Quantum Mechanics II

Norman Christ

Transcribed by Ron Wu

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Contents

1 Time Dependent Hamiltonian

1.1 General Results: Time Order Product

Lecture 1 (1/22/14)

Solve

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \tag{1.1}$$

It is attempting to write

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t H(t')dt'}|\Psi(0)\rangle \tag{1.2}$$

but the problem is

$$\left[\frac{dO(t)}{dt}, O(t)\right] \neq 0$$

or

$$\frac{d}{dt}e^{O(t)} \neq \frac{dO(t)}{dt}e^{O(t)}$$

(1.2) works only if the eigenstates remain the same

$$H(t)|\psi_n\rangle = E_n(t)|\psi_n\rangle$$

time independent eigenstate, so

$$\frac{dH}{dt}|\psi_n\rangle = \frac{dE_n(t)}{dt}|\psi_n\rangle$$

then the factor in (1.2) becomes

$$e^{-\frac{i}{\hbar}\int_0^t H(t')dt'} = \sum_n |\psi_n\rangle\langle\psi_n| e^{-\frac{i}{\hbar}\int_0^t E_n(t')dt'}$$

if furthermore $H(t)$ is time independent, E_n is constant, we have old

$$|\Psi_n(t)\rangle = |\psi_n\rangle e^{-\frac{i}{\hbar}E_n t}$$

Unfortunately for time dependent Hamilton, separation of variable doesn't work. More mysterious, even the exponential in (1.2) doesn't make sense. It will be replaced by time order product. First show why (1.2) is hopeless. What is

$\frac{d}{dt}e^{O(t)}$? Claim

$$\frac{d}{dt}e^{O(t)} = \int_0^1 d\alpha e^{\alpha O(t)} \frac{dO}{dt} e^{(1-\alpha)O(t)} \tag{1.3}$$

Proof by Taylor expansion. Compare one of the expansion terms of RHS of (1.3)

$$\begin{aligned}\int_0^1 d\alpha \frac{[\alpha O(t)]^{n_1}}{n_1!}\frac{dO}{dt}\frac{[(1-\alpha)O(t)]^{n_2}}{n_2!} &= \int_0^1 d\alpha[\alpha^{n_1}(1-\alpha)^{n_2}]\frac{[O(t)]^{n_1}}{n_1!}\frac{dO}{dt}\frac{[O(t)]^{n_2}}{n_2!} \\ &= \frac{\Gamma(n_1+1)\Gamma(n_2+1)}{\Gamma(n_1+n_2+2)}\frac{[O(t)]^{n_1}}{n_1!}\frac{dO}{dt}\frac{[O(t)]^{n_2}}{n_2!} \\ &= \frac{1}{(n_1+n_2+1)!}[O(t)]^{n_1}\frac{dO}{dt}[O(t)]^{n_2}\end{aligned}$$

There are n_1+n_2+1 number of terms such that n_1+n_2+1 =fixed. Consider one of terms of LHS of (1.3)

$$\frac{d}{dt}\frac{[O(t)]^{n_1+n_2+1}}{(n_1+n_2+1)!}$$

Using product rule and induction show

$$\frac{d}{dt}\frac{[O(t)]^{n_1+n_2+1}}{(n_1+n_2+1)!} = \frac{1}{(n_1+n_2+1)!}\left(\frac{dO}{dt}O^{n_1+n_2} + O\frac{dO}{dt}O^{n_1+n_2-1} + ... + O^{n_1+n_2}\frac{dO}{dt}\right)$$

proving (1.3). So the exponential method involving doing derivative and integral with exponential in (1.2) do not work.

But there is a formal Green function method.

Consider time evolution $U(t,t')$ s.t.

$$|\psi(t)\rangle = U(t,t')\,|\psi(t')\rangle$$

so U satisfies

$$\begin{aligned} i\hbar\frac{d}{dt}U(t,t') &= HU(t,t') \\ U(t',t') &= I \end{aligned}$$

Write U in the power expansion of H

$$U(t,t') = \sum_{n=0}^{\infty} U^{(n)}(t,t')$$

where $U^{(n)}(t,t')$ is the n power of H, meaning that

in 0th order

$$\begin{aligned} i\hbar\frac{d}{dt}U^{(0)}(t,t') &= 0 \ \left(\sim H^0\right) \\ U^{(0)}(t',t') &= I \end{aligned}$$

so

$$U^{(0)}(t,t') = I$$

1st order

$$\begin{aligned} i\hbar\frac{d}{dt}U^{(1)}(t,t') &= HU^{(0)}(t,t') \ \left(\sim H^1\right) \\ U^{(1)}(t',t') &= 0 \end{aligned}$$

so

$$U^{(1)}(t,t') = -\frac{i}{\hbar}\int_{t'}^{t} H(t_1)dt_1$$

2nd order

$$\begin{aligned} i\hbar\frac{d}{dt}U^{(2)}(t,t') &= HU^{(1)}(t,t') \ \left(\sim H^2\right) \\ U^{(2)}(t',t') &= 0 \end{aligned}$$

so

$$U^{(2)}(t,t') = \left(-\frac{i}{\hbar}\right)^2 \int_{t'}^{t} dt_2 H(t_2) \int_{t'}^{t_2} dt_1 H(t_1)$$

So nth order

Lecture 2 (1/27/14)

$$U^{(n)}(t,t') = \left(-\frac{i}{\hbar}\right)^n \int_{t'}^{t} dt_n H(t_n) \int_{t'}^{t_n} dt_{n-1} H(t_{n-1}) ... H(t_2) \int_{t'}^{t_2} dt_1 H(t_1)$$

so

$$
\begin{aligned}
U(t,t') &= \sum_{n=0}^{\infty} U^{(n)}(t,t') \\
&= \sum \left(-\frac{i}{\hbar}\right)^n \int_{t'}^{t} dt_n H(t_n) \int_{t'}^{t_n} dt_{n-1} H(t_{n-1}) \cdots H(t_2) \int_{t'}^{t_2} dt_1 H(t_1) \qquad (1.4) \\
&= \sum \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{t'}^{t} dt_n \int_{t'}^{t} dt_{n-1} \cdots \int_{t'}^{t} dt_1 T(H(t_n), H(t_{n-1}), ..., H(t_1)) \qquad (1.5) \\
&= T\{e^{-\frac{i}{\hbar}\int_{t'}^{t} H(s)ds}\} \qquad (1.6)
\end{aligned}
$$

where

$$
T(O_1, O_2) = O_1(t_1)O_2(t_2)\theta(t_1-t_2) + O_2(t_2)O_1(t_1)\theta(t_2-t_1) = \begin{cases} O_1(t_1)O_2(t_2) & t_1 > t_2 \\ O_2(t_2)O_1(t_1) & t_2 > t_1 \end{cases}
$$

i.e. later time on the right.

$$
|\Psi(t)\rangle = T\{e^{-\frac{i}{\hbar}\int_{t'}^{t} H(s)ds}\}\,|\Psi(t')\rangle \qquad (1.7)
$$

The reason there is $n!$ in (1.5) is because there are $n!$ different way to order $H(t_n), H(t_{n-1}), ..., H(t_1)$ and all the same. (1.6) should not be treated literately: integrate H, exponentiation it, then time order, as we have showed in (1.3). Exponential doesn't work. So as far as calculation is concerned, we should think (1.6) as (1.5) or more usefully think as (1.4). However it is possible to do manipulation directly on (1.6), if we think the integration as Riemann sum.

Let $t_0 = t'$, $t_N = t$, $\Delta t = (t - t')/N$, assume H is constant in the interval Δt,

$$
U(t,t') = \lim_{N\to\infty} T\{e^{-\frac{i}{\hbar}\sum_{n=0}^{N-1} H(t_n)\Delta t}\}
$$

then the ordering is easy

$$
\begin{aligned}
U(t,t') &= \lim_{N\to\infty} \prod_{n=0}^{N-1} \{e^{-\frac{i}{\hbar}\sum_{n=0}^{N-1} H(t_n)\Delta t}\} \\
&= \lim_{N\to\infty} U(t_N, t_{N-1})U(t_{N-1}, t_{N-2}) \cdots U(t_1, t_0) \qquad (1.8)
\end{aligned}
$$

1.2 Sudden Change Hamilton

Consider $H(t)$ is constant for $t < t_1$ and $t > t_2$, but it changes rapidly for $t_1 \leq t \leq t_2$, and the time interval is very small. Question: how does system evolve?

Looking at (1.7), if $t_2 \to t_1$, although $\dot{H}$ is quite big, we say the exponential

$$\int_{t_1}^{t_2} H(t)dt \to 0$$

provided

$$\frac{1}{\hbar} \langle \psi_n | H | \psi_m \rangle (t_2 - t_1) \ll 1$$

So

$$U(t_2, t_1) = I$$

states don't change.

E.g. SHO, we sudden shift the origin

$$H(t) = \frac{p^2}{2m} + \frac{1}{2} m w^2 (x - x_0(t))$$

States don't change provided

$$\frac{1}{\hbar} \hbar w (n - m)(t_2 - t_1) \ll 1$$

hence the frequency of SHO is small compare to the time interval in which sudden change in H.

This example also illustrates a general fact: although states don't change, the ground state of H before, may not be the ground state of H later.

1.3 Adiabatic Approximation

Slow change H. We use adiabatic approximation. We will show that the condition of validity is

$$\frac{\hbar}{(E_{n_1} - E_{n_2})^2} \frac{dH}{dt} \ll 1 \tag{1.9}$$

or

$$\frac{dH}{dt} \ll \frac{E_{n_1} - E_{n_2}}{\frac{\hbar}{E_{n_1} - E_{n_2}}}$$

hence $H(t)$ changes slowly compare to the relevant energy difference. We further impose that for the time dependent eigenstates that

$$H(t) \left|\psi_{t,n}\right\rangle = E_{t,n} \left|\psi_{t,n}\right\rangle$$

obeying

$$\langle \psi_{t,n} | \psi_{t,n'} \rangle = \delta_{nn'} \tag{1.10}$$

and

$$\left\langle \psi_{t,n} \middle| \frac{d}{dt} \middle| \psi_{t,n} \right\rangle = 0 \tag{1.11}$$

and assume $H(t)$ is not degenerated. Otherwise (1.9) is not absolutely well defined.

We will show that (1.11) is required by the perturbation theory that we are going to use. Let's see what (1.11) implies. Take

$$\frac{d}{dt} \left[\langle \psi_{t,n} | \psi_{t,n} \rangle = 1 \right]$$

gives

$$\left(\frac{d}{dt} \left|\psi_{t,n}\right\rangle , \left|\psi_{t,n}\right\rangle \right) + \left(\left|\psi_{t,n}\right\rangle , \frac{d}{dt} \left|\psi_{t,n}\right\rangle \right) = 0$$

so automatically

$$\Re \left\langle \psi_{t,n} \middle| \frac{d}{dt} \middle| \psi_{t,n} \right\rangle = 0$$

Hence (1.11) is equivalent to

$$\Im \left\langle \psi_{t,n} \middle| \frac{d}{dt} \middle| \psi_{t,n} \right\rangle = 0 \tag{1.12}$$

So (1.11) implies that if at $t = t$, we find some eigenstates $\left|\psi_{t,n}\right\rangle$. Being satisfied by (1.10) is not enough. We need to add an extra phase

$$\left|\psi_{t,n}\right\rangle \to e^{i\theta_n(t)} \left|\psi_{t,n}\right\rangle$$

Since

$$\frac{d}{dt}\left(e^{i\theta_n(t)}\left|\psi_{t,n}\right\rangle\right) = e^{i\theta}\frac{d}{dt}\left|\psi_{t,n}\right\rangle + i\frac{d\theta}{dt}e^{i\theta}\left|\psi_{t,n}\right\rangle,$$

by (1.11)

$$0 = \left\langle \psi_{t,n}\middle|\frac{d}{dt}\middle|\psi_{t,n}\right\rangle + i\frac{d\theta}{dt}$$

or

$$\frac{d\theta}{dt} = \Im\left\langle \psi_{t,n}\middle|\frac{d}{dt}\middle|\psi_{t,n}\right\rangle$$

then $|\psi_{t,n}\rangle$ become good eigenstates. This additional phase is known Berry phase. Reference: Berry, Quantal phase factors accompanying adiabatic changes (1984).

We propose that the solution to (1.1) has the form

$$\begin{aligned} |\Psi(t)\rangle &= \sum_{n=0}^{\infty} b_n(t)e^{-\frac{i}{\hbar}\int_0^t E_{t',n}dt'}\left|\psi_{t,n}\right\rangle \\ |\Psi(0)\rangle &= \sum_{n=0}^{\infty} b_n(0)\left|\psi_{t=0,n}\right\rangle \end{aligned} \tag{1.13}$$

To figure out $b(t)$, plugging into (1.1)

$$\begin{aligned} LHS &= \sum_{n=0}^{\infty}\left(i\hbar b_n' + E_{t',n}b_n\right)e^{-\frac{i}{\hbar}\int_0^t E_{t',n}dt'}\left|\psi_{t,n}\right\rangle + i\hbar b_n e^{-\frac{i}{\hbar}\int_0^t E_{t',n}dt'}\frac{d}{dt}\left|\psi_{t,n}\right\rangle \\ RHS &= \sum_{n=0}^{\infty} E_{t',n}b_n e^{-\frac{i}{\hbar}\int_0^t E_{t',n}dt'}\left|\psi_{t,n}\right\rangle \end{aligned}$$

Applying $\langle\psi_{t,m}|$ to above, using (1.10), (1.11) and integrate

$$b_m(t) = b_m(0) + \int_0^t dt_2 \sum_{n\neq m} b_n(t_2)e^{-\frac{i}{\hbar}\int_0^{t_2}(E_{t_1,n}-E_{t_1,m})dt_1}\left\langle \psi_{t_2,m}\middle|\frac{d}{dt}\middle|\psi_{t_2,n}\right\rangle \tag{1.14}$$

To simplify above, we approximate the integral by Riemann sum $\Delta t_2 \to 0$, use perturbation

$$H(t+\Delta t) = H(t) + \frac{dH}{dt}\Delta t$$

we assume that

$$\left|\psi_{t+\Delta t,n}\right\rangle = \left|\psi_{t,n}\right\rangle + \frac{d}{dt}\left|\psi_{t,n}\right\rangle\Delta t$$

and relate $\frac{d}{dt}|\psi_{t,n}\rangle\Delta t$ to the perturbation $\frac{dH}{dt}\Delta t$, assume it is the 1st order correction, so

$$\frac{d}{dt}|\psi_{t,n}\rangle\Delta t=\sum_{n'\neq n}|\psi_{t,n'}\rangle\frac{\left\langle\psi_{t,n'}\middle|\frac{dH}{dt}\Delta t\middle|\psi_{t,n}\right\rangle}{E_n-E_{n'}}$$

Lecture 3 (1/29/14)

Recall when we do perturbation, we say that the 1st order correction of $|\psi_{t,n}\rangle$ contains no $|\psi_{t,n}\rangle$ term, see Griffiths footnote page 253, or equivalently last semester Quantum Mechanics I note equation (3.11), we imposed

$$S_{nn}^{(1)} \text{ to be real}$$

Hence (1.11) must be satisfied.

Go back to (1.14), we have

$$b_m(t)=b_m(0)+\int_0^t dt_2\sum_{n\neq m}b_n e^{-\frac{i}{\hbar}\int_0^{t_2}(E_{t_1,n}-E_{t_1,m})dt_1}\frac{\left\langle\psi_{t_2,m}\middle|\frac{dH}{dt}\middle|\psi_{t_2,n}\right\rangle}{E_{t_2,n}-E_{t_2,m}}$$

We want to claim that the integral is 0, even when $t\to\infty$, so adiabatic approximation can be applied to very long time interval

$$\int_0^t dt_2 b_n(t_2)e^{-\frac{i}{\hbar}\int_0^{t_2}(E_{t_1,n}-E_{t_1,m})dt_1}\frac{\left\langle\psi_{t_2,m}\middle|\frac{dH}{dt}\middle|\psi_{t_2,n}\right\rangle}{E_{t_2,n}-E_{t_2,m}}\approx\underbrace{\int_0^t dt_2 e^{-iw_{nm}t_2}}_{\sim\frac{1-e^{-iw_{nm}t}}{w_{nm}}}b_n(0)\frac{\left\langle\frac{dH}{dt}\right\rangle_{nm}}{w_{nm}\hbar}$$

hence we assumed $w_{nm}\sim(E_{t,n}-E_{t,m})/\hbar$, i.e. as eigenstates evolve, the energy spacings are bounded. The $e^{-iw_{nm}t}$ term shows that even $t\to\infty$, it doesn't grow. Applying (1.9)

$$\frac{\hbar\left\langle\frac{dH}{dt}\right\rangle_{nm}}{(E_n-E_m)^2}\ll 1$$

we get $b(t)$ is constant. This completes the adiabatic approximation.

Example. Consider a spin 1/2 particle with $\vec{\mu}=\gamma\vec{S}$ in a time varying magnetic field from $t=0$ to T. Assume $t=0$, $|\psi\rangle=\left|\frac{1}{2}\right\rangle$.

$$H(t)=-\gamma\vec{S}\cdot\vec{B}(t)$$

$$\frac{2\pi}{T} \ll \gamma B$$

change of Humiliation is much smaller than the Larmor precession frequency.

Two cases:

1)

$$\vec{B}(t) = B\hat{z}(1 - \frac{2t}{T})$$

2)

$$\vec{B}(t) = B[\hat{z}\cos\frac{2\pi t}{T} - \hat{y}\sin\frac{2\pi t}{T}]$$

For 1)

$$H\left|\frac{1}{2}\right\rangle = -\gamma B(t) S_z \left|\frac{1}{2}\right\rangle = -\gamma B(t)\frac{\hbar}{2}\left|\frac{1}{2}\right\rangle$$

Hence the eigenstate of $H(t)$ stays the same. To apply (1.13) with $b_{1/2} = 1$ and $b_{-1/2} = 0$,

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t -\frac{\gamma\hbar}{2}B(t')dt'}\left|\frac{1}{2}\right\rangle = e^{\frac{i}{2}\gamma B(t-\frac{t^2}{T})}\left|\frac{1}{2}\right\rangle$$

For 2)

To apply (1.13), we need to know $|\psi_{t,n}\rangle$, eigenstate of the time varying Hamilton. Check

$$\left|\psi_{t,\pm\frac{1}{2}}\right\rangle = e^{-i\sigma_x \frac{\pi t}{T}}\left|\pm\frac{1}{2}\right\rangle \tag{1.15}$$

Indeed, using Quantum Mechanics I note equation (2.38)

$$\left|\psi_{t,\frac{1}{2}}\right\rangle = [\cos\frac{\pi t}{T} - i\sigma_x \sin\frac{\pi t}{T}]\left|\frac{1}{2}\right\rangle = \begin{pmatrix} \cos\frac{\pi t}{T} \\ -i\sin\frac{\pi t}{T} \end{pmatrix}$$

$$\begin{aligned}
H\left|\psi_{t,\frac{1}{2}}\right\rangle &= -\gamma B[S_z\cos\frac{2\pi t}{T} - S_y\sin\frac{2\pi t}{T}]\begin{pmatrix} \cos\frac{\pi t}{T} \\ -i\sin\frac{\pi t}{T} \end{pmatrix} \\
&= -\gamma B\frac{\hbar}{2}\begin{pmatrix} \cos\frac{2\pi t}{T} & i\sin\frac{2\pi t}{T} \\ -i\sin\frac{2\pi t}{T} & -\cos\frac{2\pi t}{T} \end{pmatrix}\begin{pmatrix} \cos\frac{\pi t}{T} \\ -i\sin\frac{\pi t}{T} \end{pmatrix} \\
&= -\gamma B\frac{\hbar}{2}\begin{pmatrix} \cos\frac{\pi t}{T} \\ -i\sin\frac{\pi t}{T} \end{pmatrix}
\end{aligned}$$

We need to check (1.15) satisfies (1.11)

$$\left\langle \frac{1}{2} \middle| e^{i\sigma_x \frac{\pi t}{T}} \frac{d}{dt} e^{-i\sigma_x \frac{\pi t}{T}} \middle| \frac{1}{2} \right\rangle = \left\langle \frac{1}{2} \middle| -i\frac{\pi t}{T}\sigma_x \middle| \frac{1}{2} \right\rangle = 0$$

Now apply (1.13)

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t -\gamma B \frac{\hbar}{2} dt} \begin{pmatrix} \cos\frac{\pi t}{T} \\ -i\sin\frac{\pi t}{T} \end{pmatrix} = e^{\frac{i\gamma B}{2}t} \begin{pmatrix} \cos\frac{\pi t}{T} \\ -i\sin\frac{\pi t}{T} \end{pmatrix}$$

When $t = T/2$

$$\left| \Psi(\frac{T}{2}) \right\rangle = e^{\frac{i\gamma B}{4}t}(-i) \left| -\frac{1}{2} \right\rangle$$

When $t = T$

$$|\Psi(T)\rangle = e^{\frac{i\gamma B}{2}t}(-1) \left| \frac{1}{2} \right\rangle$$

This is shocking Berry phase. It says as $\vec{B}$ rotates, spin rotates. When $\vec{B}$ makes 2π rotation, $|\Psi\rangle$ gains extra -1.

One can even show that if the $\vec{B}$ fields rotates like a cone. The Berry phase of a full rotation is not -1, it will depend on the open angle of the cone. If the open angle goes to 0, Berry phase becomes 1. See HW problem 47 of problem set 13.

1.4 Time Dependent Perturbation

We now consider the case that the time dependent part of Hamilton is small

$$H(t) = H_0 + V(t) \tag{1.16}$$

H_0 constant. Solve

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = [H_0 + V(t)]\,|\Psi(t)\rangle$$

The idea is to substitute

$$|\Psi_I(t)\rangle \equiv e^{iH_0 t/\hbar}\,|\Psi(t)\rangle$$

$|\Psi_I(t)\rangle$ called interaction picture, in contrast to Schrodinger/Heisenberg pictures. So

$$\begin{aligned} i\hbar\frac{d}{dt}|\Psi_I(t)\rangle &= \left\{-H_0 e^{iH_0t/\hbar} + e^{iH_0t/\hbar}[H_0 + V(t)]\right\}|\Psi(t)\rangle \\ &= e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}|\Psi_I(t)\rangle \end{aligned}$$

Hence

$$i\hbar\frac{d}{dt}|\Psi_I(t)\rangle = V_I(t)|\Psi_I(t)\rangle \tag{1.17}$$

V_I interaction picture potential.

Now the time order product notation becomes useful, because the exponents are small

$$U_I(t_b, t_a) = T\left\{e^{-\frac{i}{\hbar}\int_{t_a}^{t_b} V_I(t')dt'}\right\} \tag{1.18}$$

Example. Consider H such that $V(t) = 0$ for $t < t_1$ and $t > t_2$. Find 1st order in V, the probability that an initial eigenstate $|\psi_n\rangle$ for $t < t_1$ becomes $|\psi_{n'}\rangle$ for $t > t_2$ where $H_0|\psi_n\rangle = E_n|\psi_n\rangle$.

Lecture 4 (2/3/14)

1st order in V means expanding (1.18) in 1st order, so it has only one term (no cross term), nothing to order,

$$|\Psi_I(t)\rangle = \left[I - \frac{i}{\hbar}\int_{t_a}^{t_b} V_I(t')dt'\right]|\Psi_I(t_a)\rangle \tag{1.19}$$

and

$$|\Psi_I(t_a)\rangle = e^{-iE_nt_a/\hbar}|\psi_n\rangle$$

The probability

$$\begin{aligned} P_{n\to n'} &= |\langle\psi_{n'}|\Psi(t_b)\rangle|^2 \\ &= \left|\left\langle\psi_{n'}\middle|e^{-iH_0t/\hbar}\middle|\Psi_I(t_b)\right\rangle\right|^2 \\ &= \left|\left\langle\psi_{n'}\middle|e^{-iE_{n'}t/\hbar}\middle|\Psi_I(t_b)\right\rangle\right|^2 \\ &= |\langle\psi_{n'}|\Psi_I(t_b)\rangle|^2 \end{aligned} \tag{1.20}$$

That is why in calculating the transition probability, we generally use interaction picture and Schrodinger picture interchangeably.

