, a_{\alpha}^\dagger] = 0
\]
\[\hat{H} = (\text{ground state energy}) + \sum \omega_a a^\dagger_a a_a \]
notice the embarrassing fact that if there are an infinity of oscillators 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

\[
H = \frac{p_i^2}{2} + \frac{1}{2} C_{ij} q_i q_j
\]

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

\[
H = \frac{p_i'^2}{2} + \frac{1}{2} Q_i^2
\]

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

\[
\begin{array}{c}
\text{(Diagram of unit cell)}
\end{array}
\]

Each cell is identified by a vector \( \mathbf{R} = m_a \mathbf{a} + m_b \mathbf{b} + m_c \mathbf{c} \)

where \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) are fundamental vectors characteristic of the crystal lattice and \( (m_a, m_b, m_c) \) 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 \( \mathbf{R} \) within a cell by \( \mathbf{R} \)

Then the total Hamiltonian for the system takes the form

\[
\sum_{\mathbf{R}} \frac{p_{\mathbf{R}}^2}{2} + \frac{1}{2} \sum C_{\mathbf{R}, s, t} q_{\mathbf{R}, s} q_{\mathbf{R}, t}
\]
where \( C_{ij} = \sum_{m,n} \left( \mathbf{N}_i - \mathbf{N}_j \right) \)

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

\[ \omega^2 q_{n,m} = \sum_{m,n} \left( \mathbf{N}_i - \mathbf{N}_j \right) q_{n,m} \]

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 \[ \frac{A}{2} \left( q_n - q_{n+1} \right)^2 \]

Differentiate with respect to \( q_n \) to get the force

\[ \omega^2 q_n = A \left( q_n - q_{n+1} \right) - A \left( q_{n-1} - q_n \right) = A \left( 2q_n - q_{n+1} - q_{n-1} \right) \]

To patch up the end points we define the conditions

\[ \mathbf{P}(-1) = 0 \quad \mathbf{P}(0) = 2 \]

Then our previous techniques would be to find the determinant of

\[
\begin{vmatrix}
2A - \omega^2 & -A \\
-A & 2A - \omega^2 - A \\
-A & 2A - \omega^2 - A \\
\end{vmatrix}
\]

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 \[ \sum_n \beta_n \left( q_n - q_{n+2} \right)^2 \]

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 \( q_m = e^{i m \delta} \).

\[
\omega_n^2 e^{i m \delta} = A \left[ 2 e^{i m \delta} - e^{i (m+1) \delta} - e^{i (m-1) \delta} \right] = \omega_n^2 = 2 A \left[ 1 - \cos \delta \right]
\]

At first sight one feels that \( \delta \) may be arbitrary and hence that there is a continuum of solutions for \( \omega_n \). 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 periodic boundary conditions is one quite standard technique in these crystal problems. It means that if \( \frac{m}{2} \) is the number of atoms in the crystal, then \( q_0 + s = q_s \).

For our example this means \( e^{i \frac{m}{2} \delta} = 1 \).

Hence \( \delta = 2\pi l \frac{\ell}{m} \) where \( \ell \) is an integer from 0 to \( \frac{m}{2} - 1 \) (or it may assume an equal number of values in an interval symmetric about zero).

Only discrete values corresponding to the integer \( \ell \)'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 \( \delta \) continued outside this fundamental interval, the frequencies would simply repeat.

Hence we always limit ourselves to the first zone constructed in the way.

If \( \delta \) should be non-zero, it is easy to see that the answer will have the form

\[
\omega = 2 \beta (1 - \omega_0 \delta) + 2 \beta (1 - \omega_0 2 \delta)
\]

and so forth for more distant interactions.
Solid state physicists do not in general talk about $\mathcal{F}$, however. The quantity normally used is $k = \frac{\delta}{\lambda} = \text{phase difference/cm}$. For a three-dimensional crystal, $k$ becomes a vector $\mathbf{k} = \left( \frac{\delta_1}{a}, \frac{\delta_2}{b}, \frac{\delta_3}{c} \right)$ in a space called reciprocal lattice space (since $\frac{1}{a}, \frac{1}{b}, \frac{1}{c}$ are the units of length along the respective crystal directions).

Because the spacing of $\mathcal{F}$ is $\frac{2\pi}{\lambda}$, the spacing of $k$ is $\frac{2\pi}{\Lambda a} = \frac{2\pi}{L \cdot a \cdot b}$. For very small $k$ (i.e., very long waves) we get from above that $\omega^2 \approx \hbar a^2 k^2 / \lambda^2$ where $c$ may be thought of as the speed of sound. Hence at long wavelengths the speed of sound is very nearly independent of the wavelength.

Given an allowed $k$, define a mode of vibration by $q_k = \sum_{\text{atoms}} e^{-i\mathbf{k} \cdot \mathbf{r}_n}$ Then the Hamiltonian assumes the form $H = \sum \left( \frac{p_k^2}{2m} + \omega_k q_k^2 \right)$ where $\omega_k(k) = \mathcal{H}(1 - \omega \cdot \mathbf{k} a)$. Notice again that just as there is only a region of $\mathcal{F}$ 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 $\text{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 importance (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.

Inserting this $\omega_k^2 q_k^4 e^{-i\mathbf{k} \cdot \mathbf{r}} = \sum_{\mathbf{r}} P_{\mathbf{r}, s} (\mathbf{k}) e^{i\mathbf{r} \cdot \mathbf{M}} q_s^4$

But $\sum_{\mathbf{r}} P_{\mathbf{r}, s} (\mathbf{k}) e^{i\mathbf{r} \cdot \mathbf{M}} = X_{\mathbf{r}, s} (\mathbf{k})$ is just a Fourier transform of the $P_{\mathbf{r}, s}$

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 magnitude 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

\[
\int d^3k \left( \text{volume factor} \right) \left( \frac{2\pi}{L_a} \right)^3
\]

For a three dimensional crystal with one atom per unit cell the simple generalization of our calculation for a one dimensional crystal yields

\[
\omega \propto k^2
\]

(projections on various axes in \( k \) space need not look alike unless the crystal is isotropic)

It is possible to prove that at \( k=0 \), \( \omega \propto k^2 \) 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 \( k \to 0 \), it is not necessary that all frequencies go through zero. One finds in fact

\[
\omega \propto k
\]

In the acoustical branch one might have, for example, the two atoms moving together

\[
\begin{align*}
&\rightarrow \rightarrow \\
&\uparrow \downarrow \uparrow \downarrow
\end{align*}
\]

with the pattern slightly displaced from cell to cell

For the optical branch they might move \( \rightarrow \leftarrow \) 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 \( k \))
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:

![Diagram of a cubic crystal]

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 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 $P = P_{out} - P_{in}$

Show that this will excite a mode of wavevector $\mathbf{k}$ where

$$\mathbf{k} = \mathbf{L} + \mathbf{l}$$

where $\mathbf{L}$ 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:

$$\sum_{\mathbf{k}} \rightarrow \int \frac{d^3 k}{(2\pi)^3}$$

We are not usually interested in all $\mathbf{k}$ values.

If the 3 fundamental translation vectors of the lattice are $\mathbf{a}, \mathbf{b}, \mathbf{c}$, then the phase in the $N$th cell is

$$e^{i \mathbf{k} \cdot \mathbf{N}}$$

for a mode with wavevector $\mathbf{k}$.

Now if $\mathbf{k}' = \mathbf{k} + \mathbf{l}$

then $e^{i \mathbf{k}' \cdot \mathbf{N}} = e^{i \mathbf{k} \cdot \mathbf{N}}$ if $e^{i \mathbf{L} \cdot \mathbf{l}} = 1$

This will be insured if

$$\mathbf{l} = L_a \frac{\mathbf{b} \times \mathbf{c}}{|a \cdot b c|} + L_b \frac{\mathbf{c} \times \mathbf{a}}{|a \cdot b c|} + L_c \frac{\mathbf{a} \times \mathbf{b}}{|a \cdot b c|}$$

where $L_a = L \cdot a = 2\pi n_1$,

$L_b = 2\pi n_2$, $L_c = 2\pi n_3$

$n_1, n_2, n_3$ are integers.
\( L_x, L_y, L_z \) are the components of \( \mathbf{L} \) along the three directions perpendicular to the 3 planes formed by choosing 2 of the 3 vectors \( a, b, c \).

\[ L_x, L_y, L_z = 2\pi \text{ (integer)} \]

The set of all such \( L \)'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 \( W_p(k) \)**

At temperature \( T \),

\[ U = \sum_{\beta} \sum_k \frac{h W_\beta(k)}{e^{\frac{h W_\beta(k)}{k_B T}} - 1} \]

\[ = V \sum_{\beta} \int \frac{d^3k}{(2\pi)^3} \frac{h W_\beta}{e^{\frac{h W_\beta}{k_B T}} - 1} \]

\[ C_V = \frac{\partial U}{\partial T} = k_B V \sum_{\beta} \int \frac{d^3k}{(2\pi)^3} \left( \frac{h W_\beta}{k_B} \right)^2 \frac{e^{\frac{h W_\beta}{k_B T}}}{(e^{\frac{h W_\beta}{k_B T}} - 1)^2} \]

The integration \( \int d^3k \) 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 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 energy in the electronic motion, 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, \( kT > \hbar \omega_n(k) \) for all \( k \) and \( \hbar \omega_n(k) \)

then \( U \approx kT \sum_{\text{modes}} \int \frac{d^3k}{(2\pi)^3} V \)

\[ V = \text{volume of unit cell} = 12 \cdot 2x \leq 1 \]

\[ \int \frac{d^3k}{(2\pi)^3} V = 1 \]

\[ U \approx k_B T (\text{no. of modes}) = 3Nk_B T \]

\( N = \text{no. of atoms in crystal} \)

\( C_v = 3R \) per degree Kelvin per mole

\( = 6 \text{ calories per deg. per mole at high } T. \)

For low T:

\[ \omega_n(k) = \frac{\hbar c}{k} \]

\( C_v \) depends slightly on direction of \( k \), for only 3 \( k \)'s exist for low \( T \) — those for which \( \omega_n(k) \to 0 \) in reciprocal space.

\[ U = k_B T V \sum_k \int \frac{d^3k}{(2\pi)^3} \left( \frac{\hbar c k}{k_B T} \right)^3 \frac{1}{\exp \left( \frac{\hbar c k}{k_B T} \right) - 1} \]

Let \( x = \frac{\hbar c k}{k_B T} \).

Then

\[ U = k_B T \int \frac{d\omega}{T^4} \left( \frac{k_B T}{\hbar c \omega} \right)^3 \frac{1}{(2\pi)^3} \int_0^x \frac{x^3 dx}{e^x - 1} \]

only a small error is introduced if we take the upper limit as \( \infty \), and then the integral \( = \frac{\pi^4}{15} \).

Then

\[ U = \left( \frac{k_B T}{C_0^3} \right)^{\frac{4}{3}} \]

where \( \frac{1}{C_0^3} = \frac{1}{3} \sum_i \frac{1}{C_i^3} \)

\[ C_v \propto T^3 \quad \text{as } T \to 0 \]

\( C_0 \) is some average speed of sound.
For very small $T$ (say $10^{-6} \, \text{K}$), $C_v$ 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

\[ C_v \]

\[ T \]

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 to each other, then we would obtain

\[ C_v \]

\[ 3k_B T \text{(no. of atoms)} \]

\[ 3k_B T \text{(no. of molecules)} \]

\[ T \]

There is a theory due to Debye, and this consists of first writing

\[ W_k = c_0 \, \text{if} \] 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 \[ U = 3k_B T \int \frac{d^3k}{(2\pi)^3} \frac{\hbar c_0 k}{k_B T} \frac{1}{\exp \left( \frac{\hbar c_0 k}{k_B T} \right) - 1} \]

Use the approximation of replacing the unit cell in the reciprocal lattice by a sphere of radius \( k_{\text{max}} \).

Then \[ \int \frac{d^3k}{(2\pi)^3} \rightarrow 4\pi \int_0^{k_{\text{max}}} \frac{d^2k}{(2\pi)^2} \frac{k^2}{k} \frac{\hbar c_0 k}{k_B T} \frac{1}{\exp \left( \frac{\hbar c_0 k}{k_B T} \right) - 1} \]

and \[ U = \left( \frac{k_B T}{\hbar c_0} \right)^4 \left( \frac{3}{2\pi^2} \int_0^{\Theta/T} \frac{x^3 dx}{e^x - 1} \right) \]

For \( T \rightarrow 0 \), we recover previous formula.

For \( T \gg \Theta \), \( \Theta \) is called the Debye temperature, it is a useful quantity to know in the case of a particular crystal.

\[ U = \left( \frac{k_B T}{\hbar c_0} \right)^4 \left( \frac{3}{2\pi^2} \int_0^{\Theta/T} \frac{x^3 dx}{e^x - 1} \right) \] \( \Rightarrow \) \( CV \) = constant independent of \( T \) and independent of c0.

Hard crystals usually have high \( \Theta \) (diamond), soft crystals generally have low \( \Theta \) (Argon).

This theory of specific heat has been widely abused. Rather than plotting \( CV \) vs. \( T \), with \( \Theta \) as an adjustable parameter, and comparing with experimental \( CV \) vs. \( T \), people have plotted \( \Theta_0 \) vs. \( T \) as a way of reporting measurements of the specific heat.

One obtains in this manner foolish curves like

\[ \Theta_0 \]

\[ T \]
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 $\omega$.

Solution: $\phi_n(x) = \frac{1}{\pi^{1/4} \sqrt{n!}} \frac{1}{\sqrt{2^n n!}} e^{-x^2/2} \frac{d^n}{dx^n} e^{-x^2/2}$

where $H_n(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2}$

(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 $H_n(x)$)

$\Sigma = \sum_{n=0}^{\infty} \frac{e^{x^2/2} \frac{d^n}{dx^n} e^{x^2/2}}{\sqrt{2^n n!}} \left( \frac{d^n}{dx^n} e^{-y^2/2} \right) \left( \frac{d^n}{dx^n} e^{-i\omega t} \right) e^{-i\omega t}$

$\frac{d^n}{dx^n} e^{-x^2} = \frac{1}{\sqrt{2^n \pi}} \frac{d^n}{dx^n} \int_{-\infty}^{\infty} e^{ixy} e^{-y^2/2} dy$

$= \frac{1}{\sqrt{2^n \pi}} \int_{-\infty}^{\infty} (i y)^n e^{ixy} e^{-y^2/2} dy$

$\Sigma = \frac{e^{x^2/2} e^{x'^2/2}}{2\pi^{3/2}} \left( \int_{-\infty}^{\infty} e^{ixy} e^{-y^2/2} \int_{-\infty}^{\infty} e^{ix'y} e^{-y'^2/2} \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} e^{-i\omega t} \right)$

The evaluation of the integrals is straightforward (though slightly tedious) the result is

$\sum_{n=0}^{\infty} = \frac{2}{\sqrt{\pi}} \frac{\exp \left( \frac{i}{2} (x^2 + x'^2) + (1 + e^{i\omega t}) \right) + 2 xx' e^{-i\omega t}}{(1 - e^{2i\omega t})^{1/2}}$
More on Neutron Scattering

The amplitude for the process takes the form

\[
\int e^{i k \cdot r} \left| \sum_i V_i (r_i - R_i) \right| e^{i q \cdot r} \right>
\]

where the sum is over the lattice sites

\[ V_i \] has different values for the different types of atoms involved

\[
\sum_j e^{-i k \cdot r} e^{i q \cdot r} \left| \int V_j (r_j - R_j) d^3 R \right|^2 = \left< f \left| \sum_j V_j (P) e^{i R_j \cdot \vec{p}} i \right> \right>
\]

Provided the wavelength for \( P \) is long compared to other dimensions, the dipole approximation can be used to evaluate the integrals and \( V_j \) is approximately independent of \( P \).

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:

\[
\left< i \left| \sum_j e^{i \vec{p} \cdot \vec{q}_i} e^{i \vec{p} \cdot \vec{R}_i} i \right> \right>
\]

where \( \vec{q}_i \) is the oscillating coordinate and \( \vec{R}_i \) is the equilibrium position.

Hence we find

\[
\sum_j V_j (P) e^{i P \cdot \vec{q}_i} \left< i \left| e^{i \vec{p} \cdot \vec{R}_i} i \right> \right>
\]

This was previously evaluated to give

\[ e^{-P^2 <q^2>/2} \]

It is obvious that if \( \frac{<q^2>}{\lambda^2} \gg 1 \), there will be almost no elastic scattering.

The probability is then just

\[
\left| \sum_j V_j (P) e^{i P \cdot \vec{R}_i} \right|^2 e^{-P^2 <q^2>/2}
\]

\( V_j (r_i - r_j) \) 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

\[
\sum_{\omega \mu \alpha} e^{i \omega \cdot \vec{R} \cdot \vec{q}} \sum_j \left< \sum_{\omega \mu \alpha} e^{i \omega \cdot \vec{R} \cdot \vec{q}} \right>_{\omega \mu \alpha}
\]

For one type this is

\[
V (P) \sum_{\omega \mu \alpha} e^{i \omega \cdot \vec{R} \cdot \vec{q}}
\]

Where \( \omega, \mu, \alpha \) are the components along the directions in reciprocal lattice space.

Hence we arrive at

\[
V (P) \left[ \frac{1 - e^{i \omega \cdot \vec{q}}} {1 - e^{i \omega \cdot P}} \right] \left[ \frac{1 - e^{i \mu \cdot \vec{q}}} {1 - e^{i \mu \cdot P}} \right] \left[ \frac{1 - e^{i \alpha \cdot \vec{q}}} {1 - e^{i \alpha \cdot P}} \right]
\]

The absolute square gives

\[
|V (P)|^2 e^{-P^2 <q^2>/2}
\]

\[
\left[ \frac{\sum \omega \mu \alpha e^{i \omega \cdot \vec{q}}} {\sum \omega \mu \alpha e^{i \omega \cdot \vec{q}}} \right] \left[ \frac{\sum \omega \mu \alpha e^{i \mu \cdot \vec{q}}} {\sum \omega \mu \alpha e^{i \mu \cdot \vec{q}}} \right] \left[ \frac{\sum \omega \mu \alpha e^{i \alpha \cdot \vec{q}}} {\sum \omega \mu \alpha e^{i \alpha \cdot \vec{q}}} \right]
\]
This approaches a product of \( N \to \infty \) functions as \( N \to \infty \) \[ \delta \left( \frac{P_{av}}{2} \right) \]

Thus \( P \) must be a reciprocal lattice vector to have any appreciable contribution.

Now consider the case of inelastic scattering
\[ \sum_j V_j (\vec{P}) \langle \mathbf{f} | e^{i \vec{P} \cdot \vec{q}_j} | i \rangle \approx e^{i \vec{P} \cdot \vec{r}_j} \]

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 \( E_0 \)
\[ T_{fi} (E_0) = \int \frac{d^3 k}{(2\pi)^3} \int (E_{kf} - E_0) \langle \mathbf{f} | e^{i \vec{P} \cdot \vec{q}_j} | i \rangle \]

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
\[ \Psi_{\text{after}} = e^{i \vec{P} \cdot \vec{r}} \Psi_{\text{before}} \]
\[ \langle \Psi_{\text{after}} | H | \Psi_{\text{after}} \rangle - \langle \Psi_{\text{before}} | H | \Psi_{\text{before}} \rangle = \frac{\hat{P}^2}{2m} + \int \rho_{\text{other momenta}} \cdot V \]
\[ \langle \Psi_{\text{after}} | e^{i \vec{P} \cdot \vec{r}} H e^{i \vec{P} \cdot \vec{r}} - H | \Psi_{\text{after}} \rangle = \frac{\hat{P}^2}{2m} + \hat{P} = \langle \Psi_{\text{after}} | \frac{\hat{P}^2}{2m} | \Psi_{\text{after}} \rangle \]

because \[ \hat{P}_{\text{pop}} \left[ e^{i \vec{P} \cdot \vec{r}} f(x) \right] = \hat{P} f(x) \rho_{\text{number}} e^{i \vec{P} \cdot \vec{r}} + e^{i \vec{P} \cdot \vec{r}} \rho_{\text{pop}} f \]

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 \[ \sum_n e^{-\beta m} |<m|e^{i \vec{P} \cdot \vec{r}} |m>|^2 \]
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

\[ Q_m = \text{displacement} = \frac{1}{\sqrt{\eta}} \sum \frac{e^{ikr}}{r} \]

where \( \eta \) 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

\[ H = \frac{1}{2} \sum \left( \frac{1}{2} \beta_m^2 + \frac{1}{2} (q_m - q_{m+1})^2 \right) \]

\[ Q_n = \frac{1}{\sqrt{\eta}} \sum q_m e^{ikr_n} \]

where \( r_n = \alpha m \) is the actual position in space of the atom

For long wavelengths \( \omega^2 = 2 \alpha (1 - \cos \alpha) \) becomes \( \omega^2 \propto \alpha a^2 k^2 \)

\( k \alpha \) small implies \( q_m \) may be replaced by the continuous \( q(x) \)

\[ Q_n = \int \frac{dx}{\alpha} e^{ikr_n} q(x) \]

defines the normal modes

Generally one redefines

\[ Q' = \int \frac{dx}{\alpha} e^{ikr_n} q'(x) \]

\[ q'(x) = \int Q_n' \frac{dx}{\alpha} e^{-ikr_n} \]

Then the formula for the energy becomes

\[ H = \sum \left[ \frac{1}{2} \left( \frac{\partial q(x)}{\partial t} \right)^2 \frac{dx}{\alpha} + \frac{1}{2} \alpha a^2 \left( \frac{\partial q(x)}{\partial x} \right)^2 \frac{dx}{\alpha} \right] \]

\( \rho = \frac{1}{\alpha} \) 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

\[ \Pi(x) = \rho_m a \]

\( q_m - q_{m+1} = -\rho a \delta_{nm} \rightarrow \Pi(x) q(x) - q(x') \Pi(x) = -\rho a \int (x - x') \]

\[ H = \int \frac{dx}{\alpha} \left( \frac{\rho^2}{2} \frac{dx}{\alpha} + \frac{\rho^2}{2} \left( \frac{\partial q}{\partial x} \right)^2 \right) \]

\[ q(x) \rightarrow \Pi(x) \]

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 $Q_n$'s, define a Fourier transform of the conjugate momentum
$$\widehat{p}(x) = \int e^{-ix\cdot\xi} \frac{\widehat{P}(\xi)}{2\pi} d\xi$$

$$P(K_1) Q(K_2) - Q(K_2) P(K_1) = -i \delta(K_1 - K_2)$$

$$H = \int \frac{d^3k}{(2\pi)^3} \left[ \frac{1}{2} p^2 + \frac{1}{2} k^2 c^2 Q(k)^2 \right]$$

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

$$K E = \frac{1}{2} \int \frac{\partial Q}{\partial x} \cdot \frac{\partial Q}{\partial x} \, dx$$

$$P E = \frac{1}{2} \int c \omega \epsilon \epsilon c \cdot c \, dx$$

$$\epsilon_{ij} = \frac{1}{2} \left[ \frac{\partial \epsilon_{j}}{\partial x_{i}} + \frac{\partial \epsilon_{i}}{\partial x_{j}} \right]$$

The tensor $\epsilon_{ij}$ 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.

\[
\begin{align*}
  & t \\
  & \begin{array}{c}
  a^*aa \\
  a^*a^*a \\
  c^*a^*a^*
  \end{array}
\end{align*}
\]

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 \( k \).

\[
\begin{array}{c}
\text{ideal} \\
\text{real}
\end{array}
\]
\[\omega\text{ with indicates lifetime of photon}\]

At the low \( k \) end of the spectrum, we can approximate reality by the previously developed continuum formalism, and try using \( \left( \frac{d^2}{dx} \right)^3 \) 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 \( \mathbf{U} \) is a reciprocal lattice vector, \( e^{i \mathbf{k} \cdot \mathbf{U}} = 1 \) \( \forall \mathbf{k} \) 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

\[
\mathbf{k}' + \mathbf{k}'' = \mathbf{k}'' + \mathbf{U} \quad \text{for } k' \neq k''
\]

For very small \( k \), no \( \mathbf{U} \) will be required. If \( \mathbf{U} \) is required, the process is called an umklapp process.

Hence we may restate the above

Problem: Explain carefully how the umklapp processes 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

\[
e^{-\frac{k}{\hbar} \Delta E \sqrt{\text{Top of acoustical branch}}}
\]

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 Mössbauer effect.

Problem: Invent a way to measure the momentum of a phonon.

Aside:

1) For an amorphous medium there are quantities analogous to phonons, but they scatter very fast and very randomly.

2) For waves the simple minded rule of thumb

\[
\frac{k}{\hbar} = \frac{\text{momentum}}{\text{energy}}
\]

will almost always give the same answers as more elaborate analyses.

Problem: Influence of impurities on the properties of crystals.

Take a low density \( \mathcal{N} \) of atoms with different masses. Assum each flaw acts independently scattering phonons into other directions

As \( T \to 0 \), for density \( \mathcal{N} \), how does the thermal conductivity depend on \( T \) and how on \( \mathcal{N} \)?