For $n \neq n'$

$$\begin{aligned}\langle \psi_{n'} | \Psi_I(t_b) \rangle &= \left\langle \psi_{n'} \middle| -\frac{i}{\hbar} \int_{t_a}^{t_b} e^{iH_0 t'/\hbar} V(t') e^{-iH_0 t'/\hbar} dt' \middle| \psi_n \right\rangle e^{-iE_n t_a/\hbar} \\ &= -\frac{i}{\hbar} \int_{t_a}^{t_b} e^{-iw_{nn'} t'/\hbar} V(t') dt' e^{-iE_n t_a/\hbar}\end{aligned}$$

where

$$w_{nn'} = \frac{E_n - E_{n'}}{\hbar}$$

Using Fourier

$$\tilde{V}(w_{nn'}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iw_{nn'} t'/\hbar} V(t') dt'$$

so

$$\langle \psi_{n'} | \Psi_I(t_b) \rangle = -\frac{i}{\hbar} \sqrt{2\pi} \tilde{V}(w_{nn'}) e^{-iE_n t_a/\hbar}$$

Thus

$$P_{n \to n'} = \frac{2\pi}{\hbar^2} \left| \tilde{V}(w_{nn'}) \right|^2 \tag{1.21}$$

1.5 Decay of an Unstable State

Last semester we studied α decay. Now we do a general study. Consider the decay of an unstable state in perturbation

$$H = H_0 + V \tag{1.22}$$

H_0 has two types of eigenstates

1) One discrete decaying state

$$H_0 |d\rangle = E_d |d\rangle$$

2) Continuous decay product from $|d\rangle$

$$H_0 |\psi_{\vec{p}}\rangle = E_{\vec{p}} |\psi_{\vec{p}}\rangle$$

and

$$\begin{aligned}
\langle d|d\rangle &= 1 \\
\langle \psi_{\vec{p}}|\psi_{\vec{p}'}\rangle &= \delta^{(3)}(\vec{p}-\vec{p}') \\
\langle d|\psi_{\vec{p}}\rangle &= 0
\end{aligned}$$

Why are $|\psi_{\vec{p}}\rangle$ continuous? That has to do with finite volume space and time. Typical

$$E_{\vec{p}} = \frac{p^2}{2m} \text{ plane wave } \gamma \text{ radiation}$$

for some erotic problem E may depend on direction of $\vec{p}$. We will see that the typical decay products are center around E_d. If $|\psi_{\vec{p}}\rangle$ are discrete, that belongs to different sets of problems, e.g. mixing.

Plug

$$|\Psi_I(t)\rangle = a(t)\,|d\rangle + \int d^3\vec{p} b_{\vec{p}}(t)\,|\psi_{\vec{p}}\rangle \tag{1.23}$$

into (1.17)

$$i\hbar\left(\dot{a}(t)\,|d\rangle + \int d^3\vec{p}\dot{b}_{\vec{p}}(t)\,|\psi_{\vec{p}}\rangle\right) = a(t)V_I(t)\,|d\rangle + \int d^3\vec{p}V_I(t)b_{\vec{p}}(t)\,|\psi_{\vec{p}}\rangle \tag{1.24}$$

Apply $\langle\psi_{\vec{p}'}|$

$$i\hbar\dot{b}_{\vec{p}}(t) = a(t)\,\langle\psi_{\vec{p}}|V_I(t)|d\rangle + \int d^3\vec{p}'\,\langle\psi_{\vec{p}}|V_I(t)|\psi_{\vec{p}'}\rangle\,b_{\vec{p}'}(t) \tag{1.25}$$

To solve b, we put zeroth order value to the right side of equation

$$a(t) \to a(0) = 1 \qquad b(t) \to b(0) = 0$$

so

$$\begin{aligned}
b_{\vec{p}}(t) &= -\frac{i}{\hbar}\,\langle\psi_{\vec{p}}|V(t)|d\rangle \int_0^t e^{-i(E_d-E_{\vec{p}})t'/\hbar}dt' \qquad (1.26)\\
&= \langle\psi_{\vec{p}}|V(t)|d\rangle\,\frac{e^{-i(E_d-E_{\vec{p}})t/\hbar}-1}{E_d-E_p}
\end{aligned}$$

$$|b_{\vec{p}}(t)|^2 = |\langle\psi_{\vec{p}}|V(t)|d\rangle|^2 \left(\frac{t}{\hbar}\right)^2 \frac{\sin^2(E_d - E_{\vec{p}})t/2\hbar}{[(E_d - E_{\vec{p}})t/2\hbar]^2} \tag{1.27}$$

The graph of $|b_{\vec{p}}(t)|^2$ v.s. $E_{\vec{p}}$ shows that in (1.23) the distribution of $|\psi_{\vec{p}}\rangle$ has width $\sim \hbar/t$, (i.e. the 1st minimum $(E_d - E_{\vec{p}})t/\hbar = \pi \implies E_d - E_{\vec{p}} \sim \hbar/t$), the high of graph $\sim (t/\hbar)^2$. Hence the decay probability

$$\int |b_{\vec{p}}(t)|^2 \, d\vec{p} \sim \frac{\hbar}{t}\left(\frac{t}{\hbar}\right)^2 \sim t$$

longer you wait, more probably it decays. It also shows that if we divide probability by time, we may get something more intrinsic, i.e. rate of decay.

It looks like if we push $t \to \infty$, we can get a sharp peak, hence decay becomes discrete, but this will break down (1.26), where we assume $b(t)$ is small, so we replace it by $b(0) = 0$ on the right.

The exact condition for t is

$$\frac{\langle\psi_{\vec{p}}|V(t)|d\rangle \, t}{\hbar} \ll 1$$

i.e. the maximum high of $|b_{\vec{p}}(t)|^2$ when $E_{\vec{p}} = E_d$ is $\ll 1$.

1.6 Fermi Golden Rule

It has calculation advantage to replace

$$\frac{\sin^2(E_d - E_{\vec{p}})t/2\hbar}{[(E_d - E_{\vec{p}})t/2\hbar]^2}$$

by δ function so that essentially the bell curve becomes a sharp peak. Since

$$\int_{-\infty}^{\infty} dz \frac{\sin^2 z}{z^2} = \pi$$

which we are going to verify

$$\lim_{\epsilon\to 0} \int dz \frac{\sin^2 z}{(z - i\epsilon)^2} = \lim_{\epsilon\to 0} \int dz \frac{-\frac{1}{4}(e^{2iz} + e^{-2iz} - 2)}{(z - i\epsilon)^2}$$

shift the pole up. For the e^{-2iz} part, we have to close the contour lower half plane, so no pole enclosed. For -2 part, we choose to close the contour lower half plane, so no pole.

$$\lim_{\epsilon\to 0^+}\int dz \frac{\sin^2 z}{(z-i\epsilon)^2} = \lim_{\epsilon\to 0^+}\int dz - \frac{1}{4}\frac{e^{2iz}}{(z-i\epsilon)^2}$$

which is a double pole. By Cauchy theorem

$$\int \frac{f(z)}{(z-z_0)^2}dz = f'(z_0)2\pi i$$

so

$$\int_{-\infty}^{\infty} dz \frac{\sin^2 z}{z^2} = -\frac{1}{4}2i(2\pi i) = \pi$$

Hence

$$\frac{\sin^2(E_d - E_{\vec{p}})t/2\hbar}{[(E_d - E_{\vec{p}})t/2\hbar]^2} = \pi\delta\left(\frac{(E_d - E_{\vec{p}})t}{2\hbar}\right) = \pi\frac{\delta(E_d - E_{\vec{p}})}{\frac{t}{2\hbar}} \tag{1.28}$$

Therefore the probability of decaying, by (1.20), (1.23), (1.27) and (1.28)

$$\begin{aligned} P_{d\to \text{all } \vec{p}} &= \int d^2\vec{p}\,|b_{\vec{p}}(t)|^2 \\ &= \int d^2\vec{p}\,|\langle\psi_{\vec{p}}|V(t)|d\rangle|^2\,\frac{2\pi}{\hbar}t\delta(E_d - E_{\vec{p}}) \end{aligned}$$

If we divide t,

$$Rate = \frac{2\pi}{\hbar}\int d^2\vec{p}\,|V_{\vec{p}d}|^2\,\delta(E_d - E_{\vec{p}})$$

or more generally

$$\begin{aligned} Rate &= \frac{2\pi}{\hbar}\sum_{\vec{p}}|V_{\vec{p}d}|^2\,\delta(E_d - E_{\vec{p}}) \\ &= \frac{2\pi}{\hbar}\sum_{\vec{p}}|\langle\vec{p}|V|d\rangle|^2\,\delta(E_d - E_{\vec{p}}) \end{aligned} \tag{1.29}$$

including all $\vec{p}$ continuous and discrete. This is known as Fermi's Golden Rule.

Example. Decay of an excited hydrogen atom.

$|d\rangle = |2p\rangle$, with energy $E = -\frac{me^2}{2\hbar^2}\frac{1}{4}$

$|\psi_{\vec{p}}\rangle = |1s, \gamma(\vec{p})\rangle$, with energy $E = -\frac{me^2}{2\hbar^2} + hpc$, the $\gamma(\vec{p})$ part requires quantization EM field involving photons energy hpc. We will do that later in the course.

Example. HW problem 48 of problem set 14: Auger Effect, is a physical phenomenon in which the filling of an inner-shell vacancy of an atom is accompanied by the emission of an electron from the same atom.

Consider Helium atom with 2 electrons at the excited states.$|d\rangle = |2s, 2p\rangle$, one electron falls in $1s$ and the other escapes, $|\psi_{\vec{p}}\rangle = |1s, e^-(\vec{p})\rangle$

$$\begin{aligned} E_d &= -\frac{me^4Z^2}{2\hbar^2 n^2} = -\frac{me^2}{2\hbar^2}\frac{4}{4}2 \\ E_{\psi_{\vec{p}}} &= -\frac{me^2}{2\hbar^2}4 + \frac{p^2}{2m} \end{aligned}$$

This can be worked out by

$$H = \frac{\vec{p}_1 + \vec{p}_2}{2m} - \frac{2e^2}{|r_1|} - \frac{2e^2}{|r_2|} + \underbrace{\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}}_{V}$$

We now solve a complete problem

Example. Consider a H atom in its ground state, immersed in a time varying EM field.

$$\vec{E}(\vec{r}, t) = \vec{\epsilon}\sin(\vec{k}\cdot\vec{r} - wt)$$

Plane wave, so charge at ∞, so $\varphi = 0$

$$\vec{E} = -\frac{1}{c}\dot{\vec{A}}(\vec{r}, t) - \nabla\varphi = -\frac{1}{c}\dot{\vec{A}}(\vec{r}, t)$$

we say

$$\vec{A}(\vec{r}, t) = -\underbrace{\frac{c}{w}}_{\frac{1}{k}}\cos(\vec{k}\cdot\vec{r} - wt)\vec{\epsilon}$$

Lowest order in field strength

$$\begin{aligned} H &= \frac{(\vec{p}+\frac{e}{c}\vec{A})^2}{2m} - \frac{e^2}{r} \\ &= \underbrace{\frac{\vec{p}^2}{2m} - \frac{e^2}{r}}_{H_0} + \underbrace{\frac{e}{mc}\vec{p}\cdot\vec{A}}_{V(t)} \end{aligned}$$

We are interested in final states,

$$\left|e^-(\vec{p})\right\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi\hbar)^{3/2}} \qquad E_{\psi_{\vec{p}}} = \frac{p^2}{2m}$$

knock

$$|1s,\gamma(w)\rangle = \frac{1}{\sqrt{\pi}}e^{-r/a_0}\frac{1}{a_0^{3/2}} \qquad E_d = -\frac{me^4}{2\hbar^2} + \hbar w$$

e^- out of atom, absorb a photon. Why does it have to absorb a photon? Why cannot it produce a photon? Then it will mean that the ejected free e^- has energy

$$-\frac{me^4}{2\hbar^2} - \hbar w$$

that is even lower than its value in the ground state of H. So not physical

Compute

$$\langle\psi_{\vec{p}}|V(t)|d\rangle = \left\langle \vec{p}\left| -\frac{e}{mc}\vec{p}\cdot\vec{\epsilon}\frac{1}{k}\frac{e^{i(\vec{k}\cdot\vec{r}-wt)}+e^{-i(\vec{k}\cdot\vec{r}-wt)}}{2}\right| 1s\right\rangle \tag{1.30}$$

Lecture 5 (2/5/14)

Let us do one of the two terms above.

$$\int d^3\vec{r} - \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}\frac{e}{mw}\vec{p}\cdot\vec{\epsilon}e^{i\vec{k}\cdot\vec{r}}\frac{1}{2}\frac{e^{-r/a_0}}{\sqrt{\pi}a_0^{3/2}}e^{-iwt} \tag{1.31}$$

First ignoring $e^{i\vec{k}\cdot\vec{r}} \approx 1$, called dipole approximation, because without it, we only have $\vec{p}\cdot\vec{\epsilon}$ that contains the angular distribution in the polarized direction, i.e. dipole momentum. To get high poles, we need to expand $e^{i\vec{k}\cdot\vec{r}}$.

Under what condition $e^{i\vec{k}\cdot\vec{r}} \approx 1$? Since r is dictated by e^{-r/a_0}, so if

$$hw \sim \frac{me^4}{\hbar^2} = \text{atomic energy} \tag{1.32}$$

i.e. ionizing H atom with visible lights, not gamma rays.

$$k = \frac{w}{c} \sim \frac{me^4}{c\hbar^3} = \underbrace{\frac{me^2}{\hbar^2}}_{\frac{1}{a_0}} \underbrace{\frac{e^2}{\hbar c}}_{\alpha} \implies \lambda \sim \frac{a_0}{\alpha}$$

so the wave length is 100 times longer than the size of atom. So

$$kr \sim ka_0 \sim \alpha \implies e^{i\alpha} \approx 1$$

Now do integral, pick $\hat{z} \parallel \vec{p}$

$$(1.31) = -\frac{1}{(2\pi\hbar)^{3/2}} \frac{e}{mw} \vec{p}\cdot\vec{\epsilon} \frac{1}{2\sqrt{\pi} a_0^{3/2}} 2\pi e^{-iwt} \underbrace{\int_{-1}^{1} d\cos\theta \int_0^\infty r^2 dr e^{-ipr\cos\theta/\hbar} e^{-r/a_0}}_{\int_0^\infty r^2 dr \frac{e^{-ipr/\hbar} - e^{ipr/\hbar}}{-ipr/\hbar} e^{-r/a_0}}$$

Put $y = r/a_0 \pm ipr/\hbar$ for the two integrals

$$\int_0^\infty \frac{ir}{p/\hbar} dr (e^{-ipr/\hbar} - e^{ipr/\hbar}) e^{-r/a_0} = \frac{i}{p/\hbar} \underbrace{\int_0^\infty y e^{-y} dy}_{1} \left[\frac{1}{(\frac{1}{a_0} + i\frac{p}{\hbar})^2} - \frac{1}{(\frac{1}{a_0} - i\frac{p}{\hbar})^2} \right]$$

so

$$(1.31) = -\frac{1}{(2\pi\hbar)^{3/2}} \frac{e}{mw} \vec{p}\cdot\vec{\epsilon} \frac{1}{2\sqrt{\pi} a_0^{3/2}} 2\pi e^{-iwt} \frac{i}{p/\hbar} a_0^2 \frac{-4i\frac{pa_0}{\hbar}}{\left[1 + (\frac{pa_0}{\hbar})^2\right]^2}$$

so

$$(1.30) = -\frac{1}{(2\pi\hbar)^{3/2}} \frac{e}{mw} \vec{p}\cdot\vec{\epsilon} \frac{1}{\sqrt{\pi} a_0^{3/2}} 2\pi \frac{i}{p/\hbar} a_0^2 \frac{-4i\frac{pa_0}{\hbar}}{\left[1 + (\frac{pa_0}{\hbar})^2\right]^2} \cos wt$$

the $\cos wt$ will be averaged to $\frac{1}{2}$.

By Fermi golden rule

$$\begin{aligned} Rate &= \frac{2\pi}{\hbar}\int d^3\vec{p}\delta(\frac{p^2}{2m}+\frac{me^4}{2\hbar^2}-\hbar w)\frac{1}{(2\pi\hbar)^3}\frac{e^2}{m^2w^2}(\vec{p}\cdot\vec{\epsilon})^2\frac{1}{\pi a_0^3}(2\pi)^2\frac{\hbar^2}{p^2}a_0^4\frac{16\left(\frac{pa_0}{\hbar}\right)^2}{\left[1+(\frac{pa_0}{\hbar})^2\right]^4}\frac{1}{2} \\ &= \frac{8a_0^3}{\pi\hbar^4}\frac{e^2}{m^2w^2}\underbrace{\int d^3\vec{p}\delta(\frac{p^2}{2m}+\frac{me^4}{2\hbar^2}-\hbar w)\frac{(\vec{p}\cdot\vec{\epsilon})^2}{\left[1+(\frac{pa_0}{\hbar})^2\right]^4}}_{2\pi\underbrace{\int_{-1}^{1}d(\cos\theta)\cos^2\theta}_{\frac{2}{3}}\int_0^\infty p^2dpp^2|\vec{\epsilon}|^2\frac{\delta(\frac{p^2}{2m}+\frac{me^4}{2\hbar^2}-\hbar w)}{\left[1+(\frac{pa_0}{\hbar})^2\right]^4}} \end{aligned}$$

so

$$\begin{aligned} Rate &= \frac{8a_0^3}{\pi\hbar^4}\frac{e^2}{m^2w^2}\frac{4\pi}{3}p^4|\vec{\epsilon}|^2\frac{1}{\frac{p}{m}\left[1+(\frac{pa_0}{\hbar})^2\right]^4} \\ &= \frac{e^2}{mw}\frac{32}{3}\left(\frac{pa_0}{\hbar}\right)^3\epsilon^2\frac{1}{\left(1+(\frac{pa_0}{\hbar})^2\right)^4} \end{aligned} \tag{1.33}$$

where

$$p=\sqrt{2m(\hbar w-\frac{me^4}{2\hbar^2})} \tag{1.34}$$

The rate (1.33) has a maximum at

$$p=\sqrt{\frac{3}{5}}\frac{\hbar}{a_0}$$

By (1.34), it corresponds to

$$\hbar w=\frac{4}{5}\frac{me^4}{\hbar^2}$$

which agrees perfectly to our dipole assumption (1.32).

One can compute the cross section from the excitation rate upon impinging photons on atoms

$$Rate=\sigma_{\text{ionization}}\times\text{flux of photons}$$

$$\text{Flux}=\frac{\text{energy density}}{\hbar w}\times c$$

$$\text{energy density} = \frac{1}{8\pi}(\vec{E}^2 + \vec{B}^2) = \frac{1}{8\pi}\epsilon^2$$

so the cross section

$$\sigma = \frac{\frac{e^2}{mw}\frac{32}{3}\left(\frac{pa_0}{\hbar}\right)^3 \epsilon^2 \frac{1}{\left(1+(\frac{pa_0}{\hbar})^2\right)^4}}{\frac{1}{8\pi}\epsilon^2 c}$$

1.7 Wigner-Weisskopf Approximation

Wigner-Weisskopf approximation is in between of adiabatic approximation and time dependent approximation. We assume similarly to adiabatic approximation (1.9),

$$\hbar \times \text{rate} \ll \text{scale of energies of the problem}$$

We also assume

$$H(t) = H_0 + V(t)$$

$V(t)$ is small, so that

$$\langle \psi_{\vec{p}} | V(t) | \psi_{\vec{p}'} \rangle = 0 \tag{1.35}$$

saying that once it decays to $\psi_{\vec{p}}$, it cannot become $\psi_{\vec{p}'}$, because V is small. Also

$$\langle d | V(t) | d \rangle = 0 \tag{1.36}$$

that is because $\dot{V}$ is small, so if $\langle d|V(t)|d\rangle$ is not 0, it must be nearly a constant, so we absorb constants to H_0.

Using Wigner-Weisskopf approximation (without formal perturbation theory) we will quickly derive the characteristic feature of the decay, given by the Lorentzian curves (1.27). From there we will re derive the Fermi golden rule.

Apply $\langle d|$ to (1.24)

$$\begin{aligned} i\hbar\dot{a}(t) &= a(t)\langle d| V_I(t) |d\rangle + \int d^3\vec{p}\, \langle d| V_I(t) b_{\vec{p}}(t) |\psi_{\vec{p}}\rangle \\ &= a(t)\langle d| V(t) |d\rangle + \int d^3\vec{p}\, \langle d| V(t) |\psi_{\vec{p}}\rangle\, b_{\vec{p}}(t) e^{-i(E_{\vec{p}}-E_d)t/\hbar} \\ &= \sum_{\vec{p}} \langle d| V(t) |\psi_{\vec{p}}\rangle\, b_{\vec{p}}(t) e^{-i(E_{\vec{p}}-E_d)t/\hbar} \end{aligned} \tag{1.37}$$

replacing $\int d^3p$ by $\sum_{\vec{p}}$ as we did in (1.29).

And (1.25) becomes

$$i\hbar\dot{b}_{\vec{p}}(t) = \langle\psi_{\vec{p}}|V|d\rangle\, a(t)e^{-i(E_d - E_{\vec{p}})t/\hbar}$$

Try the ansatz

$$a(t) = e^{-\gamma t/2}$$

so $|a(t)|^2$ implies γ is the rate of decay. Then

$$b_{\vec{p}} \;=\; \frac{1}{i\hbar}\int_0^t V_{\vec{p}d}e^{-i(E_d - E_{\vec{p}} - i\gamma\hbar/2)t/\hbar}$$

assuming $V_{\vec{p}d}$ is small,

$$b_{\vec{p}}(t) = V_{\vec{p}d}\frac{e^{-i(E_d - E_{\vec{p}} - i\gamma\hbar/2)t/\hbar} - 1}{E_d - E_{\vec{p}} - i\gamma\hbar/2}$$

so $|b(t)|^2$ shows that γ in the denominator also represents the width.

To find γ, we put it into (1.37)

$$\text{RHS} = \underbrace{\sum_{\vec{p}} |V_{\vec{p}d}|^2 \frac{e^{-\gamma t/2}}{E_d - E_{\vec{p}} - i\gamma\hbar/2}}_{I} + \underbrace{\sum_{\vec{p}} |V_{\vec{p}d}|^2 \frac{-e^{-i(E_{\vec{p}} - E_d)t/\hbar}}{E_d - E_{\vec{p}} - i\gamma\hbar/2}}_{II} \tag{1.38}$$

$$\text{LHS} = -i\hbar\frac{\gamma}{2}e^{-\gamma t/2} \tag{1.39}$$

Lecture 6 (2/10/14)

To evaluate I, we use principal value integral of $1/z$.

$$\frac{1}{z - i\epsilon} = P(\frac{1}{z}) + i\pi\delta(z) \tag{1.40}$$

Pf. Consider contours $c_1 = (-\infty, -\delta) \cup (\delta, \infty)$ and c_2 lower half circle around 0 with radius δ. Choosing lower half because as $\epsilon \to 0$, it will not touch c_2. Consider a function $f(z)$ analytic on c_1, c_2. The contour integral of c_2 is $z = \delta e^{i\phi}$,

$\phi \in [\pi, 2\pi]$, $dz = i\delta e^{i\phi} d\phi$

$$\begin{aligned}
\lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} \frac{f(z)}{z - i\epsilon} &= \lim_{\delta \to 0} \underbrace{\left(\int_{-\infty}^{-\delta} \frac{f(z)}{z} dz + \int_{\delta}^{\infty} \frac{f(z)}{z} dz \right)}_{\equiv P(\frac{f(z)}{z})} + f(0) \int_{\pi}^{2\pi} \frac{i\delta e^{i\phi} d\phi}{\delta e^{i\phi}} \\
&= P(\frac{f(z)}{z}) + i\pi f(0)
\end{aligned}$$

where

$$P(\frac{1}{z}) \text{ is also a distribution function like } \delta\text{,it means } \int_{-\infty}^{\infty} P(\frac{1}{z}) f(z) = P(\frac{f(z)}{z})$$

Hence we proved (1.40).

As $\gamma \to 0$, I in (1.38) is

$$I = P\left(\sum_{\vec{p}} |V_{\vec{p}d}|^2 \frac{e^{-\gamma t/2}}{E_d - E_{\vec{p}}} \right) + i\pi \sum_{\vec{p}} |V_{\vec{p}d}|^2 e^{-\gamma t/2} \delta(E_d - E_{\vec{p}})$$

The first term on the right looks like a 2nd order perturbation energy.

To evaluate II in (1.38), we use Jordan's lemma. Close the contour lower half plane, enclosing pole

$$E_{\vec{p}} = E_d - i\gamma\hbar/2$$

then

$$II \sim \sum_{\vec{p}} |V_{\vec{p}d}|^2 e^{-\gamma t/2} (-2\pi i)$$

this expression assumes $V_{\vec{p}d}$ is constant. Actually we add δ to above

$$II = \sum_{\vec{p}} |V_{\vec{p}d}|^2 e^{-\gamma t/2} (-2\pi i) \delta(E_d - E_{\vec{p}})$$

to enforce that $V_{\vec{p}d}$ is evaluated at the pole $E_{\vec{p}} = E_d - i\gamma\hbar/2$ where $\gamma \to 0$, called narrow width approximation.

Thus (1.39) = (1.38) gives

$$\frac{\gamma}{2} = \frac{i}{\hbar} P \left(\sum_{\vec{p}} |V_{\vec{p}d}|^2 \frac{1}{E_d - E_{\vec{p}}} \right) + \frac{\pi}{\hbar} \sum_{\vec{p}} |V_{\vec{p}d}|^2 \, \delta(E_d - E_{\vec{p}})$$

so γ has real and imaginary parts

$$\Re(\gamma) = \frac{2\pi}{\hbar} \sum_{\vec{p}} |V_{\vec{p}d}|^2 \, \delta(E_d - E_{\vec{p}})$$

which is Fermi golden rule.

$$\Im(\frac{\gamma}{2}) = \frac{1}{\hbar} P \left(\sum_{\vec{p}} \frac{|V_{\vec{p}d}|^2}{E_d - E_{\vec{p}}} \right) = \frac{\Delta E_d^{(2)}}{\hbar}$$

$\Delta E_d^{(2)}$ second energy shift. This imaginary decay rate is special to QM.

One can show that probability is conserved, i.e.

prob in one of the final state $|\vec{p}\rangle$ = 1−prob remaining in $|d\rangle$

We will use Fermi golden rule to do many problems later.

1.8 Heavy Ion Moving Through Matter

Semiclassical Treatment

First consider a heavy ion $Q = Ze$, mass M, coulomb interacting with and scattered by an atom in the matter which has Z' bound electrons circulating around the nuclei. Suppose the atom sitting at the origin and the heavy ion comes in with $\vec{v} = v\hat{x}$, and impact parameter b. Later we will assume the matter is uniformly distributed so we will integrate over b.

The momentum transfer due to the scattering, i.e. the recoil momentum the atom gained, is

$$\Delta p = \int_{-\infty}^{\infty} F(t) dt$$

F is coulomb force. The energy transfer is

$$\Delta E = \frac{(\Delta p)^2}{2m}$$

so most ΔE goes to the electrons. Also assume $\vec{v}$ is very fast compare to the e^- motion, so Q is zipping by before e^- begins to move. Since the problem has symmetry, net momentum transfer occurs only in z direction

$$\Delta p_z = \int_{-\infty}^{\infty} F_z(t)dt = \int_{-\infty}^{\infty} \frac{Ze^2}{(vt)^2 + b^2} \frac{b}{\sqrt{(vt)^2 + b^2}} dt$$

where t in the integral is initialized as when Q is right above the origin at $(0, b)$, $t = 0$.

$$\Delta p_z = Ze^2 b \int_{-\infty}^{\infty} \frac{dt}{((vt)^2 + b^2)^{3/2}}$$

set $y = vt/b$

$$\Delta p_z = \frac{Ze^2}{vb} \int_{-\infty}^{\infty} \frac{dy}{(y^2 + 1)^{3/2}} = \frac{2Ze^2}{vb} \tag{1.41}$$

which is the net momentum transfer to one e^-.

How accurate is this approximation? We need to examine the biggest simplification we made, that e^- does not change orbital motion during the collision.

$$\tau_{collision} \sim \frac{b}{v}$$

so e^- moves vertically

$$\Delta z = \frac{\Delta p_z}{m} \tau_{collision} = \frac{2Ze^2}{v^2 m}$$

we want $\Delta z \ll b$. But this does not have to be the case, since we are going to integrating all b.

Now semiclassical (mix of classical and qm) argument comes in, we say by uncertainty, we don't know exactly where the e^- is; we know it is in radius a_0. Likewise we say there is lower bound for impact parameter b

$$b > b_{min} = a_0$$

so as long as

$$\frac{\hbar^2}{me^2} = a_0 \gg \frac{2Ze^2}{v^2 m}$$

Recall speed of e^- orbiting is

$$v_{e^-} = \alpha c = \frac{e^2}{\hbar c} c$$

hence

$$v^2 \gg \frac{2Ze^4}{\hbar^2} = 2Z(v_{e^-})^2 \tag{1.42}$$

Hence if the impact speed $v \gg v_{e^-}$, the semiclassical result (1.41) is valid. There is another way to get a little stronger condition than (1.42). By Broglie, the wavelength of e^- associate with the momentum transfer

$$b_{min} = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{mv} \gg \Delta z = \frac{2Ze^2}{v^2 m} \tag{1.43}$$

$$v \gg \frac{\pi Z e^2}{\hbar} \text{ or } v^2 \gg \frac{\pi^2 Z^2 e^4}{\hbar^2} \tag{1.44}$$

Now a ∞ large slab of matter with thickness Δl, Q passes through the slab with $\vec{v}$ perpendicularly enters the slab. The impact parameter b makes a ring

$$\Delta E = \int_{b_{min}}^{\infty} (2\pi b db \Delta l)\eta Z' \frac{(\Delta p_z)^2}{2m}$$

η density of atoms in the matter. By (1.41)

$$\frac{\Delta E}{\Delta l} = \frac{Z'\pi n}{m} \int_{b_{min}}^{\infty} bdb \frac{4Z^2 e^4}{v^2 b^2} = \frac{4\pi\eta Z' Z^2 e^4}{mv^2} \ln \frac{b_{max}}{b_{min}}$$

From (1.43), $b_{min} = \hbar/mv$, we will get $b_{max} = v/w_{atom}$ from quantum mechanical treatment, adiabatic approximation, below, and w_{atom} is atomic frequency. Because we will show we will need

$$\tau_{collision} \gg w_{atom} \text{ or } \frac{b_{max}}{v} \gg \frac{1}{w_{atom}}$$

thus the energy transfer per unit length

$$\frac{\Delta E}{\Delta l} = \frac{4\pi\eta Z' Z^2 e^4}{mv^2} \ln \frac{mv^2}{\hbar w_{atom}} \tag{1.45}$$

Quantum Mechanical Treatment

Lecture 7 (2/12/14)

We will compute integral of some wave functions, so we need to set up coordinates. Put nuclei at (X, Y, Z). The ith e^-'s position is (x_i, y_i, z_i) with respect to the nuclei. Ion's coming in with position $(vt, 0, 0)$. The potential of the interaction

$$V = \sum_{i=1}^{Z'} \frac{Ze^2}{\sqrt{(X - vt + x_i)^2 + (Y + y_i)^2 + (Z + z_i)^2}}$$

t is initialized as before, i.e. $t = 0$, $X = 0$. And put $vt = \tilde{x}$, thus

$$V = \sum_{i=1}^{Z'} \frac{Ze^2}{\sqrt{(\tilde{x} - x_i)^2 + (Y + y_i)^2 + (Z + z_i)^2}}$$

By (1.19) first order perturbation, the probability of transition of the atom from ground state $|0\rangle$ to state $|n\rangle$ due to the interaction is

$$\begin{aligned} P_{0\to n} &= |\langle n|\Phi(t)\rangle|^2 = \left| -\frac{iZe^2}{\hbar} \int_{-\infty}^{\infty} dt \sum_{i=1}^{Z'} \left\langle n \middle| \frac{e^{-i(E_0-E_n)t/\hbar}}{\sqrt{(\tilde{x} - x_i)^2 + (Y + y_i)^2 + (Z + z_i)^2}} \middle| 0 \right\rangle \right|^2 \\ &= \left| -\frac{iZe^2}{v\hbar} \underbrace{\int_{-\infty}^{\infty} d\tilde{x} \sum_{i=1}^{Z'} \left\langle n \middle| \frac{e^{-i(E_0-E_n)\tilde{x}/v\hbar}}{\sqrt{(\tilde{x} - x_i)^2 + (Y + y_i)^2 + (Z + z_i)^2}} \middle| 0 \right\rangle}_{:=F(Y,Z)} \right|^2 \end{aligned} \tag{1.46}$$

and the energy transfer per unit length, or energy gained per unit length

$$\frac{dE}{dl} = \eta \int dY dZ \sum_n (E_n - E_0) P_{0\to n} \tag{1.47}$$

Recall Parseval identity

$$\int dY dZ |F(Y,Z)|^2 = \int d^2 q_\perp |\tilde{F}(q_\perp)|^2 = \frac{1}{2\pi}\int d^2 q_\perp \left| \int dY dZ e^{-iq_y Y - iq_z Z} F(Y,Z)\right|^2$$

Let

$$\vec{q}_\perp = (0, q_y, q_z)$$

i.e. conjugate momentum of the nuclei, which is also the conjugate momentum of the e^-s, because e^-'s positions are labeled using the relative coordinate.

Combine (1.47), (1.46), using Parseval

$$\begin{aligned} \frac{dE}{dl} &= \frac{\eta Z^2 e^4}{v^2 \hbar^2} \sum_n (E_n - E_0) \frac{1}{2\pi} \int d^2 q_\perp \\ & \left| \underbrace{\int \frac{dY dZ}{2\pi} \int_{-\infty}^{\infty} d\tilde{x} \sum_{i=1}^{Z'} \left\langle n \left| \frac{e^{-i(E_0 - E_n)\tilde{x}/v\hbar - iq_y Y - iq_z Z}}{\sqrt{(\tilde{x}-x_i)^2 + (Y+y_i)^2 + (Z+z_i)^2}} \right| 0 \right\rangle}_{:=F(\vec{q}_n)} \right|^2 \end{aligned} \tag{1.48}$$

Let

$$\vec{q}_n = (\frac{E_n - E_0}{v\hbar}, q_y, q_z) \tag{1.49}$$
$$\vec{r}_i = (x_i, y_i, z_i)$$

put $\tilde{x} = -X$,

$$\begin{aligned} F(\vec{q}_n) &= \int d^3\vec{r} \frac{1}{2\pi} \sum_{i=1}^{Z'} \left\langle n \left| \frac{e^{-i\vec{q}_n \cdot \vec{r}}}{|\vec{r} + \vec{r}_i|} \right| 0 \right\rangle \\ &= \int d^3\vec{r} \frac{1}{2\pi} \sum_{i=1}^{Z'} \left\langle n \left| \frac{e^{-i\vec{q}_n \cdot (\vec{r} + \vec{r}_i)}}{|\vec{r} + \vec{r}_i|} e^{i\vec{q}_n \cdot \vec{r}_i} \right| 0 \right\rangle \end{aligned}$$

Recall

$$\int d^3 r \frac{e^{-i\vec{q}\cdot\vec{r}}}{|\vec{r}|} = \frac{4\pi}{q^2}$$

Pf

$$\int d^3\vec{r}\frac{e^{-i\vec{q}\cdot\vec{r}}}{|\vec{r}|}q^2 = \int d^3\vec{r}e^{-i\vec{q}\cdot\vec{r}}\underbrace{\nabla^2\frac{1}{|\vec{r}|}}_{4\pi\delta^3(\vec{r})} = 4\pi$$

Therefore (1.48) becomes

$$\begin{aligned}\frac{dE}{dl} &= \frac{\eta Z^2e^4}{v^2\hbar^2}\sum_n(E_n-E_0)\int d^2q_\perp\left|\sum_{i=1}^{Z'}\left\langle n\middle|2\frac{e^{i\vec{q}_n\cdot\vec{r}_i}}{q_n^2}\middle|0\right\rangle\right|^2 \\ &= \frac{4\eta Z^2e^4}{v^2\hbar^2}\sum_n(E_n-E_0)\int d^2q_\perp\sum_{i,j=1}^{Z'}\frac{1}{q_n^4}\left\langle 0\middle|e^{-i\vec{q}_n\cdot\vec{r}_i}\middle|n\right\rangle\left\langle n\middle|e^{i\vec{q}_n\cdot\vec{r}_j}\middle|0\right\rangle\end{aligned} \tag{1.50}$$

From definition of q_n (1.49), q_n^2 depends on n. This makes things complicated. We divide the integral to two regions

$$\int d^2q_\perp = \int_{\mathrm{I}} d^2q_\perp + \int_{\mathrm{II}} d^2q_\perp$$

There is a $\bar{q}$ that separates two regions

Region I

$$0 \le q_\perp \le \bar{q}$$

Region II

$$\bar{q} \le q_\perp$$

What should be $\bar{q}$? As we will see, we want

$$\frac{Z'e^2m}{\hbar^2} \ll \bar{q} \ll \frac{mv}{\hbar} \tag{1.51}$$

For region II, we suppose that $q_\perp$ is so high that e^- leaves the atom, so

$$w_{n0}\hbar = E_n - E_0 \approx E_n = \frac{\hbar^2q_n^2}{2m} \tag{1.52}$$

this also defines w_{n0}. And

$$E_n \text{ is almost the ionization energy} \tag{1.53}$$

Since

$$q_n = (\frac{w_{n0}}{v}, q_y, q_z)$$

(1.52) implies

$$w_{n0} = \frac{\hbar}{2m}[q_\perp^2 + (\frac{w_{n0}}{v})^2]$$

or

$$(\frac{w_{n0}}{v})^2 - \frac{2mv}{\hbar}(\frac{w_{n0}}{v}) + q_\perp^2 = 0$$

so

$$q_x = \frac{w_{n0}}{v} = \frac{mv}{\hbar} \pm \sqrt{\frac{m^2v^2}{\hbar^2} - q_\perp^2} := \frac{w_\pm}{v} \tag{1.54}$$

this relates w_n to $q_\perp$. Now we see why we enforce (1.51), so that the square root is positive. So in region II

$$\left(\frac{dE}{dl}\right)_{\text{II}} = \frac{4\eta Z^2 e^4}{v^2\hbar^2} \int_{\text{II}} d^2 q_\perp \left(\frac{\hbar w_+}{q_+^4} + \frac{\hbar w_-}{q_-^4}\right) \sum_{i,j=1}^{Z'} \sum_n \left\langle 0 \middle| e^{-i\vec{q}_n\cdot\vec{r}_i} \middle| n \right\rangle \left\langle n \middle| e^{i\vec{q}_n\cdot\vec{r}_j} \middle| 0 \right\rangle$$

By (1.53), we further assume that $\vec{q}_n$ in the bracket is independent of n, so

$$\left(\frac{dE}{dl}\right)_{\text{II}} = \frac{4\eta Z^2 e^4}{v^2\hbar^2} \int_{\bar{q}}^{\frac{mw}{\hbar}} \underbrace{d^2 q_\perp}_{2\pi q_\perp dq_\perp} \left(\frac{\hbar w_+}{q_+^4} + \frac{\hbar w_-}{q_-^4}\right) \underbrace{\sum_{i,j=1}^{Z'} \left\langle 0 \middle| e^{-i\vec{q}_\pm\cdot(\vec{r}_i - \vec{r}_j)} \middle| 0 \right\rangle}_{Z'}$$

the sum is non-zero only when $\vec{r}_i = \vec{r}_j$.

$$\frac{\hbar w_+}{q_+^4} = \frac{\frac{\hbar^2 q_\pm^2}{2m}}{q_+^4} = \frac{\hbar^2}{2m} \frac{1}{q_\perp^2 + \left(\frac{mv}{\hbar} + \sqrt{\frac{m^2v^2}{\hbar^2} - q_\perp^2}\right)^2}$$

so

$$\left(\frac{dE}{dl}\right)_{\text{II}} = \frac{4\pi\eta Z' Z^2 e^4}{v^2 m}\int_{\bar{q}}^{\frac{mw}{\hbar}} q_\perp dq_\perp \underbrace{\frac{1}{q_\perp^2+\left(\frac{mv}{\hbar}+\sqrt{\frac{m^2v^2}{\hbar^2}-q_\perp^2}\right)^2}+\frac{1}{q_\perp^2+\left(\frac{mv}{\hbar}-\sqrt{\frac{m^2v^2}{\hbar^2}-q_\perp^2}\right)^2}}_{\frac{1}{q_\perp^2}}$$

$$= \frac{4\pi\eta Z' Z^2 e^4}{v^2 m}\ln\frac{mv}{\hbar\bar{q}} \tag{1.55}$$

Lecture 8 (2/17/14)

Now study region I. We have

$$q_\perp \le \bar{q} \ll \frac{mv}{\hbar} \tag{1.56}$$

there are two probabilities. Case 1: suppose $q_\perp$ is large enough to ionize the atoms. We have (1.54)

$$q_{x\pm} = \frac{mv}{\hbar} \pm \sqrt{\frac{m^2v^2}{\hbar^2}-q_\perp^2}$$

Using (1.56),

$$q_{x-} = \frac{1}{2}q_\perp^2\frac{\hbar}{mv} \sim q_\perp\frac{q_\perp}{\frac{mv}{\hbar}} \ll q_\perp$$

$$q_{x+} = 2\frac{mv}{\hbar} \gg q_\perp$$

this is kind of head on collision, so deflection angle is very small.

Case 2: if the atom is not ionized, then by (1.51)

$$q_x = \frac{E_n - E_0}{\hbar v} = \frac{Z'^2 m e^4}{2\hbar^2}\left(1-\frac{1}{n^2}\right)\frac{1}{\hbar v} \sim \underbrace{\frac{Z'e^2}{\hbar}\frac{1}{v}}_{\ll 1}\underbrace{\frac{Z'e^2 m}{\hbar^2}}_{\le q_\perp} \ll q_\perp$$

now we understand why we put a lower bound in (1.51), and the condition

$$\frac{Z'e^2}{\hbar} \ll v$$

agrees semiclassical condition (1.44).

Therefore we can divide region I into two subregions I_a and I_b depending on whether $q_x \gg q_\perp$ or $q_x \ll q_\perp$ respectively.

Let $\bar{q}'$ be the separation

$$0 \leq q_{\perp a} \leq \bar{q}' \leq q_{\perp b} \leq \bar{q}$$

so

$$q_x \ll \bar{q}' \tag{1.57}$$

In region I_b we can neglect q_x to $q_\perp$i.e. $q_\perp \approx q_n$; in region I_a we use the dipole approximation.

So (1.50) gives

$$\left(\frac{dE}{dl}\right)_{\mathrm{I}_b} = \frac{4\eta Z^2 e^4}{v^2\hbar^2} \int d^2 q_\perp \frac{1}{q_\perp^4} \underbrace{\sum_n (E_n - E_0) \sum_{i=1}^{Z'} \left|\left\langle n \middle| e^{i\vec{q}_\perp \cdot \vec{r}_i} \middle| 0 \right\rangle\right|^2}_{=M}$$

$$\begin{aligned}
M &= \sum_n (\langle n|H|n\rangle - E_0) \sum_{i=1}^{Z'} \left|\left\langle n \middle| e^{i\vec{q}_\perp \cdot \vec{r}_i} \middle| 0 \right\rangle\right|^2 \\
&= \sum_{i,j} \left\langle 0 \middle| e^{-i\vec{q}_\perp \cdot \vec{r}_j} H e^{i\vec{q}_\perp \cdot \vec{r}_i} \middle| 0 \right\rangle - \sum_{i,j} \left\langle 0 \middle| E_0 e^{-i\vec{q}_\perp \cdot \vec{r}_j} e^{i\vec{q}_\perp \cdot \vec{r}_i} \middle| 0 \right\rangle \\
&= \frac{1}{2} \sum_{i,j} \left\langle 0 \middle| \left\{ e^{-i\vec{q}_\perp \cdot \vec{r}_j} \left(H e^{i\vec{q}_\perp \cdot \vec{r}_i} - e^{i\vec{q}_\perp \cdot \vec{r}_i} H \right) + \left(e^{-i\vec{q}_\perp \cdot \vec{r}_j} H - H e^{-i\vec{q}_\perp \cdot \vec{r}_j} \right) e^{i\vec{q}_\perp \cdot \vec{r}_i} \right\} \middle| 0 \right\rangle
\end{aligned}$$

$$H = \sum_i \frac{p_i^2}{2m} - \frac{Z' e^2}{|\vec{r}_i|}$$

ignoring $\frac{Z'e^2}{|\vec{r}|}$ because it commutes with $e^{i\vec{q}_\perp \cdot \vec{r}}$, hence cancel. So

$$\begin{aligned}
\left[H, e^{i\vec{q}_\perp \cdot \vec{r}_i}\right] f(\vec{r}_i) &= \frac{\hbar^2 \vec{q}_\perp^2}{2m} e^{i\vec{q}_\perp \cdot \vec{r}_i} f + 2i\vec{q}_\perp \hbar \frac{1}{2m} f' e^{i\vec{q}_\perp \cdot \vec{r}_i} \\
&= e^{i\vec{q}_\perp \cdot \vec{r}_i} \left(\frac{\hbar^2 \vec{q}_\perp^2}{2m} - \frac{2\vec{q}_\perp \cdot \vec{p}_i}{2m} \right) f(\vec{r}_i)
\end{aligned}$$

so

$$
\begin{aligned}
M &= \frac{1}{2}\sum_{i,j}\left\langle 0\left| e^{-i\vec{q}_\perp\cdot(\vec{r}_j-\vec{r}_i)}\left(\frac{\hbar^2\vec{q}_\perp^2}{2m}-\frac{2\vec{q}_\perp\cdot\vec{p}_i}{2m}\right)-e^{-i\vec{q}_\perp\cdot\vec{r}_j}\left(\frac{\hbar^2\vec{q}_\perp^2}{2m}+\frac{2\vec{q}_\perp\cdot\vec{p}_j}{2m}\right)e^{i\vec{q}_\perp\cdot\vec{r}_i}\right|0\right\rangle \\
&= \frac{1}{2}\sum_{i,j}\left\langle 0\left| -e^{-i\vec{q}_\perp\cdot(\vec{r}_j-\vec{r}_i)}\frac{2\vec{q}_\perp\cdot\vec{p}_i}{2m}-e^{-i\vec{q}_\perp\cdot\vec{r}_j}\frac{2\vec{q}_\perp\cdot\vec{p}_j}{2m}e^{i\vec{q}_\perp\cdot\vec{r}_i}\right|0\right\rangle \\
&= \frac{1}{2}\left\langle 0\left| -\sum_{i\neq j}\underbrace{e^{-i\vec{q}_\perp\cdot(\vec{r}_j-\vec{r}_i)}\frac{2\vec{q}_\perp\cdot(\vec{p}_i+\vec{p}_j)}{2m}}_{M_1}+\sum_{i=j}\left(\underbrace{-\frac{2\vec{q}_\perp\cdot\vec{p}_i}{2m}}_{M_2}+\frac{2\hbar^2\vec{q}_\perp^2}{2m}\right)\right|0\right\rangle
\end{aligned}
$$

M_1 gives 0, because it is odd in the integration over $\vec{q}_\perp$, because $\vec{q}_\perp\cdot(\vec{p}_i+\vec{p}_j)$ is odd, and $e^{-i\vec{q}_\perp\cdot(\vec{r}_j-\vec{r}_i)}$ is even if we exchange $\vec{r}_j\leftrightarrow\vec{r}_i$, when $\vec{q}_\perp\to-\vec{q}_\perp$. Likewise M_2 gives 0. Therefore

$$
\left(\frac{dE}{dl}\right)_{\mathrm{I}_b}=\frac{4\eta Z^2e^4}{v^2\hbar^2}\int_{\bar{q}'}^{\bar{q}}d^2q_\perp\frac{1}{q_\perp^4}\frac{1}{2}Z'\frac{\hbar^2\vec{q}_\perp^2}{m}=\frac{4\pi\eta Z'Z^2e^4}{v^2m}\ln\frac{\bar{q}}{\bar{q}'} \tag{1.58}
$$

similar result as (1.55).