(give just a power law dependence, since that would be the first thing you'd measure)
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

$$ q_n \rightarrow q(x) $$

$$ \frac{p_n}{\hbar} \rightarrow \pi(x), \quad a = \text{spacing between atoms in discrete case} $$

then

$$ \left[ q_n, p_m \right] = i \hbar \delta_{nm} \implies \left[ \pi(x), q(x') \right] = -i \hbar \delta(x-x') \quad \ldots \quad (1) $$

In terms of $q(x), \pi(x)$,

$$ \text{kinetic energy} = \frac{1}{2} \int \frac{(\pi(x))^2}{\hbar^2} dx = \frac{1}{2} \int \pi^2(x) dx $$

$$ \text{potential energy} = \frac{c}{2} \int \left( \frac{\partial q}{\partial x} \right)^2 dx $$

i.e.,

$$ H = \frac{1}{2} \int \left[ \pi^2(x) + c \left( \frac{\partial q}{\partial x} \right)^2 \right] dx \quad \ldots \quad (2) $$

Write

$$ q(x) = \sum_k \frac{1}{\sqrt{2\omega_k}} \left( a_k^* + a_k \right) e^{-ikx} $$

$$ \pi(x) = \sum_k \frac{i \sqrt{\omega_k}}{2} \left( a_k^* - a_k \right) e^{-ikx} \quad \ldots \quad (3) $$

then with the substitution

$$ \sum_k \rightarrow \frac{i}{(2\pi)^2} \int dk $$
the commutation rules of the $a$'s are found to be:

\[ [a_k, a^*_l] = \delta(k-l), \quad [a_k, a_l] = 0 = [a^*_k, a^*_l] \quad - - - (4) \]

One may verify the equivalence of (4) and (1) by using (4) and (3) to obtain the CR's of $\Pi(x), q(y)$:

\[ q(x) \Pi(y) - \Pi(y) q(x) \]
\[ = \sum_k \frac{i}{\sqrt{\omega_k}} \left( a^*_k + a_k \right) (q^*_k - q_k) \]
\[ - (q^*_k - q_k) (a^*_k + a_k) \left( e^{-ikx} - e^{iky} \right) \]
\[ = \sum_k i e^{-ik(x-y)} = i \int \frac{dk}{2\pi} e^{-ik(x-y)} \]
\[ = i \delta(x-y) \]

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

\[ H = \frac{1}{2} \int \left( q^2 + c^2 \frac{\partial^2 q}{\partial x^2} \right) dx = \sum_k \omega_k (a^*_k a_k + \frac{1}{2}) \]

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

\[ \dot{q}(y) = +\frac{i}{\hbar} \int dx \left[ \Pi^2(x) q(y) + c^2 \frac{\partial^2 q(y)}{\partial x^2} \right] \]
\[ = +\frac{i}{\hbar} \int dx \left[ \Pi^2(x) q(y) - \Pi(x) \Pi(y) - \Pi(x) q(y) \Pi(x) \right. \]
\[ - \left. q(y) \Pi^2(x) \right] \]
\[ = +\frac{i}{\hbar} \int dx \left[ \Pi(x) (-i \delta(x-y)) + (\cdot i \delta(x-y)) \pi(x) \right] \]
or, \( \dot{q}(y) = \Pi(y) \) as expected.

Also, \( \dot{\Pi}(y) = i \left[ H, \Pi(y) \right] \)

\[
= c^2 \frac{\partial^2 \dot{q}}{\partial y^2}
\]
upon integrating by parts.

For a 3-dimensional scalar field (only one disturbance at each point in space)

\[
\dot{\Pi} = c^2 \nabla^2 \dot{q} = \ddot{q}
\]

**Vibrations of a three-dimensional solid:**

There are 3 different disturbances (3 independent displacements) at each point — label by \( i \).

Then

\[
\left[ \Pi_i(x), \dot{q}_j(y) \right] = -i \delta(x-y) \delta_{ij}
\]

**Kinetic energy**

\[
\frac{1}{2} \int \frac{\partial q_i}{\partial x} \frac{\partial q_j}{\partial x} \, dx
\]

**Potential energy**

\[
\frac{1}{2} \int_{ij, kl} C_{ij, kl} \frac{\partial q_i}{\partial x_j} \frac{\partial q_k}{\partial x_l} \, dx
\]

where the coefficients \( C_{ij, kl} \) are symmetric under any of the following interchanges

\[
i \leftrightarrow j
\]

\[
k \leftrightarrow l
\]

\[
i j \leftrightarrow kl
\]

This gives the equations of motion

\[
\ddot{q}_i = \sum_{j, k, l} C_{ij, kl} \frac{\partial^2}{\partial x_j \partial x_l} q_j(x)
\]
The general case is rather formidable. A simpler case would be

$$\ddot{\phi} = \lambda_1 \nabla^2 \phi + \lambda_2 \nabla (\nabla \phi)$$

with $\lambda_1, \lambda_2$ 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, $L = L(\phi)$ such $L$ may depend on $\dot{\phi}$, $\ddot{\phi}$.

Then $S = \int L \, dx$ is an extremum for arbitrary variations $\delta \phi$ in the fields $\phi$.

The Euler-Lagrange equations are then

$$\frac{\partial L}{\partial \phi} - \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{\phi}} \right) + \sum_k \frac{\partial}{\partial x^k} \left( \frac{\partial L}{\partial \dot{\phi} \partial \phi} \right)$$

**Example:** For $L = \frac{1}{2} \dot{\phi}^2 - \frac{c^2}{2} (\nabla \phi)^2$

the equation of motion is $\ddot{\phi} = -c^2 \nabla^2 \phi$.

For classical electromagnetism (free field),

$$L = \frac{1}{2} (E^2 - B^2)$$

(in presence of sources, add $\frac{1}{2} \mu_0 \nabla \cdot (\nabla \phi)$)
Writing $S$ in terms of $A$, $\phi$, the action principle becomes
\[
\frac{1}{\hbar} \int \left\{ \left[ \frac{\partial A}{\partial t} + \nabla \phi \right]^2 - \left( \nabla A \right)^2 \right\} d^3x = 0
\]
Expanding and integrating by parts
\[
\frac{1}{\hbar} \int \left\{ \left( \frac{\partial A}{\partial t} \right)^2 + (\nabla \phi)^2 - \frac{\nabla \cdot A}{\partial t} - (\nabla A)^2 \right\} d^3x = 0
\]
Choose gauged gauge so that $\nabla \cdot A = 0$ (Coulomb gauge)
Integrating $(\nabla \phi)^2 = -\Delta^2 \phi + \nabla \cdot (\nabla \phi \phi)$ by parts and making use of the result $\nabla^2 \phi = 0$ for free fields as a shortcut
\[
\frac{1}{\hbar} \int \left( \frac{\partial A}{\partial t} \right)^2 - (\nabla A)^2 \right\} d^3x = 0 \Rightarrow \delta \left( \frac{\partial \tilde{A}}{\partial t} - \nabla \cdot \tilde{A} \right) = 0
\]
Let $\Pi = \frac{\partial A}{\partial t}$
Then using the quantum mechanical condition
\[
\left[ \Pi_i (x), A_j (y) \right] = -i \delta_{ij} \delta^3 (x - y) \delta_{ij}
\]
and
\[
H = \int \mathcal{H} d^3x = \frac{1}{\hbar} \int \left( \left( \frac{\Pi^2}{2} \right)^2 + (\nabla A)^2 \right) \right\} d^3x
\]
Or, when sources are present
\[
H = \frac{1}{\hbar} \int \left\{ \frac{\Pi^2}{2} + (\nabla A)^2 + J \cdot A - \phi \frac{\hbar^2}{2} \right\} d^3x
\]
Problems (Do not hand in — no assignment this week)

1. Derive Maxwell's Equations as operator equations from

\[ \mathbf{\Pi} = i [H, \mathbf{\Pi}] \]
\[ \mathbf{A} = i [H, \mathbf{A}] \]

2. a. Evaluate \([A_2(x, t), A_m(x', t')]\) for free fields.

b. Write \(A_2(x) = \sum_{k, \omega} \frac{1}{\sqrt{2W_k}} \left[ a_k^+ \alpha \varepsilon^2 e^{-i k \cdot x} + \varepsilon^* a_k \alpha \varepsilon e^{i k \cdot x} \right]\)

and interpret the \(\alpha\)'s. (Find CR's, etc.)

Remarks:

In our treatment of elasticity, we began with real atoms, 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 wave-like properties of light caused people to treat light as the elastic vibrations of a solid, since that was where wave-like 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.

**Election in Metals**

Let us work out the consequences of making the following wild approximations:

1) Disregard the potential of the electron due to the ion core.

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.

Then \( N = \int \frac{d^3k}{(2\pi)^3} \text{Vol.} = \frac{2V}{(2\pi)^3} \frac{4\pi}{3} k_f^3 \)

\(2\) possible momenta,

\[
n = \frac{k_f^3}{3\pi^2}
\]
And the total energy
\[ E = 2 \int_{\text{sphere}} \frac{d^3k}{(2\pi)^3} \frac{V \cdot k^2}{2m} = \frac{k^5 V}{10\pi^2 m} \]

This is a completely degenerate electron gas—electron gas at 0 temperature.

Energy/unit volume \( \propto \pi \frac{V}{3} \)

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:

\[ T = 0 \] (the temperature assumption is not important)

\[ \text{no. of neutrons} \approx \text{no. of protons} \]

Electrons get pushed up as the nucleons are pulled together, so that they are approximately free.

\[ \rho = \rho(x) \]

\[ \text{Find } \rho = \rho(e) \]

2) Weak magnetic field \( B^2 \) 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 \( B^2 \)—what happens?

Find energy \( E \) vs. field strength \( B \). \( X = \frac{\partial E}{\partial B} \) = magnetic susceptibility.
We obtained the energy of a system of free electrons. What is the wave-function \( \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_i, \ldots) \)?

These are non-interacting e's. Consider electrons with spin "up", wavefunction \( \Psi \)

\[
\Psi = e^{i \mathbf{k}_1 \cdot \mathbf{r}_1} e^{i \mathbf{k}_2 \cdot \mathbf{r}_2} \cdots
\]

Let there be \( N \) electrons with spin up, then the requirements of Pauli Principle are satisfied if

\[
\Psi = \frac{1}{\sqrt{N!}} \sum_{\text{permutations}} (-1)^P \prod P i e^{i \mathbf{k}_\alpha \cdot \mathbf{r}_\alpha}
\]

where \( P \) is the permutation that takes \( \alpha_1 \) into \( \alpha_P \).

This can also be written as a (Slater) determinant:

\[
\Psi = \frac{1}{\sqrt{N!}} \det \begin{bmatrix}
\phi_{\alpha_1}(R_1) & \phi_{\alpha_1}(R_2) & \cdots & \phi_{\alpha_1}(R_n) \\
\phi_{\alpha_2}(R_1) & \phi_{\alpha_2}(R_2) & \cdots & \phi_{\alpha_2}(R_n) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_{\alpha_n}(R_1) & \phi_{\alpha_n}(R_2) & \cdots & \phi_{\alpha_n}(R_n)
\end{bmatrix}
\]

Incidentally, all the \( \phi_{\alpha_k} \)'s are different — otherwise \( \Psi \) would vanish.

What is the probability of finding an electron at \( \mathbf{r}_b \)? We expect this to be a function of \( r = |\mathbf{r}_a - \mathbf{r}_b| \) only, starting at 0 for \( r = 0 \) and leveling off to a constant as \( r \to \infty \)

\[
f(r)
\]

Find instead the probability of finding one \( \mathbf{a}^\prime \) at \( \mathbf{a}^\prime \) and one electron at \( \mathbf{b} \). This is proportional to finding the probability of finding one at \( \mathbf{b} \).
When one has been found at "b".

\[ \text{Prob. (one e at "a", one e at "b")} \]

\[ = \langle \Psi | \prod_i \delta(R_i - R_i^*) \sum_j \delta(R_j^* - R_j^*) \Psi \rangle \]

Typical term in this matrix element is

\[ \langle e^{ik_1 \cdot R_1} e^{ik_2 \cdot R_2} \ldots e^{ik_n \cdot R_n} | \delta(R_1 - R_1^*) \delta(R_2 - R_2^*) \ldots e^{ik_n \cdot R_n} \rangle \]

integrating over all variables except \( R_1, R_2 \)

obtain either \( k_1 = R_1 \)

\[ \begin{align*}
    k_2 &= R_2 \\
    k_2 &= R_1
\end{align*} \]

Contributes matrix element = 1

Contribution to matrix element

\[ = -e^{i (k_2 - k_1) \cdot (R_2 - R_1)} \]

\[ = -e^{i R \cdot \Gamma} \]

\[ \Gamma = k_2 - k_1, \]

\[ R = R_2 - R_1 \]

So that probability \( \propto \int d^3k \left( e^{i R \cdot \Gamma} - 1 \right)^2 \)

Integrating

\[ K_f = \text{fermi energy} \]

\[ \text{Prob.} \propto \left| \int_0^{2K_f^2} \frac{dk}{4\pi} (\frac{\sin RR}{RR}) k^2 dk \right|^2 \]

Notice that as \( R \to 0 \), prob. \( \to 0 \)

Let \( x = 2K_f R \)

Then prob. \( \propto \sum \frac{1 + \frac{3}{x^2} (r_0 x - \sin x)}{x^3} \]

Normalize so that prob. \( \to 1 \) as \( x \to \infty \)

Prob. \( \sim \) \[
\begin{array}{c}
0 \\
K_f R \to
\end{array}
\]
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 \( V \)

\[
\begin{array}{c}
E_0 - \phi \\
E_0 - \epsilon_i
\end{array}
\]

\[ \uparrow \]

Energy

Let \( \phi \) be the 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 \( e^{-\frac{E}{kT}} \), 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

\[
e^{-\frac{\epsilon' - \phi}{kT}}
\]

\[
\epsilon_f = E_0 - \phi
\]

\[
\epsilon_a = E_0 - \epsilon'
\]

\[
e^{-\frac{(\epsilon_a - \epsilon_f)}{kT}} = e^{-\frac{(E_a - E_f)}{kT}}
\]
Yorc Accurate View

The above is not strictly correct - the energy levels should be measured relative to the chemical potential $\mu$, 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 $\Phi_T$ be the energy necessary to remove some "average" electron from the metal; $\mu_T = \nu - \Phi_T$; weighting factor $e^{-\beta(E_0 - \mu_T)}$.

We will soon discover just what is meant by "average" in this context; and that $\Phi_T$ is just the work function of the metal involved.

Suppose that there are $N_a^i$ particles in energy state $m_a^i$, for a given configuration $i$ of the $N$ electrons in the system. Then the probability of this configuration is $e^{-\beta \sum_{a}\sum_{\text{all } N_a^i} E_a^i}$.

the net probability that the system is in some state is $\sum_{i} e^{-\beta \sum_{a} m_a^i E_a^i}$.

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 $E_a^i \rightarrow E_a^i - \mu$ for some $\mu$ and sum as if there were no constraint on the total number of particles in the system. $\mu$ is then picked to make the total number come out right, i.e. from now on all energies are written relative to $\mu$ 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 $\sum \sum_{i} e^{-\beta \sum_{a} m_a^i (E_a^i - \mu)} = e^{-\beta \sum_{a} \mu}$

A bit of experimentation will show that if you have no constraint on the total number of particles then $\sum_{\text{configurations}} e^{-\beta \sum_{a} m_a^i (E_a^i - \mu)} = \frac{1}{a} \left[ \sum_{\text{configurations}} e^{-\beta (m_a^i)(E_a^i - \mu)} \right]$ each configuration has either $m_a^i = 0 \text{ or } 1$. Then this becomes $\prod_{a} \left[ 1 + e^{-\beta (E_a^i - \mu)} \right]$

From $e^{-\beta \sum_{a} m_a^i E_a^i} = \prod_{a} \left[ 1 + e^{-\beta (E_a^i - \mu)} \right]$ we find $\sum_{a} \frac{1}{a} \prod \left[ 1 + e^{-\beta (E_a^i - \mu)} \right]$

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 $\zeta = \frac{1}{2} m$ for the electron.

$g = \frac{1}{\beta} \int \frac{d^3 \rho}{(2\pi^3)^3} \left[ 1 + e^{-\beta (\frac{1}{2} m \rho - \mu)} \right] = \frac{2}{(2\pi)^3} \rho \text{ Volume}$
Calculation of Statistical Quantities

\[ \langle N \rangle = \text{average number in the box} = \frac{\sum \alpha \langle n_\alpha \rangle \exp\left(-\frac{\beta}{\alpha} (\mu_\alpha)(E_{\alpha} - \mu)\right)}{\sum \exp\left(-\frac{\beta}{\alpha} (\mu_\alpha)(E_{\alpha} - \mu)\right)} \]

\[ = \frac{1}{\beta} \frac{\partial}{\partial \mu} e^{-\beta \mu} = -\frac{\partial g}{\partial \mu} \]

This shows how the number in the box is related to the chemical potential.

We can also calculate the density \( \rho = \frac{1}{V} \) and the average number in a given energy state

\[ \langle m_\alpha \rangle = \frac{\sum \langle n_\alpha \rangle \exp\left(-\frac{\beta}{\alpha} (E_{\alpha} - \mu)\right)}{\sum \exp\left(-\frac{\beta}{\alpha} (E_{\alpha} - \mu)\right)} = \frac{0 + \exp(-\beta (E_{\alpha} - \mu))}{1 + \exp(-\beta (E_{\alpha} - \mu))} \]

\[ \langle m_\alpha \rangle = \frac{1}{1 + \exp(-\beta (E_{\alpha} - \mu))} = \frac{1}{1 + \exp(-\beta (E_{\alpha} - \mu))} \]

It is easy to remember the \(+\) sign in the denominator, because \( \langle n_\alpha \rangle \) must be a number between 0 and 1.

We can now define "average" energy as that energy at which \( \langle m_\alpha \rangle = \frac{1}{2} \). This defines \( \mu + \beta \frac{\rho}{\beta} \).

Notice that if \( T = 0 \) \( \beta \rightarrow \infty \)

\[ \epsilon < \mu \Rightarrow e^{\beta (E_{\alpha} - \mu)} = 1 \]

\[ \epsilon > 0 \Rightarrow e^{\beta (E_{\alpha} - \mu)} \rightarrow \infty \]

\[ \langle m_\alpha \rangle \]

As the temperature gets higher and higher, \( \langle m_\alpha \rangle \rightarrow \frac{1}{2} \exp\left(-\frac{\beta}{\alpha} (E_{\alpha} - \mu)\right) \), which has the shape \( e^{-\frac{E_{\alpha}}{T}} \) 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 \( \mu \) is the same

\[ \frac{1}{\sum \exp(-\beta (E_{\alpha} - \mu))} = \frac{1}{1 + \exp(-\beta (\mu - E_{\alpha}))} \]

\[ |A| = |B| \]

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

$$I = \int_0^\infty \frac{g(\epsilon) \, d\epsilon}{1 + e^{b(\epsilon - \mu)}} = \int_0^\infty f(\epsilon) \, d\epsilon$$

There is a handy way to get at these:

$$I = \int_0^\infty f(\epsilon) \, d\epsilon + \int_0^\infty f(\epsilon) = \int_0^\infty g(\epsilon) \, d\epsilon - \int_0^\infty \frac{g(\epsilon) \, d\epsilon}{1 + e^{b(\epsilon - \mu)}} + \int_0^\infty \frac{g(\epsilon) \, d\epsilon}{1 + e^{b(\epsilon - \mu)}}$$

$$\int_0^\infty \frac{g(\epsilon) \, d\epsilon}{1 + e^{b(\epsilon - \mu)}} = \frac{1}{b} \int_0^\infty \frac{g(\mu - \frac{y}{b}) \, dy}{1 + e^{y}}$$

$$\int_0^\infty \frac{g(\epsilon) \, d\epsilon}{1 + e^{b(\epsilon - \mu)}} = \frac{1}{b} \int_0^\infty \frac{g(\mu + x/b) \, dx}{1 + e^{x}}$$

For most applications

$$\int_0^{\beta \mu} = \int_0^\infty g(\mu - \frac{y}{b}) \approx g(\mu - \frac{y}{b}) \approx g(\mu) \approx g(u + \frac{x}{b}) \approx g(u)$$

To do $$\int_0^\infty \frac{x \, dx}{1 + e^x}$$, expand $$\frac{x \, e^{-x}}{1 + e^{-x}}$$ in a power series and sum. You should find

$$\int_0^\infty \frac{x \, dx}{1 + e^x} = \frac{\pi^2}{12}$$

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

$$C_V = 2 \gamma' T + \alpha T^3 \quad U_0 \quad T$$

$$2 \gamma' T + 3 \alpha \quad \frac{h}{k} \quad T$$

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 $$g(\epsilon)$$ 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 = $$4\pi k^2 d_k = 4\pi k E \, dE \approx 4\pi k^2 E$$

Phonon contribution: The number of phonons which will contribute to the specific heat is the number of lattice vibrations that can be excited = all those up to $$\frac{\omega}{k}$$
Look in $k$ space for the phonons. We know now have the whole volume of the sphere

$$\sim k^3_{outside} \sim \omega^3_{n, k \neq 0} \sim \frac{1}{T^3}$$

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 $\mu$.

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. Let's 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, let's 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, $E_d$. 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

$$\begin{array}{c}
\text{apart} \\
\text{Together}
\end{array}$$

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.

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 $\text{Phase difference } = 0$

The highest energy state will have a phase difference of $\pi$.

PROBLEM: Why does a phase difference of $\pi$ always give the same energy as $-\varepsilon$? 

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 $\frac{E}{k}$ whereas for the next band it may look like $\frac{E}{k}$.

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 Schrödinger equation for the system:

$$
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = \varepsilon \psi(\vec{r})
$$

$$V(\vec{r}) = V(\vec{r} + \vec{N})$$

where $\vec{N}$ is any lattice vector.

Substitute $\vec{r}' = \vec{r} + \vec{N}$

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r} + \vec{N}) \right] \psi(\vec{r} + \vec{N}) = \varepsilon \psi(\vec{r} + \vec{N})$$

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r} + \vec{N}) = \varepsilon \psi(\vec{r} + \vec{N})$$

Hence $\psi(\vec{r} + \vec{N})$ is a solution with the same energy as $\psi(\vec{r})$, for any lattice vector $\vec{N}$.

Define $\mathcal{M}(\vec{r}) = \sum_{\vec{N}} \psi(\vec{r} + \vec{N}) e^{-i \vec{N} \cdot \vec{N}}$

This is then a solution of the Schrödinger equation with the same energy as $\psi(\vec{r})$.

It has the property $\mathcal{M}(\vec{r} + \vec{N}_0) = \mathcal{M}(\vec{r}) e^{-i \vec{N} \cdot \vec{N}_0}$

Thus solutions of the Schrödinger equation with a periodic potential can be constructed to satisfy $\psi(\vec{r} + \vec{N}) = \psi(\vec{r}) e^{-i \vec{k} \cdot \vec{N}}$ for some $\vec{k}$.

Then Floquet's theorem says that the solutions take the form $\psi(\vec{r}) = u(\vec{r}) e^{i \vec{k} \cdot \vec{r}}$. 

Expand the \( u(\vec{r}) \) in a Fourier series 
\[
  u(\vec{r}) = \sum L \vec{e}^{i \vec{L} \cdot \vec{r}}
\]
(\( \vec{L} \) is a vector in the reciprocal lattice space). Then plug this back into
\[
  \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] u(\vec{r}) e^{i \vec{L} \cdot \vec{r}} = \varepsilon u(\vec{r}) e^{i \vec{L} \cdot \vec{r}}
\]
We then find
\[
  \sum L \left[ \frac{\hbar^2}{2m} (\vec{L} + \vec{\omega})^2 + V(\vec{r}) \right] \vec{A}_{\vec{L}} e^{i (\vec{L} + \vec{\omega}) \cdot \vec{r}} = \varepsilon \sum L \vec{A}_{\vec{L}} u(\vec{r}) e^{i (\vec{L} + \vec{\omega}) \cdot \vec{r}}
\]
Hence
\[
  \left[ \frac{\hbar^2}{2m} (\vec{\omega} + \vec{L})^2 - \varepsilon \right] \vec{A}_{\vec{L}} = - \sum L \nabla L - \vec{\omega} \vec{A}_{\vec{L}}
\]
The point is to solve this for the energy levels \( \varepsilon \) and the wave function pieces \( \vec{A}_{\vec{L}} \).
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**

\[
  V_\omega - \vec{L} \rightarrow \text{small}; \quad \nabla \vec{L} = 0
\]
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 
\[
  V(\vec{r}) \approx -V_0 \quad \text{and} \quad \frac{\hbar^2}{2m} (\vec{L} + \vec{\omega})^2 - \varepsilon \approx 0 \quad \vec{L} \neq 0
\]

\[
  \vec{L} \neq 0 \Rightarrow \vec{A}_{\vec{L}} = -\frac{V_0 \hbar^2}{2m (\vec{L} + \vec{\omega})^2 - \varepsilon}
\]
We can substitute this back to find the correction to \( \varepsilon \)

\[
  \varepsilon = \frac{\hbar^2}{2m} - \sum L \frac{V_0 \hbar^2}{2m (\vec{L} + \vec{\omega})^2 - \varepsilon}
\]
However for \( \vec{L} \neq 0 \)

\[
  (\vec{L} + \vec{\omega})^2 \approx \vec{\omega}^2 \Rightarrow \vec{A}_{\vec{L}} \text{ is large and not } \propto 0 \quad \text{as we assumed. Thus in this case the approximation breaks down and the analysis has to be redone.}
\]
The trouble comes for 
\[
  2 \vec{L} \cdot \vec{L} + \vec{\omega}^2 = 0 \quad \vec{L} \cdot (\vec{\omega} + \vec{L}) = 0
\]

This equation defines a set of troublesome vectors \( \vec{L} \) - a plane of \( \vec{L} \) which goes through \( \vec{\omega}/2 \).
Hence each \( \vec{L} \) gives a plane of singular points in \( \vec{k} \) space. The set of all such planes divides \( \vec{k} \) space up into Brillouin zones. Thus we see that at the edge of the Brillouin zone
the energy will probably deviate from \( \frac{k^2}{2m} \).

To find out quantitatively what is happening, pick one particular \( L_i \neq 0 \):

\[
(k + L_i)^2 - k^2 \sim V
\]

Then \( A_\omega, A_{L_i} \) are not small, but all the other terms are. Returning to the original set of equations gives:

\[
\left[ \frac{\hbar^2 k^2}{2m} - \epsilon \right] A_\omega = -V_{-L_i} A_{L_i},
\]

\[
\left[ \frac{\hbar^2 (k + L_i)^2}{2m} - \epsilon \right] A_{L_i} = -V_{L_i} A_\omega
\]

(\( V_{-L} = V_L \))

Define \( \omega(p) = \frac{p^2}{2m} \)

Then equations can be solved only for:

\[
\epsilon = \frac{\omega(k + L_i) + \omega(k)}{2} \pm \sqrt{\left( \frac{\omega(k + L_i) - \omega(k)}{2} \right)^2 + \left| V_{L_i} \right|^2}
\]

\( \epsilon \) small \( \left| V_{L_i} \right|^2 \Rightarrow \)

\[
\epsilon = \omega(k) - \frac{\left| V_{L_i} \right|^2}{\omega(k + L_i) - \omega(k)}
\]

\[
\epsilon = \omega(k + L_i) + \frac{\left| V_{L_i} \right|^2}{\omega(k + L_i) - \omega(k)}
\]

Thus the edge of the zone leads to a gap in the energy curve.

\[ \text{gap} \]

ASIDE: ONE DIMENSIONAL MODELS OF SOLIDS TO PLAY WITH

a) Cosine potential - leads to Mathieu's equation

b) \[ \text{\begin{array}{c}
\vspace{0.5cm}
\end{array}} \]

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 BONDING APPROXIMATION

Here the potential wells are taken as relatively deep and far apart.

If \( f(x) \) is the solution around one of the wells, try as a solution

\[
\sum_N c_n e^{i \mathbf{p}_n \cdot \mathbf{r}} f \left( \mathbf{r} - \mathbf{R}_n \right)
\]

It there is only one atom per unit cell of a given kind,

\[
V = \sum_N \mathbf{V} (\mathbf{R} - \mathbf{R}_n) \frac{1}{2m} \nabla^2 f + \mathbf{V}(\mathbf{r}) f = \epsilon_0 f
\]

To get an idea of the energy levels, use the formula

\[
\mathcal{E} = \frac{N}{V} = \frac{\int \mathbf{V} \mathbf{\phi} \mathbf{\psi} \mathbf{\phi} dV}{\int \mathbf{\psi} \mathbf{\psi} dV}
\]
\[ D = \sum_{N \neq N'} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \int f^*(\mathbf{r} - \mathbf{r}') f(\mathbf{r} - \mathbf{r}') \, d^3r \]
\[ = 1 + \sum_{M} e^{i\mathbf{k} \cdot \mathbf{M}} \int f^*(\mathbf{r} - \mathbf{M}) f(\mathbf{r} - \mathbf{M}) \, d^3r = 1 + \sum_{M} e^{i\mathbf{k} \cdot \mathbf{M}} \mathcal{I}(M) \]
\[ \mathcal{I}(M) = \int f^*(\mathbf{r} - \mathbf{M}) f(\mathbf{r}) \, d^3r \]

should probably be computed for only those \( M \) corresponding to nearest neighbors

\[ N = \sum_{N' \neq N} \sum_{M} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{M})} \int f^*(\mathbf{r} - \mathbf{M}) \left[ \frac{-\hbar^2}{2m} \nabla^2 + \sum_{l} \nu(\mathbf{r} - \mathbf{M}) \right] f(\mathbf{r} - \mathbf{M}) \, d^3r \]

Then

\[ E = E_0 + \frac{N}{D} \]

Define

\[ \mathcal{J}(M) = \int f^*(\mathbf{r} - \mathbf{M}) \left[ V(\mathbf{r}) - N(\mathbf{r}) \right] f(\mathbf{r}) \, d^3r \]

\[ E = E_0 + \left[ \frac{\mathcal{J}_0 + \sum_{M \neq 0} \mathcal{J}(M) e^{i\mathbf{M} \cdot \mathbf{r}}}{1 + \sum_{M \neq 0} \mathcal{I}(M) e^{i\mathbf{M} \cdot \mathbf{r}}} \right] \]

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

\[ E = E_0 + \left\{ \frac{\mathcal{J}_0 + 2 \mathcal{J}_{\infty} \left[ \cos k_x a + \cos k_y a + \cos k_z a \right]}{1 + 2 \mathcal{I}_{\infty} \left[ \cos k_x a + \cos k_y a + \cos k_z a \right]} \right\} \]
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 have been 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 $c_i^+$ 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 $l$

This is produced by an interaction like

$$\sum_{k,k'} \Gamma_{k,k',k'} c_{k}^{} c_{k'}^{} c_{k''}$$

However if this $\Delta$ is part of a Hamiltonian operator, its Hermitian conjugate must be included also

$$\Delta^\dagger c_{k}^{} = \sum_{k,k',k''} \Gamma_{k,k',k''} c_{k'}^{} c_{k''}^{} c_{k}^{} + \sum_{k,k',k''} \Gamma_{k,k',k''}^* c_{k}^{} c_{k''}^{} c_{k'}^{}$$

Knowledge of the $\Gamma$'s would then allow perturbation theory calculations of all sorts of processes, with $\Delta^\dagger$ as perturbation

To perform such calculations, one must know the properties of these $c_{k,i}$'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

$$c_{1}^{+1} = \{1\} \Rightarrow c_{1}^{+1} = 0$$

By taking the adjoint,

$$c_{1}^{1} = 10$$

$$c_{1}^{1} = 0$$
Similarly \( C C^+ + C^* C = 1 \)
(test by applying to all possible states)
and \( C_i^+ C_i = N_i \) (where \( N_i \) is either 0 or 1)

Puzzle: Suppose you know only that an operator \( C \) obeys
\( C^* C = 0 \) \hspace{1cm} C C = 0 \hspace{1cm} 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.
\( C_{a^+} C_{b^+} /0> = 1 \alpha \beta > \)

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
\( |ab> = - |ba> \quad \Rightarrow \quad C_{a^+} C_{b^+} /0> = - C_{b^+} C_{a^+} /0> \)

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 \( C_a C_{b^+} = - C_b C_{a^+} \)

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 \( |a> \) and \( |b> \) are states, a perfectly allowable state is
\( |a> + \beta |b> = |c> \exists |\alpha|^2 + |\beta|^2 = 1 \)

\( C_C^+ = \alpha C_{a^+} + \beta C_{b^+} \)

Hence
\( (\alpha C_{a^+} + \beta C_{b^+})(\alpha^* C_a + \beta^* C_b) + C_{a^+} C_{a^+} + C_{b^+} C_{b^+}) = 1 \)

Expand. Use \( |\alpha|^2 + |\beta|^2 = 1 \)

Then
\( \beta \alpha^* C_{b^+} C_a + \alpha \beta^* C_{a^+} C_b + \beta^* \alpha \) \hspace{1cm} C_C^+ C_C = 0 \hspace{1cm} C_C C_C^+ = 0 \)

\( C_{b^+} C_C + C_C C_{b^+} = 0 \)
We thus have a set of anticommutation relations for fermions which parallel the commutation relations previously derived for bosons

$$\begin{align*}
[c_a, c_b^+]_+ &= 0 \\
[c_a^+, c_b^+]_+ &= \delta_{ab}
\end{align*}$$

if \( a \neq b \) are orthogonal

Exercise: figure out what these relations are if \( a \) and \( b \) are not orthogonal.

Above we determined the operator \( c_b^+ = \alpha c_a^+ + \beta c_b^+ \) which creates an electron with amplitude \( \alpha \) to be in state \( a \) and amplitude \( \beta \) to be in state \( b \). Likewise,

\[
c_b^+ = \sum_p \langle p | c_b^+ | \psi_p \rangle \sqrt{\frac{2}{\pi \hbar^2}} e^{i \mathbf{p} \cdot \mathbf{x}} \delta (\mathbf{p})
\]

creates an electron with amplitude \( \langle p | c_b^+ | \psi_p \rangle \) to have momentum \( \mathbf{p} \).

This means its wave function must have the form

\[
\sum_p \langle \mathbf{p} | \psi \rangle \begin{pmatrix} c_a^+ \rangle & \langle c_b^+ \rangle \end{pmatrix} \begin{pmatrix} \psi \rangle \cdot \end{pmatrix} = \psi (x)
\]

And \( c_b^+ = \sum_p \langle \mathbf{p} | c_b^+ | \psi \rangle \begin{pmatrix} c_a^+ \rangle & \langle c_b^+ \rangle \end{pmatrix} \begin{pmatrix} \psi \rangle \cdot \end{pmatrix} \). If we symbolize the creation operator by \( \langle \mathbf{k} | \rangle \),

then \( c_b^+ = \sum_p \langle \mathbf{p} | c_b^+ | \psi \rangle \begin{pmatrix} c_a^+ \rangle & \langle c_b^+ \rangle \end{pmatrix} \begin{pmatrix} \psi \rangle \cdot \end{pmatrix} \).

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 \( \psi (x) \) be an operator which creates an electron at \( x \). Then

\[
\psi (x) = \sum_p \langle \mathbf{p} | c_b^+ | \psi \rangle \begin{pmatrix} c_a^+ \rangle & \langle c_b^+ \rangle \end{pmatrix} \begin{pmatrix} \psi \rangle \cdot \end{pmatrix} \]

Exercise: using the properties of the \( c_b^+ \)'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 \( \psi^* (x) = \int \frac{d^3 \mathbf{p}}{\pi^{\frac{3}{2}}} e^{-i \mathbf{p} \cdot \mathbf{x}} \psi^* (\mathbf{p}) \)

and \( \psi^* (x) = \sum_p \langle \mathbf{p} | c_b^+ \rangle \begin{pmatrix} c_a^+ \rangle & \langle c_b^+ \rangle \end{pmatrix} \begin{pmatrix} \psi \rangle \cdot \end{pmatrix} \).

Then

\[
\psi^* (x) = \int \frac{d^3 \mathbf{p}}{\omega \hbar} \frac{\psi^* (\mathbf{p})}{\mathbf{p} \cdot \mathbf{p}}
\]

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 \( f_k (r) = e^{i \mathbf{k} \cdot \mathbf{r}} u_k (r) \)

is the wave function for an electron of propagation vector \( \mathbf{k} \), then the operator which creates such a particle is

\[
\hat{c}_k^+ = \int f_k (r) \psi^* (r) \, d^3 \mathbf{r}
\]

Thus, for an arbitrary number of non-interacting electrons, the Hamiltonian of the system can be written as

\[
\hat{H} = \sum_k E_k \hat{n}_k = \sum_k E_k \hat{c}_k^+ \hat{c}_k
\]

But \( \psi^* (x) = \sum_k \hat{c}_k^+ f_k^* (r) \psi^* (x) \)

and if \( \hat{H} \) is the Hamiltonian for the individual electron wave function, then

\[
\hbar \psi^* (x) = \sum_k \hat{H} \hat{c}_k^+ f_k^* (r) \psi^* (x) = \sum_k E_k \hat{c}_k^+ \psi^* (x)
\]
\[
\int \psi^+ \psi d^3x = \int d^3x \sum_{k} \sum_{k'} \epsilon_{k} \gamma^{k'} \gamma^k \psi_{k'}^*(k) \psi_{k}^*(k) \\
= \sum_{k} \epsilon_{k} \gamma^k \gamma^k
\]

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

\[
\hat{H} = \int \psi^+ (x) \hbar \psi (x) d^3x
\]

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

\[
\hat{H} = \sum_{k} \epsilon_{k} \gamma^k \gamma^k + \sum_{k} \frac{\hbar}{2} \omega_{k} a_{k}^+ a_{k} \\
+ \sum_{k,k'} \left[ \gamma^k \gamma^{k'} a_{k} \right] \left[ \gamma^{k} \gamma^{k'} a_{k}^+ \right]
\]

This formalism can be used to treat any system in which electrons interact only by exchange of phonons. If, in addition to this, there is some direct electron-electron interaction, a further development is necessary.

If the electrons interact through some potential \(V(R, R')\) then the amplitude for scattering by this potential will be proportional to \(V(Q) = \int V(k) e^{-i Q \cdot k} d^3k\).

Then the definitions of the creation operators imply that the Hamiltonian should contain terms of the form

\[
\sum_{\rho} \left( \frac{p_{2m}}{2} \right) \psi_{\rho}^+ \psi_{\rho} + \sum_{Q} V(Q) \int \left( \rho_{1+} \rho_{2-} - \rho_{1-} \rho_{2+} \right) \psi_{\rho}^+ \psi_{\rho} \psi_{\rho+} \psi_{\rho-} \psi_{\rho},
\]

Use of the relation

\[
\psi_{\rho}^+ \psi_{\rho} = \int e^{i \rho \cdot x} \psi^*(x) dx
\]

allows us to rewrite the interaction term as

\[
\int \psi^+ (x) \psi^+ (y) V(x-y) \psi (x) \psi (y) d^3x d^3y = \int \psi^+ (x) \psi (x) V(0) d^3x
\]

To understand this, we compare it with the classical expression for interaction of two charge densities.

\[
G_{\text{classical}} = \frac{1}{2} \int \int \rho(x) \rho(x) V(x-y) \rho(y) dx dy
\]

By doing this we discover:

a) we should have defined the interaction as \(\int V(Q) \int \psi_{\rho}^+ \psi_{\rho} \psi_{\rho} \psi_{\rho}^+ dx dy\)

b) There seems to be an extra term \(\int \psi^+ (x) \psi (x) V(0) d^3x\)

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
\[ H = \int \psi^*(x) \left[ -\frac{\hbar^2}{2m} \left( \nabla - e \mathcal{A}(x) \right)^2 + e^2 \phi(x) \right] \psi(x) \, d^3x 
+ \frac{1}{2} \int \int \psi^*(x) \psi^*(y) \frac{e^2}{|x-y|} \psi(y) \psi(x) \, d^3x \, d^3y \]
where the $\psi$'s are field operators.

With this Hamiltonian, the Schrödinger equation for such a system is
\[ -\frac{i}{\hbar} \frac{\partial \Phi}{\partial t} = H \Phi \]
Notice that there is no reason for the solution $\Phi$ to be composed of a definite number
of electrons. However, because this particular Hamiltonian commutes with the
particle number operator $N = \int \psi^* \psi \, d^3x$
it is possible to choose solutions which do have the property $N \Phi = n \Phi$
In general, this interaction will not mix subspaces with different $n$. 
Let $c_k^\dagger$ be the operator that creates an electron in state $k$. Then $\sum_k c_k^\dagger c_k = \delta_{kk'}$ and $\sum_k c_k^\dagger c_k = 0$.

A simple Hamiltonian that permits discussion of electron scattering in a crystal is

$$H = \sum_k E_k c_k^\dagger c_k + \sum_{kk'} t_{kk'} c_k^\dagger c_{k'}^\dagger c_{k'} c_k.$$

An unoccupied electron state in an energy band is called a "hole." Electron creation operators are hole destruction operators and vice versa.

The formal identification is $c_k = b_k^\dagger$, consequently

$$\sum_k b_k^\dagger b_k^\dagger = \delta_{kk'} \quad \sum_k b_k^\dagger b_k = 0.$$

Rewrite the Hamiltonian:

$$H = \sum_k E_k c_k^\dagger c_k + \sum_k \delta_{kk'} b_k^\dagger b_k^\dagger$$

$$+ \sum_{kk'} \lambda_{kk'} c_k^\dagger c_{k'}^\dagger c_{k'} c_k$$

$$+ \sum_{kk'} \lambda_{kk'} b_k^\dagger b_{k'}^\dagger b_{k'} b_k.$$
The 4 terms bilinear in the creation and destruction operators yield the following processes in first order:

\[ \begin{array}{c}
\text{Time} \\
1. \quad \langle j' | \hat{a}_j \hat{a}_j' | j \rangle \\
2. \quad \langle k' | \hat{a}_k \hat{a}_e \rangle \\
3. \quad \langle k' | \hat{a}_k' \hat{a}_e \rangle \\
4. \quad \langle k' | \hat{a}_k' \hat{a}_e \rangle 
\end{array} \]

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.

2\textsuperscript{nd} order contributions

Consider the following. We have 2 diagrams that contribute in 2\textsuperscript{nd} order:

\[ \begin{array}{c}
\text{and} \\
(A) \\
(B) 
\end{array} \]

Now to conserve energy, in the initial state there is a phonon of energy \( w_1 \), and in the final state there is a phonon of energy \( w_2 \), where

\[ E_1 + w_1 = E_2 + w_2 \]

\( E_1 = \text{energy of electron 1} \), \( E_2 = \text{energy of electron 2} \).
From the perturbation theory of last term, the 2nd-order contribution to the amplitude is

\[ \sum_{r} \frac{\langle f | V | r \rangle \langle r | V | i \rangle}{E_i - E_r + i\varepsilon} \]

where the sum runs over all intermediate states.

Evaluating (A) and (B):

(A): \[ \sum_{k} \frac{\langle 2 | \lambda_k \Lambda_{k} C_k^* \Lambda_{k} | k \rangle \langle k | \lambda_{k} \Lambda_{k} C_k^* \Lambda_{k} | i \rangle}{E_i - E_k + i\varepsilon} \]

\[ = \sum_{k} \frac{\lambda_{2k} \Lambda_{k} \Lambda_{1}}{E_i + \omega_1 - E_k + i\varepsilon} \]

(B): \[ \sum_{k} \frac{\langle 2 | \lambda_{k} \Lambda_{k} b_k c_k^* b_k^* c_k^* | 1 \rangle \langle 1 | \lambda_{k} \Lambda_{k} b_k c_k^* b_k^* c_k^* | 0 \rangle}{E_k - (E_2 + \omega_1) + i\varepsilon} \]

\[ = -\sum_{k} \frac{\lambda_{2k} \Lambda_{k} \Lambda_{1}}{E_k - \omega_1 - E_1 + i\varepsilon} \]

\[ = \sum_{k} \frac{\lambda_{2k} \Lambda_{k} \Lambda_{1}}{E_i + \omega_1 - E_k - i\varepsilon} \]

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 not 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 

\[ A_k(x) = \int \phi_k^*(x) A(x) \phi_k(x) \, dx \]

then the contribution of (A) may be written

\[
\int dx_2 \, dx_1 \, dt_2 \, dt_1 \, \phi_2^*(x_2) \, A(x_2) \, K(2,1) \, A(x_1) \, \phi(x_1)
\]

and if we redefine where

\[ K_2(2,1) = \Theta(t_2-t_1) \sum_{\text{electrons}} e^{-i \omega_k (t_2-t_1)} \phi_k^*(x_2) \phi_k(x_1) \]

\[ \Theta(t_2-t_1) = \begin{cases} 1, & t_2 > t_1 \\ 0, & t_2 < t_1 \end{cases} \]

if we define for \( t_2 < t_1 \),

\[ K_1(2,1) = -\sum_{\text{holes}} e^{-i \omega_k (t_2-t_1)} \phi_k^*(x_2) \phi_k(x_1) \]

(A) + (B) may be written in the same form as (A) alone:

\[
\int dx_2 \, dx_1 \, dt_2 \, dt_1 \, \phi_2^*(x_2) \, A(x_2) \, K(2,1) \, A(x_1) \, \phi(x_1)
\]
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 those 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 asymmetrical 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's may be derived from a Lagrangian \( L \) that gives the action

\[
\text{action} = \int \left[ (\nabla \phi - \frac{\partial A}{\partial t})^2 - (\nabla \times A)^2 \right] dx^3 dt
\]
Interaction with matter is handled by adding the additional term $\int g_{\mu}(x) A^\mu(x) dx$ to the Lagrangian.

In the renormalize non-covariant Coulomb gauge $\nabla \cdot A = 0$, the interaction of charged particles through the electromagnetic field is equivalent to

1. Instantaneous Coulomb interaction $\frac{e^2}{r_{ij}}$

2. $H = \sum_k \omega_k a^+_k a_k + \int g_{\mu}(x) A^\mu(x) dx + H_{\text{matter}}$

$$A(x) = \sum_{k,i} \frac{1}{\sqrt{2\omega_k}} \left[ \epsilon_{k,i} e^{ik \cdot x} a_{k,i} + \epsilon^*_{k,i} e^{-ik \cdot x} a^*_k a^*_i \right]$$

Let us write down the classical relativistic relations for particles.

$$E = m_0 \gamma \quad p = m_0 \gamma v \quad \gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2}$$

(C is taken to be 1)

So

$$E^2 = p^2 + m_0^2$$

or

$$p^2 = m^2$$

where $p^\mu = (E, p)$

and if $A^\mu = (A_0, A)$, $B^\mu = (B_0, B)$

then $A \cdot B = A_\mu B^\mu = A_0 B_0 - A \cdot B$

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 $\nabla_{\mu} = (\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}) = (\frac{\partial}{\partial t}, -\nabla_x)$

(Notice the minus sign in the definition of $\nabla_{\mu}$)

Another useful vector is $X^\mu = (t, x)$.
Non-relativistically the phase of a free particle of momentum $k$ frequency (energy) $\omega$ is

$$e^{i(p \cdot x - \omega t)}$$

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: $E = \sqrt{p^2 + m^2}$

we obtain $\frac{d\Psi}{dt}$ - group $= \frac{dE}{dp} = $ classical $= \frac{P}{E}$

The Schrödinger equation 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

$$i \frac{\partial \Psi}{\partial t} = \sqrt{E^2 - p^2} \Psi$$

which, horrible as it looks, can be made to work out.

But the equation in the presence of an external field:

$$(i \frac{\partial}{\partial t} - eA) \Psi = \sqrt{m^2 - (p - ieA)^2} \Psi$$

presents difficulties.

a second-order equation suggests itself

$$\left[ (i \frac{\partial}{\partial t} - eA)^2 - \nabla \cdot \nabla ( - i \nabla - eA)^2 \right] \Psi = m^2 \Psi$$
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 non-relativistic 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 $H \psi = i \partial \psi / \partial t$, where he permitted the wave-function $\psi$ to have several components, and the Hamiltonian was permitted to be a matrix operator on these components.

Guessed

$H = \frac{\mathbf{p}^2}{2m} + \frac{\mathbf{e} \cdot \mathbf{A}}{c} + \frac{\mathbf{p} \cdot \mathbf{p}}{2m} + \beta m$

where $\mathbf{p}, \beta$ are matrices.

i.e.,

$H = \mathbf{p} \cdot \mathbf{p} + \beta m$

$\mathbf{p}, \beta$ hermitean

an external

with an electric field present,

$H = \mathbf{p} \cdot (p = eA) + \beta m$

$p = -i\partial / \partial t$

and $i\partial / \partial t \rightarrow i\partial / \partial t$. 

Look for a sol'n of the form \( \psi = u e^{-i k x} \) (free particle)

then \( u \) satisfies the equation

\[
E \ u = (x \cdot k + \beta m) u
\]

\[
E^2 u = (x \cdot k + \beta m)^2 u
\]

\[
E^2 = k_x^2 + k_y^2 + k_z^2 + m^2
\]

\[
\Rightarrow \quad \alpha_x^2 = 1 = \alpha_y^2 = \alpha_z^2
\]

\[
dx \ dx + dy \ dy + dz \ dz = 0, \ etc.
\]

\[
\beta d_x + dx \beta = 0
\]

and \( \beta = 1 \)

In 4 dimensions an explicit set of \( \alpha \)'s and \( \beta \) that satisfy these equations is

\[
\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 6x \\ 6x & 0 \end{pmatrix}
\]

\[
\alpha_y = \begin{pmatrix} 0 & 6y \\ 6y & 0 \end{pmatrix} \quad \alpha_z = \begin{pmatrix} 0 & 6z \\ 6z & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}
\]

Where \( 6x, 6y, 6z \) are the usual Pauli spin matrices. \( I : 2 \times 2 \) identity matrix \( O : 2 \times 2 \) zero matrix.

Write the 4 component wavefunction

\[
\begin{pmatrix} u_x \\ u_y \\ u_z \\ u_\epsilon \end{pmatrix} e^{-i k x} \quad \text{as} \quad \begin{pmatrix} U_a \\ U_b \end{pmatrix} e^{-i k x}
\]

where \( U_a, U_b \)

are 2 component objects.
In an external field \( \left( \frac{i}{\hbar} \frac{\partial}{\partial t} + eA \right) \Psi = \frac{\epsilon}{\hbar} \left( \frac{\partial}{\partial x} - eA \right) \Psi + \beta m \Psi \)

"Multiply" by \( \beta \):

\[
\beta \left( \frac{i}{\hbar} \frac{\partial}{\partial t} - eA \right) + \beta e \left( i \frac{\partial}{\partial x} + eA \right) \Psi = m \Psi
\]

Define another set of matrices:

\[
\chi = \chi_0 = \beta, \quad \chi = \beta \gamma
\]

Then the equation becomes

\[
\chi \left( \frac{i}{\hbar} \frac{\partial}{\partial \mu} - eA_\mu \right) \Psi = m \Psi
\]

where \( \chi_\mu \chi_\nu + \chi_\nu \chi_\mu = 2 \delta_\mu_\nu \)

These commutation rules are invariant under fourier transformations.