Lastly we do region I_a. Using dipole, (1.50) gives

$$
\left(\frac{dE}{dl}\right)_{\mathrm{I}_a} = \frac{4\eta Z^2e^4}{v^2\hbar^2}\int d^2q_\perp\frac{1}{q_n^4}\sum_n(E_n-E_0)\sum_{i,j=1}^{Z'}\underbrace{\langle 0|\vec{q}_n\cdot\vec{r}_j|n\rangle\langle n|\vec{q}_n\cdot\vec{r}_i|0\rangle}_{q_n^2\sum_{i,j}\langle 0|\vec{r}_j|n\rangle\langle n|\vec{r}_i|0\rangle}
$$

Define the oscillator strength for the state $|n\rangle$

$$
f_n=\frac{2m}{3\hbar^2}(E_n-E_0)\sum_{i,j}\langle 0|\vec{r}_j|n\rangle\langle n|\vec{r}_i|0\rangle \tag{1.59}
$$

$$
\begin{aligned}
\left(\frac{dE}{dl}\right)_{\mathrm{I}_a} &= \frac{4\pi\eta Z^2 e^4}{v^2 m}\sum_n \int_0^{\bar{q}'} q_\perp dq_\perp \frac{1}{q_n^2} f_n \\
&= \frac{4\pi\eta Z^2 e^4}{v^2 m}\sum_n f_n \int_0^{\bar{q}'} dq_\perp \frac{q_\perp}{q_\perp^2 + (\frac{E_n - E_0}{\hbar v})^2} \\
&= \frac{4\pi\eta Z^2 e^4}{v^2 m}\sum_n f_n \ln \sqrt{1 + \left(\frac{\bar{q}'}{\frac{E_n - E_0}{\hbar v}}\right)^2}
\end{aligned}
$$

By (1.57)

$$
\left(\frac{dE}{dl}\right)_{\mathrm{I}_a} = \frac{4\pi\eta Z^2 e^4}{v^2 m}\sum_n f_n \ln \frac{\bar{q}'}{\frac{E_n - E_0}{\hbar v}}
$$

To go further, we have to compute f_n. Luckily f_n has a nice property

$$
\sum_n f_n = Z'
$$

called Thomas-Reiche-Kuhn sum rule. We will study this more when we study photon decay.

So we define an average atomic frequency

$$
w_{atom} = \frac{\overline{E_n - E_0}}{\hbar} \tag{1.60}
$$

such that

$$
\sum_n f_n \ln \frac{E_n - E_0}{\hbar} = Z' \ln w_{atom}
$$

so

$$
\left(\frac{dE}{dl}\right)_{\mathrm{I}_a} = \frac{4\pi\eta Z' Z^2 e^4}{v^2 m} \ln \frac{v\bar{q}'}{w_{atom}} \tag{1.61}
$$

Therefore combining (1.55), (1.58), and (1.61)

$$
\frac{dE}{dl} = \frac{4\pi\eta Z' Z^2 e^4}{v^2 m}\left(\ln \frac{mv}{\hbar\bar{q}} + \ln \frac{\bar{q}}{\bar{q}'} + \ln \frac{v\bar{q}'}{\bar{w}}\right) = \frac{4\pi\eta Z' Z^2 e^4}{v^2 m} \ln \frac{mv^2}{\hbar w_{atom}}
$$

agrees the semiclassical result (1.45).

2 Identical Particles

2.1 Spin Statistics

Lecture 9 (2/19/14)

The concept of identical particles is intrinsically quantum mechanic. Classical particles can be traced as the system evolves, because they are distinguishable. Quantum mechanically all e^-s are the same.

If we have a quantum state $\psi(\vec{r}_1, m_1, \vec{r}_2, m_2)$ which describes particles with identical characteristics then we can consider an exchange operator P_{12} defined as

$$P_{12}\psi = \psi(\vec{r}_2, m_2, \vec{r}_1, m_1)$$

m is another label e.g. spin in z direction.

$$1\&2 \text{ being identical} \iff [O, P_{12}] = 0 \text{ for each operator } O$$

in particular

$$[H, P_{12}] = 0 \tag{2.1}$$

thus we can work with eigenstates of P_{12}.

Theorem. *In nature all particles with integer spin (Boson) have $P_{12} = +1$; all particles with half integer spin (Fermion) have $P_{12} = -1$.*

This is consequence of qft, positivity, and local character action.

For example, for 2 Bosons, if we have a wave function

$$\psi(\vec{r}_1, \vec{r}_2)$$

but

$$\psi(\vec{r}_1, \vec{r}_2) \neq \psi(\vec{r}_2, \vec{r}_1)$$

We have to symmetrize it

$$\psi_s = N(\psi(\vec{r}_1, \vec{r}_2) + \psi(\vec{r}_2, \vec{r}_1))$$

and N is found by

$$1 = |N|^2 \left(2 + 2\Re \underbrace{\int d\vec{r}_1 d\vec{r}_2 \psi^*(\vec{r}_1, \vec{r}_2)\psi(\vec{r}_2, \vec{r}_1)}_{\text{exchange term}} \right)$$

The one of the real physical effect of symmetrization is that it changes energy. Suppose we have a potential because of (2.1)

$$V(\vec{r}_1, \vec{r}_2) = V(\vec{r}_2, \vec{r}_1)$$

then

$$\langle \psi_s | V | \psi_s \rangle = |N|^2 \left(2 \int d\vec{r}_1 d\vec{r}_2 |\psi|^2 V + 2\Re \underbrace{\int d\vec{r}_1 d\vec{r}_2 \psi^*(\vec{r}_1, \vec{r}_2) V(\vec{r}_1, \vec{r}_2) \psi(\vec{r}_2, \vec{r}_1)}_{\text{exchange energy}} \right)$$

Clearly if $\psi^*(\vec{r}_1, \vec{r}_2)$ and $\psi(\vec{r}_2, \vec{r}_1)$ have no overlap, i.e. $\psi(\vec{r}_1, \vec{r}_2)$ is non-zero on $\vec{r}_1 \in R_1, \vec{r}_2 \in R_2$ and $R_1 \cap R_2$, then symmetrization has no effect. If the number of indistinguishable particles is larger than 2, the symmetrization becomes headache. However there is a nice formulation: second quantization. We'll show they have similar structure as SHO whose occupation number is analogous to the number of photons in each mode. Fermion is a lot harder than Bosons, because of the nightmare minus sign.

2.2 Bosons

Consider states formed of products of single particle wave functions. Introduce an ordered basis of single particle states

$$\{\psi_k(\vec{r}, m)\}_{k=1}^{\infty}$$

such that

$$\sum_{m=-j}^{j}\int d^3r\psi_k^*\psi_{k'} = \delta_{kk'} \tag{2.2}$$

and construct N-particle state as

$$\Psi(\vec{r}_1, m_1, ..., \vec{r}_N, m_N) = \prod_{i=1}^{N}\psi_{k_i}(\vec{r}_i, m_i)$$

and

$$\psi_{k_i} \in \{\psi_k(\vec{r}, m)\}_{k=1}^{\infty}$$

Clearly $\langle\Psi|\Psi\rangle = 1$. We should symmetrize it, which can be done by summing over all permutations of the arguments (don't change the order of the basis)

$$\Psi_s(\vec{r}_1, m_1, ..., \vec{r}_N, m_N) = \eta\sum_{\{\sigma\}}\psi_{k_1}(\vec{r}_{\sigma_1}, m_{\sigma_1})\cdot ... \cdot\psi_{k_N}(\vec{r}_{\sigma_N}, m_{\sigma_N}) \tag{2.3}$$

σ is a bijection from $\{1, 2, ..., N\}$ to $\{1, 2, ..., N\}$. E.g. $N = 3$, there are $3! = 6$ permutations

σ_1	σ_2	σ_3
1	2	3
1	3	2
2	1	3
2	3	1
3	1	2
3	2	1

Find normalization η

$$\begin{aligned}\langle\Psi_s|\Psi_s\rangle &= \eta^2\left(\int d^3r_1 ... \int d^3r_N\sum_{m_1} ... \sum_{m_N}\right)\left(\sum_{\{\sigma'\}}\psi_{k_1}(\vec{r}_{\sigma'_1}, m_{\sigma'_1})\cdot ... \cdot\psi_{k_N}(\vec{r}_{\sigma'_N}, m_{\sigma'_N})\right) \\ &\quad \left(\sum_{\{\sigma\}}\psi_{k_1}(\vec{r}_{\sigma_1}, m_{\sigma_1})\cdot ... \cdot\psi_{k_N}(\vec{r}_{\sigma_N}, m_{\sigma_N})\right)\end{aligned}$$

If all k_i's are distinct, e.g.

$$
\begin{aligned}
\Psi_s &= \psi_1(x_1)\psi_2(x_2)\psi_3(x_3) + \psi_1(x_1)\psi_2(x_3)\psi_3(x_2) + \psi_1(x_2)\psi_2(x_1)\psi_3(x_3) \\
&\quad + \psi_1(x_2)\psi_2(x_3)\psi_3(x_1) + \psi_1(x_3)\psi_2(x_1)\psi_3(x_2) + \psi_1(x_3)\psi_2(x_2)\psi_3(x_1)
\end{aligned} \tag{2.4}
$$

By (2.2)

$$\langle \Psi_s | \Psi_s \rangle = \eta^2 N!$$

In general let n_k be the number of times the state ψ_k appears in the product (2.3), e.g.

$$
\begin{aligned}
\Psi_s &= \psi_1(x_1)\psi_2(x_2)\psi_2(x_3) + \psi_1(x_1)\psi_2(x_3)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\psi_2(x_3) \\
&\quad + \psi_1(x_2)\psi_2(x_3)\psi_2(x_1) + \psi_1(x_3)\psi_2(x_1)\psi_2(x_2) + \psi_1(x_3)\psi_2(x_2)\psi_2(x_1) \\
&= 2\left(\psi_1(x_1)\psi_2(x_2)\psi_2(x_3) + \psi_1(x_2)\psi_2(x_1)\psi_2(x_3) + \psi_1(x_3)\psi_2(x_1)\psi_2(x_2)\right)
\end{aligned} \tag{2.5}
$$

By (2.2)

$$\langle \Psi_s | \Psi_s \rangle = \eta^2 N! \prod_k (n_k!)$$

n_k is called the occupation number of the state ψ_k. So a better way to label $\Psi_s(\vec{r}_1, m_1, ..., \vec{r}_N, m_N)$ in (2.3),

$$|n_1, n_2, ..., n_k, ...\rangle = \frac{1}{\sqrt{N! \prod_k (n_k!)}} \sum_{\{\sigma\}} \psi_{k_1}(\vec{r}_{\sigma_1}, m_{\sigma_1}) \cdot ... \cdot \psi_{k_N}(\vec{r}_{\sigma_N}, m_{\sigma_N}) \tag{2.6}$$

we choose the phase of η to be 1 by choice. $n_1, n_2, ..., n_k, ...$ are the occupation numbers of all elements in the basis, so many of the $n_1, n_2, ..., n_k, ...$ are 0, and by convention $0! = 1$, and

$$\sum n_k = N$$

those wavefunction with non-zero occupation numbers appear on the right of (2.6). They appear in the same order in the basis with the multiplicities n_k. So the permutation σ only permutes finitely many terms.

2.3 Free Theory & Second Quantization

Now consider a non-interacting potential

$$V_N(\vec{r}_1, ..., \vec{r}_N) = \sum_{i=1}^{N} V(\vec{r}_i) \tag{2.7}$$

We would like to find the matrix element of it, because of perturbation,

$$\begin{aligned}\langle n_1', n_2', ..., n_k', ...|V_N|n_1, n_2, ..., n_k, ...\rangle &= \prod_{l=1}^{N}\left\{\int d^3r_l \sum_{m_l=-j}^{j}\right\}\frac{1}{N!\prod_k(n_k!)} \qquad (2.8)\\ &\left(\sum_{\{\sigma'\}}\psi_{k_1}^*(\vec{r}_{\sigma_1'}, m_{\sigma_1'})\cdot ... \cdot \psi_{k_N}^*(\vec{r}_{\sigma_N'}, m_{\sigma_N'})\right)\\ &\left(\sum_{i=1}^{N} V(\vec{r}_i)\right)\left(\sum_{\{\sigma\}}\psi_{k_1}(\vec{r}_{\sigma_1}, m_{\sigma_1})\cdot ... \cdot \psi_{k_N}(\vec{r}_{\sigma_N}, m_{\sigma_N})\right)\end{aligned}$$

Using orthogonality of $\psi_k(\vec{r}, m)$, we first expand the function $V(\vec{r})\psi_k(\vec{r}, m)$ in the basis of $\psi_k(\vec{r}, m)$

$$V(\vec{r})\psi_k(\vec{r}, m) = \sum \psi_{k'}(\vec{r}, m)V_{k'k} \tag{2.9}$$

where $V_{k'k}$ are constants independent of $(\vec{r}, m)$, and are given by

$$V_{k'k} = \langle\psi_{k'}|V|\psi_k\rangle = \int d^3r \sum_m \psi_{k'}^*(\vec{r}, m)V(\vec{r})\psi_k(\vec{r}, m) \tag{2.10}$$

Lecture 10 (2/24/14)

Now we are back to (2.8). The easiest case is when $n_i' = n_i\ \forall i$, e.g. $N = 3$ cf (2.5)

$$|1, 2, 0, 0, ...\rangle = \frac{1}{\sqrt{3}}\left(\psi_1(x_1)\psi_2(x_2)\psi_2(x_3) + \psi_1(x_2)\psi_2(x_1)\psi_2(x_3) + \psi_1(x_3)\psi_2(x_1)\psi_2(x_2)\right)$$

$$
\begin{aligned}
V_N\,|1,2,0,0,...\rangle \;=\; & \frac{1}{\sqrt{3}}\{[\psi_1(x_1)V_{11}+\psi_2(x_1)V_{21}+\psi_3(x_1)V_{31}+...]\,\psi_2(x_2)\psi_2(x_3) \\
& +\psi_1(x_1)\,[\psi_1(x_2)V_{12}+\psi_2(x_2)V_{22}+\psi_3(x_2)V_{32}+...]\,\psi_2(x_3) \\
& +\psi_1(x_1)\psi_2(x_2)\,[\psi_1(x_3)V_{12}+\psi_2(x_3)V_{22}+\psi_3(x_3)V_{32}+...] \\
& +[\psi_1(x_2)V_{11}+\psi_2(x_2)V_{21}+\psi_3(x_2)V_{31}+...]\,\psi_2(x_1)\psi_2(x_3) \\
& +\psi_1(x_2)\,[\psi_1(x_1)V_{12}+\psi_2(x_1)V_{22}+\psi_3(x_1)V_{32}+...]\,\psi_2(x_3) \\
& +\psi_1(x_2)\psi_2(x_1)\,[\psi_1(x_3)V_{12}+\psi_2(x_3)V_{22}+\psi_3(x_3)V_{32}+...] \\
& +[\psi_1(x_3)V_{11}+\psi_2(x_3)V_{21}+\psi_3(x_3)V_{31}+...]\,\psi_2(x_1)\psi_2(x_2) \\
& +\psi_1(x_3)\,[\psi_1(x_1)V_{12}+\psi_2(x_1)V_{22}+\psi_3(x_1)V_{32}+...]\,\psi_2(x_2) \\
& +\psi_1(x_3)\psi_2(x_1)\,[\psi_1(x_2)V_{12}+\psi_2(x_2)V_{22}+\psi_3(x_2)V_{32}+...]\}
\end{aligned} \tag{2.11}
$$

Among those terms that have non-zero contributions to $\langle 1,2,0,0,...|V_N|1,2,0,0,...\rangle$ are

$$
\begin{aligned}
V_N\,|1,2,0,0,...\rangle \;\to\; & \frac{1}{\sqrt{3}}\{\psi_1(x_1)V_{11}\psi_2(x_2)\psi_2(x_3) \\
& +\psi_1(x_1)\psi_2(x_2)V_{22}\psi_2(x_3) \\
& +\psi_1(x_1)\psi_2(x_2)\psi_2(x_3)V_{22} \\
& +\psi_1(x_2)V_{11}\psi_2(x_1)\psi_2(x_3) \\
& +\psi_1(x_2)\psi_2(x_1)V_{22}\psi_2(x_3) \\
& +\psi_1(x_2)\psi_2(x_1)\psi_2(x_3)V_{22} \\
& +\psi_1(x_3)V_{11}\psi_2(x_1)\psi_2(x_2) \\
& +\psi_1(x_3)\psi_2(x_1)V_{22}\psi_2(x_2) \\
& +\psi_1(x_3)\psi_2(x_1)\psi_2(x_2)V_{22}\} \\
= \; & \frac{1}{\sqrt{3}}(V_{11}+2V_{22})\,\{\psi_1(x_1)\psi_2(x_2)\psi_2(x_3) \\
& +\psi_1(x_2)\psi_2(x_1)\psi_2(x_3) \\
& +\psi_1(x_3)\psi_2(x_1)\psi_2(x_2)\} \\
= \; & (V_{11}+2V_{22})\,|1,2,0,0,...\rangle
\end{aligned}
$$

so

$$
\langle 1,2,0,0,...|V_N|1,2,0,0,...\rangle = V_{11}+2V_{22}
$$

Suppose we want to find

$$\langle 1,1,1,0,...|V_N|1,2,0,0,...\rangle$$

Among those terms in (2.11) that have non-zero contributions to $\langle 1,1,1,0,...|V_N|1,2,0,0,...\rangle$ are

$$\begin{aligned} V_N\,|1,2,0,0,...\rangle \;\; &\rightarrow \;\; \frac{1}{\sqrt{3}}\{\psi_1(x_1)\psi_3(x_2)V_{32}\psi_2(x_3) \\ &\quad +\psi_1(x_1)\psi_2(x_2)\psi_3(x_3)V_{32} \\ &\quad +\psi_1(x_2)\psi_3(x_1)V_{32}\psi_2(x_3) \\ &\quad +\psi_1(x_2)\psi_2(x_1)\psi_3(x_3)V_{32} \\ &\quad +\psi_1(x_3)\psi_3(x_1)V_{32}\psi_2(x_2) \\ &\quad +\psi_1(x_3)\psi_2(x_1)\psi_3(x_2)V_{32}\} \\ &= \frac{V_{32}}{\sqrt{3}}(2.4) \\ &= \frac{V_{32}}{\sqrt{3}}\sqrt{6}\,|1,1,1,0,...\rangle \end{aligned}$$

thus

$$\langle 1,1,1,0,...|V_N|1,2,0,0,...\rangle = \sqrt{2}V_{32}$$

Clearly from the expansion in (2.11) to see that e.g. if we compute

$$\langle 1,0,2,0,...|V_N|1,2,0,0,...\rangle = 0$$

Therefore in general

$$\langle n_1',n_2',...,n_k',...|V_N|n_1,n_2,...,n_k,...\rangle = \begin{cases} \sum_k^\infty n_k V_{kk} & n_i' = n_i\,\forall i \\ \sqrt{n_l'}\sqrt{n_k}V_{lk} & \begin{matrix} n_l' = n_l+1\; n_k' = n_k-1 \\ n_i' = n_i' \text{ for other } i \neq k,l \end{matrix} \\ 0 & \text{otherwise} \end{cases} \tag{2.12}$$

We want to justify the factor $\sqrt{n_l'}\sqrt{n_k}V_{lk} = \sqrt{n_l'}\frac{n_k}{\sqrt{n_k}}V_{lk}$.

0) the V_{lk} term is the matrix element of the 1 particle potential, not matrix

element of V_N. Also notice that in (2.12), occupation number of k index decreases and occupation number of l index increases. This cannot be switched, i.e. $V_{lk} \neq V_{kl}$ and ultimately as we'll see in (2.13) creation operator is on the left and annihilation operator is on the right.

1) the n_k term counts the number of terms in $\sum_i V(r_i)$ where r_i is an argument of the state $\psi_k(r_i)$

2) the $\sqrt{n_k}$ term is taken out from the normalization $\sqrt{n_k!}$ which becomes extra when $n_k \to n_k - 1$

3) the $\sqrt{n_l'} = \sqrt{n_l + 1}$ term is due to adding the missing $n_l + 1$ into the normalization $\sqrt{n_l!}$ of the new state.

Therefore

$$V_N = \sum_{l,k} a_l^+ V_{lk} a_k \tag{2.13}$$

where a_k, annihilation operator, similar to lowering SHO operator, defined as

$$\langle n_1', n_2', ..., n_k', ...|a_k|n_1, n_2, ..., n_k, ...\rangle = \begin{cases} \sqrt{n_k} & n_k' = n_k - 1 \; n_i' = n_i \; \forall i \neq k \\ 0 & \text{otherwise} \end{cases} \tag{2.14}$$

or

$$a_k \left|n_1, n_2, ..., n_k, ...\right\rangle = \sqrt{n_k} \left|n_1, n_2, ..., n_k - 1, ...\right\rangle \tag{2.15}$$

a_k^+ is a_k hermitian conjugate so

$$\langle n_1', n_2', ..., n_k', ...| \left(a_k \left|n_1, n_2, ..., n_k, ...\right\rangle\right) = \left(a_k^+ \left|n_1', n_2', ..., n_k', ...\right\rangle, \left|n_1, n_2, ..., n_k, ...\right\rangle\right)$$

so

$$a_k^+ \left|n_1, n_2, ..., n_k, ...\right\rangle = \sqrt{n_k + 1} \left|n_1, n_2, ..., n_k + 1, ...\right\rangle \tag{2.16}$$

a_k^+ is called creation operator, similar to raising SHO operator. This analogy will become more clear later. It is equivalent in EM sense to say that counting number of photons in the field.

Using the definitions (2.14), (2.16), one can check that (2.13) is indeed a correct representation of (2.12).

To be more precise, we say that a_k, a_k^+ are defined in Fock space, the direct sum of states with all total number of particles N

$$\mathcal{H}_N = \bigotimes_{i=1}^{N} \mathcal{H}^{\text{1-particle}}$$

where (2.6) lives, then

$$\mathcal{H}_{\text{Fock}} = \bigoplus_{N=1}^{\infty} \mathcal{H}_N$$

More generally if V depends on m, we write (2.13), by (2.10)

$$V_N = \sum_{k'k} a_{k'}^+ \sum_{mm'} \int d^3\vec{r} \psi_{k'}^*(\vec{r}, m') V(\vec{r})_{m'm} \psi_k(\vec{r}, m) a_k$$

Define

$$\Psi(\vec{r}, m) = \sum_k \psi_k(\vec{r}, m) a_k \tag{2.17}$$

which is an operator living in Fork space.

$$V_N = \sum_{mm'} \int d^3r \Psi^+(\vec{r}, m') V(\vec{r})_{m'm} \Psi(\vec{r}, m) \tag{2.18}$$

This is called second quantization. "second" means people are tired of old qm quantization, now we quantize wave function further. One special feature of this space is that representation of V_N in (2.18) is no long in position space $V_N(\vec{r})$. V_N itself becomes an operator, through a_k, acting on $|n_1, n_2, ..., n_k, ...\rangle$. One can trace back to position space via ψ_k from (2.6).

Two important commutations

$$[a_{k'}, a_k^+] = \sqrt{n_k + 1}\sqrt{n_k + 1} - \sqrt{n_k}\sqrt{n_k} = 1\delta_{kk'} \tag{2.19}$$

$$\begin{aligned}
[\Psi(\vec{r}', m'), \Psi^+(\vec{r}, m)] &= \sum_{kk'} \psi_{k'}(\vec{r}', m')[a_{k'}, a_k^+]\psi_k(\vec{r}, m) = \sum_k \langle \vec{r}', m' | \psi_{k'} \rangle \langle \psi_k | \vec{r}, m \rangle \\
&= \langle \vec{r}', m' | \vec{r}, m \rangle = \delta(\vec{r}' - \vec{r})\delta_{mm'}
\end{aligned} \tag{2.20}$$

It is also easy to show from (2.15)

$$[a_{k'}, a_k] = [a^+_{k'}, a^+_k] = 0 \tag{2.21}$$

Besides non-interacting potential (2.7), there is another common potential, cf PS#16, problem 54.

$$V_N = \frac{1}{2} \sum_{i \neq j}^{N} V(\vec{r}_i, \vec{r}_j) \tag{2.22}$$

Similar to (2.9), we put

$$V(\vec{r}_i, \vec{r}_j)\psi_{k_i}(\vec{r}_i, m)\psi_{k_j}(\vec{r}_j, m) = \sum_{k'_i k'_j} \psi_{k'_i}(\vec{r}_i, m)\psi_{k'_j}(\vec{r}_j, m)V_{k'_i k'_j k_i k_j}$$

Following the argument above, to compute

$$\langle n'_1, n'_2, ..., n'_k, ...|V_N|n_1, n_2, ..., n_k, ...\rangle \tag{2.23}$$

one can express V_N in Fork space

$$V_N = \frac{1}{2} \sum_{mm'} \int d^3r \int d^3r' \Psi^+(\vec{r}', m')\Psi^+(\vec{r}, m)V(\vec{r}, \vec{r}')_{m'm}\Psi(\vec{r}', m')\Psi(\vec{r}, m) \tag{2.24}$$

where $\Psi(\vec{r}', m')$ is in (2.17), and a_k is the same in (2.15). So (2.23) is not zero unless 1) $\forall k \; n_k = n'_k$ or 2) $n_k = n'_k$ for all k except for the four distinct states whose $k = a, b, c, d$ and

$$n'_a = n_a + 1 \quad n'_b = n_b + 1 \quad n'_c = n_c - 1 \quad n'_d = n_d - 1$$

Later when we do quantization of EM field and study photon coherence state, we will come back to Bosons.