Let \( \Psi = \begin{pmatrix} \Psi_a \\ \Psi_b \end{pmatrix} \)

Then

\[
\left( \frac{-\hbar}{\beta} \frac{\partial}{\partial t} - eA \right) \Psi_a = \beta \left( \frac{\partial}{\partial x} - eA \right) \Psi_a + m \Psi_a
\]

and

\[
\left( \frac{-\hbar}{\beta} \frac{\partial}{\partial t} - eA \right) \Psi_b = \beta \left( \frac{\partial}{\partial x} - eA \right) \Psi_b - m \Psi_b
\]

For a routine, check equations are

\[\frac{-\hbar}{\beta} \frac{\partial}{\partial t} \Psi_a = 6 \left( \frac{\partial}{\partial x} \right) \Psi_b \]

\[\frac{-\hbar}{\beta} \frac{\partial}{\partial t} \Psi_b = 6 \left( \frac{\partial}{\partial x} \right) \Psi_a \]
DIRAC EQUATION

\[-\frac{\beta}{\hat{c}} \frac{\partial \psi}{\partial t} = H \psi\]

where

\[H = \beta m + eV + \hat{A} \cdot (\hat{p} - e\hat{A})\]

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 \(\alpha_i\) must anticommute, and

\[\alpha_i \beta = -\beta \alpha_i\]

One representation of these commutation relations is

\[\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \alpha = \begin{pmatrix} \hat{r} & \hat{s} \\ \hat{s}^\dagger & \hat{r}^\dagger \end{pmatrix}\]

Hence if \(\psi\) 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 \(\psi\) is Hermitian, \(\frac{\partial}{\partial t} \int \psi^\dagger \psi \, dv = \int \left[ \frac{\partial}{\partial t} \psi^\dagger \psi + \psi^\dagger \frac{\partial}{\partial t} \psi \right] \, dv = 0\)

Thus \(\psi^\dagger \psi\) can be thought of as a probability density.

Expectation values take the usual form \(\langle \alpha \rangle = \int \psi^\dagger \alpha \psi \, dv\).

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 \(\alpha\) and \(\beta\) matrices. Then the new representation can be related to the old as follows:

\[\alpha' = S \alpha S^{-1}, \quad \beta' = S \beta S^{-1}\]

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 \(\psi_a\) and \(\psi_b\) looks like

\[(E - eV) \psi_a - \hat{A} \cdot \hat{p} \psi_b = m \psi_a\]

\[(E - eV) \psi_b - \hat{A} \cdot \hat{p} \psi_a = -m \psi_b\]

for \(\psi_s = \psi_a + \psi_b\), \(\psi_d = \psi_a - \psi_b\)

these may be rewritten as

\[(E - eV) \psi_s - \hat{A} \cdot \hat{p} \psi_s = m \psi_s\]

\[(E - eV) \psi_d + \hat{A} \cdot \hat{p} \psi_d = m \psi_d\]
\[(E-eV+\vec{\alpha}.\vec{\beta})(E-eV-\vec{\alpha}.\vec{\beta})\psi_s = m^2 \psi_s\]
\[(E-eV-\vec{\alpha}.\vec{\beta})(E-eV+\vec{\alpha}.\vec{\beta})\psi_d = m^2 \psi_d\]

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 $\beta$ decay is created as pure $\psi_s$, 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 $\beta$

\[\{\beta\left[-\frac{\hbar}{c} \frac{2}{i\hbar} - eV\right] - \beta \vec{\alpha}.(\vec{\beta} - \vec{\alpha}.\vec{\beta})\} \psi = m \psi\]

Define $\gamma_0 = \beta, \quad \vec{\gamma} = \beta \vec{\alpha} = \left(\begin{array}{c} \frac{\hbar}{c} \\ -i \frac{\hbar}{c} \end{array}\right)$

because $p_0 = -\hbar \frac{2}{i\hbar}$, we can write

\[\left[\gamma_0(p_0 - eV) - \vec{\gamma}.(\vec{\beta} - \vec{\alpha}.\vec{\beta})\right] \psi = m \psi\]

For any four vector $\vec{\beta}$, define $\vec{B} = B_0 \gamma_0 - \vec{B}.\vec{\gamma}$

then the Dirac equation takes the form

\[\left(\vec{\gamma} - \frac{e}{\hbar} \vec{A} - m\right) \psi = 0\]

i.e., because $p_0 = i \frac{\hbar^2}{\hbar^2}, \vec{p} = \frac{\hbar}{\hbar^2}$, define $\nabla = \left(\frac{\hbar^2}{\hbar^2}, -\frac{\hbar^2}{\hbar^2}\right)$

then

\[(i \vec{\gamma} - \frac{e}{\hbar} \vec{A}) \psi = m \psi\]

**SOLUTIONS OF THE DIRAC EQUATION**

a) Particle at rest, no field

\[(p_0 \gamma_0 - m) \psi = 0 \Rightarrow \begin{pmatrix} \gamma_0 \\ \gamma \end{pmatrix} \begin{pmatrix} e^{-m} & 0 \\ 0 & e^{im} \end{pmatrix} \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = 0\]

For $\psi_a, E=m$

$\varphi_a = \begin{pmatrix} \phi \\ 0 \end{pmatrix} e^{-imt}$

For $\psi_b, E=-m$

$\psi_b = \begin{pmatrix} \phi \\ -i \chi \end{pmatrix} e^{imt}$

Here $\phi$ and $\chi$ can be any 2 component spinor 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 $e^{-iEt+i\vec{p}.\vec{x}}$

\[\left(\vec{\gamma} - m\right) \psi = 0\]
\[ (E - m) \phi - \frac{\vec{p} \cdot \vec{\sigma}}{E + m} \phi = 0 \]
\[ \vec{p} \cdot \vec{\sigma} \phi - (E + m) \phi = 0 \]

Solution 1)
\[ \phi = \left( \frac{\vec{p} \cdot \vec{\sigma}}{E + m} \right) \phi \]

\[ \psi = \begin{pmatrix} \phi \\ \frac{\vec{p} \cdot \vec{\sigma}}{E + m} \phi \end{pmatrix} \]

By substituting this back we see that
\[ (E - m) \phi - \frac{\vec{p} \cdot \vec{\sigma}}{E + m} \phi = 0 \]
\[ E^2 = \vec{p}^2 + m^2 \]

Hence in position space
\[ \chi = \left( \frac{\vec{p} \cdot \vec{\sigma}}{E + m} \phi \right) e^{i(\pm \sqrt{E^2 - m^2} t) + i \vec{p} \cdot \vec{x}} \]

Choose the sign such that as \( \vec{p} \rightarrow 0 \), this approaches
\[ \chi = \left( \frac{\vec{p} \cdot \vec{\sigma}}{E + m} \phi \right) e^{i \sqrt{E^2 - m^2} t + i \vec{p} \cdot \vec{x}} \]

Solution 2)
\[ \phi = \frac{\vec{p} \cdot \vec{\sigma} \chi}{E - m} \]

Here again \( \vec{p}^2 = m^2 + \vec{p}^2 \), but we choose the square root such that as \( \vec{p} \rightarrow 0 \), the solution approaches
\[ \begin{pmatrix} 0 \\ \chi \end{pmatrix} e^{i m t} \]

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
\[ \begin{pmatrix} \frac{-\vec{p} \cdot \vec{\sigma} \chi}{E + m} \\ \chi \end{pmatrix} e^{-i E t + i \vec{p}' \cdot \vec{x}} \]

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, let's forget about this and just try to understand the nonrelativistic limit of the Dirac equation in a field
\[(p - E \cdot \mathbf{n} - m)\chi = 0\]

reduces to the set of coupled equations

\[
\begin{align*}
(E - m - \mathbf{e}_\nu \cdot \mathbf{v}) \phi - (\mathbf{p} - E \cdot \mathbf{n} \mathbf{e}_\nu) \cdot \mathbf{\nabla} \chi &= 0 \\
\mathbf{\nabla} \cdot (\mathbf{p} - E \cdot \mathbf{n} \mathbf{e}_\nu) \phi - (E + m - \mathbf{e}_\nu \cdot \mathbf{v}) \chi &= 0 \\
\chi &= \left(\frac{1}{(E + m - \mathbf{e}_\nu \cdot \mathbf{v})}\right) \mathbf{\nabla} \cdot (\mathbf{p} - E \cdot \mathbf{n} \mathbf{e}_\nu) \phi
\end{align*}
\]

Substitute this into the first equation. It is important to preserve the order of operators, because the \(\mathbf{p}\) and \(E\) are differential operators which don't commute with \(\mathbf{\nabla}\).

\[
(E - m - \mathbf{e}_\nu \cdot \mathbf{v}) \phi = \left(\mathbf{p} - E \cdot \mathbf{n} \mathbf{e}_\nu\right) \cdot \mathbf{\nabla} \left(\frac{1}{(E + m - \mathbf{e}_\nu \cdot \mathbf{v})}\right) \mathbf{\nabla} \cdot (\mathbf{p} - E \cdot \mathbf{n} \mathbf{e}_\nu) \phi
\]

Use \(E = M + W\)

\[
\frac{1}{2M + W - \mathbf{e}_\nu \cdot \mathbf{v}} \approx \frac{1}{2M} - \frac{(W - \mathbf{e}_\nu \cdot \mathbf{v})^2}{(2M)^2}
\]

\[
(W - \mathbf{e}_\nu \cdot \mathbf{v}) \phi = \frac{1}{2M} \mathbf{\nabla} \cdot \mathbf{\nabla} \phi - \frac{(W - \mathbf{e}_\nu \cdot \mathbf{v})^2}{(2M)^2} \phi
\]

Rewrite the equation by adding and subtracting the same thing on both sides

\[
\left[1 + \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2}\right] (W - \mathbf{v}) \left[1 + \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2}\right] \phi = \frac{1}{2M} \left(\mathbf{\nabla} \cdot \mathbf{\nabla}\right)^2 \phi +
\]

\[
+ \frac{1}{8M^2} \left[(\mathbf{\nabla} \cdot \mathbf{\nabla})^2 (W - \mathbf{v}) - 2 \mathbf{\nabla} \cdot \mathbf{\nabla} (W - \mathbf{v}) \mathbf{\nabla} \cdot \mathbf{\nabla} + (W - \mathbf{v}) (\mathbf{\nabla} \cdot \mathbf{\nabla})^2\right] \phi
\]

To really be able to consider the non-relativistic limit, we should write everything in terms of a non-relativistic wave function. \(\phi\) is not the non-relativistic wave function in the case where the fields are present. Define \(\Phi = \left[1 + \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2}\right] \phi\)

Then to lowest non-trivial order

\[
\phi = \Phi - \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2} \Phi
\]

hence \(\nabla^2 \phi + \nabla^2 \chi \approx \nabla^2 \Phi \left[1 + \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2}\right] \approx \Phi \nabla^2 \Phi\)

\(\Phi\) contains the major effects of the "small" components as well as the large ones. Thus we can think of \(\Phi\) as a non-relativistic wave function and imagine the problem of finding the energy eigenvalues to be the same as that of minimizing

\[
\int \left(\nabla^2 \Phi\right)^2 \text{ (mass) }\Phi \text{ dual} + \int \left(\nabla^2 \Phi\right)^2 \text{ dual}
\]

Upon substituting this expression for \(\phi\) we obtain an equation of the form

\[
\left[1 + \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2}\right] (W - \mathbf{v}) \Phi = \left(\mathbf{g}/\text{tch}\right)
\]

which we unravel again to first order by

\[
(W - \mathbf{v}) \Phi \approx \left(\mathbf{g}/\text{tch}\right) - \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^2}{8M^2} \left(\mathbf{g}/\text{tch}\right)
\]

Keeping lowest order terms, we arrive at

\[
(W - \mathbf{v}) \Phi = \frac{1}{2M} \left(\mathbf{e}_\nu \cdot \mathbf{v}\right)^2 \Phi - \frac{(\mathbf{e}_\nu \cdot \mathbf{v})^4}{8M^3} \Phi
\]

\[
+ \frac{1}{8M^2} \left[(\mathbf{e}_\nu \cdot \mathbf{v})^2 (W - \mathbf{v}) - 2 \mathbf{e}_\nu \cdot \mathbf{v} (W - \mathbf{v}) \mathbf{e}_\nu \cdot \mathbf{v} + (W - \mathbf{v}) (\mathbf{e}_\nu \cdot \mathbf{v})^2\right] \Phi
\]
For any two operators $A$ and $B$,

$$A^2B - 2AABA + BA^2 = \left[ A, [A, B] \right]$$

set $A = \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}$  \hspace{1cm} B = \gamma - v'$

Calculate $\left[ \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, E - m - eV \right] = \left[ \frac{\sigma \cdot (\hat{p} - \gamma \hat{A})}{\sqrt{\gamma}}, E - m - eV \right]$

Assume for simplicity that $\frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}$ (This is not necessary. For fun and practice try working the whole mess through without assuming this)

Thus we get $-e \left[ \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, V \right] = -e \sigma \cdot \left[ \frac{\rho}{\sqrt{\gamma}}, V \right] = -i e \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}}$

$$\left\{ \right\} = \left[ \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, -i e \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right]$$

$$= -i e \left[ \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right] + i \frac{e^2}{c} \left( \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right)$$

use $\frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} = \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} + i \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} \left( \frac{\sigma \times \hat{E}}{\sqrt{\gamma}} \right)$

$$\left[ \frac{\sigma \cdot \hat{A}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right] = 2 i \frac{\sigma \cdot \hat{A} \times \hat{E}}{\sqrt{\gamma}}$$

$$\left[ \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right] = -i \frac{\sigma \cdot \hat{A} \times \hat{E}}{\sqrt{\gamma}} + i \frac{\sigma \cdot \hat{p} \times \hat{E}}{\sqrt{\gamma}} - i \frac{\sigma \cdot (\hat{E} \times \hat{p})}{\sqrt{\gamma}}$$

$$\frac{\sigma \cdot (\hat{p} \times \hat{E})}{\sqrt{\gamma}} f = E_{\gamma} \sigma \cdot \left( \frac{\sigma \cdot (\hat{E} \times \hat{p})}{\sqrt{\gamma}} \right) f$$

But $E_{\gamma} = -\frac{\gamma}{c^2} \frac{\partial}{\partial x} j \cdot \frac{\sigma \times \hat{p}}{\sqrt{\gamma}} f = -\frac{\sigma \cdot (\hat{E} \times \hat{p})}{\sqrt{\gamma}} f + \frac{\gamma}{c} \left[ \frac{\partial E_{\gamma}}{\partial x} - \frac{\partial E_{\gamma}}{\partial x} \right] f$

and

$$-i e \left[ \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right] = -e \left[ \frac{\sigma \cdot \hat{A} \times \hat{E}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right]$$

In similar fashion we calculate

$$\frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} = \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} + i \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} \left( \frac{\sigma \times \hat{p}}{\sqrt{\gamma}} \right)$$

Hence we obtain (to lowest order)

$$\mathcal{W} = \mathcal{U} + \frac{1}{2M} \left( \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} \right)^2 - \frac{\sigma \cdot \hat{p}}{2M} \left( \frac{\sigma \cdot \hat{p}}{\sqrt{\gamma}} \right)^2$$

$$-\frac{e^2}{8M^2} \left\{ \frac{\sigma \cdot \hat{A} \times \hat{E}}{\sqrt{\gamma}}, \frac{\sigma \cdot \hat{E}}{\sqrt{\gamma}} \right\}$$

The individual terms can now be interpreted

$$\mathcal{U}$$ \hspace{1cm} ordinary potential energy

$$\frac{\sigma \cdot \hat{p}}{2M}$$ \hspace{1cm} non-relativistic kinetic energy

$$-\frac{e^2}{2M}$$ \hspace{1cm} Pauli spin effect (magnetic moment $\frac{e}{2M}$ due to spin)

$$-\frac{(\sigma \cdot \hat{p})^2}{8M^2}$$ \hspace{1cm} first relativistic correction to the kinetic energy

$$\left( \frac{p^2 + m^2}{\sqrt{p^2 + m^2}} = m \left[ 1 + \frac{1}{2} \frac{p^2}{m^2} - \frac{1}{8} \frac{p^4}{m^4} + \cdots \right] \right.$$

$$\ldots$$

$$\ldots$$
We are left only with the term \( \frac{e}{2m} \left\{ \frac{\mathbf{\nabla} \cdot \mathbf{E}}{4m} + \frac{\mathbf{\nabla} \times (\mathbf{E} \times \mathbf{\hat{n}})}{2m} \right\} \).

\( \frac{e}{m} \) is like \( \frac{e}{2m} \)

a particle in motion in an electric field sees a magnetic field

\[- \frac{\mathbf{\nabla} \times \mathbf{E}}{c} = \mathbf{E} \times \frac{\mathbf{\hat{n}}}{m}\]

Then the energy of interaction of the electron's spin magnetic moment with this field will be \[- \frac{e}{2m} \frac{\mathbf{\hat{s}} \cdot (\mathbf{E} \times \mathbf{\hat{n}})}{m} \]

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 \(-\mathbf{u} \times \mathbf{\hat{u}}\), which then interacts with the electric field via \(-\mathbf{u} \times \mathbf{\hat{u}} \cdot \mathbf{E}\).

Within an atom, the electric field of the nucleus has the form \( \frac{e^n}{r^3} \). Then \( \mathbf{\hat{S}} \cdot (\mathbf{\nabla} \times \mathbf{E}) = \frac{2e^2}{4\pi M^2} \frac{\mathbf{r} \times \mathbf{\hat{S}}}{r^3} \) is the orbital angular momentum \( \mathbf{\hat{L}} \mathbf{\hat{S}} = \mathbf{\hat{L}} \mathbf{\hat{S}} \).

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 \( \frac{e}{2m} \). 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
\[
\frac{d}{dt} \mathbf{\mathbf{\nu}} - e \mathbf{\mathbf{A}} - \frac{\gamma}{2} \mathbf{\sigma} \cdot \mathbf{\mathbf{F}} \mathbf{\mathbf{\nu}} - m \mathbf{\nu} = 0
\]
where
\[
\mathbf{\sigma} = \frac{1}{2} \left[ \gamma \gamma_1 \gamma \right]
\]
\[
\mathbf{\mathbf{F}}_{uv} = \frac{2}{\partial x_u} \mathbf{A}_v - \frac{2}{\partial x_v} \mathbf{A}_u
\]

Figure out how to work this through to a non-relativistic equation and show that
\[
\mathbf{\mathbf{\mu}} = \frac{\nu'}{2m} \mathbf{\mathbf{J}} + (\mathbf{\mu} - \frac{e}{2m} \mathbf{\nu}) \mathbf{\sigma} \cdot \mathbf{\beta} \mathbf{\mathbf{J}} - \frac{\mathbf{\mathbf{P}} \cdot \mathbf{\mathbf{P}}}{\gamma m^3} \mathbf{\mathbf{J}}
\]
\[
+ \frac{1}{2} (\mathbf{\mu} - \frac{e}{2m}) \left( \mathbf{\nabla} \cdot \mathbf{\mathbf{\nu}} + 2 \mathbf{\mathbf{\sigma}} \cdot (\mathbf{\mathbf{E}} \times \mathbf{\mathbf{B}}) \right)
\]

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
\[
\frac{1}{2} (\mathbf{\mu} - \frac{e}{2m}) \left( \mathbf{\nabla} \cdot \mathbf{\mathbf{\nu}} + \frac{e}{2m} \mathbf{\mathbf{J}} \right)
\]

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 \( \mathbf{\mu} \)).

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 \( \frac{e}{2m} \). 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.
Anomalous magnetic moment of the electron:

An electron is described by a wave function $\Psi$ that satisfies the Dirac Equation:

$$\gamma_{\mu} \left( i \partial_{\mu} - e A_{\mu} \right) \Psi = m \Psi \quad \text{(1)}$$

where $A_{\mu} = A_{\mu}^{\text{total}}$ is made up of an external field $A_{\mu}^{\text{ext}}$ together with $A_{\mu}^{\text{r}}$, the field due to the electron itself.

$$A_{\mu} = A_{\mu}^{\text{ext}} + A_{\mu}^{\text{r}}$$

Classically, an electron satisfies

$$m \frac{d^2 x_{\mu}}{dt^2} = \gamma_{\mu} F_{\mu\nu}$$

where $F_{\mu\nu} = F_{\mu\nu}^{\text{ext}} + F_{\mu\nu}^{\text{r}}$

Then

$$m \frac{d^2 x_{\mu}}{dt^2} = \gamma_{\mu} F_{\mu\nu}^{\text{ext}}$$

and the term $\gamma_{\mu} F_{\mu\nu}^{\text{r}}$ 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 in the full $A_{\mu}$ instead of $A_{\mu}^{\text{ext}}$ into eq. (1) we obtain the anomalous magnetic moment of the electron as a term in the non-relativistic reduction of eq. (12) Hamiltonian derived from eq. (1). The term would look like

$$e q \gamma_{\mu} F_{\mu\nu}^{\text{ext}}$$

where the anomalous moment $q$ 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 reduction of the Dirac equation with the Pauli term there appeared the term

\[ \frac{e}{8m} \nabla \mathbf{E} \]

which came mathematically from \([6\mathbf{p}, 6\mathbf{E}]\).

   Explain the physical origin of the term.

2. For entertainment, you might try to examine the Dirac Equation in Hamiltonian form with

\[ H_D = \mathbf{p} \cdot \mathbf{E} \mathbf{p} - e \mathbf{A} + \beta m \]

and using the operator equation of motion

\[ \Theta^* = i [H, \Theta] \]

evaluate \( \mathbf{j} \) and \( \mathbf{p}^* \).

Find the velocity operator for the Dirac electron.

3. How many different matrices can you make from products of \( \mathbf{L} \)'s and \( \beta \) ? (The purpose of this exercise is to gain familiarity with the commutation laws).
Solutions to the Dirac Equation for a Free Particle

Let \( \Psi = e^{-i(Et - \mathbf{p} \cdot \mathbf{x})} \left( \begin{array}{c} \psi_a' \\ \psi_b' \end{array} \right) \); \( \Psi = \left( \begin{array}{c} \psi_a \\ \psi_b \end{array} \right) \)

Then with our choice of \( \alpha = \left( \begin{array}{c} 0 \\ \frac{1}{\sqrt{2}} \end{array} \right) \), \( \beta = \left( \begin{array}{c} \frac{1}{\sqrt{2}} \\ 0 \end{array} \right) \) the Dirac equation becomes

\[
\begin{align*}
(E + m) \psi_b' &= 6 \cdot p \cdot \psi_a' \\
(E - m) \psi_a' &= 6 \cdot p \cdot \psi_b'
\end{align*}
\]

\[
\begin{align*}
(E^2 - m^2) \psi_a' &= (E^2 - m^2) 6 \cdot p \cdot \psi_b' = 6 \cdot p \cdot (E + m) \psi_b = 6 \cdot \frac{p^2}{m} \psi_a
\end{align*}
\]

So that \( E^2 = m^2 + p^2 \) or \( \Psi = 0 \).

\[
\Rightarrow E = \pm E_p \quad \text{where} \quad E_p = \sqrt{m^2 + p^2}
\]

A. For \( E = E_p \)

\[
\psi_b' = \frac{6 \cdot p}{m + E_p} \psi_a'
\]

Let us choose our axes so that \( \mathbf{p} \) is in \( \hat{z} \) direction.

\[
\text{Spin up (positive helicity)} \quad \text{then} \quad \hat{z} \cdot \psi_a = + \psi_a = \delta \quad \text{(1)} \quad \text{where} \quad \delta = \text{some number chosen for convenient normalization}
\]

\[
\text{then} \quad \psi_b = \frac{p \hat{z} \cdot \psi_a}{m + E_p} = \frac{6 \cdot p}{E + m} \psi_a \quad \text{(1)}
\]

Choosing the normalization \( \psi^* \psi = \psi^*_b \psi_b + \psi^*_a \psi_a = 1 \)

we have \( \delta = \sqrt{\frac{2E}{E + m}} \) or \( \delta = \sqrt{\frac{2E}{2E + m}} \)

or \( \psi = \sqrt{\frac{E + m}{2E}} \left( \begin{array}{c} 0 \\ \frac{p}{E_p + m} \end{array} \right) = \frac{1}{\sqrt{2E}} \frac{E_p + m}{E_p - m} \left( \begin{array}{c} \frac{p}{E_p + m} \\ 0 \end{array} \right) \)
Spin down (negative helicity)

\[ e_y \psi_a = -\psi_a \]

Then \[ e_y \psi_b = -\psi_b \]

and

\[
\psi = \frac{1}{\sqrt{2E_p}} \begin{pmatrix} 0 \\ V E_p + m \\ 0 \\ -V E_p + m \end{pmatrix}
\]

Now, if we want an eigenstate of \( e_x \) instead of \( e_y \), we try

\[ e_x \psi_a = \psi_a \]

\[ \psi_a = \frac{1}{\sqrt{2}} (1) \]

but then \[ \psi_b = \frac{\rho}{\sqrt{2}(E_p + m)} \] \((-1)\) is not an eigenstate of \( e_x \).

This is because the operator \( \begin{pmatrix} 0 & 0 \\ 0 & e_x \end{pmatrix} \) does not commute with the hamiltonian. Only the operator \( \begin{pmatrix} e_y & 0 \\ 0 & e_y \end{pmatrix} \) commutes with \( H \) when the momentum \( \vec{p} \) is in the \( z \) direction.