2.4 Fermions

We will see that the quantization of Fermions uses anti commutator. This is a deep consequence in QFT when general relativity meets quantum mechanics. Recall commutation relationship allows converting classical variables, e.g. real x real p, to quantum operators. What about anti commutator? This leads to reformulate classical mechanics with Grassmann variables and our discussion of Grassmann variables will be useful when we study path integral for Fermions.

First we do anti symmetrization, similar to (2.6)

$$|n_1, n_2, ..., n_k, ...\rangle = \frac{1}{\sqrt{N!}} \sum_{\{\sigma\}} \mathrm{sgn}(\sigma) \psi_{k_1}(\vec{r}_{\sigma_1}, m_{\sigma_1}) \cdot ... \cdot \psi_{k_N}(\vec{r}_{\sigma_N}, m_{\sigma_N}) \tag{2.25}$$

$\mathrm{sgn}(\sigma)$ will give a $-$ if two indices are exchanged. So $n_k = 0$ or 1. Those wave-function with 1 occupation numbers appear on the right of (2.25). They appear in the same order in the basis. E.g.

$$|1, 1, 0, ...\rangle \;\; = \tfrac{1}{\sqrt{2}} \;\; (\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)) \tag{2.26}$$

Define

$$\mathrm{sgn}(\sigma) = \frac{\prod_{i>j}^{N}(x_{\sigma_i} - x_{\sigma_j})}{\prod_{i>j}^{N}(x_i - x_j)} \tag{2.27}$$

numerators and denominators are polynomials in the N variables $x_1, ..., x_N$.

(2.27) makes easy to show that the sgn of composition of two permutation is the product of the sgns of the two permutations, i.e.

$$\mathrm{sgn}(\sigma \circ \tau) = \mathrm{sgn}\sigma \mathrm{sgn}\tau$$

Proof

$$\mathrm{sgn}(\sigma \circ \tau) = \frac{\prod_{i>j}^{N}(x_{\sigma_{\tau_i}} - x_{\sigma_{\tau_j}})}{\prod_{i>j}^{N}(x_{\tau_i} - x_{\tau_j})} = \frac{\prod_{i>j}^{N}(x_{\sigma_{\tau_i}} - x_{\sigma_{\tau_j}})}{\prod_{i>j}^{N}(x_{\tau_i} - x_{\tau_j})} \frac{\prod_{i>j}^{N}(x_{\tau_i} - x_{\tau_j})}{\prod_{i>j}^{N}(x_i - x_j)}$$

and set $\tau_i = l$ and order l in the same order of τ_i. QED

This definition also accomplishes the requirement that it will give a $-$ if two indices are exchanged.

Proof. First swap 2 neighboring indexes

$$\begin{cases} \sigma_i = j \\ \sigma_j = i \\ j = i+1 \\ \sigma_k = k \qquad k \neq i, j \end{cases}$$

then clearly (2.27) gives $-$. Then use the product rule proved above

$$\begin{cases} \sigma_i = j \\ \sigma_j = i \\ j = i+m \\ \sigma_k = k \qquad k \neq i, j \end{cases}$$

To do that first swap neighboring indexes $(i, i+1)$, $(i, i+2)$,..., (i, j) so after m swaps

$$1, 2, 3, ..., i, ..., j, ..., N$$

becomes

$$1, 2, 3, ..., i-1, i+1, ..., j-1, j, i, j+1, ..., N$$

Then we swap neighboring indices $(j, j-1)$, $(j, j-2)$,..., $(j, i+1)$ so after $m-1$ swaps,

$$1, 2, 3, ..., j, ..., i, ..., N$$

so total $(-1)^{2m-1}$. QED

There is a Slater matrix determinant representation of (2.25)

$$|n_1, n_2, ..., n_k, ...\rangle = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \psi_{k_1}(\vec{r}_1, m_1) & \psi_{k_1}(\vec{r}_2, m_2) & ... & \psi_{k_1}(\vec{r}_N, m_N) \\ \psi_{k_2}(\vec{r}_1, m_1) & \ddots & & \\ \vdots & & & \\ \psi_{k_N}(\vec{r}_1, m_1) & \psi_{k_N}(\vec{r}_2, m_2) & ... & \psi_{k_N}(\vec{r}_N, m_N) \end{pmatrix}$$

Lecture 11 (2/26/14)

Similar to Boson, we define non-interacting potential

$$V_N = \sum_{i=1}^{N} V(\vec{r}_i) \tag{2.28}$$

Similar to (2.9), expand

$$V(\vec{r})\psi_k(\vec{r}, m) = \sum \psi_{k'}(\vec{r}, m) V_{k'k}$$

and

$$V_{k'k} = \langle \psi_{k'} | V | \psi_k \rangle = \int d^3r \sum_m \psi^*_{k'}(\vec{r}, m) V(\vec{r}) \psi_k(\vec{r}, m)$$

Similar to (2.8), we find

$$\begin{aligned}
\langle n'_1, n'_2, ..., n'_k, ... | V_N | n_1, n_2, ..., n_k, ... \rangle \quad &= \quad \prod_{l=1}^{N} \left\{ \int d^3 r_l \sum_{m_l=-j}^{j} \right\} \frac{1}{N!} \\
&\left(\sum_{\{\sigma'\}} \mathrm{sgn}(\sigma') \psi^*_{k_1}(\vec{r}_{\sigma'_1}, m_{\sigma'_1}) \cdot ... \cdot \psi^*_{k_N}(\vec{r}_{\sigma'_N}, m_{\sigma'_N}) \right) \\
&\left(\sum_{i=1}^{N} V(\vec{r}_i) \right) \left(\sum_{\{\sigma\}} \mathrm{sgn}(\sigma) \psi_{k_1}(\vec{r}_{\sigma_1}, m_{\sigma_1}) \cdot ... \cdot \psi_{k_N}(\vec{r}_{\sigma_N}, m_{\sigma_N}) \right)
\end{aligned}$$

The easiest case is when $n'_i = n_i \; \forall i$, e.g. $N = 2$ cf (2.26)

$$\frac{1}{\sqrt{2}} \left(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1) \right)$$

$$\begin{aligned}
V_N \left| 1, 1, 0, 0, ... \right\rangle \quad = \quad & \frac{1}{\sqrt{2}} \left\{ \left[\psi_1(x_1)V_{11} + \psi_2(x_1)V_{21} + \psi_3(x_1)V_{31} + ... \right] \psi_2(x_2) \right. \\
& + \psi_1(x_1) \left[\psi_1(x_2)V_{12} + \psi_2(x_2)V_{22} + \psi_3(x_2)V_{32} + ... \right] \\
& - \left[\psi_1(x_2)V_{11} + \psi_2(x_2)V_{21} + \psi_3(x_2)V_{31} + ... \right] \psi_2(x_1) \\
& \left. - \psi_1(x_2) \left[\psi_1(x_1)V_{12} + \psi_2(x_1)V_{22} + \psi_3(x_1)V_{32} + ... \right] \right\}
\end{aligned} \tag{2.29}$$

Among those terms that have non-zero contributions to $\langle 1, 1, 0, 0, ... | V_N | 1, 1, 0, 0, ... \rangle$

are

$$
\begin{aligned}
V_N\,|1,1,0,0,...\rangle \;\; &\rightarrow \;\; \frac{1}{\sqrt{2}}\,\{\psi_1(x_1)V_{11}\psi_2(x_2) \\
&\quad +\psi_1(x_1)\psi_2(x_2)V_{22} \\
&\qquad -\psi_1(x_2)V_{11}\psi_2(x_1) \\
&\qquad -\psi_1(x_2)\psi_2(x_1)V_{22}\} \\
&= \;\; (V_{11}+V_{12})\,|1,1,0,0,...\rangle
\end{aligned}
$$

so

$$\langle 1,1,0,0,...|V_N|1,1,0,0,...\rangle = V_{11}+V_{22}$$

Suppose we want to find

$$\langle 0,1,1,0,...|V_N|1,1,0,0,...\rangle$$

Among those terms in (2.29) that have non-zero contributions to $\langle 0,1,1,0,...|V_N|1,1,0,0,...\rangle$ are

$$
\begin{aligned}
V_N\,|1,1,0,0,...\rangle \;\; &\rightarrow \;\; \frac{1}{\sqrt{2}}\,\{\psi_3(x_1)V_{31}\psi_2(x_2) \\
&\qquad -\psi_3(x_2)V_{31}\psi_2(x_1)\}
\end{aligned} \tag{2.30}
$$

thus

$$\langle 0,1,1,0,...|V_N|1,1,0,0,...\rangle = -V_{31} \tag{2.31}$$

Clearly from the expansion in (2.29) to see that e.g. if we compute

$$\langle 0,0,1,1,...|V_N|1,1,0,0,...\rangle = 0$$

With experience we can say that

$$\langle n_1', n_2', ..., n_k', ...|V_N|n_1, n_2, ..., n_k, ...\rangle = \begin{cases} \sum_k^{\infty} n_k V_{kk} & n_i' = n_i \,\forall i \\ V_{lk}(-1)^{\gamma_l(\{n'\})}(-1)^{\gamma_k(\{n\})} & \begin{matrix} n_l' = 1 \, n_l = 0 \, n_k' = 0 \, n_k = 1 \\ n_i' = n_i' \text{ for other } i \neq k, l \end{matrix} \\ 0 & \text{otherwise} \end{cases} \tag{2.32}$$

where

$$\gamma_k(\{n\}) = \sum_{i<k} n_i$$

e.g. in (2.31)

$$\gamma_k(\{n\}) = \gamma_1(\{n\}) = 0 \qquad \gamma_l(\{n'\}) = \gamma_3(\{n'\}) = 0 + 1 = 1$$

The nasty thing for Fermion is the (-1) factor, while as the nasty thing for Boson is the permutation factor. Where does the nasty γ come from? It comes from, e.g. in (2.30), the order of the wave functions changed, it becomes $\psi_3\psi_2$, so the (-1) sign doesn't cancel when we do $\langle 0, 1, 1, 0, ...|V_N|1, 1, 0, 0, ...\rangle$. This was not a problem for Boson.

Therefore we do similarly thing as (2.13)

$$V_N = \sum_{l,k} a_l^+ V_{lk} a_k \tag{2.33}$$

a_k, annihilation operator, defined as

$$\langle n_1', n_2', ..., n_k', ...|a_k|n_1, n_2, ..., n_k, ...\rangle = \begin{cases} (-1)^{\gamma_k(\{n\})} & n_k' = 0, n_k = 1 \; n_i' = n_i \,\forall i \neq k \\ 0 & \text{otherwise} \end{cases} \tag{2.34}$$

or

$$a_k \left|n_1, n_2, ..., n_k, ...\right\rangle = (-1)^{\gamma_k(\{n\})} \left|n_1, n_2, ..., n_k - 1, ...\right\rangle$$

a_k^+ is a_k hermitian conjugate, creation operator, so

$$\langle n_1', n_2', ..., n_k', ...| \left(a_k |n_1, n_2, ..., n_k, ...\rangle\right) = \left(a_k^+ |n_1', n_2', ..., n_k', ...\rangle, |n_1, n_2, ..., n_k, ...\rangle\right)$$

so

$$a_k^+ |n_1, n_2, ..., n_k, ...\rangle = (-1)^{\gamma_k(\{n\})} |n_1, n_2, ..., n_k + 1, ...\rangle \tag{2.35}$$

Using the definitions (2.34), (2.35), one can check that (2.33) is indeed a correct representation of (2.32).

Since (2.33) looks exactly the same as (2.13), we should have (2.18) as well. What about two important commutation relations (2.19) and (2.20)? They turn out to become anticommutators

$$\{a_{k'}, a_k^+\} = 1\delta_{kk'}$$

$$\{\Psi(\vec{r}', m'), \Psi^+(\vec{r}, m)\} = \sum_{kk'} \psi_{k'}(\vec{r}', m')\{a_{k'}, a_k^+\}\psi_k(\vec{r}, m) = \delta(\vec{r}' - \vec{r})\delta_{mm'}$$

Proof. WLOG assume $k' < k$

$$\begin{aligned} a_{k'} a_k^+ |n_1, n_2, ..., n_{k'}, ..., n_k, ...\rangle &= a_{k'} (-1)^{\gamma_k(\{n\})} |n_1, n_2, ..., n_{k'}, ..., n_k + 1, ...\rangle \\ &= (-1)^{\gamma_{k'}(\{n\})} (-1)^{\gamma_k(\{n\})} |n_1, n_2, ..., n_{k'} - 1, ..., n_k + 1, ...\rangle \end{aligned}$$

$$\begin{aligned} a_k^+ a_{k'} |n_1, n_2, ..., n_{k'}, ..., n_k, ...\rangle &= a_k^+ (-1)^{\gamma_{k'}(\{n\})} \left| n_1, n_2, ..., \underbrace{n_{k'} - 1}_{n'_{k'}}, ..., n_k, ... \right\rangle \\ &= (-1)^{\gamma_k(\{n'\})} (-1)^{\gamma_{k'}(\{n\})} |n_1, n_2, ..., n_{k'} - 1, ..., n_k + 1, ...\rangle \end{aligned}$$

They are off by a -1 sign, so

$$a_{k'} a_k^+ + a_k^+ a_{k'} = \{a_{k'}, a_k^+\} = 0$$

If $k' = k$. If $n_k = 1$, then

$$a_k^+ a_k = 1 \quad a_k a_k^+ = 0$$

If $n_k = 0$, then

$$a_k^+ a_k = 0 \quad a_k a_k^+ = 1$$

In sum

$$\{a_{k'}, a_k^+\} = 1\delta_{kk'}$$

QED.

This proof works exactly the same to show that

$$\{a_{k'}, a_k\} = 0$$

Besides non-interacting potential (2.28), there is another common potential, which we will use when we study Coulomb gas.

$$V_N = \frac{1}{2}\sum_{i\neq j}^{N} V(\vec{r}_i, \vec{r}_j) \tag{2.36}$$

same as (2.22), we should get (2.24) too.

2.5 Grassmann Variables

We replace the real numbers of classical mechanics with anti-commuting Grassmann numbers, and we are interested to see how qm can be derived from such classical mechanics through anti commutation relation.

Consider a complex algebra generated by $\bar{N}$ anti commuting variables

$$\hat{z}_1, \hat{z}_2, ..., \hat{z}_{\bar{N}}$$

and

$$\{\hat{z}_i, \hat{z}_j\} = 0 \quad \forall i, j$$

a general element of this algebra is

$$g = \sum_{n=0}^{\bar{N}} \sum_{i_n > i_{n-1} > \ldots > i_1} c_{i_n i_{n-1} \ldots i_1} \hat{z}_{i_1} \hat{z}_{i_2} \ldots \hat{z}_{i_n} \qquad c_{i_n i_{n-1} \ldots i_1} \in \mathbb{C}$$

no power of $\hat{z}_i$, because $\hat{z}_i^2 = 0$. g is a vector in a vector space of dimension $2^{\bar{N}}$.

Lecture 12 (3/3/14)

We need only elements of the form

$$q = \sum_{j=1}^{\bar{N}} a_j \hat{z}_j$$

We want N of these to represent classical variables for the N particles

$$q_i = \sum_{j=1}^{\bar{N}} a_{ij} \hat{z}_j \qquad 1 \le i \le N$$

we assume $N \ll \bar{N}$, because we don't want them to interfere each other. We want q_i to satisfy

$$\{q_i, q_j\} = 0 \qquad \text{and} \qquad \prod_{i=1}^{N} q_i \neq 0$$

The first condition is automatically satisfied, and the second condition is important for taking products like in (2.37), in (2.39) and ultimately in the denominator of (2.41). But if $N = \bar{N}$, it is very like that the second condition will not be satisfied, e.g. $N = 3$

$$q_1 = z_1 + z_2 \; q_2 = z_2 + z_3 \; q_3 = z_1 - z_3$$

then

$$q_1 q_2 q_3 \;=\; (z_1 z_2 + z_1 z_3 + z_2 z_3)(z_1 - z_3) = z_2 z_3 z_1 - z_1 z_2 z_3 = 0$$

Consider wave function depends on these q_i's.

$$\psi(q_1, \ldots, q_N)$$

which must be a polynomial in product of the q_i

$$\psi(q_1, ..., q_N) = \sum_{n=0}^{N} \sum_{i_n > i_{n-1} > ... > i_1} c_{i_n i_{n-1} ... i_1} q_{i_1} q_{i_2} ... q_{i_n} \tag{2.37}$$

Now define the derivative

$$\frac{\partial}{\partial q_i}$$

from the Taylor formula.

$$\Delta q_i \frac{\partial}{\partial q_i} \psi(q_1, ..., q_N) \equiv [\psi(q_1, ..., q_i + \Delta q_i, ..., q_N) - \psi(q_1, ..., q_i, ..., q_N)]$$

This $\equiv$ is exact because higher order terms $O(\Delta q^2) = 0$ for q are Grassmann variables.

Claim:

$$q_i \frac{\partial}{\partial q_j} + \frac{\partial}{\partial q_j} q_i = \delta_{ij} \tag{2.38}$$

This will be the analogy of $[x_i, \partial/\partial x_j] = \delta_{ij}$

Pf. Consider

$$\Delta q_j \left(q_i \frac{\partial}{\partial q_j} + \frac{\partial}{\partial q_j} q_i \right) \psi \tag{2.39}$$

If $i \neq j$,

$$\begin{aligned} \Delta q_j \left(q_i \frac{\partial}{\partial q_j} + \frac{\partial}{\partial q_j} q_i \right) \psi &= -q_i \Delta q_j \frac{\partial}{\partial q_j} \psi + \Delta q_j \frac{\partial}{\partial q_j} (q_i \psi) \\ &= -q_i [\psi(q_j + \Delta q_j) - \psi(q_j)] + [q_i \psi(q_j + \Delta q_j) - q_i \psi(q_j)] = 0 \end{aligned}$$

If $i = j$,

$$\begin{aligned} \Delta q_i \left(q_i \frac{\partial}{\partial q_i} + \frac{\partial}{\partial q_i} q_i \right) \psi &= -q_i [\psi(q_i + \Delta q_i) - \psi(q_i)] + [(q_i + \Delta q_i) \psi(q_i + \Delta q_i) - q_i \psi(q_i)] \\ &= \Delta q_i \psi(q_i + \Delta q_i) = \Delta q_i \psi(q_i) \end{aligned}$$

because $O(\Delta q^2) = 0$. QED

Looks like from (2.39), we are going to associate

$$q_i \to x_i \quad \frac{\partial}{\partial q_i} \to p_i$$

but we actually need anti commutation relation, this reminds us

$$\{a_k, a^+_{k'}\} = \delta_{kk'}$$

We put

$$\begin{aligned} |n_1, n_2, ..., n_k, ...\rangle &\to \prod_{k=1}^{\bar{N}} q_k^{1-n_k} \quad (2.40) \\ &= \frac{\prod_{k=1}^{\bar{N}} q_k}{q_1 q_2 ... q_N} \quad (2.41) \end{aligned}$$

we should take (2.40) as the definition, while as (2.41) just an intuitive expression.

Then consider

$$q_k |n_1, n_2, ..., n_k, ...\rangle$$

e.g.

$$q_3 |0, 1, 0, 1, 0, ...\rangle = q_3(q_1 q_3 q_5 q_6 ...) = 0$$

e.g.

$$\begin{aligned} q_4 |0, 1, 0, 1, 0, ...\rangle &= q_4(q_1 q_3 q_5 q_6 ...) \\ &= (-1) q_1 q_4 q_3 q_5 q_6 ... \\ &= (-1)(-1) q_1 q_3 q_4 q_5 q_6 ... = |0, 1, 0, 0, 0, ...\rangle \end{aligned}$$

In general

$$q_k |n_1, n_2, ..., n_k, ...\rangle = \begin{cases} (-1)^{\sum_{l<k}(1-n_l)} |n_1, n_2, ..., n_k - 1, ...\rangle & n_k = 1 \\ 0 & n_k = 0 \end{cases}$$

so q_k annihilates. Compare this to the definition of a_k (2.34), we can express a_k in term of Grassmann variables

$$a_k = q_k(-1)^{\sum_{l<k} 1} = q_k(-1)^{k-1} \tag{2.42}$$

Using the proof of the anti commutation (2.38), we can see that

$$a_k^+ = \frac{\partial}{\partial q_k}(-1)^{\sum_{l<k} 1} = \frac{\partial}{\partial q_k}(-1)^{k-1}$$

Indeed multiply q_k means a_k remove a particle and derivative means add a particle.

2.6 Coulomb Gas

Consider a volume of $\Omega = L^3$ filled with a uniform background of positive charges (which is just shifting up the groundstate so we don't have to consider it for now) and essentially free electrons (no external forces because the background force is uniform). Our task is to find 1st order correction to the ground state energy in the Coulomb repulsion between the e^-'s.

Look like they should completely cancel out but because e^-'s are Fermions, they don't get too close to either other, it's not same as the uniform distributed positive background, so we will get some net energy.

$$H = \underbrace{\sum_{i=1}^{N} \frac{p_i^2}{2m}}_{H^0} + \underbrace{\frac{1}{2}\sum_{i\neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}}_{V}$$

We are going to do perturbation, so the groundstates are plane waves

$$\psi_{\vec{p}_{\vec{n}}}(\vec{r}) = \frac{e^{i\vec{p}_{\vec{n}}\cdot\vec{r}/\hbar}}{\sqrt{\Omega}} \qquad \vec{p}_{\vec{n}} = (n_1, n_2, n_3)\frac{2\pi\hbar}{L} \qquad (\Delta p)^3 = (\frac{2\pi\hbar}{L})^3$$

we want to find

$$E_{grd}^{(1)} = \left\langle \psi_{\vec{p}_{\vec{n}_1}}, \psi_{\vec{p}_{\vec{n}_2}}, \ldots \middle| V \middle| \psi_{\vec{p}_{\vec{n}_1}}, \psi_{\vec{p}_{\vec{n}_2}}, \ldots \right\rangle = \langle p_f | V | p_f \rangle \tag{2.43}$$

(need to antisymmetrize $\left|\psi_{\vec{p}_{\vec{n}_1}}, \psi_{\vec{p}_{\vec{n}_2}}, \ldots\right\rangle$)

This looks like exact what we have been building up to. The ground state of N electrons, denoted $|p_f\rangle$, is the state where all single particle states are filled up to a Fermi momentum p_f, i.e. $n_{\vec{p}} \neq 0$ for all $|\vec{p}| \leq p_f$ and

$$E \leq E_f = \frac{p_f^2}{2m}$$

so $E_{grd}^{(0)}$ is simply

$$E_{grd}^{(0)} = \langle n_1, n_2, ...| H^0 |n_1, n_2, ...\rangle = \sum_k n_k E_k$$

To solve (2.43), we first find a relation between p_f and N.

$$N = 2\sum_{|\vec{p}|\leq p_f} 1 = 2\int_{|\vec{p}|\leq p_f} d^3p (\frac{2\pi\hbar}{L})^3 = (\frac{2\pi\hbar}{L})^3 8\pi \int_0^{p_f} p^2 dp = L^3 \frac{1}{3\pi^2}(\frac{p_f}{\hbar})^3$$

2 counts for spin. Write N differently

$$N = 2\frac{\left(\frac{4\pi p_f^3}{3}\right)}{(2\pi\hbar)^3}\Omega$$

2 counts for the spin, the $\left(\frac{4\pi p_f^3}{3}\right)/(2\pi\hbar)^3$ gives number of particles per state in phase space.