The form of the \( 4 \times 4 \) matrices that represent the spin operators are \( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \) with our choice of \( \alpha, \beta \), and more generally, \( e_x = -i \frac{\partial}{\partial z} \)

\( e_y = -i \frac{\partial}{\partial x} \)

\( e_z = -i \frac{\partial}{\partial y} \)

Momentum in arbitrary direction

Suppose the spherical angles describing the direction of \( \vec{p} \) relative to fixed coordinate axes are \( \theta, \phi \). Then \( e_x \psi = \psi \) where \( \psi = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\phi} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix} \)
Then \( \psi = \frac{1}{2} \) and \( \psi = \left( \frac{\psi}{\psi} \right) = \frac{1}{\sqrt{2E_P}} \left( \begin{array}{c}
\sqrt{E_P+m} \cos\theta e^{i\phi} \\
v E_P+m \sin\theta e^{-i\phi} \\
v E_P-m \cos\theta e^{i\phi} \\
v E_P-m \sin\theta e^{-i\phi}
\end{array} \right)

(positive helicity spinor)

and negative helicity spinor is \( \psi = \frac{1}{\sqrt{2E_P}} \left( \begin{array}{c}
-\sqrt{E_P+m} \sin\theta e^{i\phi} \\
\sqrt{E_P+m} \cos\theta e^{i\phi} \\
\sqrt{E_P-m} \sin\theta e^{-i\phi} \\
\sqrt{E_P-m} \cos\theta e^{-i\phi}
\end{array} \right)\)

For \( E = -E_P \) 

let \( \mathbf{p} \) be in \( \hat{z} \) direction. For helicity \( (h) = + \) \( \Psi = \frac{1}{\sqrt{2E_P}} \left( \begin{array}{c}
-V_E - m \\
0 \\
V_E - m \\
0
\end{array} \right) \)

\( h = -\) \( \Psi = \frac{1}{\sqrt{2E_P}} \left( \begin{array}{c}
0 \\
V_E - m \\
0 \\
V_E + m
\end{array} \right) \)

Dirac proposed that the negative energy states exist, but are all filled with riddles. 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 absence of an electron with negative energy from the negative energy sea of \( \frac{e^2}{\hbar c} \) electrons is physically the same as the creation of an electron and a positron, both with positive energy.

Example of the use of Dirac Equation — Scattering in a Coulomb Potential (first Born approximation)

The scattering cross section \( \sigma \) is given by

\[
\sigma = 2\pi \delta(E_f - E_i) \int \frac{d^4 p_f}{(2\pi)^3} |M_{ef}|^2
\]
\[ m_{ci} = \int \psi_i^* V(r) \psi_i(x) \, d^3 x \]
\[ \psi_i(x) = e^{i(B \cdot x - E_i t)} u \]
\[ m = \int u_i^+ e^{i(x \cdot p - E_i t)} \frac{Z e^2}{r} u_i \, d^3 x \]
\[ = (u_i^+ u_i) \frac{4 \pi Z e^2}{\alpha^2} \]
\[ \Delta = p_i^+ - p_i^- \]

\[ \delta(E_i - E_f) \text{ insures that } |P_i| = |P_f| = \rho \]

then,
\[ g u_i = \frac{2 \pi}{(2\pi)^3} \int \frac{d \omega}{4} \delta(\sqrt{p_i^+ m^2 - \omega^2 + m^2}) \rho \, d^3 p' \left( \frac{4 \pi^2 e^2}{Q^2} \right)^2 |u_i^* u_i|^2 \]
\[ = (2\pi)^2 \rho \left( \frac{16 \pi^2}{Q^2} \right)^2 (E_i - E_f) \, d\omega \left( \frac{u_i^+ u_i}{Q^2} \right)^2 \]

\[ g(\theta) = \frac{4Z e^2 (m_i^2 + p_i^2) |u_i^+ u_i|^2}{16 \rho^4 \sin^4 \theta \alpha^2} \]

We must still evaluate \( u_i^+ u_i \).
There are 4 cases:
\[ h = + \rightarrow k^+ \text{ or } k^- \]
\[ h = - \rightarrow k^+ \text{ or } k^- \]

\[ u_i : \quad h = +, \quad u_i = \begin{pmatrix} \frac{V_{E+m}}{V_{E-m}} \frac{1}{V_{2E}} \end{pmatrix}, \quad h = -, \quad u_i = \begin{pmatrix} 0 \\ \frac{V_{E+m}}{V_{E-m}} \end{pmatrix} \]

\[ u_i : \quad h = +, \quad u_i = \begin{pmatrix} \frac{V_{E+m} \cos \theta}{V_{E-m} \cos \theta} \\ \frac{V_{E+m} \sin \theta}{V_{E-m} \sin \theta} \end{pmatrix}, \quad h = -, \quad u_i = \begin{pmatrix} \frac{V_{E+m} \sin \theta}{V_{E-m} \sin \theta} \\ \frac{V_{E+m} \cos \theta}{V_{E-m} \cos \theta} \end{pmatrix} \]
\[ h^+ \rightarrow h^+, \quad u^+ u_1 = \cos \theta_2 \]
\[ h^+ \rightarrow h^-, \quad u^+ u_1 = -\frac{m}{E} \sin \theta_2 \]
\[ h^- \rightarrow h^-, \quad u^- u_1 = \cos \theta_2 \]
\[ h^- \rightarrow h^+, \quad u^- u_1 = \frac{m}{E} \sin \theta_2 \]

If the helicity of the incoming electron is \(+\), then the scattering cross section is

\[
\frac{Z^2 e^4}{4} \frac{(m^2 + p^2)}{E^2} \left( \frac{m^2 \sin^2 \theta_2}{E^2} \right)
\]

The cross-section is the same with incoming electron of \(-\), 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 \(k\), \( e^- \rightarrow p_1 \) \( \rightarrow \) outgoing photon \(k'\), outgoing electron \(p_2\)

\( (a \text{ special coordinate system}) \)
CALCULATION OF THE COMPTON EFFECT

\[ \gamma + e^- \rightarrow \gamma + e^- \]

(notice that the process \( \gamma + e^- \rightarrow e^- \) 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 \((A_0, A_n, A_y, k_2)\) associated with the problem:

\[
\begin{align*}
P_1 &= (m, 0, 0, 0) \\
\gamma_1 &= v_1(1, 0, 0, 1) \\
P_2 &= (E_2 - p_2 \sin \theta, 0, p_2 \cos \theta) \\
\end{align*}
\]

Final state quantities are constrained by

\[
\begin{align*}
P_1 + \gamma_1 &= P_2 + k_2 \\
\text{energy-momentum conservation} \\
P_2 &= m^2 = (P_1 + \gamma_1 - k_2) = m^2 + 2P_1 \cdot k_2 - 2P_1 \cdot k_2 = 2P_1 \cdot k_2
\end{align*}
\]

This gives the well known formula for change of \(\gamma\) ray frequency

\[
\begin{align*}
f' &= f - \frac{m}{c \omega'} \left( \frac{m}{c \omega} \right) \\
\end{align*}
\]

Must also consider the possible polarizations of the \(\gamma\) ray

\[
\begin{align*}
\perp \quad \text{plane of scattering (0,0,1,0)} \\
\parallel \quad \text{plane of scattering} \\
\text{use } e \cdot k = 0 \text{ to get possibilities} \\
e_1 &= (0,1,0,0) \\
e_2 &= (0, \cos \theta, 0, -\sin \theta)
\end{align*}
\]

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.

\[ \text{Probability of transition/sec} = 2\pi \int \left( E_0 \delta - E^i \right) \frac{d^3 k^2}{(2\pi)^3} \left| M \right|^2 \]

(Notice: this formula always holds, relativistic kinematics or no relativistic kinematics. It is the change in the way you write $\delta$ inside the $\int$ function which changes the ultimate form for the phase space)

\[ H = \beta \gamma + \sum \left( \rho - \bar{\alpha} \gamma \right) \bar{H} + H_{\text{int}} \]

\[ H_{\text{int}} = -\bar{\gamma} \bar{\alpha} \sum \bar{A} \bar{A} \]

(notice that Dirac theory contains no $\bar{A} \bar{A}$ terms)

\[ \bar{A} = \sum \bar{\alpha}_k \sqrt{\gamma} \left[ a_k^i \bar{\epsilon}_k^i e^{ik \cdot x} + a_k^i \bar{\epsilon}_k^i e^{-ik \cdot x} \right] \]

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.

\[ \text{Prob/sec} = 2\pi \int \left( \frac{\gamma m^2 + (\vec{k}_1^2 - \vec{k}_2^2)^2 + \omega_2 - m - \omega_1}{2\pi} \right) \frac{k^2_2}{(2\pi)^3} \frac{d\omega_2}{d\omega_2} \frac{1}{\left| M \right|^2} \]

If we cancel the $\int$ 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 (there are of course related by *)

Generally one measures angular distributions.

\[ f(x) = \frac{\Delta(x-a)}{f'(a)} \]

if $f=0$ at $x=a$

Here

\[ f(k_2) = \sqrt{m^2 + \omega_1^2 + \omega_2^2 - 2\omega_1 \omega_2 \cos \theta + \omega_2 - m - \omega_1} \]

\[ f'(k_2) = \frac{\omega_2 - \omega_1 \cos \theta}{E_2^2} + 1 \]

This must be evaluated at

\[ \omega_2 = m + \omega_1 - E_2 \]

\[ f'(a) = \frac{\omega_1 m}{\omega_2 E_2} \]

Thus

\[ \text{Prob/sec} = \sigma \text{C} = \frac{\omega_1^2 E_2}{m \omega_1 (2\pi)^3} \frac{d\omega_2}{d\omega_2} \left| M \right|^2 = \frac{\text{cross section}}{m + \text{relative velocity}} \]

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 mass 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 $\bar{\gamma}_1$, then create $\bar{\gamma}_2$

\[ A = \sum \left< 2 \middle| \bar{\gamma}_2^i \bar{\epsilon}_2^i e^{-ik_1 \cdot x} \right| 1 \times \left< 1 \middle| \bar{\gamma}_1^i \bar{\epsilon}_1^i e^{ik_1 \cdot x} \right| 0 \right> \]

\[ E_1 + \omega_1 - E_2 \]
\[ B = \sum_2 \frac{\langle x | \alpha, e^{-i k_x x} | \beta \rangle \langle \beta | \alpha, e^{i k_x x} \rangle}{E_1 + \omega_1 - (E_j + \omega_1 + \omega_2)} \]

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 \( u e^{i k \cdot x} \), where \( u \) is a 4-component spinor. Everyone knows what to do with the \( e^{i k \cdot x} \) 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

\[ A = \sum_{\text{energy}} \frac{\langle u_x | d_x | u_i \rangle \langle u_i | d_i | u_i \rangle}{E_1 + \omega_1 - |E_1| - \varepsilon} + \sum_{\text{energy}} \frac{\langle u_x | d_x | u_i \rangle \langle u_i | d_i | u_i \rangle}{E_1 + \omega_1 + |E_1| - \varepsilon} \]

\[ B = \sum_{\text{energy}} \frac{\langle u_x | u_i \rangle \langle u_i | u_i \rangle}{E_1 - \omega_2 - |E_j| - \varepsilon} + \sum_{\text{energy}} \frac{\langle u_x | u_i \rangle \langle u_i | u_i \rangle}{E_1 - \omega_2 + |E_j| - \varepsilon} \]

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 can 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

\[ E_1 + \omega_1 - (E_1 + |E_k| + E_z) - \varepsilon = -(E_1 - \omega_2 + |E_k|) - \varepsilon \]

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.

\[
\sqrt{\frac{2 \omega_i^2 \omega_j^2}{\epsilon^2}} \frac{1}{A} = \sum \frac{\langle u_2 | d_2 | u_i \rangle \langle u_i | d_1 | u_1 \rangle}{E_i + \omega_i - \epsilon E_i^*} + \sum \frac{\langle u_2 | d_2 | u_i \rangle \langle u_i | d_1 | u_1 \rangle}{E_i + \omega_i - \epsilon E_i^* + i \epsilon}
\]

\[
\sqrt{\frac{2 \omega_i^2 \omega_j^2}{\epsilon^2}} \frac{1}{B} = \sum \frac{\langle u_2 | d_1 | u_j \rangle \langle u_j | d_1 | u_1 \rangle}{E_j - \omega_j - \epsilon E_j^*} + \sum \frac{\langle u_2 | d_1 | u_j \rangle \langle u_j | d_1 | u_1 \rangle}{E_j - \omega_j - \epsilon E_j^* + i \epsilon}
\]

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 Mishina becomes quite clear!

Casimir invented an improvement to do the sum over intermediate states

\[
\sum_i (u_i \times d_i u_i) = \sum_i (\sigma^t)_{\lambda \mu} (u_i \times d_i u_i)_{\beta \alpha} = \nu \pi \lambda^t \omega
\]

where

\[
\lambda^t_{\alpha \beta} = \sum_{\text{energies}} (u_i \times d_i u_i)_{\alpha} (u_i \times d_i u_i)_{\beta}
\]

Explicit computation with the \( u_i \)'s shows that

\[
\lambda^t = \frac{1}{2E} \left[ E + m \beta^2 \& \beta + \frac{\alpha^2}{\beta} \right]
\]

\[
\lambda^t = \frac{1}{2E} \left[ E - m \beta - \frac{\alpha^2}{\beta} \right]
\]

These can be obtained more simply:

\[
\sum_{\text{all states}} u_i \times u_i^* = \frac{1}{\hbar}
\]

\[
\sum_{\text{energies}} u_2 \times \frac{(H + \epsilon E_i)}{2E_i} u_i \times M u_i = \sum_{\text{all energies}} \frac{u_2 \times N (H + \epsilon E_i) u_i \times M u_i}{2E_i}
\]

\[
= \frac{u_2 \times N (H + \epsilon E_i) M u_1}{2E_i}
\]
Likewise \[ \lambda = \frac{H - LE_i l}{2 E_i} \approx \frac{L E_i l - H}{2 E_i l} \]

We thus see that any sum over positive energy intermediate states is got by inserting \( \lambda^+ \); similarly for \( \lambda^- \) and negative energy intermediate states.

Hence we have

\[
A = \frac{u_2^* \lambda_2 (|E_i| + m \beta + \overrightarrow{P}_1) \alpha_1 u_1}{2|E_i| (E_i + w_1 - |E_i|)} + \frac{u_2^* \lambda_2 (|E_i| - m \beta - \overrightarrow{P}_1) \alpha_1 u_1}{2|E_i| (E_i + w_1 + |E_i|)}
\]

\[
= \frac{u_2^* \lambda_2 (\overrightarrow{P}_1 + \overrightarrow{k}_1 + m \beta)}{(E_i + w_1)^2 - (\overrightarrow{P}_1 + \overrightarrow{k}_1)^2 - m^2} \alpha_1 u_1
\]

Define \( \overline{u}^* \beta = \overline{u} \)

Thus if \( u^* = (u_1^*, u_2^*, u_3^*, u_4^*) \) then \( \overline{u} = (u_1^*, u_2^*, -u_3^*, -u_4^*) \)

The final form for our A matrix element is then

\[
\overline{u}_2 \lambda_2 (\overrightarrow{P}_1 + \overrightarrow{k}_1 + m \beta) \alpha_1 u_1
\]

Likewise B is

\[
\overline{u}_2 \lambda_1 (\overrightarrow{P}_1 - \overrightarrow{k}_2 + m \beta) \alpha_1 u_1
\]

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 41: Effect of two time inversions on a spin J system

\[
T^2 \mid J = m + \frac{1}{2} \rangle = \frac{1}{\sqrt{2}} \mid J = m \rangle
\]

\[
\text{(m < - + in revers)}
\]

How to find answer:

from element from element from element from element

\[
\begin{align*}
\text{a) } T |J, m\rangle &= \text{phase } |J, -m\rangle \\
\text{b) } T (\alpha |1\rangle + \beta |2\rangle) &= \alpha^* T |1\rangle + \beta^* T |2\rangle \\
\text{c) Integral spin, mass } 0 &\Rightarrow \exists \text{ state } \exists S_z = 0 \\
T |0\rangle &= e^{i\delta T |0\rangle} \\
T^2 |0\rangle &= e^{-i\delta T |0\rangle} = 10 \rangle \\
\text{d) Half integral spin } \\
T |+\rangle &= e^{i\delta} |+\rangle \\
T |-\rangle &= e^{-i\delta} |+\rangle \\
T\frac{1}{\sqrt{2}}[|+\rangle + |\rangle - |\rangle] &\text{ must be spin down in } \times \text{ direction} \\
&= \frac{e^{i\delta}}{\sqrt{2}} [1 \rangle - \rangle - \rangle] = \frac{1}{\sqrt{2}} \left[ e^{i\delta} |+\rangle + \eta \left(e^{i(\delta - \delta')} |+\rangle - \rangle \right) \right]
\end{align*}
\]

\[
= \frac{1}{\sqrt{2}} e^{i(\delta - \delta')} = -1
\]
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
\[ e^{i\frac{p}{m}} |0, i\rangle = \left( m_0 \begin{pmatrix} v_{x0} & v_{y0} \end{pmatrix} i \right) = |3 \text{ momentum}, i\rangle \]

The general "boost" operator has the form
\[ e^{i\frac{p}{m} \cdot \hat{N}} \]

Other operators work as expected
\[ \mathbf{P}^2 \left| \mathbf{p}, \mathbf{p}_0, i \rightangle = \mathbf{P}^2 \left| \mathbf{p}, \mathbf{p}_0, i \rightangle \]
\[ \tan \theta = \frac{\mathbf{P}^2}{E} \quad \sin \theta = \frac{p}{m} \]

defines the parameter v for the transformation
\[ p_+ |0, i\rangle = \frac{p}{m} |0, i\rangle \]

The operator $\frac{p_+^2}{m^2} = p^2 - \frac{p_y^2}{p_x^2}$ 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
\[ \mathbf{J}_z = i \left[ \mathbf{p}_x \frac{\partial}{\partial \mathbf{y}} - \mathbf{p}_y \frac{\partial}{\partial \mathbf{x}} \right] + \mathbf{J}_z \rightarrow \text{(intrinsic spin)} \]
\[ \mathbf{N}_z = i \left[ \mathbf{p}_z \frac{\partial}{\partial \mathbf{p}_z} - \mathbf{p}_r \frac{\partial}{\partial \mathbf{p}_r} \right] + \left[ \frac{\mathbf{p}_x \times \mathbf{p}_y}{E + m} \right] \]

The most general wave function can then be written in the form
\[ |\Psi\rangle = \sum \left( a_+ |1\rangle + a_- |\rangle \right) \]

and the most general scattering operator can be put as
\[ f(a_1, a_2) + \frac{\overline{a}_+}{\overline{a}_-} (\overline{a}_1 \overline{a}_2) \]

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
\[ \frac{\sqrt{2m(E_1 + m)} - \mathbf{p}_1 \cdot \mathbf{p}_2 + i \cdot (\mathbf{p}_1 \times \mathbf{p}_2)}{\sqrt{2m(E_2 + m) - \mathbf{p}_1 \cdot \mathbf{p}_2}} \]

and in a pseudoscalar potential would look like
\[ \frac{\overline{a}_+}{\overline{a}_-} (E_1 + m) - \frac{\overline{a}_+}{\overline{a}_-} (E_2 + m) \]

Question: If you scatter twice in a scalar potential according to the graph
\[ \begin{array}{c}
\text{t} \quad \text{t} \\
\end{array} \]

can you prove from the amplitude resulting that electron and positron must have opposite intrinsic spins?
Differential cross-section for Compton scattering in lab ($p^2=0$):

\[ d\sigma = \frac{1}{16\pi E_2} \frac{1}{(2\pi)^2} \frac{1}{m^2} \frac{1}{m + 2E_2\sin^2 \theta/2} \frac{dE_2}{d\Omega} \]

\[ = \frac{d\Omega}{6\pi m^2} \frac{w_2}{m w_1} \frac{1}{m + 2w_2\sin^2 \theta/2} \]

From kinematics:

\[ \frac{w_2}{w_1} = \frac{m}{m + 2w_2\sin^2 \theta/2} \]

\[ \Rightarrow \frac{d\sigma}{d\Omega} \bigg|_{\text{lab}} = \frac{1}{6\pi m^2} \frac{1}{m^2} \frac{\frac{w_2^2}{w_1^2}}{m + 2w_2\sin^2 \theta/2} \]

\[ \Rightarrow (1) \]

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 helicities 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. Therefore, 16 polarized differential amplitudes $M$ that occur in Compton Scattering.

Kinematics of scattering in the lab system:

Initial state spinors

\[ u_1 = u_{1+} = \sqrt{2m} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{or} \quad u_1 = u_{1-} = \sqrt{2m} \begin{pmatrix} 0 \\ i \end{pmatrix} \]

(recall: normalization is $2E$ particles/unit volume)
Final state spinors:

\[
\begin{align*}
\mathbf{U}_2 &= \mathbf{U}_{2+} = 
\begin{pmatrix}
\sqrt{E + m} \cos \frac{\gamma}{2} \\
-\sqrt{E + m} \sin \frac{\gamma}{2} \\
\sqrt{E - m} \cos \frac{\gamma}{2} \\
-\sqrt{E - m} \sin \frac{\gamma}{2}
\end{pmatrix}, \\
\text{or} \quad \mathbf{U}_2 &= \mathbf{U}_{2-} = 
\begin{pmatrix}
\sqrt{E + m} \sin \frac{\gamma}{2} \\
\sqrt{E + m} \cos \frac{\gamma}{2} \\
-\sqrt{E - m} \sin \frac{\gamma}{2} \\
-\sqrt{E - m} \cos \frac{\gamma}{2}
\end{pmatrix}.
\end{align*}
\]

\[
\begin{align*}
\mathbf{U}_{2-} &= (\sqrt{E + m} \mathbf{e}_6, \sqrt{E + m} \mathbf{e}_\Gamma, \sqrt{E - m} \mathbf{e}_6, \sqrt{E - m} \mathbf{e}_\Gamma) \\
\mathbf{U}_{2+} &= (\sqrt{E + m} \mathbf{e}_\Gamma, -\sqrt{E + m} \mathbf{e}_6, -\sqrt{E - m} \mathbf{e}_\Gamma, \sqrt{E - m} \mathbf{e}_6)
\end{align*}
\]

where \[
\begin{pmatrix}
\mathbf{e}_6 \\
\mathbf{e}_\Gamma
\end{pmatrix} = \begin{pmatrix}
\sin \frac{\gamma}{2} \\
\cos \frac{\gamma}{2}
\end{pmatrix}
\]

There are 2 possibilities for \(e_1\), the polarization of the beam \(X\):

(i) polarized in plane of scattering \(e_1 = (1, 0, 0, 0) = e_{1a}\)

(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 scattering \(e_2 = (0, 1, 0, 0) = e_{2b}\)

Now we carry out the computation of \(M\) for the 16 different processes:

In each case, \(U_\alpha\):

\[
\begin{align*}
\frac{M}{\sqrt{E^*}} &= \mathbf{U}_2 \cdot \mathbf{F}_2 \left( \frac{p_1 + k_1 + m}{(p_1 + k_1)^2 - m^2} \right) \mathbf{U}_1 + \mathbf{U}_2 \cdot \mathbf{F}_1 \left( \frac{p_1 - k_1 + m}{(p_1 - k_1)^2 - m^2} \right) \mathbf{U}_1 \\
&= \mathbf{U}_2 \left( \frac{k_1 \mathbf{e}_1 + k_2 \mathbf{e}_2}{2mW_1} + \frac{k_2 \mathbf{e}_1 - k_1 \mathbf{e}_2}{2mW_2} \right) \mathbf{U}_1 \quad \text{since} \quad \mathbf{F}_1 \mathbf{e}_1 = -\mathbf{F}_1 \mathbf{e}_2 \\
&= \mathbf{U}_2 \left( \frac{k_1 \mathbf{e}_1 + k_2 \mathbf{e}_2}{2mW_1} \right) \mathbf{U}_1 \\
\end{align*}
\]

\[
\begin{align*}
k_1 &= W_1 (\frac{k_1}{p_1} - \frac{k_2}{p_2}) \\
k_2 &= W_2 (\frac{k_1}{p_1} - \frac{k_2}{p_2} \cos \theta - \frac{k_2}{p_2} \sin \theta)
\end{align*}
\]
Case 1: \[ u_1 = e_1 + u_2 \]
\[ e_1 = e_2 \]

Then \[-\frac{e_f}{x} = e_f \]
\[-\frac{e_d}{x} = (C - S_S) = x(C - z_S) \]

According to the abbreviations:
- \( x_f \rightarrow x \)
- \( y_f \rightarrow y \)
- \( z_f \rightarrow z \)
- \( t_f \rightarrow t \)

Then \[ M_1 \cdot 2m = \frac{\bar{u}_2}{4\pi e^2} \left[ (x_c - S_S)(1 - 2t) + x_c (t_c - z_c - x_c - z_c - S_S) \right] u_1 \]

\[ = \bar{u}_2 \left[ t_c - x_c - t_c z_c - x_c z_c + t_c z_c - x_c z_c - z_c^2 - S_S - z_c^2 \right] u_1 \]

where repeated use has been made of the commutation rules for the \( S \): \( x t + t x = 0 \)
\( x^2 = -1 \), etc.

\[ = \bar{u}_2 \left[ 2t c - x S - z (1 + C) \right] u_1 \]

To evaluate \( [2t c - x S - z (1 + C)] u_1 \), we make use of the table of \( S \)-matrices on page 8.

\[ M_1 \cdot \frac{2m}{4\pi e^2} = \frac{\bar{u}_2}{4\pi e^2} \left[ \begin{array}{c} 2t c \\ 0 \\ 0 \end{array} \right] u_1 \]

\[ = \bar{u}_2 \left[ 2 t e + m c + m (6 s - t c) - 1 \sqrt{e - m} \right] u_1 \]

\[ = 2 t e + m c \cos \theta m \sqrt{e - m} - m (1 + t c) m (1 + t c) - 1 \sqrt{e - m} \cdot \cos \theta m \sqrt{e - m} \]

Or, \[ M_1 = \frac{4\pi e^2}{\bar{u}_2} \left[ 2 t e + m c \cos \theta m \sqrt{e - m} - m (1 + t c) m (1 + t c) - 1 \sqrt{e - m} \cdot \cos \theta m \sqrt{e - m} \right] \]
Table of Independent $\gamma$-matrices:

We write this out in a particular representation defined by

\[
\gamma = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

Then \( \gamma = \beta \gamma \beta = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \chi = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \)

\[
\gamma_x \gamma_y = -i \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}
\]

\[
\gamma_x \gamma_y = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \quad \chi_5 = \chi_x \chi_y \chi_t = +i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

\[
\gamma_y \gamma_t = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}
\]

\[
\gamma_t \chi_x = \chi_x = \begin{pmatrix} 0 & i \chi_x \\ i \chi_x & 0 \end{pmatrix}
\]

\[
\gamma_t \gamma_y = \begin{pmatrix} 0 & i \chi_y \\ i \chi_y & 0 \end{pmatrix}
\]

\[
\gamma_5 \gamma_x = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \chi_x \gamma_y \chi_y
\]

\[
\gamma_5 \gamma_y = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \gamma_t \gamma_x \chi_x \gamma_t
\]

\[
\gamma_5 \gamma_y = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \chi_x \gamma_y \chi_y
\]

\[
\gamma_5 \gamma_t = \begin{pmatrix} 0 & i \chi_t \\ i \chi_t & 0 \end{pmatrix} = \psi_x \psi_y \psi_y
\]

\[
\psi_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \psi_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \psi_t = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]
2. \[ u_{1+} \rightarrow u_{2+} \]
\[ e_{1a} \rightarrow e_{2b} \]
\[-\xi = \xi \]
\[-\eta = 0 \]
\[ M_{2x2m} = \bar{u}_{2} \left\{ -\frac{y}{2} (t-z)x + x(t-zc-xc) y s \right\} u_{1} \]
\[ = \bar{u}_{2} \left\{ \begin{array}{c}
ty/2 -xy -ty -xyxc + ycs \end{array} \right\} u_{1} \]
\[ = \sqrt{\sin u_{2}} \left( \begin{array}{c}
0 \\
is \end{array} \right) \]
\[ = i \sqrt{\sin u_{2}} \left\{ 1 - l C - csc^{2} \right\} \]
\[ M_{2} \overline{\text{VEM}} = i \sqrt{\sin u_{2}} \left\{ \cos \eta_{2} - \cos(\theta - \eta_{2})^{2} \right\} \]

3. \[ u_{1+} \rightarrow u_{2-} \]
\[ e_{1a} = e_{2a} \rightarrow e_{2} = e_{2a} \]
\[-\xi_{1} = \xi \]
\[-\eta_{2} = 0 \]
\[ M_{3} \overline{2m} = \bar{u}_{2} \left\{ \begin{array}{c}
tc - zc -txs -x + t - zc - zc^{2} + xcs + tc zc \end{array} \right\} u_{1} \]
\[ = \bar{u}_{2} \left\{ \begin{array}{c}
tc - zc -txs -x + t - zc - zc^{2} + xcs + tc zc \end{array} \right\} u_{1} \]
\[ = \bar{u}_{2} (2tc - zc - zc - xs) u_{1} \]
\[ M_{3} \overline{\text{VEM}} = \bar{u}_{2} \left( \begin{array}{c}
2c \\
0 \\
rc \end{array} \right) \]
\[ = \left\{ 2\sqrt{\text{VEM}} \cos \xi - \sqrt{\text{VEM}} \sin \theta - \xi + \eta \right\} \]
\[ M_{3} \overline{\text{VEM}} = \sqrt{\sin u_{2}} \left\{ \cos \eta_{2} - \cos(\theta - \eta_{2})^{2} \right\} \]

4. \[ u_{1+} \rightarrow u_{2-} \]
\[ e_{1a} \rightarrow e_{2b} \]
\[ a \text{ in } \theta_{a2}, M_{4x4} = \bar{u}_{2} (xys(c-1) + yss) u_{1} \]
\[ M_{4} \overline{\text{VEM}} = -i \sqrt{\text{VEM}} \left\{ \sin(\theta - \eta_{2}) + \sin \eta_{2} \right\} \]

5. \[ u_{1-} \rightarrow u_{2-} \]
\[ e_{1a} \rightarrow e_{2a} \]
\[ M_{5} \overline{\text{VEM}} = \bar{u}_{2} \left\{ 2\sqrt{\text{VEM}} \cos \xi \cos \eta_{2} - \sqrt{\text{VEM}} \cos(\theta + \xi) - \sqrt{\text{VEM}} \cos \eta_{2} \right\} \]
Notice that $M_5 = M_1$. This can be seen to be a consequence of the invariance of the coupling $\gamma + A^\mu$ under parity transformation $P$.

Under $P$, $\hat{S}$ (spin), like $\hat{J}$ (orbital angular momentum), is invariant. $\hat{P}$, however, changes sign, so $\hat{S} \cdot \hat{P}$ 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.

Putting these together, we see that

$$M_1 (u_1^+ \to u_2^+) = M_2 (u_1^- \to u_2^-) = M_5 (u_1^- \to u_2^-)$$

Similarly,

$$M_6 (u_1^- \to u_2^-) = M_2 (u_1^+ \to u_2^+)$$

$$M_7 (u_1^- \to u_2^+) = M_5 (u_1^+ \to u_2^-)$$

$$M_8 (u_1^- \to u_2^+) = M_4 (u_1^+ \to u_2^-)$$

9. $\quad u_1^+ \to u_2^+
\quad e_1 \to e_2$
\quad $-\theta_1 = x$
\quad $-\theta_2 = y$
\quad $M_q \frac{\sqrt{2m}}{4\pi e^2} = \left\{ 2 \sqrt{E+m \cos \theta_2} - \sqrt{E-m \cos \theta_2} \right\}$

10. $\quad u_1^+ \to u_2^+
\quad e_1 \to e_2$
\quad $-\theta_1 = y$
\quad $-\theta_2 = x C - z S$
\quad $M_q \frac{\sqrt{2m}}{4\pi e^2} = \frac{\bar{u}_2}{\sqrt{2m}} \left( x y z C - y S - x y z \right) u_1 = i \sqrt{E-m \cos \theta_2 \cos \theta} \left( C + z S \right)$
11. \( u_1^- \rightarrow u_2^- \quad \text{By parity} \quad M_{11} = M_9 \)

12. \( u_1^- \rightarrow u_2^- \quad \text{By parity} \quad M_{12} = M_{10} \)

13. \( u_1^+ \rightarrow u_2^- \quad \quad 14. \quad u_1^- \rightarrow u_2^+ \)
\( E_{1b} \rightarrow E_{2b} \quad \quad E_{1b} \rightarrow E_{2b} \)

\[ M_{13} = M_{14} \]

\[ \frac{\sqrt{2}m}{4\pi \hbar} M_{13} = 2 \left( \sqrt{E^2 - m^2} \sin \frac{\theta}{2} + \sqrt{E_m} \sin \frac{\theta}{2} \right) \]

15. \( u_1^+ \rightarrow u_2^- \quad \quad 16. \quad u_1^- \rightarrow u_2^+ \)
\( E_{1b} \rightarrow E_{2a} \quad \quad E_{1b} \rightarrow E_{2a} \)

\[ M_{15} = M_{16} \]

\[ \frac{\sqrt{2}m}{4\pi \hbar} M_{15} = \frac{1}{\sqrt{2}m} \left( \frac{x y z}{E^2 - m^2} \right) \quad \text{(Sommerfeld 10.)} \]

\[ = \frac{i}{\sqrt{2}m} \left( \cos \frac{\theta}{2} - \cos \left( \theta + \frac{\pi}{2} \right) \right) \]

\[ = i \left( \sqrt{E_m} \sin \left( \theta + \frac{\pi}{2} \right) - \sqrt{E^2 - m^2} \sin \frac{\theta}{2} \right) \]

The various polarized cross sections are obtained by the replacement \( M \rightarrow M_k \), \( k = 1, 2, \ldots, 16 \) in Equation (1).
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.

$$\mathcal{H} = \frac{1}{8\pi} \int (E^2 + B^2) d\text{vol} + \int \psi^*(x) \left[ \beta m + e \phi(x) + \frac{1}{c} \left( \tau \cdot \nabla - \frac{e}{c} A \right) \right] \psi(x) \, d^3x$$

Energy of Free Electron-magnetic Field

where the $\psi$'s are operators which create and annihilate electrons.

This may be broken down further into the energy of the free electron-positron field

$$\int \psi^*(x) \left[ \beta m + \gamma_0 \frac{1}{c} \nabla \right] \psi(x) \, d^3x$$

and a term which represents the interaction between the electric field and the matter fields

$$e \int \psi^*(x) \left[ \phi(x) - \frac{\gamma_5}{2} \vec{A} \right] \psi(x) \, d^3x = \int j_\mu(x) A_\mu(x) \, d^3x$$

where

$$j_\mu = e \psi^* \gamma_\mu \psi = e \overline{\psi}(x) \gamma_\mu \psi(x)$$

and it is important to keep in mind that each of $\psi$, $\psi^*$, $A_\mu$ 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

$$\nabla \cdot A = 0 \quad j = \nabla^2 \phi = \rho$$

(a point charge has $\phi(r) = \frac{Q}{r}$)

Thus the $e \int \psi^* \phi(x) \psi(x) \, d^3x$ term can be written

$$\frac{e^2}{2} \int \psi^*(x) \psi(x) \psi^*(y) \psi(y) \, d^3x \, d^3y$$

up to $\infty$

and we have managed to express this piece of the interaction without use of photon creation and annihilation operators. The $\infty$ mentioned above comes from the $\int$ 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

\[-e \int A^\mu(x) \frac{\partial}{\partial x^\mu} \psi(x) \cdot \bar{A}^\mu(x) \, d^3x\]

where

\[\bar{A}^\mu(x) = \sum_{i=1}^{\infty} \sqrt{\frac{n!}{2n!}} \left[ e^{i\mathbf{k} \cdot \mathbf{x}} + e^{-i\mathbf{k} \cdot \mathbf{x}} \right] \hat{e}_{i,\mu}^\nu \hat{a}_{\mu,\nu}^i e^{-iE_i x} \]

where \(\hat{e}_{i,\mu}^\nu\) is the polarization vector for a photon of polarization type 1 (helicity \(\pm 1\)) and

\[\psi(x) = \sum_{\rho, \lambda} u_{\rho, \lambda} \, c_{\rho, \lambda} \, e^{i \mathbf{p} \cdot \mathbf{x}}\]

\(u_{\rho, \lambda}\) is a 4-component spinor for a solution of the Dirac equation of momentum \(\mathbf{p}\), type \(\lambda\) (\(\mathbf{p}\) runs over 4 possibilities - positive energy spin up and spin down, and negative energy spin up and spin down)

\[(\beta \mathbf{m} + \mathbf{\alpha} \cdot \mathbf{p}) u_{\rho, \lambda} = \mathcal{E} u_{\rho, \lambda}\]

\(\mathcal{E} = \pm E_+ = \sqrt{m^2 + \mathbf{p}^2}\) or \(\mathcal{E} = \mp E_+ = -\sqrt{m^2 + \mathbf{p}^2}\)

Likewise

\[\psi^{\lambda\ast} = \sum_{\rho, \lambda} c_{\rho, \lambda}^{\ast} \, u_{\rho, \lambda}^{\ast} \, e^{-i \mathbf{p} \cdot \mathbf{x}}\]

Change notation:

let \(u_{\rho, \kappa}\) stand for those solutions such that \(\mathcal{E} = + E_{\rho, \kappa}\)

where \(\kappa\) is a spin index with two possible values

\(u_{\rho, \kappa} = u_{-\rho, \kappa}\) for those solutions with \(\mathcal{E} = - E_{\rho}\)

Then we have

\[(\beta \mathbf{m} + \mathbf{\alpha} \cdot \mathbf{p}) u_{\rho, \kappa} = E_{\rho} u_{\rho, \kappa}\]

\[(\beta \mathbf{m} - \mathbf{\alpha} \cdot \mathbf{p}) u_{\rho, \kappa} = -E_{\rho} u_{\rho, \kappa}\]

And the free Hamiltonian takes the form

\[H_{\text{free}, \rho, \kappa} = \sum_{\rho, \lambda} E_{\rho} \, c_{\rho, \kappa}^{\ast} \, c_{\rho, \lambda} = \sum_{\rho, \lambda} E_{\rho} \left[ c_{\rho, \kappa}^{\ast} \, c_{\rho, \lambda} - c_{\rho, \kappa} \, c_{\rho, \lambda}^{\ast} \right]\]

where

\[c_{\rho, \kappa}^{\ast} \, c_{\rho, \lambda} + c_{\rho, \lambda}^{\ast} \, c_{\rho, \kappa} = \delta_{\rho, \rho'} \, \delta_{\kappa, \lambda'}\]

In accordance with our new terminology for the spinors, define a new terminology for the annihilation operators of negative energy states

If \(c_{\rho, \kappa}\) annihilates an electron of momentum \(\mathbf{p}\), spin type \(\kappa\), then \(c_{\rho, \lambda}\) creates a positron with momentum \(-\mathbf{p}\).

Then

\[H_{\text{free}} = \sum E_{\rho} \left[ c_{\rho, \kappa}^{\ast} \, c_{\rho, \lambda} + d_{\rho, \kappa}^{\ast} \, d_{\rho, \lambda} \right] = \sum_{\rho} E_{\rho} \]

another \(\mathbf{p}\)
This is the energy of the full sea of negative energy states. We measure relative energies away from it.

Now \( \Psi = \sum_{\rho, \eta} \left[ c_{\rho, \eta} u_{\rho, \eta} e^{i\rho \cdot x} + d_{\rho, \eta}^+ v_{\rho, \eta} e^{-i\rho \cdot x} \right] \)

notice that creation of positron in initial state (i.e. annihilation of positron in final state) gives a column vector \( \sum_{\rho, \eta} u_{\rho, \eta} \) whereas annihilation of electron in final state (by \( \Psi^+ \)) gives a row vector \( \sum_{\rho, \eta} v_{\rho, \eta} \).

Hence a positron in the initial state leads to \( \underline{\Psi} \) on the left side of the matrix element, whereas an electron in the initial state leads to \( \Psi \) on the right side of the matrix element.

Use this to expand out the interaction Hamiltonian

\[
\hat{A} = \sum \frac{\mu_{\eta}}{2w_{\eta}} \left[ \tilde{e}_{\eta, \kappa}^+ a_{\kappa} e^{i\h \cdot x} + \tilde{\tilde{e}}_{\eta, \kappa}^+ a_{\kappa}^* e^{-i\h \cdot x} \right]
\]

\[
\Psi = \sum [ c_{\rho, \eta} u_{\rho, \eta} e^{i\rho \cdot x} + d_{\rho, \eta}^+ v_{\rho, \eta} e^{-i\rho \cdot x} ]
\]

to obtain

\[
\hat{A} = \sum \frac{\mu_{\eta}}{2w_{\eta}} \int \left[ c_{\rho, \eta}^* u_{\rho, \eta} e^{-i\rho \cdot x} + d_{\rho, \eta}^+ v_{\rho, \eta} e^{i\rho \cdot x} \right] \left[ \tilde{\tilde{e}}_{\eta, \kappa}^+ a_{\kappa} e^{i\h \cdot x} + \tilde{\tilde{e}}_{\eta, \kappa}^+ a_{\kappa}^* e^{-i\h \cdot x} \right]
\]

\[
\hat{A} \sum [ c_{\rho, \eta} u_{\rho, \eta} e^{i\rho \cdot x} + d_{\rho, \eta}^+ v_{\rho, \eta} e^{-i\rho \cdot x} ]
\]

In every case the spatial integration will give only a \( \int \) function of the momenta (because the exponentials are the only functions of \( \mathbf{x} \) present)

We then obtain a sum of the following pieces:

\[
\sqrt{\frac{4\pi e^2}{2\omega}} c_{\rho, \kappa}^* a_{\kappa} \cdot \tilde{e}_{\kappa, \eta} + \tilde{\tilde{e}}_{\kappa, \eta}^+ u_{\rho, \eta}^* \cdot \mathbf{D}(-\mathbf{P} + \mathbf{K} + \mathbf{\rho}^1)
\]

\[
\sqrt{\frac{4\pi e^2}{2\omega}} c_{\rho, \kappa}^* a_{\kappa} \cdot \tilde{e}_{\kappa, \eta}^+ v_{\rho, \eta}^* \cdot \mathbf{D}(-\mathbf{P} + \mathbf{K} - \mathbf{\rho}^1)
\]

\[
\sqrt{\frac{4\pi e^2}{2\omega}} c_{\rho, \kappa}^* a_{\kappa} \cdot \tilde{e}_{\kappa, \eta}^+ v_{\rho, \eta}^* \cdot \mathbf{D}(\mathbf{P} + \mathbf{K} - \mathbf{\rho}^1)
\]

\[
\sqrt{\frac{4\pi e^2}{2\omega}} c_{\rho, \kappa}^* a_{\kappa} \cdot \tilde{e}_{\kappa, \eta}^+ v_{\rho, \eta}^* \cdot \mathbf{D}(\mathbf{P} + \mathbf{K} + \mathbf{\rho}^1)
\]
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
\[ i \frac{\partial \Psi}{\partial t} = \mathbf{\gamma} \Psi - \Psi \mathbf{\eta} \]
tells you about the operator \( \gamma \)
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 elements above.

Consider scattering to order \(\sigma^2\)

\[
\begin{align*}
\int & \sum_{\text{internal polarizations}} \frac{4\pi e^2}{2w_q} \frac{(u_{3\sigma}^* \gamma_1 u_2)(u_{4\sigma}^* \gamma_2 u_1)}{(E_1 + E_2) - (E_3 + E_4 + w_q) + i\varepsilon} \\
= & \sum_{\text{internal polarizations}} \frac{4\pi e^2}{2w_q} \frac{(u_{3\sigma}^* \gamma_1 u_2)(u_{4\sigma}^* \gamma_2 u_1)}{(E_1 + E_2) - (E_3 + E_4 + w_q) + i\varepsilon} 
\end{align*}
\]

for \( \quad q = (q_t, q_y, 0, 0) \) the contributions are

1) Coulomb interaction

\[
\frac{4\pi e^2}{Q^2} (u_{3\sigma}^* u_1) (u_{4\sigma}^* u_2)
\]

2) Virtual transverse photons

\[
\frac{4\pi e^2}{2w_q} \frac{(u_{3\sigma}^* \gamma_1 u_2)(u_{4\sigma}^* \gamma_2 u_1)}{(E_1 + E_2) - (E_3 + E_4 + w_q) + i\varepsilon}
\]

from \( \nu_3\)

Notice that if there were 3 directions of polarization (two \( \perp \nu \) and one \( \parallel \nu \) )

then \( \sum_{\text{all 3}} (\not{A} \cdot \not{c}_3) (\not{B} \cdot \not{c}_3) = \not{A} \cdot \not{B} \)

Hence \( \sum_{\text{transverse}} (\not{A} \cdot \not{c}_3) (\not{B} \cdot \not{c}_3) = \not{A} \cdot \not{B} - \not{A} \cdot \nu \not{B} \cdot \nu \)

Thus combination of the two transversely polarized pieces gives

\[
\frac{4\pi e^2}{2w_q} \left[ \frac{(u_{3\sigma}^* \gamma_1 u_2)(u_{4\sigma}^* \gamma_2 u_1)}{Q} - \frac{(u_{3\sigma}^* \gamma_1 u_2)(u_{4\sigma}^* \gamma_2 u_1)}{Q} \right] \left[ \frac{1}{E_1 - E_3 - w_q + i\varepsilon} + \frac{1}{E_2 - E_4 - w_q + i\varepsilon} \right]
\]

But \( \frac{1}{E_1 - E_3 - w_q} + \frac{1}{E_2 - E_4 - w_q} = \frac{2w_q}{E_0^2} \)

Then the sum of these terms gives

\[
4\pi e^2 \left\{ \frac{1}{\not{q}^2} (u_{4\sigma} \not{y} u_2) \cdot (u_{3\sigma} \not{q} u_1) + \frac{1}{Q^2} (u_{3\sigma} \not{y} u_2) (u_{4\sigma} \not{y} u_2) - \frac{(u_{3\sigma} \not{y} u_2) (u_{4\sigma} \not{y} u_2)}{Q^2} \right\}
\]

But \( q_4 u_4 \not{y} u_2 = u_4 (\not{p}_x - \not{p}_y) u_2 = u_4 (m - m) u_2 = 0 \)

(current conservation)

Hence \( u_4 \not{q} \cdot \not{y} u_2 = q_4 u_4 \not{y} u_2 \)

and we arrive at

\[
\left\{ - \frac{(u_{4\sigma} \not{y} u_2) (u_{3\sigma} \not{y} u_1)}{\not{q}^2} + \frac{(u_{4\sigma} \not{y} u_2) (u_{3\sigma} \not{y} u_1)}{\not{q}^2} + \frac{(u_{3\sigma} \not{y} u_2) (u_{4\sigma} \not{y} u_2)}{Q^2} - \frac{q_4^2 (u_{4\sigma} \not{y} u_2)}{Q^2 \not{q}^2} \right\}
\]

But \( \frac{1}{\not{q}^2} + \frac{1}{Q^2} - \frac{q_4^2}{Q^2 \not{q}^2} = 0 \)
Hence we have shown that all the lowest order interactions due to charge coalesce into one manifestly covariant matrix element

\[ -\frac{4\pi e^2}{q^2} \left( \frac{\overline{u}_3}{q} \gamma^\mu u_2 \right) \left( \frac{\overline{u}_3}{q} \gamma^\mu u_1 \right) \]

which can be symbolized by the picture

\[ \gamma^\mu \]

For the charge current \( j_\mu = \overline{u}_3 \gamma^\mu u_1 \), we have

\[ \frac{1}{q^2} j_\mu \]

Interaction with \( j'_\mu = \overline{u}_4 \gamma^\mu u_2 \) 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 \( \frac{1}{p-m} \) or \( \frac{1}{p^2} \), it is no longer necessary to draw two graphs which differ by time ordering.

It is only necessary to draw one graph. This is always the convention used in applications.

**Applications and Discussion**

It happens that \( \mu \) 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 \( \mu \) particles shot in (in the lab frame). The \( \mu \) and \( e \) will scatter into new momentum states because of the interaction of their charges.

\[ \sigma = \frac{G \mu^2}{(2\pi)^4} \int (2\pi) d^4 p_\mu \int (2\pi) d^4 p_\nu \int (2\pi) d^4 p_\delta \int (2\pi) d^4 p_\xi \frac{d^4 p_\mu}{(2\pi)^4} \frac{d^4 p_\nu}{(2\pi)^4} \frac{1}{2m_e 2\varepsilon_{\mu\nu}} |M|^2 \]

The \( \int \) 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 \( \mu \) 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-
It is easy to see that the largest contributions to the cross section come from \( p_z = p_1 \) (forward scattering in the center of mass system). When \( q^2 \) 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 \( q^2 \) behavior of the matrix element. But \( q^2 \) for this particular experiment is extremely small even for high energy \( \mu^+e^- \)

Question: if it were possible to have a target of \( \mu^+e^- \) and shoot electrons at them, would it be easier to explore the large \( q^2 \) 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 \( \gamma_\mu \rightarrow -\gamma_\mu \)?

Why?