Or in term of number density

$$n = \frac{N}{L^3} = \frac{1}{3\pi^2}(\frac{p_f}{\hbar})^3 \tag{2.44}$$

From (2.36), we have

$$\begin{aligned} E_{grd}^{(1)} &= \langle p_f | V | p_f \rangle \\ &= \left\langle p_f \middle| \frac{1}{2}\int d^3r \int d^3r' \sum_{ss'} \Psi^+(\vec{r}', s')\Psi^+(\vec{r}, s)\frac{e^2}{|\vec{r} - \vec{r}'|}\Psi(\vec{r}', s')\Psi(\vec{r}, s) \middle| p_f \right\rangle \end{aligned}$$

Since we first destroy particles $\Psi(\vec{r}', m')\Psi(\vec{r}, m)$ at $\vec{r}'$ and $\vec{r}$ then create them $\Psi^+(\vec{r}', m')\Psi^+(\vec{r}, m)$, we don't have to worry that itself-interaction, i.e. when $\vec{r}' = \vec{r}$,

V blows up. This also shows that it is not okay to switch $\Psi^+(\vec{r}, s)$ and $\Psi(\vec{r}', s')$ or switch $\Psi^+(\vec{r}, s)$ and $\Psi(\vec{r}, s)$

Lecture 13 (3/5/14)

Therefore we can define 4-point Green's function

$$G_{ss'}(r, r') = \left\langle p_f \middle| \Psi^+(\vec{r}', s')\Psi^+(\vec{r}, s)\Psi(\vec{r}', s')\Psi(\vec{r}, s) \middle| p_f \right\rangle \tag{2.45}$$

then

$$E^{(1)}_{grd} = \frac{1}{2}e^2 \int d^3r \int d^3r' \frac{1}{|\vec{r} - \vec{r}'|} \sum_{ss'} G_{ss'}(r, r') \tag{2.46}$$

that is because Ψ or Ψ^+ contents a which acts only on Fork space, we can move $\frac{1}{|\vec{r}-\vec{r}'|}$ outside. And because $|p_f\rangle$ has only states whose momentum below p_f, we can replace Ψ by Ψ^{p_f}

$$\Psi^{p_f}(\vec{r}, s) = \sum_{|\vec{k}| \le p_f} \psi_k(\vec{r}, s) a_k$$

thus

$$G_{ss'}(r, r') = \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}', s')\Psi^{p_f +}(\vec{r}, s)\Psi^{p_f}(\vec{r}', s')\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle$$

we will rewrite above in two different ways:

$$G_{ss'}(r, r') = \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}', s')\Psi^{p_f +}(\vec{r}, s) \middle| p_f \right\rangle \left\langle p_f \middle| \Psi^{p_f}(\vec{r}', s')\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle$$

because $|p_f\rangle \langle p_f|$ is now complete set of states

Or

$$G_{ss'}(r, r') = \frac{1}{2} \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}', s')\Psi^{p_f}(\vec{r}', s') \middle| p_f \right\rangle \times \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}, s)\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle$$

because $\vec{r}$ and $\vec{r}'$ are independent variables after removal $1/|\vec{r} - \vec{r}'|$

In sum

$$\begin{aligned} G_{ss'}(r, r') &= \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}', s')\Psi^{p_f}(\vec{r}', s') \middle| p_f \right\rangle \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}, s)\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle \\ &\quad - \left\langle p_f \middle| \Psi^{p_f +}(\vec{r}', s')\Psi^{p_f +}(\vec{r}, s) \middle| p_f \right\rangle \left\langle p_f \middle| \Psi^{p_f}(\vec{r}', s')\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle \end{aligned}$$

that is we decompose 4-point function into product of 2-point functions.

Let's evaluate them separately

$$\left\langle p_f \middle| \Psi^{p_f +}(\vec{r}, s)\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle = 2\sum_{|\vec{p}|\le p_f} \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{\sqrt{\Omega}} \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{\sqrt{\Omega}} = 2\sum_{|\vec{p}|\le p_f} \frac{1}{\Omega} = \frac{N}{\Omega} = n \quad (2.47)$$

2 counts for spin. So we can interpret n as an operator acting on Fork space

$$n = \Psi^{p_f +}(\vec{r}, s)\Psi^{p_f}(\vec{r}, s) \quad (2.48)$$

Does this make sense? Indeed we would say

$$n(\vec{r}_0, s_0) = \sum_{i=1}^{N} \sum_{ss'} \underbrace{\delta^3(\vec{r}_0 - \vec{r})\delta_{s_0 s}\delta_{s_0 s'}}_{V_{ss'}}$$

recall V_N in the 2-point function acting on Fork space

$$\begin{aligned} n = V_N = \sum_{i=1}^{N} V_{ss'}(\vec{r}) &= \sum_{ss'} \int d^3 r \Psi^+(\vec{r}, s') V(\vec{r})_{ss'} \Psi(\vec{r}, s) \\ &= \sum_{ss'} \int d^3 r \Psi^+(\vec{r}, s') \delta^3(\vec{r}_0 - \vec{r})\delta_{s_0 s}\delta_{s_0 s'} \Psi(\vec{r}, s) = \Psi^+(\vec{r}_0, s_0)\Psi(\vec{r}_0, s_0) \end{aligned}$$

proving (2.48).

Next

$$\left\langle p_f \middle| \Psi^{p_f +}(\vec{r}', s')\Psi^{p_f}(\vec{r}, s) \middle| p_f \right\rangle = \left(\frac{L}{2\pi\hbar}\right)^3 \int_{|\vec{p}|\le p_f} d^3 p \frac{e^{-i\vec{p}\cdot\vec{r}'/\hbar}}{\sqrt{\Omega}} \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{\sqrt{\Omega}} \delta_{ss'} \quad (2.49)$$

The $(L/2\pi\hbar)^3 = 1/(\Delta p)^3$ is necessary when summation is converted into integral. Choose polar $\hat{z} \parallel (\vec{r} - \vec{r}')$

$$\begin{aligned} (2.49) &= \frac{1}{(2\pi\hbar)^3} 2\pi \int_0^{p_f} dp p^2 \int_{-1}^{1} d(\cos\theta) e^{ip|\vec{r}-\vec{r}'|\cos\theta/\hbar} \delta_{ss'} \\ &= \frac{1}{(2\pi\hbar)^3} 4\pi \int_0^{p_f} dp p \frac{\hbar}{|\vec{r}-\vec{r}'|} \sin\frac{p|\vec{r}-\vec{r}'|}{\hbar} \delta_{ss'} \end{aligned}$$

put $x = \frac{p_f|\vec{r}-\vec{r}'|}{\hbar}$ $\quad y = \frac{p|\vec{r}-\vec{r}'|}{\hbar}$

$$\begin{aligned}
(2.49) \quad &= \frac{1}{(2\pi\hbar)^3} 4\pi \frac{p_f^3}{x^3} \underbrace{\int_0^x yydy \sin y}_{\sin x - x\cos x} \delta_{ss'} \\
&= \frac{1}{2} \underbrace{\frac{p_f^3}{\pi^2\hbar^3}}_{3n} \frac{1}{x^3} (\sin x - x\cos x) \delta_{ss'} \qquad (2.50)
\end{aligned}$$

This has no singularity at $x = 0$

$$\frac{1}{x^3}(\sin x - x\cos x) \sim \frac{1}{x^3}(x - \frac{x^3}{6} - x + \frac{x^3}{2} + ...) \sim \frac{1}{3}$$

Now back to (2.46), by (2.47) and (2.50)

$$E_{grd}^{(1)} = \frac{1}{2}e^2 \int d^3r \int d^3r' \frac{1}{|\vec{r}-\vec{r}'|} \sum_{ss'} \left[\frac{n^2}{4} - \frac{n^2}{4}\delta_{ss'} \left(3\frac{1}{x^3}(\sin x - x\cos x) \right)^2 \right]$$

the extra 4 in $n^2/4$ from (2.47) is to count for the summation $\sum_{ss'} = 2 \times 2$. In writing this way, we can see if x went to 0, we would have $E_{grd}^{(1)} = 0$. But it cannot, because it's Fermion.

Now we add in background of positive change of uniform density n. This will cancel the self energy term (2.47), so

$$E_{grd}^{(1)} = \frac{1}{2}e^2 \int d^3r \int d^3r' \frac{1}{|\vec{r}-\vec{r}'|} \left[-\frac{n^2}{4} 2 \left(3\frac{1}{x^3}(\sin x - x\cos x) \right)^2 \right]$$

Let $R = |\vec{r}-\vec{r}'|$, or $x = p_f R/\hbar$, then $\vec{r}$ and $\vec{R}$ are independent integrations

$$\begin{aligned}
E_{grd}^{(1)} &= -e^2 \int d^3r \int d^3R \frac{1}{R} (\frac{3n}{2})^2 [\frac{1}{x^3}(\sin x - x\cos x)]^2 \\
&= -e^2 \Omega 4\pi \int RdR (\frac{3n}{2})^2 [\frac{1}{x^3}(\sin x - x\cos x)]^2
\end{aligned}$$

Let $L \to \infty$, $x \in [0, \infty)$

$$E_{grd}^{(1)} = -e^2 \Omega 4\pi (\frac{3n}{2}\frac{\hbar}{p_f})^2 \underbrace{\int_0^\infty xdx[\frac{1}{x^3}(\sin x - x\cos x)]^2}_{\frac{1}{3}}$$

so by (2.44)

$$\frac{E_{grd}^{(1)}}{N} = -e^2 \frac{1}{\pi}(\frac{p_f}{\hbar})$$

so if we impose that the average energy of one e^- is

$$\left|\frac{E_{grd}^{(1)}}{N}\right| \ll \frac{p_f^2}{2m} \tag{2.51}$$

we have

$$\underbrace{\frac{e^2 m}{\hbar}}_{\hbar/a_0} \ll p_f$$

i.e.

$$\hbar \ll p_f a_0$$

In other word, the condition (2.51) is saying that not to put too many e^- in the box or atoms will be formed.

2.7 Thomas-Fermi Atom

The line of attack is that for a large Z atom, we know that the e^- cloud is not like the free e^- in box we discussed above, we borrow (2.44) anyway

$$n = \frac{1}{3\pi^2}(\frac{p_f}{\hbar})^3 \tag{2.52}$$

Thus the potential that e^-s experiencing, i.e. outside of nuclear is

$$\nabla^2 \Phi(\vec{r}) = -4\pi\rho(\vec{r}) = 4\pi e n \tag{2.53}$$

Use Schrodinger for the radial wave functions.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - e\Phi(\vec{r})\right)\psi_E(\vec{r}) = E\psi_E(\vec{r}) \tag{2.54}$$

where

$$E = \frac{p^2(r)}{2m} - e\Phi(r) + \frac{l(l+1)\hbar^2}{2mr^2}$$

so

$$p(r) = \sqrt{2m[E + e\Phi(r)] - \frac{l(l+1)\hbar^2}{r^2}} \tag{2.55}$$

in particular

$$p_f(r) = \sqrt{2m[E_f + e\Phi(r)]} \tag{2.56}$$

hence it is largest when $l = 0$. Therefore combining with (2.52) and (2.53), we can solve for Φ and from there we can solve (2.54) to obtain wave functions.

Lecture 14 (3/10/14)

To see under what condition (2.52) is valid, we need to derive (2.52). First using WKB in 1D, we suppose e^{-}s are bounded in some 1D potential $V(x)$, with left and right tuning points x_1 and x_2. We have

$$\left(-\frac{\hbar^2 d^2}{2mdx^2} + V(x)\right)\psi_n(x) = E_n\psi_n(x) \tag{2.57}$$

the WKB for ψ_E in the bound region is

$$\psi_E = \frac{N_E}{\sqrt{v_E(x)}}\sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx'\right)$$

To find the normalization N_E, we assume outside the bound region $\psi_E \to 0$, i.e.

$$1 = N_E^2\int_{x_1}^{x_2}\frac{1}{v_E}\sin^2\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx'\right)dx$$

Assuming

$$\sin^2\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx'\right) \to \frac{1}{2} \tag{2.58}$$

for large oscillations, which is the basic assumption for WKB to work. Let

$$\tau = 2\int_{x_1}^{x_2} \frac{1}{v_E} dx = \oint \frac{1}{v_E} dx$$

we get

$$N_E = \frac{2}{\sqrt{\tau}}$$

Next use Bohr quantization

$$\oint p(x)dx = 2\pi\hbar(n + \frac{1}{2})$$

then the number of state per unit distance per energy

$$\frac{dn}{dE} = \frac{1}{2\pi\hbar}\oint \frac{dp(x)}{dE} dx = \frac{\tau}{2\pi\hbar}$$

This can be used to determine the electrons density up to Fermi energy

$$\rho(x) = -2e \sum_{\substack{n \text{ s.t.} \\ E_n \leq E_f}} |\psi_n(x)|^2 = -2e \int dE \frac{dn}{dE} \left| \frac{N}{\sqrt{v}} \right|^2 \frac{1}{4} \tag{2.59}$$

assuming (2.58), and 2 counts for moving in $\pm p$ directions. So

$$\rho(x) = -e \int dE \frac{1}{\pi\hbar} \frac{1}{v} = -e \int_0^{p_f} dp \frac{1}{\pi\hbar} = -e \frac{p_f}{\pi\hbar} \tag{2.60}$$

Now in 3D, write

$$\psi_{l,m}(\vec{r}) = \frac{1}{r} u_r(r) Y_{lm}(\theta, \phi)$$

where

$$-e\,|u_r(r)|^2 \sim \rho(x) \text{ of } (2.60)$$

with p_f is just (2.55), because $u_r(r)$ satisfies the same Schrodinger

$$\left(-\frac{\hbar^2 d^2}{2mdr^2} - e\Phi(r) + \frac{\hbar^2 (l+1)l}{r^2} \right) u_{nl}(r) = E_{nl} u_{nl}(r)$$

as (2.57), but the Fermi momentum of 1D is not the same as 3D.

Similar to (2.59)

$$\begin{aligned}\rho(r) &= -2e\int \sum_{\substack{n \text{ s.t.} \\ E_n \le E_f}} \left|\psi_{l,m}(\vec{r})\right|^2 d\Omega \\ &= -2e\int \sum_{0}^{l_{max}} \sum_{m=-l}^{l} \left|\frac{u_{n,l}}{r} Y_{lm}\right|^2 d\Omega\end{aligned}$$

2 for spins. And

$$\int \left|Y_{lm}\right|^2 d\Omega = \frac{1}{4\pi}$$

then

$$\rho(r) = -2e \sum_{0}^{l_{max}} (2l+1) \frac{1}{r^2} \frac{\sqrt{2m[E_f + e\Phi(r)] - \frac{l(l+1)\hbar^2}{r^2}}}{\pi\hbar} \frac{1}{4\pi} \tag{2.61}$$

where l_{max} is such that the square root is near 0. Put

$$x = \frac{l(l+1)\hbar^2}{r^2} \qquad dx = \frac{(2l+1)\hbar^2}{r^2}$$

so

$$\begin{aligned}\rho(r) &= \int_0^{2m[E_f+e\Phi(r)]} dx \frac{-e}{2\pi^2\hbar^3} \sqrt{2m[E_f + e\Phi(r)] - x} \\ &= \frac{-e}{2\pi^2\hbar^3} \frac{2}{3} \left(2m(E_f + e\Phi(r))\right)^{3/2} \\ &= \frac{-ep_f^3}{3\pi^2\hbar^3}\end{aligned}$$

by (2.56). This proves (2.52).

Now back to (2.53) and write Laplace in spherical coordinate with only radial dependence

$$\nabla^2\Phi(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr}\Phi(r)\right)$$

define ϕ such that

$$\frac{e^2 Z\phi(r)}{r} = E + e\Phi(r)$$

the boundary conditions

$$\lim_{r\to 0} r\Phi(r) = eZ$$

becomes

$$\lim_{r\to 0} \phi(r) = 1 \tag{2.62}$$

and

$$\nabla^2\Phi(r) = \frac{eZ}{r}\frac{d^2\phi}{dr^2} \tag{2.63}$$

so (2.53) becomes

$$\frac{eZ}{r}\frac{d^2\phi}{dr^2} = 4\pi\frac{e}{3\pi^2\hbar^3}\left(2m\frac{e^2 Z\phi(r)}{r}\right)^{3/2}$$

or

$$\frac{d^2\phi}{dr^2} = \frac{1}{r^{1/2}}\phi^{3/2}\frac{4\cdot 2^{3/2}\cdot m^{3/2}\cdot Z^{1/2}\cdot e^3}{3\pi\hbar^3}$$

let $r = \lambda x$

$$\begin{aligned}\frac{d^2\phi}{dx^2} &= \frac{1}{x^{1/2}}\phi^{3/2}\underbrace{\lambda^{3/2}\frac{4\cdot 2^{3/2}\cdot m^{3/2}\cdot Z^{1/2}\cdot e^3}{3\pi\hbar^3}}_{=1} \\ &= \frac{\phi^{3/2}}{x^{1/2}} \end{aligned} \tag{2.64}$$

if choose

$$\lambda = (\frac{3\pi}{4})^{2/3}\underbrace{\frac{\hbar^2}{me^2}}_{a_0}\frac{1}{2Z^{1/3}}$$

dimension works out nicely.

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(2.64) is a non-linear ode so we have no hope of solving it. But we use software we find the asymptotic behavior is denominated by

$$\phi = \frac{144}{x^3} \tag{2.65}$$

which is actually one of the solutions away from the origin. One can also find numerically that

$$x\phi(x) \leq 0.486 \tag{2.66}$$

is bounded.

From (2.65) we see that Φ never goes to 0. So we compute the radius of the atom as the radius $R = R_{Z-1}$ that encloses $Z-1$ electrons. That is

$$Z - 1 = \int_{r<R} d^3 r n(r) = \int_{r<R} d^3 r \frac{1}{4\pi e} \nabla^2 \Phi$$

By (2.63), (2.62)

$$Z-1 = \int_0^R r dr Z \frac{d^2\phi}{dr^2} = Z \left(r \left. \frac{d\phi}{dr} \right|_0^R - \int_0^R \frac{d\phi}{dr} dr \right) = Z \left(R \left. \frac{d\phi}{dr} \right|_R - \phi(R) + \underbrace{\phi(0^+)}_{1} \right)$$

so

$$-1 = Z \left(R(-3)\lambda^3 \frac{144}{R^4} - \lambda^3 \frac{144}{R^3} \right)$$

that is

$$R_{Z-1} = ((4)(144)Z)^{1/3} (\frac{3\pi}{4})^{2/3} a_0 \frac{1}{2Z^{1/3}} \approx 7.3 a_0$$

hence the size of large atoms does not grow with Z.

The second beautiful result is the following. We can find l_{max} the largest l exists for given Z, by following the discussion after (2.61).

$$\begin{aligned} l_{max}(l_{max}+1) &\leq \frac{2m}{\hbar^2} r^2 [E + e\Phi(r)] \\ &= \frac{2m}{\hbar^2} r e^2 Z \phi(r) \\ &= \frac{2m}{\hbar^2} e^2 Z \lambda \underbrace{x\phi(x)}_{\leq 0.486} \\ &\leq 0.861 Z^{3/2} \end{aligned}$$

We would like to replace $l(l+1)$ by $(l+\frac{1}{2})^2$, which is what it should be if we do 1D WKB more carefully when we compute $l(l+1)\hbar^2/r^2$ at $r=0$. Thus

$$1.252(l + \frac{1}{2})^2 \leq Z$$

	l_{max}	compute $1.252(l+\frac{1}{2})^2$	experiment find the smallest Z
s	0	0.156	1
p	1	4.22	4
d	2	19.55	19
f	3	53.6	57
g	4	113.9	> 118?(unknown, highly unstable)

This table says e.g. for $l = 2$ e^- can only exist in atoms with $Z \geq 20$ and experiment finds $Z \geq 19$.

2.8 Hartree-Fock Molecules

Speaking of molecules, there are three energy scales:

1) electronic scale (Rydberg)

$$E_{elec} \sim \frac{me^4}{\hbar^2}$$

recall hydrogen energy $E_n = -\frac{me^4}{2\hbar^2 n^2}$.

2) vibrational energy of the nuclei (SHO)

Suppose $\Delta R \sim a_0$ is the displacement of a nucleus (with mass M) from the position of lowest electron energy, we expect

$$\Delta E = \frac{1}{2}k(\Delta R)^2 = \frac{1}{2}Mw^2 a_0^2 \sim \frac{me^4}{\hbar^2}$$

so

$$E_{vib} \sim \hbar w \sim \frac{me^4}{\hbar^2}\sqrt{\frac{m}{M}}$$

3) rotation of nuclear

$$E_{rot} \sim \frac{L^2}{2I} \sim \frac{\hbar^2}{Ma_0^2} = \frac{me^4}{\hbar^2}\frac{m}{M}$$

So we can easily see the energy hierarchies.

A molecule has N nucleus and n electrons. Let $\Phi_E(\vec{R}_1, ..., \vec{R}_N, \vec{r}_1, ..., \vec{r}_n)$ be energy eigenstates of

$$[\underbrace{\sum_{i=1}^{N}\frac{P_i^2}{2M_i}}_{0}+\sum_{j=1}^{n}\frac{p_j^2}{2m}+V(R_i,r_j)]\Phi_E(\vec{R}_1,...,\vec{R}_N,\vec{r}_1,...,\vec{r}_n)=E\Phi_E(\vec{R}_1,...,\vec{R}_N,\vec{r}_1,...,\vec{r}_n) \tag{2.67}$$

with leading term to be neglected. This is called Born-Oppenheimer approximation. Why can we neglect $P_i^2/2M_i$? Because typically

$$P_i^2/2M_i \sim E_{vib}$$

whiles

$$p_j^2/2m_j \sim E_{elec}$$

Therefore in H, R_i is cyclic, so

$$[R_i, H] = 0$$

So for given $\vec{R}_1,...,\vec{R}_N$, we can define $\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$ to be the eigenstates of H and the eigenstates of R_i, $1 \le i \le N$, where k is an additional label, i.e.

$$[\sum_{j=1}^{n}\frac{p_j^2}{2m}+V(R_i,r_j)]\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)=E_{\vec{R}_1,...,\vec{R}_N,k}\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n) \tag{2.68}$$

Using the fact that $\{\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)\}_k$ is a complete set of states for fixed $\vec{R}_1,...,\vec{R}_N$, we expand

$$\Phi_E(\vec{R}_1,...,\vec{R}_N,\vec{r}_1,...,\vec{r}_n)=\sum_k \phi_k(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n) \tag{2.69}$$

Now back to (2.67)

$$\left(\sum_{i=1}^{N}\frac{P_i^2}{2M_i}+\sum_{j=1}^{n}\frac{p_j^2}{2m}+V(R_i,r_j)\right)\sum_k \phi_k(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$$

$$=E\sum_k \phi_k(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n) \tag{2.70}$$

The P_i only operates on $\phi_k(\vec{R}_1,...,\vec{R}_N)$ not on $\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$, because $\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$ doesn't know the motion of nuclei, because it comes from (2.68). Thus we have

$$\sum_k \left[\left(\sum_{i=1}^N \frac{P_i^2}{2M_i} + E_{\vec{R}_1,...,\vec{R}_N,k}\right)\phi_k(\vec{R}_1,...,\vec{R}_N)\right]\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$$
$$= E\sum_k \phi_k(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$$

then

$$\left(\sum_{i=1}^N \frac{P_i^2}{2M_i} + E_{\vec{R}_1,...,\vec{R}_N,k}\right)\phi_k(\vec{R}_1,...,\vec{R}_N) = E\phi_k(\vec{R}_1,...,\vec{R}_N) \tag{2.71}$$

$E_{\vec{R}_1,...,\vec{R}_N,k}$ comes from (2.68), which may or may not be exactly solvable. If not, use variational principle to find the approximated minimum energy of $E_{\vec{R}_1,...,\vec{R}_N,k}$ as a function of $(\vec{R}_1,...,\vec{R}_N)$ from the electron problem (2.68). Anyway the E in (2.71) only counts the energy of electron problem $E_{\vec{R}_1,...,\vec{R}_N,k}$ and the kinetic energy of the nuclei $\frac{P_i^2}{2M_i}$, and it doesn't count the distortion energy of the electrons cloud due to the motion of the nuclei, translation or rotation. This whole discussion is known as Hartree-Fock approximation.