One of the most precise experiments to date along this line is the scattering \( e^-p \rightarrow e^-p \). Here the matrix element is again proportional to \( \overline{J}_\mu \gamma_\mu \frac{\mathcal{H}_3 \gamma_\mu}{(p_z-p_1)^2} \), where \( \overline{J}_\mu \) now represents the electromagnetic current of the proton. It can be shown that the most general form of \( \overline{J}_\mu \) is

\[
\overline{J}_\mu = \overline{u}_3 \left[ e \gamma_\mu F_1 + F_2 (\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu) q^\nu \right] u_1
\]

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 (\( q^2 \))

(Justify this form for \( \overline{J}_\mu \) by fiddling with others)

It is found empirically that both \( F_1 \) and \( F_2 \) have the shape

\[
\frac{K_{l,2}}{(q^2 - x^2)^2}
\]

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.
Differential cross-section for Compton Scattering in lab ($p^2 = 0$):

$$d\sigma = \frac{1}{16mE_2 w_1 w_2} \frac{1}{(2\pi)^2} \frac{1}{m^2 - w_2^2} \frac{E_2}{m + 2w_2 \sin \theta / 2} \frac{d\Omega}{d\omega}$$

$$= \frac{d\sigma}{d\Omega} \frac{w_2}{64\pi^2} \frac{1}{m^2 - w_2^2} \frac{E_2}{m + 2w_2 \sin \theta / 2}$$

From kinematics, $w_2 = \frac{m}{m + 2w_2 \sin \theta / 2}$

$$\therefore \quad \frac{d\sigma}{d\Omega} \frac{1}{64\pi^2} \frac{1}{m^2 - w_2^2} \frac{E_2}{m^2 - w_2^2} \frac{w_2^2}{w_1^2}$$

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 helicities 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

$$u_1 = u_{1+} = \sqrt{2m} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{or} \quad u_1 = u_{1-} = \sqrt{2m} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$
Final state spinors:

\[ U_2 = U_{2+} = \begin{pmatrix} \sqrt{E+m}\cos\delta/2 \\ \sqrt{E+m}\sin\delta/2 \\ \sqrt{E-m}\cos\delta/2 \\ \sqrt{E-m}\sin\delta/2 \end{pmatrix}, \quad \text{or} \quad U_2 = U_{2-} = \begin{pmatrix} \sqrt{E+m}\sin\delta/2 \\ \sqrt{E+m}\cos\delta/2 \\ -\sqrt{E-m}\sin\delta/2 \\ -\sqrt{E-m}\cos\delta/2 \end{pmatrix} \]

\[ \bar{U}_{2-} = (\sqrt{E+m} \ 0 \ \sqrt{E-m} \ \sqrt{E-m}) \]
\[ \bar{U}_{2+} = (\sqrt{E+m} \ 0 \ -\sqrt{E-m} \ \sqrt{E-m}) \]

where \[ \delta = \sin\delta/2 \]
\[ \Gamma = \cos\delta/2 \]

There are 2 possibilities for \( \delta \), the polarisation of the incoming \( \gamma \):

(i) polarized in plane of scattering, \( \delta = (1, 0, 0, 0) = \theta 0 \)

(ii) polarized perpendicular to plane of scattering, \( \delta = (0, 1, 0, 0) = \theta 0 \)

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 scatter, \( E_2 = (0, 1, 0, 0) = E_{2b} \)

Now we carry out the computation of \( M \) for the 16 different processes:

In each case, \( \frac{M}{4\pi} \)

\[ \frac{M}{4\pi} = \frac{\bar{U}_2 \sigma \cdot (p_1 + k_1 + m) \sigma_1 U_1}{(p_1 + k_1)^2 - m^2} + \frac{\bar{U}_2 \sigma \cdot (p_1 - k_1 + m) \sigma_1 U_1}{(p_1 - k_1)^2 - m^2} \]

\[ = \frac{\bar{U}_2 (\frac{\sigma_1 \cdot k_1}{2m} + \frac{\sigma_2 \cdot k_2}{2m})}{2m} \]

\[ \frac{\sigma_1 \cdot k_1}{2m} = -\frac{\sigma_1 \cdot k_1}{2m} \]

\[ \frac{\sigma_2 \cdot k_2}{2m} = -\frac{\sigma_2 \cdot k_2}{2m} \]

\[ K_1 = W_1 (x_1 - y_1) \]

\[ K_2 = W_2 (x_2 - Y_2 \cos\theta - Z_2 \sin\theta) \]
Case 1: \[ u_1 = u_+ \quad u_2 = u_- \]
\[ e_1 = e_+ \quad e_2 = e_- \]

Then \[ \begin{align*}
-\xi_1 &= \xi_1 \\
-\xi_2 &= \xi_2 \quad x \quad &= xC - zS \\
\xi_1 C - \xi_2 S &= xC - zS
\end{align*} \]

according to the abbreviations:
\[ \begin{align*}
\xi_1 &\rightarrow x \\
\xi_2 &\rightarrow y \\
\xi_1 &\rightarrow z \\
\xi_2 &\rightarrow t
\end{align*} \]

Then \[ \begin{align*}
M_1 \cdot \frac{2m}{4\pi e^2} &= \bar{u}_2 \left[ (xC - zS)(t - z)x + x(t - zC - xS)(xC - zS) \right] u_1 \\
&= \bar{u}_2 \left[ xC - zC - txzS - xS + tC + txzS - zC - xS \right. \\
&\quad \left. + xS - zS \right] u_1
\end{align*} \]

where repeated use has been made of the commutation rules for the \( \delta \)'s: \[ x^2 = -1 \quad etc. \]

= \[ \bar{u}_2 \left[ 2xC - xS - z(1+C) \right] u_1 \]

To evaluate \([2xC - xS - z(1+C)]u_1\), we make use of the table of \( \delta \) matrices on page 4.

Obtain \[ M_1 \cdot \frac{2m}{4\pi e^2} = \bar{u}_2 \left( \begin{matrix} 2C & \sqrt{2m} i \{E+i\Gamma, -E+i\Gamma, i\sqrt{E-m}\} / 2C \\
0 & \sqrt{1+C} \end{matrix} \right) \]

\[ M_1 \cdot \frac{2m}{4\pi e^2} = 2 \sqrt{E+m} \Gamma + \sqrt{E-m} (6S-\Gamma C) - \sqrt{E-m} \]

\[ = 2 \sqrt{E+m} \cos \theta \cos \theta_2 - \sqrt{E-m} \cos \theta (\theta_2 + \theta) - \sqrt{E-m} \cos \theta_2 \]

or, \[ M_1 = \frac{4\pi e^2}{\sqrt{2m}} \left( 2 \sqrt{E+m} \cos \theta \cos \theta_2 - \sqrt{E-m} \cos \theta (\theta_2 + \theta) - \sqrt{E-m} \cos \theta_2 \right) \]
Table of Independent $\gamma$-matrices:

We write this out in a particular representation defined by

$$\gamma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Then

$$\gamma = \beta \gamma \beta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \delta = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\gamma_1 \gamma_2 = -i \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\gamma_3 \gamma_4 = \begin{pmatrix} -i \gamma & 0 \\ 0 & -i \gamma \end{pmatrix}$$

$$\gamma_5 \gamma_6 = \begin{pmatrix} -i \gamma & 0 \\ 0 & -i \gamma \end{pmatrix}$$

$$\gamma_7 \gamma_8 = -i \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\gamma_9 = \gamma_7 \gamma_8 \gamma_9 = +i \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\gamma_{10} \gamma_{11} = \gamma_x = \begin{pmatrix} 0 & \gamma_x \\ \gamma_x & 0 \end{pmatrix}$$

$$\gamma_1 \gamma_2 = \gamma_{12} = \begin{pmatrix} 0 & \gamma_x \\ \gamma_x & 0 \end{pmatrix}$$

$$\gamma_3 \gamma_4 = \gamma_{13} = \begin{pmatrix} 0 & \gamma_y \\ \gamma_y & 0 \end{pmatrix}$$

$$\gamma_5 \gamma_6 = \gamma_{14} = \begin{pmatrix} 0 & \gamma_z \\ \gamma_z & 0 \end{pmatrix}$$

$$\gamma_7 \gamma_8 = \gamma_{15} = \begin{pmatrix} -i \gamma_x & 0 \\ 0 & i \gamma_x \end{pmatrix}$$

$$\gamma_{16} = \gamma_7 \gamma_8 \gamma_{15} = \gamma_{15} \gamma_{16} = \gamma_{17} = \gamma_{18} = \gamma_{19} = \gamma_{20}$$

$$\delta_x = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \delta_y = \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix}, \quad \delta_z = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}$$
\[
M_2 \frac{\text{vem}}{\text{te}} = \bar{u}_2 \left( \frac{z}{t} \frac{y}{x} \right) + x(t - yC - xS)u_i
= \bar{u}_2 \left( \frac{tC - yC}{tC - zC} \right) - yS + xC + tC - zC^2 + xCS + yS^2
- yS^2
= \bar{u}_2 \left( 2tC - yC - zC - xS \right) u_i
\]

\[
M_3 \frac{\text{vem}}{\text{te}} = \bar{u}_2 \left( \frac{2tC}{1 + tC} \right) + \frac{2VE\text{m} \cos \theta \sin \frac{\alpha}{2} + VE\text{m} \sin (\theta + \frac{\alpha}{2}) + VE\text{m} \sin \frac{\alpha}{2}}{\text{te}}
\]

\[
M_4 \frac{\text{vem}}{\text{te}} = \frac{2VE\text{m} \cos \theta \sin \frac{\alpha}{2} + VE\text{m} \sin (\theta + \frac{\alpha}{2}) + VE\text{m} \sin \frac{\alpha}{2}}{\text{te}}
\]

\[
M_5 \frac{\text{vem}}{\text{te}} = \frac{2VE\text{m} \cos \theta \cos \frac{\alpha}{2} - VE\text{m} \cos (\theta + \frac{\alpha}{2}) - VE\text{m} \cos \frac{\alpha}{2}}{\text{te}}
\]
Notice that \( M_5 = M_1 \). This can be seen to be a consequence of the invariance of the coupling \( g \mu \cdot A \mu \) under parity transformation \( P \).

Under \( P \), \( S^z \) (spin), like \( B \) (orbital angular momentum) is invariant. \( P \), however, changes sign, so \( S^z \cdot B \) 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 direction of polarization of both photons leaves the lowest order amplitude.

Putting these together, we see that

\[
M_1 \left( u_1^+ \rightarrow u_2^+ \right) = M \left( u_1^- \rightarrow u_2^- \right) = M_5 \left( u_1^- \rightarrow u_2^- \right) = M_5 \left( u_1^+ \rightarrow u_2^- \right)
\]

Similarly,

\[
M_6 \left( u_1^- \rightarrow u_2^- \right) = M_7 \left( u_1^+ \rightarrow u_2^+ \right) = M_8 \left( u_1^- \rightarrow u_2^+ \right)
\]

\[
M_7 \left( u_1^- \rightarrow u_2^- \right) = M_5 \left( u_1^+ \rightarrow u_2^- \right)
\]

\[
M_8 \left( u_1^- \rightarrow u_2^+ \right) = M_4 \left( u_1^+ \rightarrow u_2^- \right)
\]

\[
\begin{align*}
\theta_1 & \equiv \frac{\sqrt{2m}}{\gamma m e^2} \left\{ 2i \sqrt{E+m} \cos \alpha \gamma - i \sqrt{E-m} \cos \alpha \gamma - i \sqrt{E-m} \cos (\theta + \alpha \gamma) \right\} \\
\end{align*}
\]

\[
\begin{align*}
\phi_1 & = \gamma \\
\psi_2 & = \gamma
\end{align*}
\]

\[
M_9 \frac{\sqrt{2m}}{\gamma m e^2} \left\{ 2i \sqrt{E+m} \cos \alpha \gamma - i \sqrt{E-m} \cos \alpha \gamma - i \sqrt{E-m} \cos (\theta + \alpha \gamma) \right\} \\
\]

\[
\begin{align*}
\theta_1 & \equiv \frac{\sqrt{2m}}{\gamma m e^2} \left\{ 2i \sqrt{E+m} \cos \alpha \gamma - i \sqrt{E-m} \cos \alpha \gamma - i \sqrt{E-m} \cos (\theta + \alpha \gamma) \right\} \\
\end{align*}
\]

\[
\begin{align*}
\phi_1 & = \gamma \\
\psi_2 & = \gamma
\end{align*}
\]

\[
M_9 \frac{\sqrt{2m}}{\gamma m e^2} \left\{ 2i \sqrt{E+m} \cos \alpha \gamma - i \sqrt{E-m} \cos \alpha \gamma - i \sqrt{E-m} \cos (\theta + \alpha \gamma) \right\} \\
\]

\[
\begin{align*}
\theta_1 & \equiv \frac{\sqrt{2m}}{\gamma m e^2} \left\{ 2i \sqrt{E+m} \cos \alpha \gamma - i \sqrt{E-m} \cos \alpha \gamma - i \sqrt{E-m} \cos (\theta + \alpha \gamma) \right\} \\
\end{align*}
\]

\[
\begin{align*}
\phi_1 & = \gamma \\
\psi_2 & = \gamma
\end{align*}
\]
11. \( u_{1-} \rightarrow u_{2-} \)  
   \( E_b \rightarrow E_{2b} \)  
   By parity  \( M_{11} = M_9 \)

12. \( u_{1-} \rightarrow u_{2-} \)  
   \( E_{1b} \rightarrow E_{2a} \)  
   By parity  \( M_{12} = M_{10} \)

13. \( u_{1+} \rightarrow u_{2-} \)  
   \( E_{1b} \rightarrow E_{2b} \)

\[ M_{13} = M_{14} \]

\[ \frac{\sqrt{2m}}{4\pi e^2} M_{13} = 2 \frac{\sqrt{E+m \sin \theta}}{\sqrt{E-m \sin \theta}} + \frac{\sqrt{E-m \sin (\theta + \frac{\pi}{2})}}{\sqrt{E+m \sin \theta}} \]

15. \( u_{1+} \rightarrow u_{2-} \)  
   \( E_{1b} \rightarrow E_{2a} \)

\[ M_{15} = M_{16} \]

\[ \frac{\sqrt{2m}}{4\pi e^2} M_{15} = \frac{1}{\sqrt{2m}} \bar{u}_e \left( x y z C - y z S - x y S \right) u_i \]  
   \( \text{(Same as 10.)} \)

\[ = \frac{i}{\sqrt{2m}} \left( \cos \frac{\theta}{2} - \cos (\theta + \frac{\pi}{2}) \right) \]

\[ = i \left( \sqrt{E+m \sin (\theta + \frac{\pi}{2})} - \sqrt{E-m \sin \theta} \right) \]

The various polarized cross sections are obtained by
the replacement  \( M \rightarrow M_k \), \( k = 1, 2, \ldots, 16 \) in Equation (1).
Pair production in matter

A photon may create an $e^+e^-$ pair in the presence of a proton according to the following diagram:

\[ p_1 = 4 \text{ momentum of } e^+ \]
\[ p_2 = 4 \text{ momentum of } e^- \]

The piece of the matrix element that is represented by this diagram is

\[
\left( \sqrt{4\pi\alpha e^2} \right)^3 \left\{ \frac{J_\mu}{q^2} \right\} \left[ \overline{u}_2 \gamma_\mu \left( \frac{1}{p_1 + k - m} \right) u_1 \right] \]

where $J_\mu$ = 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

\[
J_\mu = e \overline{u}_2 \left\{ \gamma_\mu F_1(q^2) + \frac{1}{4M} \left[ q_\mu \sigma_{\nu \lambda} \right] F_2(q^2) \right\} u_1 \]

where $F_1$ and $F_2$ are functions of $q^2$.

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
the non-relativistic limit of the coupling of this $J^m$ to an external static field $A_\mu = (\phi, \vec{A})$, and identifying terms in the classical formula

$$H_{NR}^I = e\phi + \mu \cdot \vec{B}$$

In this manner, one obtains

$$F_1(0) = 1$$

$$\mu = \frac{e}{2M} (F_1(0) + F_2(0))$$

$$\Rightarrow F_2(0)$$ 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: $\gamma + p \rightarrow \gamma + p + e^+ + e^-$, and that is

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.  \[ P_1 - P_2 \text{ (a)} \]

\[ P_1 + k \to P_1^' + q \]

\[ P_1^' = P_1 + k + q \]

or \[ q = P_2 - P_1 - k \]

II.  \[ P_1 \text{ (a)} \]

\[ P_1 + k \to P_1^' + q \]

\[ q' = q = P_2 - P_1 - k \]
The amplitudes associated with these diagrams, \( M_I, M_{II} \), are

\[
M_I = \overline{u}_2 \phi(q) \frac{1}{p^2 - k^2 - m} \phi u_1 \sqrt{\pi e^2}
\]

and

\[
M_{II} = \overline{u}_2 \phi \frac{1}{p^2 - k^2 - m} \phi(q) u_1 \sqrt{\pi e^2}
\]

where

\[
\phi(x) = \int \phi(x) e^{ix} \, dx
\]

\[
A_\mu = \left( \frac{Ze^2}{R}, 0 \right)
\]

\[
\chi \phi(x) = \chi \delta(x) e^{\delta(x)}
\]

\[
= 2\pi \delta(q^2) \frac{Ze^2}{R} \frac{4\pi}{Q^2} \delta
\]

If we took into consideration the effect of electron shielding of the field of the nucleus by \( \nu(x) = \frac{Ze^2}{R} e^{-br} \)

we'd obtain

\[
\Phi(q) = 2\pi \delta(q^2) \frac{4\pi e^2}{Q^2 + \frac{1}{2} \nu}
\]

Substituting \( \Phi \) into \( M_I + M_{II} \), and 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.

One simple result is that if the e\text{e} - pair are produced with relativistic energies, they are created primarily in the forward direction within the cone defined by the angle \( \Theta = \frac{m}{k} \).

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.

β's create pairs which emit β's by bremsstrahlung, which in turn create pairs, ... thus creating a "shower."

The "common sense" infinity of quantum electrodynamics

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

\[
\text{Rate} = \frac{2\pi \delta(E+\omega-E_1)}{(2\pi)^3 2E_1 2E_2} \frac{d^3 p_2}{2\omega (2\pi)^3} |M|^2
\]

\[
M = \sum \left\{ \frac{\bar{u}_2 \gamma}{p_2 + k - m} \gamma \frac{u_1 + \bar{u}_2 \gamma}{p_1 - k - m} \right\} \sqrt{\frac{4\pi \alpha e^2}{m_0 c^2}}
\]
\[ M = \sum_{\ell} \left( \frac{\left( p_\ell + k + m \right)}{2p_\ell \cdot k} \right) \frac{1}{2} \left( \frac{p_\ell \cdot e}{p_\ell \cdot k} \right) \left( \frac{u_1}{u_1 \sqrt{4m^2}} \right) \]

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 \[ M = \bar{u}_2 \left( -\frac{1}{2} \right) \left( \frac{p_2 \cdot e}{p_2 \cdot k} \right) \left( \frac{k \cdot e}{k \cdot k} \right) \bar{u}_1 \left( \frac{p_2 \cdot e}{p_2 \cdot k} - \frac{p_1 \cdot e}{p_1 \cdot k} \right) \left( \sqrt{4m^2} \right) \]

(The \( \lambda \)'s indicate terms that cancel)

\[ = \bar{u}_2 \bar{u}_1 \left( \frac{p_2 \cdot e}{p_2 \cdot k} \right) \left( \frac{p_2 \cdot e}{p_2 \cdot k} - \frac{p_1 \cdot e}{p_1 \cdot k} \right) \left( \sqrt{4m^2} \right) \]

\[ = \frac{1}{2} \left( \frac{p_2 \cdot e}{p_2 \cdot k} \right) \left( \frac{p_2 \cdot e}{p_2 \cdot k} - \frac{p_1 \cdot e}{p_1 \cdot k} \right) \left( \sqrt{4m^2} \right) \]

Rate \[ = \frac{2\pi}{\lambda} \delta (E_f - E_i) \frac{d^3 p_2}{(2\pi)^3 2E_2E_i} \left( \frac{1}{2} \bar{u}_2 \bar{u}_1 \right) \left( \sqrt{4m^2} \right) \]

\[ x \frac{d\omega}{\omega} \left( \frac{dS}{2(2\pi)^3} \right) \]

A is the probability of scattering with no photons emitted, in lowest order.

to the approximation we've made \( g = p_2 - p_1 \)

The term \( \xi \) may be simplified

\[ \xi = \frac{p_2 \cdot e}{1 - v_1 \cos \Theta_1} - \frac{p_1 \cdot e}{1 - v_2 \cos \Theta_2} = \frac{v_1 \sin \Theta_1}{1 - v_1 \cos \Theta_1} - \frac{v_2 \sin \Theta_2}{1 - v_2 \cos \Theta_2} \]

\[ = 0 \] if \( \xi \) is perpendicular to the plane of scattering.

 photons polarized in the plane of the collision.
Energy/unit time emitted in range $dw$

$$= \text{Same formula (without the factor of } \frac{1}{w})$$

which is the same as the classical expression

**Problem:** Two soft photon emission ($k, l$)

Show that $\text{rate} = \text{Probability of scattering without emission of no photon} \times \text{probability of emitting one photon } (k) \times \text{probability of emitting other photon } (l)$

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 $Z_\mu (\tau)$

the current density

$$j_\mu (x) = e \int \delta^4 (x - Z (\tau)) \frac{\partial}{\partial \tau} \bar{Z}_\mu (\tau) \ d\tau$$

vector potential satisfies the equation

$$\square A_\mu = j_\mu (x)$$

Take the fourier transform of both sides

$$k^2 a_\mu (k) = \int e^{-i k \cdot x} j_\mu (x) \ dx$$

$$= \int e^{-i k \cdot x} \int \bar{Z}_\mu (\tau) \delta^4 (x - Z (\tau)) \ d\tau \ dx$$

$$= \int e^{-i k \cdot x} \bar{Z}_\mu (\tau) \ d\tau = j_\mu (k)$$
Let the deflection take place at \( x = 0 \), then
\[
\begin{align*}
\lambda>0 & \quad Z_\mu(x) = \bar{p}_\mu x \\
\lambda<0 & \quad Z_\mu(x) = p_\mu x \\
\end{align*}
\]
then \( \tilde{p}(k) = \int_0^\infty p_\mu e^{-ikp_\mu} \, d\mu + \int_{-\infty}^0 p_\mu e^{ikp_\mu} \, d\mu \\
= i \left( \frac{p_\mu}{k \cdot k} - \frac{\bar{p}_\mu}{\bar{k} \cdot \bar{k}} \right) \text{, so } \tilde{q}(k) = \frac{i}{k} \left( \frac{p_\mu}{k \cdot k} - \frac{\bar{p}_\mu}{\bar{k} \cdot \bar{k}} \right)
\]
This gives the classical expected energy in dw = \( e^2 C(w) \, dw \)
\[
= \frac{\text{mean energy liberated in dw}}{\text{quantum-mechanically}}
\]
\[
= \text{mean no. of photons emitted} = e^2 C(w) \, dw
\]

**Emission of Many Soft Photons:**

Rate for one photon emission = \( A \left[ \omega \left( \frac{\sin \Theta_1}{1 - \nu_1 \cos \Theta_1} \right) - \frac{\sin \Theta_2}{1 - \nu_2 \cos \Theta_2} \right] \left( \frac{d\sigma}{dw} \right) \, dw \cdot \frac{4 \pi e^2}{(2\pi)^3 \nu}
\]

Now to the same order in \( e^2 \), the cross-section for emitting no photons is
\[
\sigma_A = \sigma_A(C + 1)
\]
where \( C \) is a correction factor that comes from interference between the two diagrams

\[
6 \text{ for 1 photon emission} = 6_A \times (1 + C) \left( \frac{d\sigma}{dw} f(\theta_1) \, d\Omega_1 \right)
\]
\[
6 \text{ for 2 photon emission} = 6_A \times (1 + C) \frac{1}{2} \left( \frac{d\sigma}{dw} f(\theta_1) \, d\Omega_1 \right) \left( \frac{d\sigma}{dw} f(\theta_2) \, d\Omega_2 \right)
\]
\[
6 \text{ for 3 photon emission} = 6_A \times (1 + C) \frac{1}{3!} \left( \frac{d\sigma}{dw} f(\theta_1) \, d\Omega_1 \right) \left( \frac{d\sigma}{dw} f(\theta_2) \, d\Omega_2 \right) \left( \frac{d\sigma}{dw} f(\theta_3) \, d\Omega_3 \right)
\]
\etc.
\[ \text{: Geattering with any } \not\gamma \text{ is removed} \]

\[ = 6A \, C' \, e^{\int \frac{dw}{w} f(w) dw} \]

The divergence ("infrared catastrophe") comes from the fact that the integral \( \int_{\text{low energy}} \) doesn't converge.

However \( C' = e^{\int \frac{dw}{w} f(w) dw} \) is the contribution of the low energy virtual photons, so \( 6A \, C' \) is finite.

The analysis implies that \( 6A \, C' = 0 \).

Experientially, there is an energy \( \Delta \) such that photons with a total energy \( \Delta \) are not observed. So we measure \( 6 \) of emitting no photons with energy \( \Delta \).

\[ 6(\mathcal{E}(\omega) < \Delta) = 6 \, \text{no photon} + 6 \, \omega \text{ photon} + 6 \frac{\Delta}{\omega} \text{ photon} + \ldots \]

\[ = 6A \, C' \left( 1 + \int_{\Delta}^{\omega} \frac{dw}{w} f(w) + \frac{1}{2} \int_{\Delta}^{\omega} \frac{dw}{w^2} \left[ \int_{\Delta}^{\omega} \frac{dw'}{w'} f(w') f(w') + \ldots \right] \right) \]

\[ = 6A \, e^{\int_{\Delta}^{\omega} \frac{dw}{w} f(w)} \left( 1 + \frac{2}{\pi} \log \frac{\Delta}{\omega} + \frac{1}{2} \left( \frac{2}{\pi} \right)^2 (\log \frac{\Delta}{\omega})^2 + \ldots \right) \]

\[ = 6A \, e^{-\frac{2}{\pi} (\log \frac{\omega}{\Delta} - \log \frac{\Delta}{\omega})} \]

\[ = 6A \, e^{-\frac{2}{\pi} \log \frac{\omega}{\Delta}} = 6A \left( \frac{\omega}{\Delta} \right)^{-\frac{2}{\pi}} \]

This can be a large correction.

We will show later how to calculate \( C' \).
Additional rules for calculating diagrams: \( e^- e^- \) scattering

\[ M_A = \left( \frac{1}{2\pi e^2} \right) \frac{\bar{u}_2 \gamma \mu_1 \bar{u}_1 \gamma \mu_2}{(p_1 - p_3)^2} \]

\( A \) is the full amplitude for \( e^- \mu^- \) scattering but not for \( e^- e^- \) scattering because there is the exchange possibility:

\[ M_B = -\left( \frac{1}{2\pi e^2} \right) \frac{\bar{u}_4 \gamma \mu_1 \bar{u}_3 \gamma \mu_2}{(p_1 - p_3)^2} \]

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

\[ -p_4 = 4 \text{ momentum of incoming } e^+ \]

The matrix element is the same as \( A \) above.

What corresponds to the exchange diagram for \( e^- \) \( e^- \) scattering?

The analogy is the annihilation diagram:

\[ \text{This is the same as the first diagram rotated } 90^\circ \text{ together with the exchange of two electron exit lines (3 and 4).} \Rightarrow \text{relative minus sign in the amplitude.} \]
That the 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:

\[
\text{Rate} = \frac{\langle \bar{u}_2 N U_1 \rangle^2}{2}
\]

Suppose the incoming particle is unpolarized and the spin of the final particle is not measured.