One can go beyond Hartree-Fock, instead of (2.69). For each $\phi_k(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)$ term, we add one correction to it

$$\begin{aligned}\phi_k(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n) &= \phi_{k_0}(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k}(\vec{r}_1,...,\vec{r}_n)\\ &\quad + \sum_{k'\neq k_0}\phi_{k'}^{(1)}(\vec{R}_1,...,\vec{R}_N)\psi_{\vec{R}_1,...,\vec{R}_N,k'}(\vec{r}_1,...,\vec{r}_n)\end{aligned}$$

then plug back in (2.67). This will change (2.70) and (2.71).

Lecture 16 (3/24/14)

Example. Hydrogen Molecules

First solve the electron problem, try

$$\psi_\pm(\vec{r}) = N_\pm(\psi_{1s}(\vec{r}) \pm \psi_{1s}(\vec{r}-\vec{R}))$$

then use variational principle. For H_2^+ uses one e^- in the ψ_+ state. For H_2 uses two e^-s in the ψ_+ state with singlet spins. If one uses ψ_- (which looks better than

ψ_+ because it is correct to be antisymmetric), but one finds no bond state.

3 Scattering

We will study two methods: S-matrix approach and Schrodinger stationary wave approach. The former one is like Fermi Golden rule, works for field theory and good for perturbation theory. The latter one does not. But the two methods overlap when angular momentum is conserved, i.e. hard collisions. We will see that in that case and use spherical harmonics, the phase shift will be the same by the 2 methods.

3.1 Differential Cross Section

Recall (1.16)

$$H = H_0 + V$$

and (1.18)

$$U_I(t_f, t_i) = T\left\{e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} V_I(t')dt'}\right\}$$

The strategy is not to treat V as small but as something that can be neglected when the scattering particles are far separated. We will only study $2 \to N$ scattering. Initial state b for beams and t for target. When V is neglected, we get plane waves

$$H_0 \left|\vec{p}_b, \vec{p}_t\right\rangle = \left(\frac{p_b^2}{2m_b} + \frac{p_t^2}{2m_t}\right)\left|\vec{p}_b, \vec{p}_t\right\rangle = E_i \left|\vec{p}_b, \vec{p}_t\right\rangle$$

final state

$$H_0 \left|\vec{p}_1, ..., \vec{p}_N\right\rangle = \left(\sum_{j=1}^{N} \frac{p_j^2}{2m_j}\right)\left|\vec{p}_1, ..., \vec{p}_N\right\rangle = E_f \left|\vec{p}_1, ..., \vec{p}_N\right\rangle$$

and

$$\begin{aligned}\langle\vec{p}_b', \vec{p}_t'|\vec{p}_b, \vec{p}_t\rangle &= \delta^3(\vec{p}_b' - \vec{p}_b)\delta^3(\vec{p}_t' - \vec{p}_t) \\ \langle\vec{p}_1', ..., \vec{p}_N'|\vec{p}_1, ..., \vec{p}_N\rangle &= \prod_{j=1}^{N} \delta^3(\vec{p}_j' - \vec{p}_j)\end{aligned} \tag{3.1}$$

To connect the initial and final states, we define

$$S = \lim_{\substack{t_f \to \infty \\ t_i \to -\infty}} U_I(t_f, t_i)$$

The virtual of this formalism is that for perturbation, where U can be expanded according to the order of H, then do time order.

We also define T matrix, basically S with $\delta(E)\delta(p)$ extracted,

$$\langle \vec{p}_1, ..., \vec{p}_N | S - I | \vec{p}_b, \vec{p}_t \rangle = \delta(E_f - E_i)\delta^3(\vec{p}_f - \vec{p}_i) \langle \vec{p}_1, ..., \vec{p}_N | T | \vec{p}_b, \vec{p}_t \rangle \tag{3.2}$$

The $-I$ term will get rid of unscatterred part of final product. And

$$\vec{p}_i = \vec{p}_t + \vec{p}_b \qquad \vec{p}_f = \sum_{j=1}^{N} \vec{p}_j$$

Then we claim the measurable quantity $d\sigma$ is given by similar to Fermi golden rule cf (1.29),

$$d\sigma = \frac{(2\pi\hbar)^2}{v_b} \prod_{j=1}^{N} (\Delta p_j)^3 \delta(E_f - E_i)\delta^3(\vec{p}_f - \vec{p}_i) \left| \langle \vec{p}_1, ..., \vec{p}_N | T | \vec{p}_b, \vec{p}_t \rangle \right|^2 \tag{3.3}$$

Before we prove this, let's see what $d\sigma$ is. Suppose we have incident beam with flux F and speed v_b moving in one direction, colliding on to the target which has $\vec{\vec{p}}_t = 0$ with respect to the lab frame. By placing spectrometer with high resolution at angle (θ, ϕ), we can measure the final products $\vec{\vec{p}}_j$ go into volume $(\Delta p_j)^3$ in momentum space i.e. with uncertainty Δp_j. So the rate into final volume $(\Delta p_i)^3$ for scattering into final state is

$$F d\sigma \tag{3.4}$$

If we want to integral over a larger volume, there may be problem with interpretation of quantum measurement. Does it take into account of the interference or just adding up momentum?

By (3.4) $d\sigma$ has unit of area. Check that from (3.3)

$$[(3.3)] = \frac{(E \cdot T)^2}{L/T} P^3 \frac{1}{E} \frac{1}{P^3} \underbrace{\frac{1}{P^{3N}} \frac{1}{P^6} E^2 P^6}_{\text{by (3.1)}} = L^2$$

First step in proving (3.3), we write down the transition probability

$$\begin{aligned} P_{i \to f} &= \left| \left\langle f_1, ..., f_N \left| \underbrace{e^{iH_0 t_f/\hbar} \underbrace{U(t_f, t_i)}_{H_0+V} e^{-iH_0 t_i/\hbar}}_{U_I = S} \right| \psi_b, \psi_t \right\rangle \right|^2 \\ &= \left| \prod_{j=1}^{N} \int d^3 p_j \tilde{f}_j(p_j) \int d^3 p_b \int d^3 p_t \tilde{\psi}_t(p_t) \tilde{\psi}_b(p_b) \delta(E_f - E_i) \delta^3(\vec{p}_f - \vec{p}_i) \right. \\ &\qquad \left. \langle \vec{p}_1, ..., \vec{p}_N | T | \vec{p}_b, \vec{p}_t \rangle \right|^2 \qquad (3.5) \end{aligned}$$

$\tilde{}$ means Fourier transform. We choose to evaluate it in Fourier which is similar to what we did in (1.21) and (1.46). That is because in the above expression we have introduced target and beam wave functions at the time collision happens

$$\psi_t(\vec{r}_t) \qquad \psi_b(\vec{r}_b)$$

that both are localized around $\vec{r} = 0$ and have accurate momenta with average

$$\vec{\bar{p}}_t = 0 \qquad \vec{\bar{p}}_b = \bar{p}_b \hat{z}$$

For the final state particles, we introduce wave function $\tilde{f}_j(p_j)$ which are sharply peaked about $\vec{\bar{p}}_j$ and localized at $\vec{r}_j = 0$. Hence all wave functions are on top of each other.

First deal with final states. Assume that in the integral (3.5) any function F that has p_j argument behind $\tilde{f}_j(p_j)$ can be replaced by $\bar{p}_j$ because $\tilde{f}_j(p_j)$ is sharply peaked about $\vec{\bar{p}}_j$. That is

$$(3.5) \to \int d^3p_j \tilde{f}_j(p_j)F(\vec{\bar{p}}_j) = \int d^3p_j \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r_j f_j(r_j) e^{-i\vec{p}_j\cdot\vec{r}_j} F(\vec{\bar{p}}_j) = (2\pi\hbar)^{3/2} f_i(0) F(\vec{\bar{p}}_j)$$

or more carefully put

$$\tilde{f}_j(r_j) \sim e^{\frac{(p_j-\bar{p}_j)^2}{(\Delta p_j)^2}}$$

then

$$\int d^3p_j \tilde{f}_j(p_j) F(\vec{\bar{p}}_j) = (\Delta p_j)^{3/2} F(\vec{\bar{p}}_j)$$

In other words

$$(3.5) \quad = \quad \prod_{j=1}^{N} (\Delta p_j)^3 \left| \int d^3p_b \int d^3p_t \tilde{\psi}_t(\vec{p}_t)\tilde{\psi}_b(\vec{p}_b)\delta(\bar{E}_f - E_i)\delta^3(\vec{\bar{p}}_f - \vec{p}_i) \langle \vec{\bar{p}}_1, ..., \vec{\bar{p}}_N | T | \vec{p}_b, \vec{p}_t \rangle \right|^2 \quad (3.6)$$

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The $\delta(\bar{E}_f - E_i)$ part requires some work. Suppose

$$\vec{p}_b = (\vec{p}_b)_\perp + p_b^z \hat{z}$$

then

$$E_b = \frac{(\vec{p}_b)_\perp^2 + (\vec{p}_b)_z^2}{2m_b} = \frac{(\vec{p}_b)_z^2}{2m_b}$$

Thus

$$\delta(\bar{E}_f - E_i) = \delta(\bar{E}_f - \frac{(\vec{p}_b)_z^2}{2m_b} - \underbrace{\frac{(\vec{\bar{p}}_f - \vec{p}_b)^2}{2m_t}}_{\approx 0}) = \delta(p_b^z - \sqrt{2m_b E_f}) \underbrace{\frac{1}{\frac{\sqrt{2m_b E_f}}{m_b}}}_{\frac{1}{v_b}}$$

so we compute (3.6)

$$\left| \int d^3p_b \int d^3p_t \tilde{\psi}_t(\vec{p}_t)\tilde{\psi}_b(\vec{p}_b)\delta(\bar{E}_f - E_i)\delta^3(\vec{\bar{p}}_f - \vec{p}_i) \right|^2 \quad (3.7)$$

$$= \left| \int d^2p_b^\perp \tilde{\psi}_t(\vec{\bar{p}}_f^\perp - \vec{p}_b^\perp, \bar{p}_f^z\hat{z} - \sqrt{2m_b E_f}\hat{z}) \tilde{\psi}_b(\vec{p}_b^\perp, \vec{p}_b^z = \hat{z}\sqrt{2m_b E_f}) \frac{1}{v_b} \right|^2$$

so $\tilde{\psi}_t$ and $\tilde{\psi}_b$ in RHS of (3.7) are only functions of $\vec{p}_b^\perp$, and they look like convolution.

Using convolution theorem

$$\int \tilde{f}_1(P)\tilde{f}_2(p-P)dP = \sqrt{2\pi\hbar}[\widetilde{f_1(x)f_2(x)}](p)$$

Proof

$$\text{LHS} = \int dP \int dx_1 f_1(x_1)\frac{e^{-iPx_1/\hbar}}{\sqrt{2\pi\hbar}} \int dx_2 f_2(x_2)\frac{e^{-i(p-P)x_2/\hbar}}{\sqrt{2\pi\hbar}} = \int dx f_1(x)f_2(x)e^{-ipx/\hbar} = \text{RHS}$$

QED.

So

$$\text{RHS of (3.7)} \quad = \quad \left(\frac{2\pi\hbar}{v_b}\right)^2 \left| \int d^2r^\perp \psi_t(\vec{r}^\perp, \widetilde{\bar{p}_f^z - p_b^z})\psi_b(\vec{r}^\perp, \widetilde{p_b^z})\frac{e^{-i\vec{p}_b^\perp \cdot \vec{r}_b^\perp/\hbar}}{2\pi\hbar}\right|^2 \quad (3.8)$$

This shows beautifully that if $\psi_t(\vec{r}_t^\perp, \widetilde{\bar{p}_f^z - p_b^z})\psi_b(\vec{r}_b^\perp, \widetilde{p_b^z}) = 0$ i.e. not overlapped when in the argument $\vec{r}_t^\perp = \vec{r}_b^\perp$ are the same, they will not collide to each other. So the probability is 0. (3.8) is a function of p_b^z and $\vec{p}_b^\perp$, and we know $p_b^z = \sqrt{2m_b E_f}$, so if we add integral $\int E_b \int d^3p_f$ and $\delta(E_f - E_i)\delta^3(\vec{p}_f - \vec{p}_i)$ to (3.8), we change nothing.

$$\int dE_b \int d^3p_f \left| \int d^2r^\perp \psi_t(\vec{r}^\perp, \widetilde{\bar{p}_f^z - p_b^z})\psi_b(\vec{r}^\perp, \widetilde{p_b^z})\frac{e^{-i\vec{p}_b^\perp \cdot \vec{r}_b^\perp/\hbar}}{2\pi\hbar}\right|^2 \delta(E_f - E_i)\delta^3(\vec{p}_f - \vec{p}_i)$$

and pretend that in the delta functions $E_f = \bar{E}_f$, $\vec{p}_f = \vec{\bar{p}}_f$ as we derived before, so $\int E_f \int d^3p_f$ as only on the square, so we can now use Parseval, i.e.

$$\int |f(x)|^2 dx = \int \left|\tilde{f}(p)\right|^2 dp$$

so

$$\int dp_b^z \underbrace{\frac{dE_b}{dp_b^z}}_{v_b} \int dp^z \int d^2p^\perp \left| \underbrace{\int d^2r^\perp \psi_t(\vec{r}^\perp, \widetilde{p_f^z - p_b^z}) \psi_b(\vec{r}^\perp, \widetilde{p_b^z}) \frac{e^{-i\vec{p}_b^\perp \cdot \vec{r}_b^\perp/\hbar}}{2\pi\hbar}}_{F(p_f^z, p_b^z, \vec{p}_b^\perp)} \right|^2$$

$$= v_b \underbrace{\int d^3r \left|\psi_t(\vec{r}^\perp, r_t^z)\right|^2}_{1} \underbrace{\int dz_b \left|\psi_t(\vec{r}^\perp, r_b^z)\right|^2}_{1/A}$$

$1/A$ means the area perpendicular to the incident flux that contributes to the transition probability $P_{i\to f}$, therefore

$$P_{i\to f} = \frac{(2\pi\hbar)^2}{v_b} \prod_{j=1}^{N} (\Delta p_j)^3 \delta(E_f - E_i) \delta^3(\vec{p}_f - \vec{p}_i) \left|\langle \vec{p}_1, ..., \vec{p}_N | T | \vec{p}_b, \vec{p}_t \rangle\right|^2 \frac{1}{A}$$

Since

$$d\sigma = AP_{i\to f}$$

we proved (3.3).

3.2 Example: Rutherford Scattering

Suppose incident beam has mass m, charge e, with momenta p, and the target has mass M, charge Ze, with momenta P, After the scattering same particles come out with momenta p', P'. Let r, R be the position of the beam and target. To use (3.3), we need to compute T or S matrix.

$$\left\langle p', P' \middle| T \left\{ e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} V_I(t')dt'} \right\} \middle| p, P \right\rangle \tag{3.9}$$

$$V_I = e^{iH_0t/\hbar} V e^{-iH_0t/\hbar} = e^{iH_0t/\hbar} \frac{Ze^2}{\left|\vec{R} - \vec{r}\right|} e^{-iH_0t/\hbar}$$

1st order perturbation

$$
\begin{aligned}
(3.9) \quad &= -\frac{i}{\hbar}\left\langle p', P'\left|\int dt \frac{Ze^2}{\left|\vec{R}-\vec{r}\right|} e^{-i(E_i-E_f)t/\hbar}\right| p, P\right\rangle \\
&= -i2\pi\delta(E_f-E_i)Ze^2 \int d^3R \int d^3r \frac{e^{-i\vec{p}'\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} \frac{e^{-i\vec{P}'\vec{R}/\hbar}}{(2\pi\hbar)^{3/2}} \frac{1}{\left|\vec{R}-\vec{r}\right|} \frac{e^{i\vec{p}\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} \frac{e^{i\vec{P}\vec{R}/\hbar}}{(2\pi\hbar)^{3/2}}
\end{aligned}
$$

Put

$$\vec{p}_i = \vec{p} + \vec{P} \quad \vec{p}_f = \vec{p}' + \vec{P}' \quad \tilde{r} = \vec{r} - \vec{R}$$

then

$$
\begin{aligned}
(3.9) \quad &= \frac{-i2\pi\delta(E_i-E_f)Ze^2}{(2\pi\hbar)^6} \underbrace{\int d^3R e^{i\vec{R}(\vec{p}_i-\vec{p}_f)/\hbar}}_{(2\pi\hbar)^3\delta^3(\vec{p}_i-\vec{p}_f)} \underbrace{\int d^3\tilde{r}\frac{1}{|\tilde{r}|} e^{i\tilde{r}(\vec{p}-\vec{p}')/\hbar}}_{\frac{4\pi}{\left(\frac{\vec{p}-\vec{p}'}{\hbar}\right)^2}} \\
&= \underbrace{-i\frac{Ze^2}{\pi\hbar}\frac{1}{(\vec{p}-\vec{p}')^2}}_{\langle p', P'|T|p, P\rangle} \delta(E_i-E_f)\delta^3(\vec{p}_i-\vec{p}_f)
\end{aligned}
$$

So

$$
\begin{aligned}
d\sigma &= \frac{(2\pi\hbar)^2}{v_b} d^3p' d^3P' \delta(E_i-E_f)\delta^3(\vec{p}_i-\vec{p}_f) \frac{Z^2e^4}{(\pi\hbar)^2} \frac{1}{|\vec{p}-\vec{p}'|^4} \\
&= \frac{4Z^2e^4}{v_b} d^3p' d^3P' \delta(E_i-E_f)\delta^3(\vec{p}_i-\vec{p}_f) \frac{1}{|\vec{p}-\vec{p}'|^4}
\end{aligned}
$$

$\hbar$ is nicely gone, we get a classical result.

Suppose we want to measure cross section of the scattering beam p'. Integrating over d^3P' gets rid of $\delta^3(\vec{p}_i - \vec{p}_f)$, then write

$$d^3p' = p'^2 d\Omega dp'$$

so $d\Omega$ is the measuring angle, we also integrate over dp', so

$$d\sigma = \frac{4Z^2e^4 d\Omega}{v_b}\int dp'\delta(\frac{p'^2}{2m} - \frac{p^2}{2m} + \underbrace{\frac{P'^2}{2M} - \frac{(\vec{p}' + \vec{P}' - \vec{p})^2}{2M}}_{\approx 0})\frac{p'^2}{|\vec{p} - \vec{p}'|^4}$$

assuming $M \gg m$. Then essentially the delta function says

$$|\vec{p}| = |\vec{p}'| \tag{3.10}$$

so

$$\frac{d\sigma}{d\Omega} = \frac{4Z^2e^4}{v_b^2}\frac{p^2}{|\vec{p} - \vec{p}'|^4}$$

another v_b comes from the delta function. Combining (3.10) and some simple geometry, we can show if θ is the scattering angle between $\vec{p}$ and $\vec{p}'$

$$|\vec{p} - \vec{p}'| = 2p\sin\frac{\theta}{2}$$

so $p = v_b m$

$$\frac{d\sigma}{d\Omega} = \frac{Z^2e^4m^2}{4p^4\sin^4\frac{\theta}{2}} \tag{3.11}$$

Positron Scatters a Hydrogen Atom

Lecture 18 (4/2/14)

A second example. Consider elastic scattering of a positron from a hydrogen atom

$$H = \underbrace{\frac{P^2}{2M} + \frac{p_-^2}{2m} + \frac{p_+^2}{2m} - \frac{e^2}{|r_- - R|}}_{H_0} + \underbrace{\frac{e^2}{|r_+ - R|} - \frac{e^2}{|r_+ - r_-|}}_{V}$$

P,M, R for proton, p_-, r_- for electron, and p_+, r_+ for positron. In H_0, the states of atom and positron are separated.

Similar to (3.9), we do 1st order perturbation

$$\left\langle 1s(\vec{P}'_{atom}), \vec{p}'_+ \middle| -\frac{i}{\hbar}\int dte^{-i(E_i - E_f)t/\hbar}\left(\frac{e^2}{\left|\vec{r}_+ - \vec{R}\right|} - \frac{e^2}{|\vec{r}_+ - \vec{r}_-|}\right)\middle| 1s(\vec{P}_{atom}), \vec{p}_+\right\rangle$$

$$= -i\delta(E_i - E_f)\int d^3R\int d^3r_-\int d^3r_+\frac{e^{-\left|\vec{r}_- - \vec{R}\right|/a_0}}{\sqrt{\pi}a_0^{3/2}}\frac{e^{-i\vec{p}'_{atom}R_{COM}/\hbar}}{(2\pi\hbar)^{3/2}}\frac{e^{-i\vec{p}'_+\vec{r}_+/\hbar}}{(2\pi\hbar)^{3/2}}$$
$$\left(\frac{e^2}{\left|\vec{r}_+ - \vec{R}\right|} - \frac{e^2}{|\vec{r}_+ - \vec{r}_-|}\right)\frac{e^{-\left|\vec{r}_- - \vec{R}\right|/a_0}}{\sqrt{\pi}a_0^{3/2}}\frac{e^{i\vec{p}_{atom}R_{COM}/\hbar}}{(2\pi\hbar)^{3/2}}\frac{e^{i\vec{p}_+\vec{r}_+/\hbar}}{(2\pi\hbar)^{3/2}} \tag{3.12}$$

where
$$R_{COM} = \frac{\vec{r}_- m + \vec{R}M}{m+M}$$

Let $\vec{r} = \vec{r}_- - \vec{R}$, $\tilde{r} = \vec{r}_+ - \vec{R}$,

$$R_{COM} = \frac{\vec{r}m}{m+M} + \vec{R}$$

So

$$(3.12) = -i\delta(E_i - E_f)\int d^3R\int d^3\vec{r}\int d^3\tilde{r}\frac{e^{-2|\vec{r}|/a_0}}{\pi a_0^3}\frac{e^{i(\overbrace{-\vec{p}'_{atom} + \vec{p}_{atom} - \vec{p}'_+ + \vec{p}_+}^{-\vec{p}_f+\vec{p}_i})R/\hbar}}{(2\pi\hbar)^3}$$
$$\left(\frac{e^2}{|\tilde{r}|} - \frac{e^2}{|\vec{r}-\tilde{r}|}\right)\frac{e^{i(\vec{p}_{atom}-\vec{p}'_{atom})\vec{r}m/(m+M)\hbar}}{(2\pi\hbar)^{3/2}}\frac{e^{i(\vec{p}_+-\vec{p}'_+)\tilde{r}/\hbar}}{(2\pi\hbar)^{3/2}}$$
$$= \frac{-i\delta(E_i - E_f)\delta(\vec{p}_f - \vec{p}_i)}{(2\pi\hbar)^3}\int d^3\vec{r}\int d^3\tilde{r}\left(\frac{e^2}{|\tilde{r}|} - \frac{e^2}{|\vec{r}-\tilde{r}|}\right)\frac{e^{-2|\vec{r}|/a_0}}{\pi a_0^3}$$
$$e^{i(\vec{p}_+-\vec{p}'_+)(\tilde{r}-\overbrace{\vec{r}m/(m+M)}^{\approx 0})/\hbar}$$