Then \( \langle \bar{u}_2 N U_1 \rangle^2 = \langle \bar{u}_2 N U_1 \rangle \langle \bar{u}_2 N U_1 \rangle^* \)

Let \( \bar{N} \) be defined by \( (\bar{g} N f)^* = (\bar{f} \bar{N} g) \) (it is easy to see \( \bar{N} = \gamma^\mu N \gamma^\nu \gamma^\tau \))

Then \( \langle \bar{u}_2 N U_1 \rangle^2 = \sum_{\text{spins}} \langle \bar{u}_2 N U_1 \rangle^2 \)

\[
X = \sum_{\text{spins}} \frac{\langle \bar{u}_2 N U_1 \rangle \langle \bar{u} \bar{N} U_2 \rangle}{2m} = \sum_{\text{spins}} \frac{\bar{u} \bar{N} U_2}{2m} \bar{u} \bar{N} U_2
\]

\[
= \sum_{r=1}^{s_m} \bar{u}_2 N (\bar{g}^r + m) U_r \bar{u}_r \bar{N} U_2
\]

Since \( (\bar{g}^r + m) U_2 = 0 = (\bar{g}^r + m) U_2 \)

Now \( \bar{u}_r \bar{u}_r = 2m I \), \( I = \) identity matrix

So \( X = \sum_{\text{spins}} \frac{\bar{u}_2 N (\bar{g}^r + m) \bar{N} U_2}{2m} = \sum_{r=1}^{s_m} \frac{\bar{u}_r \bar{N} (\bar{g}^r + m) \bar{u}_r}{2m} \)

\[
= \text{trace} \left( (\bar{N} (\bar{g}^r + m) \bar{N} (\bar{g}^r + m) \right) \bar{u}_r \bar{u}_r \bar{N} U_2
\]

Adding:
\[
\text{Tr} - I = 4 \gamma^\mu = 0, \quad \text{Tr} \gamma^x \gamma^y = 0, \quad \text{Tr} (\text{product of gamma}) = 0, \quad \text{Tr} \gamma^5 = 0
\]
INTENSITY DISTRIBUTION OF BREMSSTRAHLUNG RADIATION

Consider the factor $\frac{p_1 \cdot \mathbf{e}}{P_1 \cdot k} - \frac{p_2 \cdot \mathbf{e}}{P_2 \cdot k}$, which may be interpreted as the probability that an electron emit a soft photon of momentum $k$ in going from momentum $P_1$ to momentum $P_2$.

$$p_1 \cdot \mathbf{e} = -p_{1x}e_x - p_{1y}e_y = P_1 \cdot \mathbf{e}$$

Hence we obtain a function of shape

$$\frac{U_1 \cdot s \sin \Theta_1}{1 - v_1 \cdot \mathbf{e} \cdot \Theta_1} = \frac{U_2 \cdot s \sin \Theta_2}{1 - v_2 \cdot \mathbf{e} \cdot \Theta_2}$$

A non-relativistic interpretation of this is to examine the electron before and after $p_1$.

The electron is accelerated in the direction $\Delta \mathbf{v}$ 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 an exercise for the student.

In the highly relativistic region, where $v \sim c$, $P = \sqrt{E^2 - m^2} \rightarrow E - \frac{m^2}{2E}$

Thus $\frac{p \cdot \sin \Theta}{E - \gamma \cdot \mathbf{e} \cdot \Theta} \rightarrow \frac{E \cdot \Theta}{\frac{E}{2} \left( \Theta^2 + \frac{m^2}{E^2} \right)} \sim \frac{\Theta}{\Theta^2 + \left( \frac{m}{E} \right)^2}$

This takes on the shape

$$\phi = \frac{m}{E} = \frac{1}{\gamma}$$

When the deflection angle due to scattering is big compared to $\frac{1}{\gamma}$, 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 $\mathcal{N}_1$ is $\frac{d\sigma}{d\mathcal{N}_1}$ - 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 $\mathcal{N}_2$ gives the cross section to measure the emission of some photon into angle $d\mathcal{N}_1$. 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 $\mathcal{N}_1$, we are summing cases like

\[ \begin{array}{ccc}
\includegraphics[width=0.2\textwidth]{case1} & \\ & \includegraphics[width=0.2\textwidth]{case2} & \\
where 1 and 2 have been assigned simply on the basis of the counter position.
\end{array} \]

These cases are indistinguishable.

To get a total rate, all we want is the probability that the reaction went.

$$\int d\mathcal{N}_1 d\mathcal{N}_2$$

gives twice this probability. Hence, in obtaining a total rate, we must divide the final integral by $n!$, where $n$ is the number of indistinguishable particles in the final state.

MORE ABOUT THE DIRAC EQUATION

Velocity in Dirac language

$$\mathcal{H} = \beta m + \frac{\mathbf{\mathcal{P}}}{c} \cdot (\mathbf{\mathcal{P}} - \mathbf{A}) t \mathcal{V} \quad \Rightarrow \quad \mathbf{\dot{x}} = i \left[ \mathbf{\mathcal{H}}, \mathbf{x} \right] = \alpha \mathbf{x}$$

Hence one would like to find some interpretation for $\alpha$ in terms of particle velocity

However, $\alpha^2 = 1$; thus the eigenvalues are $\pm 1$, and this seems to imply that a measurement of the velocity in the $x$ direction would yield $\pm c$

This has caused some concern.

Dirac's 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

$$v^2 = \left( \frac{\langle x_0 + t \rangle - \langle x_t \rangle}{t} \right)^2$$

would give roughly

$$\left( \frac{\langle x \rangle}{\sqrt{\langle p^2 + m^2 \rangle}} \right)^2$$

(can you show this?) but measurement of the instantaneous value would come out wrong.

Feynman's explanation

Dirac's logic is wrong. For $[\alpha_x, \beta_x] = 0$ 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 $\alpha_x$ and $\beta_x$; 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 $\alpha_x$ 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 $\alpha_x \alpha_z, \beta_x \alpha_y \alpha_z$ 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 $\gamma$ matrices. But we have assigned a Lorentz index to these matrices and treated them like a 4 vector. Now, then, do we know we are using the right $\gamma$'s? Why don't we use some $\gamma'_\nu = \alpha_\nu \gamma_\mu$ with the transformation $\alpha_\nu$ 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 $\gamma_\mu$ and $\gamma_\nu$ 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.
\[
\left[ \gamma_n (i \nabla_n - A_n) + m \right] \gamma = 0
\]

Define \( \gamma'' = S \gamma' \), where \( S \) is a matrix of constants

Then
\[
\left[ \gamma''(i \nabla_n - A_n) + m \right] \gamma'' = 0
\]

will be equivalent to the above if
\[
S \gamma_n S^{-1} = \gamma''
\]

\( \gamma_n = S^{-1} \gamma'' S \)

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, \( \bar{\gamma} A \gamma = \bar{\gamma}'' A'' \gamma'' \)

Hence \( \bar{\gamma} = \gamma_0 S^+ \gamma_0 \) must equal \( \bar{\gamma}^{-1} \)

Then an equivalence transformation by any \( S \) such that \( \bar{\gamma} = s^{-1} \) leaves everything unchanged.

**Relativistic Adjoints**

\( (\bar{F}_M g)^+ = \bar{g}_M f \) defines \( \bar{M} = \beta M^+ \beta \)

For matrices \( A, B, C \) and constants \( \alpha \),

\[
\begin{pmatrix}
\alpha & A & B \\
C & D & E \\
F & G & H
\end{pmatrix} = \alpha^+ \begin{pmatrix}
D & E & F \\
G & H & I \\
J & K & L
\end{pmatrix}
\]

\( \bar{\gamma}_n = \gamma_m \)

Hence the relativistic adjoint of any number of \( \gamma \) matrices is got simply by reversing their order.

**Examples of Useful Equivalence Transformations**

1) Define \( w \) by \( \gamma_c = \gamma_{\text{cmhw}} \)

Then the velocity transformations assume a form similar to that for rotations

For the velocity transform in \( z \) direction,

\[
\begin{align*}
\gamma_x & \rightarrow (\cosh w) \gamma_x - \gamma_t \sinh w \\
\gamma_y & \rightarrow \gamma_y \\
\gamma_t & \rightarrow (\cosh w) \gamma_t - (\sinh w) \gamma_x \\
\end{align*}
\]

If \( S = e^{-w_2} \gamma_x \gamma_z \), then \( S^{-1} = e^{-w_2} \gamma_x \gamma_t \gamma_z = S \)

\[
\begin{align*}
\bar{\gamma} = \gamma_0 s^{-1} \gamma_0 = \gamma_0 e^{-w_2} \gamma_x^+ \gamma_z^+ \gamma_t^+ \gamma_0 = e^{-w_2} \gamma_x \gamma_z \gamma_t \gamma_0 = e^{-w_2} \gamma_x \gamma_z \gamma_t = \gamma_0
\end{align*}
\]

\[
\begin{align*}
C = 1 + A + \frac{1}{2} A^2 A + \frac{1}{3!} A A A + \ldots
\end{align*}
\]

Expansion shows that

\[
S = e^{-w_2} \gamma_x \gamma_z \gamma_t
\]

2) Show that the corresponding rotation operator is \( S = e^{\frac{i}{2} \gamma_x \gamma_t \gamma_z} \)

Then
\[ \psi'(x,y,z,t) = e^{\frac{\partial}{\partial t} \int dx dy \psi(x,\omega \beta + \gamma \omega \epsilon, y, \omega \gamma, z, t)} \]

\[ \psi_{\text{order}} = (1 + i \int_d \theta) \psi \Rightarrow \mathcal{J}_z = L_z + \frac{1}{2} \beta \dot{z} \]

(work through the algebra to get some familiarity)

Using this definition of \( \mathcal{J}_z \), one can show for the Dirac equation that

if there is no vector potential, and if \( V(\nabla) = V(\nu) \), 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

\[ 2m \Delta m = (\text{const}) e^2 4 \pi \int \frac{[\bar{u} \gamma_\mu (p - k + m) \gamma_{\nu} u]}{(p - k)^2 - m^2} (\nu \nabla)^4 k \]

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 \( \gamma_k \) piece. There is also a longitudinal contribution to the self energy, which looks like \( \frac{e^2}{r_{\nu}^4} \)

**Computational Aids**

Spin summation for electrons and positrons

\[ \sum_{\text{spins}} \bar{u}_\alpha A u, \bar{u}_\beta u_\gamma = \sum_{\text{spins}} \bar{u}_\alpha A \{ u_\beta (\gamma^\alpha + m) u_\gamma \} \]

Thus

\[ \sum_{\text{spins}} |\bar{u}_\alpha M u_\gamma|^2 = \sum_{\text{spins}} \bar{u}_\alpha M \{ u_\beta (\gamma^\alpha + m) u_\gamma \} \]

To calculate the traces:

\[ T_4 1 = 4 \quad T_4 \gamma_5 = 0 \]

Trace of any odd number of \( \gamma \)'s is 0

**Terminology**

\[ \text{Trace}(X) = \text{Spur}(X) \]

\[ T_4 (AB) = T_4 (BA) \quad T_4 (ABC) = T_4 (BCA) \]

\[ \text{Sp} (a \beta \gamma) = 4 a \beta \gamma \quad \text{Sp} \beta = 0 = \text{Sp}(a \beta \gamma) \]

\[ \text{Sp} (a \beta \gamma \phi) = 4 [a \cdot b \cdot c \cdot d - a \cdot c \cdot b \cdot d + a \cdot d \cdot b \cdot c] \]

Always try to use the Dirac equation \( \gamma \partial \psi = m \psi \quad \gamma \psi = -m \psi \)

To reduce the number of \( \gamma \) matrices in the matrix element before taking traces

There are tricks for taking traces of any number of \( \gamma \) matrices, but in practice even 6 \( \gamma \) matrices in a row lead to headaches. If you find you have to take traces of more than 4 \( \gamma \)'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

\[ \sum_{\text{polarizations}} S_p \left[ \begin{array}{c} \varepsilon_i \\ \varepsilon_i \end{array} \right] \]

Provided you have not used special properties of \( \varepsilon_i \) in some gauge (like assuring it has no time component) then the summation over transverse directions of the light can be replaced by

\[ \varepsilon_i \rightarrow \gamma_\mu \gamma^\mu \]

where summation is implied (also multiply the mess by -1)

Reason:

Gauge invariance implies that replacing \( \varepsilon_i \) by \( k_i \) should give 0. If \( e_i \leftrightarrow (\omega, e_x, e_y, \omega) \) then \( k_i = (k_x, \omega, \omega, k) \)

and gauge invariance says

\[ k \left[ \begin{array}{c} \gamma_t \\ \gamma_t \end{array} \right] = 0 \]

Hence \( \gamma_\mu \gamma^\mu \) boils down to \( -\frac{1}{2} \left( \gamma_x \gamma_x + \gamma_y \gamma_y \right) \)

which is what you expect from the property \( \frac{1}{2} \text{Tr} \varepsilon \varepsilon^\dagger = \delta^{ij} \gamma_i \gamma_j \)

(\( i \) and \( k \) are spacelike)

Once the quantity is in the form

\[ \gamma_\mu \gamma^\mu \]

one then uses

\[ \gamma_\mu \gamma^\mu = 4 \]

\[ \gamma_\mu \gamma^\mu \gamma_\mu \gamma^\mu = -2 \gamma \]

\[ \gamma_\mu \gamma^\mu \gamma_\nu \gamma^\nu = 4 \gamma \cdot \gamma \]

Thus each summation over photon polarizations reduces the number of \( \gamma \) matrices in the trace by 2.

**SUMMARY OF RULES**

\[ \frac{\text{Prob of Transition}}{\text{sec}} = \frac{2\pi}{M} f(E) \frac{1}{M} \left[ \frac{1}{2E_i} \right] \frac{1}{M} \left[ \frac{1}{2E_i} \right] |M|^2 \]

\[ = (2\pi)^4 \int \varepsilon_i (\varepsilon_i - \varepsilon_m) \left[ \frac{1}{M} \left( \frac{1}{2E_i} \right) \frac{1}{M} \left( \frac{1}{2E_i} \right) \right] |M|^2 \]

where \( |M| \) is a relativistically invariant matrix

Using the normalization \( \overline{u} u = 2m \)

\[ e_i e_m = -1 \]

gives as the sum over states

\[ \sum_i \left\{ (\varepsilon_i^2 + m) \overline{u} u (\varepsilon_i^2 + m) \right\} \]

Calculation of \( \overline{u} u \)
Electron propagator $\frac{i}{\lambda - m + i\epsilon}$

Photon propagator $\frac{i}{\hbar^2 + i\epsilon}$

Spin 0 meson propagator $\frac{i}{p^2 - m^2 + i\epsilon}$

Couplings:

Fermions to a real photon $-i \not{\gamma} \sqrt{4\pi \rho^2}$

Fermions to a potential $\not{\gamma} \phi(x) = \int e^{-i\not{q} \cdot x} \phi(x) d^3 x$

To a virtual photon $-i \sqrt{4\pi \rho^2} \gamma\mu \cdots - \gamma\mu (-i \sqrt{4\pi \rho^2})$

To pseudoscalar meson $\sqrt{4\pi \eta^2} \gamma_5 \cdots \gamma_5 \sqrt{4\pi \eta^2}$

To scalar meson $\sqrt{4\pi \varphi^2} \cdots \sqrt{4\pi \varphi^2}$

For a closed loop of electrons, the rule is $-S\rho$

If there is an indeterminate momentum, sum by

$\int \frac{d^4 p}{(2\pi)^4}$
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.

\[
\Delta E^2 = 4\pi e^2 \int \bar{u} \frac{\gamma_\mu}{(p - k - m)^2} \gamma_\mu u \frac{d^4k}{(2\pi)^4 k^2}
\]

\[
= \frac{4\pi e^2}{(2\pi)^4} \int \bar{u} \gamma_\mu \left[ \frac{p - k + m}{(p - k)^2 - m^2 + i\varepsilon} \right] \gamma_\mu u \frac{d^4k}{k^2 + i\varepsilon}
\]

This formula may be obtained from the expression for the second order correction to the energy of a state in ordinary perturbation theory:

\[
\Delta E_\epsilon = \sum_n \frac{H_\epsilon H_\epsilon^\dagger}{E - E_n}, \quad \text{with } H' = \text{perturbation}
\]

\[
\Delta E^2 \text{ will turn out to be logarithmically divergent}
\]

\[
\Delta E^2 = 4\pi e^2 \int \frac{\bar{u} \gamma_\mu}{(2\pi)^4} (-2p^2 + 2p \cdot k + 4m) \frac{d^4k}{k^2 + i\varepsilon (p - k)^2 - m^2 + i\varepsilon}
\]

\[
= \frac{4\pi e^2}{(2\pi)^4} \int \frac{(-4m^2 + 4p \cdot k + 8m^2)}{(k^2 + i\varepsilon) \left[ (p - k)^2 - m^2 + i\varepsilon \right]} \frac{d^4k}{m}
\]
For the correction to the rest energy, put $p^2 = 0$.

Then \[ p = k = \omega m \]
\[ (p - k)^2 = k^2 + m^2 - 2\omega m \]

and

\[
\Delta m^2 = \frac{4\pi \epsilon^2}{(2\pi)^4} \int dk \frac{m(m+\omega)}{(w^2 - k^2 + i\epsilon)(w^2 - K^2 + 2\omega m + i\epsilon)}
\]

\[
= \frac{e^2}{\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{4\pi K^2 dk \, m(m+\omega)}{(w^2 - K^2 + i\epsilon)(w^2 - K^2 + 2\omega m + i\epsilon)}
\]

The integrand has poles as a function of $w$ at

\[
w = K - i\epsilon = w_1 \quad w = \frac{m}{k} + \sqrt{k^2 + m^2 - i\epsilon} = w_0 + m = w_2
\]

\[
w = -K + i\epsilon = w_3 \quad w = -\sqrt{k^2 + m^2 + i\epsilon} = w_0 - m = w_4
\]

The integral is evaluated along a contour $C$ in the $w$-plane with endpoints $w_1$ and $w_3$.

\[
\int_{-\infty}^{\infty} \frac{m+\omega}{(w-m-w_0)(w-m+w_0)\,(w-w_1)\,(w-w_2)} = \int_{C} \frac{m+\omega}{(w-m-w_0)(w-m+w_0)(w-w_1)(w-w_2)}
\]

where $C$ is the contour shown.

The contribution from the large semicircle vanishes in the limit of infinite radius.
\[ \int_{C} = 2\pi i \left( \text{sum of residues at poles of integrand inside } C \right) \]

\[ = 2\pi i \left\{ \frac{m-K}{(-2K) \left[ \sqrt{K^{2}+m^{2}}-m-K \right] \left[ -\sqrt{K^{2}+m^{2}}-m-K \right]} \right\}_{\text{res. at } \omega_{c}} \]

\[ + 2\pi i \left\{ \frac{2m-\sqrt{K^{2}+m^{2}}}{(-2 \sqrt{K^{2}+m^{2})}[m-K-\sqrt{K^{2}+m^{2}}][K+m-\sqrt{K^{2}+m^{2}}]} \right\}_{\text{res. at } \omega_{q}} \]

\[ = 2\pi i \left\{ \frac{K-m}{4K^{2}m} + \frac{1-2m}{\sqrt{K^{2}+m^{2}}} \frac{-4m}{\sqrt{K^{2}+m^{2}-m}} \right\} \]

\[ 2m \cdot \text{res.} = \frac{e^{2}}{\pi} \cdot 4m \cdot 2\pi i \int_{0}^{\infty} dK \left\{ \frac{K-m-K^{2}}{4m} \left( 1 - \frac{2m}{\sqrt{K^{2}+m^{2}}} \right) \right\} \]

\[ = \frac{2e^{2}i}{\pi} \int_{0}^{\infty} I(K)dK \]

For small \( K \), \( I(K) \) is regular.

For large \( K \), \( I(K) \approx K-m-K \left( 1-\frac{2m}{K} + \frac{m^{2}}{K^{2}} \right) \)

\[ \left( 1 - \frac{m}{K} + \frac{m^{2}}{2K} + \ldots \right) \]

\[ I(K) \approx K-m-K \left( 1-\frac{2m}{K} \right) \left( 1+\frac{m}{K} + \frac{m^{2}}{2K^{2}} \right) \]

\[ = K-m-K \left( 1-\frac{m}{K} - \frac{3m^{2}}{2K^{2}} \right) = \frac{3M^{2}}{2K} \]

If we integrate from \( 0 \) to \( \Lambda \), then the leading term in \( \Lambda \) 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 propagator at high energies.

\[ \frac{1}{k^2} \rightarrow \frac{C(k^2)}{k^2} \]

Where \( C(k^2) \rightarrow 1 \) when \( k^2 < \lambda^2 \)

\( \lambda = \text{cutoff} \)

We choose \( C(k^2) = \frac{-\lambda^2}{k^2 - \lambda^2} \rightarrow \frac{1}{k^2} \) as \( k^2 \rightarrow \infty \).

Suppose now that with this cutoff all integrals are convergent (they are not). If the answer for a problem depends on \( \lambda \), we consider that we don't know the answer. But if as \( \lambda \rightarrow \infty \), 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,

\[ m_{\text{exp}}^2 = m_D^2 + \frac{3e^2}{4\pi^2} \frac{m_D^2}{m_e^2} \left( \log \frac{\lambda}{m_e} \right) + O(e^4) \]

The problem is of course that \( \Delta m^2 = \infty \)

\( m_{\text{exp}} \) 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 a particular energy level of the hydrogen atom due to the possibility of virtual emission and reabsorption of a photon by the electron.

\[
\Delta E_n = E_1 + \frac{\Gamma}{2}
\]

\(E_1, \Gamma\) are real \(\quad \Gamma\) gives the lifetime of the state (rate of disintegration)

ground state:

\[
\text{Re} \, \Delta E_0 = E_1 = \Delta M_0 + \frac{m e^4}{8 \pi^2}
\]

\(\Delta M_0\) is the infinite correction to \(M_0\) to obtain \(M_{\infty}\)

If you re-express the energy in terms of the physical mass \(M_{\infty}\) rather than \(M_0\), then the correction is finite as \(1 \to \infty\).

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), Feynman & Call-Mann

There are 2 different kinds of neutrinos: \( \nu_e, \nu_\mu \)

Muon decay occurs as:

\[ \mu \rightarrow e + \bar{\nu}_e + \nu_\mu \]

The neutrinos are massless and obey Dirac's equation:

\[ p_\nu^2 = 0 \]

Muon decay, β decay, and other process are described by the weak coupling:

\[ \text{Rate} = \frac{1}{16 \pi} \left( \frac{1}{M} \right)^2 \]

where \( M \) is derived from a 4-particle point interaction:

\[ \begin{array}{c}
\begin{array}{c}
 a \\
\hline \\
 c
\end{array}
\end{array} \rightarrow \begin{array}{c}
\begin{array}{c}
 b \\
\hline \\
 d
\end{array}
\end{array} \]

\[ M = G \sqrt{8} \left( \bar{u}_d \bar{\nu}_e \bar{a} \bar{u}_c \right) \left( \bar{u}_c \bar{\nu}_\mu \bar{a} \bar{u}_b \right) = G \sqrt{8} \left( \bar{d} \bar{c} \right) \left( \bar{b} \bar{a} \right) \]

Abbreviated notation

\( \sqrt{8} \) is there for historical reasons.

\[ a = \frac{1 + \Gamma}{2} \]

\( G \) is a constant with dimensions:

\[ 6M_p^2 = 1.01 \pm 0.01 \times 10^{-5} \]

\( M_p = \text{mass of proton} \)

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 \( \nu_e + \mu \rightarrow \nu_\mu + e \).
Problem: Calculate the shape of the energy spectrum in $\mu$ decay.

Aside: There is the IVB (intermediate vector boson) theory which says that $\mu \rightarrow e + \nu_e$, for example, is

\[ e \rightarrow \mu \text{ rather than } e \rightarrow \nu_e \]

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

\[ J_\mu = (\bar{e}_\mu \gamma_\mu \mu e) + (\bar{\nu}_e \gamma_\mu \mu \mu) + J_\mu \text{ hadrons} \]

\[ J_\mu = \text{ weak current of strongly interacting particles} (\pi, \rho, \omega, \sigma, \text{ etc.}) \]

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 $\beta$ decay
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 obtained from a photon of mass \( \Lambda \) that couples
to an imaginary charge. The charge is imaginary because
what was \( 4\pi e^2 \) is now \( -4\pi e \). The imaginary charge
implies that the Hamiltonian is non-Hermitian, 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 authors always have a weak point in their arguments
where they cannot prove anything.

Question: Is the final answer consistent with unitarity?

The procedures \( \{ M_0 \to M_\exp \} \) in all calculations do not straighten
\( \frac{1}{k^2} \to \frac{C(k^2)}{k^2} \)

not straighten out all infinities.

Ex. e-e scattering in 4th order

\[
M = \sum \left\{ \begin{array}{c}
\text{Diagram 1} - \text{Diagram 2} \\
\text{Diagram 3} + \text{Diagram 4}
\end{array} \right\}
\]

The 4th order diagrams give a contribution

\[
e^2 \left( 1 + e^2 \log \frac{\Lambda^2}{m_0^2} \right) \delta \mu \ldots \delta \nu
\]
If then we identify

\[ e_{\text{exp}}^{2} = e_{\text{th}}^{2} \left( 1 + e_{\text{th}}^{2} \log \frac{M'}{M} + \ldots \right) \]

and say that \( e_{\text{exp}} \) = observed charge

\( e_{\text{th}} \) = unrenormalized ("theoretical") charge

we once again have an infinite renormalization.

If now we find the rate, in any order, of a process

\[ \Gamma (M_0, e_{\text{th}}, \Lambda, \Lambda') = G (M_{\text{exp}}, e_{\text{exp}}, \Lambda, \Lambda') \]

then

\[ \lim_{\Lambda \to \infty} \lim_{\Lambda' \to \infty} G (M_{\text{exp}}, e_{\text{exp}}, \Lambda, \Lambda') \]

exists.

The process of finding \( M_{\text{exp}} = M_{\text{exp}} (M_0, \Lambda) \)

and \( e_{\text{exp}} = e_{\text{exp}} (e_{\text{th}}, \Lambda') \)

is known as mass and charge renormalization.