Let $\check{r} = \tilde{r} - \vec{r}$

$$(3.12) = \frac{-i\delta(E_i - E_f)\delta(\vec{p}_f - \vec{p}_i)}{(2\pi\hbar)^3}\int d^3\tilde{r}\underbrace{\int d^3\vec{r}\frac{e^{-2|\vec{r}|/a_0}}{\pi a_0^3}}_{1}\frac{e^2}{|\tilde{r}|}e^{i(\vec{p}_+-\vec{p}'_+)\tilde{r}/\hbar}$$
$$-\frac{-i\delta(E_i - E_f)\delta(\vec{p}_f - \vec{p}_i)}{(2\pi\hbar)^3}\int d^3\check{r}\underbrace{\int d^3\vec{r}\frac{e^{-2|\vec{r}|/a_0}}{\pi a_0^3}e^{i(\vec{p}_+-\vec{p}'_+)\vec{r}/\hbar}}_{\frac{1}{\left(1+\frac{\left|\vec{p}_+-\vec{p}'_+\right|^2 a_0^2}{4\hbar^2}\right)^2}}\frac{e^2}{|\check{r}|}e^{i(\vec{p}_+-\vec{p}'_+)\check{r}/\hbar}$$

$$\left\langle 1s(\vec{P}'_{atom}),\vec{p}'_+\middle|T\middle|1s(\vec{P}_{atom}),\vec{p}_+\right\rangle = \frac{-ie^2}{(2\pi\hbar)^3}\frac{4\pi}{\left(\frac{|\vec{p}_+-\vec{p}'_+|}{\hbar}\right)^2}\left(1-\frac{1}{\left(1+\frac{|\vec{p}_+-\vec{p}'_+|^2 a_0^2}{4\hbar^2}\right)^2}\right)$$

thus differential cross section of the e^+ is

$$\frac{d\sigma}{d\Omega} = \frac{e^4 m^2}{(4\pi)^2 p^4 \sin^4\frac{\theta}{2}}\left(1-\frac{1}{\left(1+\frac{|\vec{p}_+-\vec{p}'_+|^2 a_0^2}{4\hbar^2}\right)^2}\right)^2$$

3.3 Stationary State Scattering

Let us consider the same situation. A plane wave beam $e^{i\vec{p}\cdot\vec{r}/\hbar}$ with momentum $\vec{p}$ coming in strikes the target. Later we will do wave packet. We want to turn the differential equation

$$(H_0+V)|\psi\rangle = E|\psi\rangle \tag{3.13}$$

into an integral equation, see below. The step is the following. Write

$$(E-H_0)|\psi\rangle = V|\psi\rangle$$

Propose

$$\left|\psi^{in}_{\vec{p}}\right\rangle = e^{i\vec{p}\cdot\vec{r}/\hbar} + \frac{V}{E-H_0}\left|\psi^{in}_{\vec{p}}\right\rangle \tag{3.14}$$

known as Lippmann–Schwinger equation. And $\psi^{in}_{\vec{p}}$ is called in-state Schrodinger equation solution, because those $\left|\psi^{in}_{\vec{p}}\right\rangle$ are the eigenfunctions to (3.13). As we will see, they have a special property that incoming plane wave momentum $|\vec{p}|$ is equal to outgoing spherical wave momentum $|\vec{p}'|$

We have

$$\begin{aligned}\psi^{in}_{\vec{p}}(\vec{r}) = \left\langle\vec{r}\middle|\psi^{in}_{\vec{p}}\right\rangle &= \underbrace{e^{i\vec{p}\cdot\vec{r}/\hbar}}_{\text{incoming/unscattered wave}} + \left\langle\vec{r}\middle|\frac{V(\vec{r})}{E-H_0}\middle|\psi^{in}_{\vec{p}}\right\rangle \\ &= e^{i\vec{p}\cdot\vec{r}/\hbar} + \int d^3r'\left\langle\vec{r}\middle|\frac{1}{E-H_0}\middle|\vec{r}'\right\rangle V(\vec{r}')\underbrace{\left\langle\vec{r}'\middle|\psi^{in}_{\vec{p}}\right\rangle}_{\psi^{in}_{\vec{p}}(\vec{r}')} \end{aligned} \tag{3.15}$$

Since $H_0 = \frac{p^2}{2m}$, we can compute

$$\left\langle \vec{r} \middle| \frac{1}{E - H_0} \middle| \vec{r}' \right\rangle$$

by putting in $\int d^3p \, |\vec{p}\rangle \langle \vec{p}|$.

$$\left\langle \vec{r} \middle| \frac{1}{E - H_0} \middle| \vec{r}' \right\rangle = \int d^3p \frac{1}{(2\pi\hbar)^3} \frac{e^{i\vec{p}\cdot(\vec{r}-\vec{r}')/\hbar}}{E - \frac{p^2}{2m}}$$

Do complex integral of p, choose $\hat{z}$ in $\vec{r} - \vec{r}'$ direction,

$$\begin{aligned} \left\langle \vec{r} \middle| \frac{1}{E - H_0} \middle| \vec{r}' \right\rangle &= \frac{2\pi}{(2\pi\hbar)^3} \int_{-1}^{1} d\cos\theta \int_0^\infty p^2 dp \frac{e^{ip|\vec{r}-\vec{r}'|\cos\theta/\hbar}}{E - \frac{p^2}{2m}} \\ &= \frac{2\pi\hbar}{(2\pi\hbar)^3 i \, |\vec{r} - \vec{r}'|} \int_{-\infty}^{\infty} pdp \frac{e^{ip|\vec{r}-\vec{r}'|/\hbar}(-2m)}{(p - \sqrt{2mE})(p + \sqrt{2mE})} \end{aligned}$$

The exponent $e^{ip|\vec{r}-\vec{r}'|/\hbar}$ enforces to close the contour upper half plane, and to avoid cross the poles, we need to shift the pole

$$\left\langle \vec{r} \middle| \frac{1}{E - H_0} \middle| \vec{r}' \right\rangle = \frac{2\pi\hbar}{(2\pi\hbar)^3 i \, |\vec{r} - \vec{r}'|} \int_{-\infty}^{\infty} pdp \frac{e^{ip|\vec{r}-\vec{r}'|/\hbar}(-2m)}{[p - (\sqrt{2mE} + i\epsilon)][p - (-\sqrt{2mE} - i\epsilon)]}$$

As we will see, such choose of $i\epsilon$ prescription will give the outgoing scattering wave, i.e. only to enclose $\sqrt{2mE}$ pole

$$\begin{aligned} \left\langle \vec{r} \middle| \frac{1}{E - H_0} \middle| \vec{r}' \right\rangle &= (2\pi i) \frac{2\pi\hbar}{(2\pi\hbar)^3 i \, |\vec{r} - \vec{r}'|} (-2m) \sqrt{2mE} \frac{e^{i\sqrt{2mE}|\vec{r}-\vec{r}'|/\hbar}}{2\sqrt{2mE}} \\ &= -\frac{2\pi m}{(2\pi\hbar)^2} \frac{e^{i\sqrt{2mE}|\vec{r}-\vec{r}'|/\hbar}}{|\vec{r} - \vec{r}'|} \end{aligned}$$

Put it back to (3.15), so this acts like a kernel

$$\psi_{\vec{p}}^{in}(\vec{r}) = e^{i\vec{p}\cdot\vec{r}/\hbar} - \frac{m}{2\pi\hbar^2} \int d^3r' \frac{e^{ip|\vec{r}-\vec{r}'|/\hbar}}{|\vec{r} - \vec{r}'|} V(\vec{r}') \psi_{\vec{p}}^{in}(\vec{r}')$$

where

$$|\vec{p}| = \sqrt{2mE}$$

To solve for $\psi^{in}_{\vec{p}}(\vec{r})$, one typically rewrite the integral iteratively, which becomes power series in V, known as Born approximation. Before we demonstrate that, we would like to examine the large r behavior of $\psi^{in}_{\vec{p}}(\vec{r})$, since $V(r')$ is non-zero for small r', so we have $r \gg r'$

For $|\vec{r}-\vec{r}'|$ in the exponent,

$$|\vec{r}-\vec{r}'| = \sqrt{(\vec{r}-\vec{r}')(\vec{r}-\vec{r}')} \to r(1-\frac{2\hat{r}\cdot\vec{r}'}{r})^{1/2} = r - \hat{r}\cdot\vec{r}'$$

For $|\vec{r}-\vec{r}'|$ in the denominator

$$|\vec{r}-\vec{r}'| \to r$$

so

$$\psi^{in}_{\vec{p}}(\vec{r}) \sim e^{i\vec{p}\cdot\vec{r}/\hbar} + \frac{e^{ipr/\hbar}}{r}\underbrace{\left(-\frac{m}{2\pi\hbar^2}\int d^3r' e^{-i\vec{p}'\cdot\vec{r}'/\hbar}V(\vec{r}')\psi^{in}_{\vec{p}}(\vec{r}')\right)}_{\equiv f(\theta,\phi)} \quad \text{for large } r \tag{3.16}$$

where $\vec{p}' = p\hat{r}$. $f(\theta,\phi)$ doesn't depend on r, so it is the scattering amplitude of the outgoing spherical wave.

Lecture 19 (4/7/14)

First we derive a relation between scattering amplitude and differential cross section

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 \tag{3.17}$$

We use wave packets

$$\psi_{\bar{\vec{p}}}(\vec{r},t) = \int d^3p\psi^{in}_{\vec{p}}(\vec{r})\tilde{F}(\vec{p})e^{-i\frac{p^2}{2m}t/\hbar}$$

Recall both plane wave and spherical wave are solutions to the free Hamiltonian (to the lowest order for spherical wave), so they have a common time evolution part $e^{-i\frac{p^2}{2m}t/\hbar}$. And $\tilde{F}(\vec{p})$ is a Gaussian centered at $\bar{\vec{p}}$ with width Δp at $t=0$

$$\tilde{F}(\vec{p}) = \left(\frac{1}{\Delta p\sqrt{\pi}}\right)^{3/2} e^{-\frac{(\vec{p}-\bar{\vec{p}})^2}{2(\Delta p)^2}}$$

For $t \gg 1$, $e^{-i\frac{p^2}{2m}t/\hbar}$ oscillates rapidly and the stationary phase dominates, i.e. the exponents

$$e^{i\vec{p}\cdot\vec{r}/\hbar}e^{-i\frac{p^2}{2m}t/\hbar} \text{ and } \frac{e^{ipr/\hbar}}{r}e^{-i\frac{p^2}{2m}t/\hbar}$$

vanish, so the spherical wave looks like a spherical shell with approximate radial location given by

$$\nabla_p(\frac{pr}{\hbar} - \frac{p^2}{2m\hbar}t)_{p=|\bar{\vec{p}}|} = 0$$

or

$$\bar{r} = t\frac{\bar{p}}{m} = vt \tag{3.18}$$

Likewise one can check for $t \ll -1$, not yet strike target, only plane wave. It is also dominated by the stationary phase condition, given by

$$\nabla_p(\frac{\vec{p}\cdot\vec{r}}{\hbar} + -\frac{p^2}{2m\hbar}t)_{p=|\bar{\vec{p}}|} = 0$$

or

$$\vec{r} = t\frac{\bar{\vec{p}}}{m}$$

agreeing behavior of a classical wave packet.

Next we compute the probability, dP, of finding the scattered particle coming outward from the scattering center within solid angle $d\Omega$, for large r

$$dP = \int_0^\infty \left|\psi_{\bar{\vec{p}}}(\vec{r},t)\_\text{only scattering part}\right|^2 r^2 dr d\Omega$$

or

$$\frac{dP}{d\Omega} = \int_0^\infty \left|\int d^3p\frac{e^{ipr/\hbar}}{r}\tilde{F}(\vec{p})f(\theta,\phi)e^{-i\frac{p^2}{2m}t/\hbar}\right|^2 r^2 dr$$

Since the Gaussian spans a very small range, we assume $f(\theta,\phi)$ is constant of p.

We decompose $\vec{p}$ in to direction parallel to the incoming beam p_z and perpendicular direction $p_\perp$. That is

$$p = \sqrt{p_z^2 + p_\perp^2} = p_z = \bar{p}_z + \delta p_z$$

where $\bar{p}_z \hat{z} = \bar{\vec{p}}$. And

$$d^3p = d\delta p_z d^2 p_\perp$$

Thus

$$\begin{aligned}
\frac{dP}{d\Omega} &= \int_0^\infty \left| \int d^3p e^{ipr/\hbar} \tilde{F}(p_z, p_\perp) f(\theta,\phi) e^{-i\frac{p^2}{2m}t/\hbar} \right|^2 dr \\
&= |f(\theta,\phi)|^2 \int_0^\infty \left| \int d\delta p_z \int d^2p_\perp e^{ipr/\hbar} \tilde{F}(p_z, p_\perp) e^{-i\frac{\bar{\vec{p}}^2}{2m}t/\hbar} \right|^2 dr \\
&= |f(\theta,\phi)|^2 \int_0^\infty \left| \int d\delta p_z \int d^2p_\perp e^{ipr/\hbar} \tilde{F}(p_z, p_\perp) \right|^2 dr
\end{aligned}$$

$\int d\delta p_z \int d^2p_\perp e^{ipr/\hbar} \tilde{F}(p_z, \vec{p}_\perp)$ is the inverse Fourier transform,

$$\vec{p}_\perp \to \vec{r}_\perp = 0$$

because $|\vec{p}_\perp| \ll p$,

$$p_z \to \delta r = r - vt$$

because of (3.18). Therefore

$$\frac{dP}{d\Omega} = |f(\theta,\phi)|^2 \int_0^\infty dr\, |F(r - vt, \vec{r}_\perp = 0)|^2$$

On the hand by the definition of cross section

$$dP = d\sigma \int_0^\infty dr\, |F(r - vt, \vec{r}_\perp = 0)|^2$$

because the probability for incident particle striking a cross sectional area $d\sigma$ located at the origin is the probability of finding the incident particle in a small cylinder of cross sectional area $d\sigma$ parallel to $\bar{\vec{p}}$ extending throughout the wave function, which is $\int_0^\infty dr\, |F(r - vt, \vec{r}_\perp = 0)|^2$, thus we proved (3.17).

Lecture 20 (4/9/14)

We now use (3.17) to re derive Rutherford scattering in a much simpler way. From (3.16), we compute $f(\theta,\phi)$ assume potential

$$V = \frac{Ze^2}{|\vec{r}|}$$

is small, we use 1st Born approximation, i.e. plugging $\psi^{in}_{\vec{p}}(\vec{r}') = e^{i\vec{p}\cdot\vec{r}/\hbar}$ into the integral

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int d^3r' e^{-i\vec{p}'\cdot\vec{r}'/\hbar}\frac{Ze^2}{|\vec{r}'|}e^{i\vec{p}\cdot\vec{r}'/\hbar} \tag{3.19}$$

with $|\vec{p}'| = |\vec{p}|$. Recall

$$\nabla^2\frac{1}{|\vec{r}|} = -4\pi\delta^3(\vec{r})$$

Do (3.19) integration by part twice,

$$\int d^3r' e^{i(\vec{p}-\vec{p}')\cdot\vec{r}'/\hbar}\frac{1}{|\vec{r}'|} = -\frac{\hbar}{i(\vec{p}-\vec{p}')}\int d^3r' e^{i(\vec{p}-\vec{p}')\cdot\vec{r}'/\hbar}\nabla_{\vec{r}'}\frac{1}{|\vec{r}'|} = \left(\frac{\hbar}{i(\vec{p}-\vec{p}')}\right)^2(-4\pi)$$

so

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\frac{4\pi\hbar^2}{(\vec{p}-\vec{p}')^2}Ze^2$$

which gives same (3.11).

This slows that the 2 methods have same common properties. We shall explore this more.

3.4 Partial Wave Expansion

Assume

$$V(\vec{r}) = V(|\vec{r}|) \tag{3.20}$$

which is a generalization of Rutherford scattering. So we have rotation symmetric, i.e. conservation of angular momentum.

We solve

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi^{in}_{\vec{p}}(\vec{r}) = E\psi^{in}_{\vec{p}}(\vec{r})$$

Express in spherical harmonics

$$\psi^{in}_{\vec{p}}(\vec{r}) = \sum_{l=0}^{\infty} c_{E,l}u_{E,l}(r)Y_{l0}(\theta) \tag{3.21}$$

no ϕ dependence because no ϕ dependence in V and no ϕ dependence in the incident beam, plane wave coming in $\hat{z}$ direction. And θ in the formula above is the azimuthal angle.

The radial Schrodinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right) u_{E,l}(r) = E u_{E,l}(r)$$

is solved by

$$j_l(kr) \quad n_l(kr)$$

for large r, $V(r) = 0$. And $k = p/\hbar$. Rayleigh's formulas give

$$\text{spherical Bessel functions } j_l(z) = (-z)^l (\frac{1}{z}\frac{d}{dz})^l \frac{\sin z}{z}$$

$$\text{spherical Neumann functions } n_l(z) = -(-z)^l (\frac{1}{z}\frac{d}{dz})^l \frac{\cos z}{z}$$

	small z (irrelevant now)	large z
$j_l(z)$	$\frac{2^l}{(2l+1)!}z^l$	$\frac{1}{z}\sin(z - \frac{\pi l}{2})$
$n_l(z)$	$\frac{-1\cdot 3\cdot \ldots \cdot (2l+1)}{(2l+1)!}\frac{1}{z^{l+1}}$	$-\frac{1}{z}\cos(z - \frac{\pi l}{2})$

Although n_l is irregular at the origin, we use them anyway, because we are only interested in large z solution. The actual $u_{E,l}$ is linear combination

$$u_{E,l} = j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l \tag{3.22}$$

for some constant δ_l. So for large r,

$$u_{E,l} \sim \frac{\sin(kr + \delta_l - \frac{\pi l}{2})}{kr} \tag{3.23}$$

Let's equate (3.21) and (3.16) in hoping to eliminate $c_{E,l}$ and find a relation between δ_l and $f(\theta, \phi)$

$$\psi_{\vec{p}}^{in}(\vec{r}) \sim \sum_{l=0}^{\infty} c_{E,l}\frac{\sin(kr + \delta_l - \frac{\pi l}{2})}{kr} Y_{l0}(\theta) = e^{i\vec{p}\cdot\vec{r}/\hbar} + \frac{e^{ipr/\hbar}}{r} f(\theta, \phi) \tag{3.24}$$

Since

$$Y_{l0} = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

we would like to express $e^{i\vec{p}\cdot\vec{r}/\hbar}$ in terms of P_l. By another Rayleigh Formula

$$\begin{aligned} e^{i\vec{p}\cdot\vec{r}/\hbar} &= e^{ipr\cos\theta/\hbar} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta) \\ &\sim \sum_{l=0}^{\infty}(2l+1)i^l \frac{\sin(kr-\frac{\pi l}{2})}{kr}P_l(\cos\theta) \end{aligned} \tag{3.25}$$

We rewrite (3.24) in two parts: incoming + outgoing waves (including scattering & reflected), and notice $\frac{e^{ipr/\hbar}}{r}f(\theta,\phi)$ has only outgoing part.

$$\begin{aligned} &\underbrace{\sum_{l=0}^{\infty} c_{E,l}\frac{e^{i(kr+\delta_l-\frac{\pi l}{2})}}{2ikr}\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)}_{\text{outgoing}}+\underbrace{\sum_{l=0}^{\infty} c_{E,l}\frac{-e^{-i(kr+\delta_l-\frac{\pi l}{2})}}{2ikr}\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)}_{\text{incoming}} \\ &= \underbrace{\sum_{l=0}^{\infty}(2l+1)i^l\frac{e^{i(kr-\frac{\pi l}{2})}}{2ikr}P_l(\cos\theta)+\frac{e^{ikr}}{r}f(\theta,\phi)}_{\text{outgoing}}+\underbrace{\sum_{l=0}^{\infty}(2l+1)i^l\frac{-e^{-i(kr-\frac{\pi l}{2})}}{2ikr}P_l(\cos\theta)}_{\text{incoming}} \end{aligned} \tag{3.26}$$

Assuming momentum conservation (or mathematically $P_l(\cos\theta)$ are orthogonal functions), so each coefficient must equal. We have from the incoming part

$$c_{E,l}e^{-i(kr+\delta_l-\frac{\pi l}{2})}\sqrt{\frac{2l+1}{4\pi}} = (2l+1)i^l e^{-i(kr-\frac{\pi l}{2})}$$

so

$$c_{E,l}\sqrt{\frac{2l+1}{4\pi}} = (2l+1)i^l e^{i\delta_l} = (2l+1)e^{i(\delta_l+\frac{\pi l}{2})}$$

Plugging this to the outgoing part

$$f(\theta,\phi) = \sum_{l=0}^{\infty}\frac{e^{i(2\delta_l)}-1}{2ik}(2l+1)P_l(\cos\theta) = \frac{1}{k}\sum_{l=0}^{\infty}e^{i\delta_l}\sin\delta_l(2l+1)P_l(\cos\theta) \tag{3.27}$$

clearly if $\delta_l=0$, $f(\theta,\phi)=0$, hence $\psi^{in}_{\vec{p}}(\vec{r})$ is plane wave, which agrees (3.25).

Lecture 21 (4/14/14)

In (3.26), we said that

$$\psi_{\vec{p}}^{in}(\vec{r}) = \underbrace{\sum_{l=0}^{\infty} c_{E,l} \frac{e^{i(kr+\delta_l-\frac{\pi l}{2})}}{2ikr}\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)}_{\text{outgoing}} + \underbrace{\sum_{l=0}^{\infty} c_{E,l} \frac{-e^{-i(kr+\delta_l-\frac{\pi l}{2})}}{2ikr}\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)}_{\text{incoming}}$$

looks like both outgoing and incoming parts gain a phase shift. But physically we prefer to say incoming wave doesn't change and outgoing wave gain $e^{2i\delta_l}$, that is

$$\psi_{\vec{p}}^{in}(\vec{r}) = e^{-i\delta_l}\left(\underbrace{\sum_{l=0}^{\infty} c_{E,l} \frac{e^{i(kr+2\delta_l-\frac{\pi l}{2})}}{2ikr}\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)}_{\text{outgoing}} + \underbrace{\sum_{l=0}^{\infty} c_{E,l} \frac{-e^{-i(kr-\frac{\pi l}{2})}}{2ikr}\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)}_{\text{incoming}}\right)$$

overall fact $e^{-i\delta_l}$ is irrelevant. We can also compute the scattering S matrix, cf (3.2),

$$\langle\text{outgoing}|S|\text{incoming}\rangle = \begin{pmatrix} e^{2i\delta_0} & & & \\ & e^{2i\delta_1} & & \\ & & \ddots & \\ & & & \ddots \end{pmatrix}$$

This kind of phase shift is manifest in the partial wave analysis, but hard to see from the early methods.

We can now derive the optical theorem

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

Since by (3.17)

$$\begin{aligned} \sigma_{tot} &= \int d\Omega\, |f(\theta,\phi)|^2 = \frac{1}{k^2}\sum_{l=0}^{\infty}\sin^2\delta_l(2l+1)^2 \underbrace{\int d\Omega P_l^2(\cos\theta)}_{\frac{4\pi}{2l+1}} \\ &= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}\sin^2\delta_l(2l+1) = \frac{4\pi}{k}\Im f(0,0) \end{aligned} \tag{3.28}$$

Likewise we can show that for scattering in a channel with specific l

$$(\sigma_{tot})_l = \frac{4\pi}{k^2}\sin^2\delta_l(2l+1) \le \frac{4\pi}{k^2}(2l+1) \tag{3.29}$$

which is uniformly bounded regardless what V is.

Example. Hard sphere scattering

$$V(r) = \begin{cases} \infty & r < a \\ 0 & r > a \end{cases}$$

so the wave function must vanish $r \le a$, so (3.22) implies

$$u_{E,l} = j_l(kr)n_l(ka) - n_l(kr)j_l(ka)$$

so by small z behavior of j_l and n_l

$$\tan\delta_l = \frac{j_l(ka)}{n_l(ka)} = \frac{(ka)^l\frac{2^l l!}{(2l+1)!}}{-\frac{1}{(ka)^{l+1}}(2l+1)!!} = -(ka)^{2l+1}\frac{2^l l!}{(2l+1)!(2l+1)!!}$$

since factorial grows much fast and if k is small, $\delta_l \ll 1$ for large l. So the δ_0 dominates, therefore by (3.28)

$$\sigma_{tot} = \frac{4\pi}{k^2}\sin^2\delta_0 = 4\pi a^2 \tag{3.30}$$

where $\delta_0 = -ka$.

This result works in general. For a general case, potential is short range, $V(r) = 0$ for $r > a$, a is called scattering length. And when k is small, energy of incident particle is small, then V looks like ∞ for $r < a$. So the above discussion applies. $\delta_0 = -ka$ dominates and by (3.23)

$$u(r) \sim \frac{\sin(k(r-a))}{kr}$$

If we change the potential to attractive $V \to -V$, then (3.16) implies $f \to -f$, then that $\delta_0 = -ka$ dominates and (3.27) imply $\delta_0 \to -\delta_0$, i.e

$$\delta_0 > 0 \qquad a \to -a$$

and

$$u(r) \sim \frac{\sin(k(r+a))}{kr}$$

A more physical explanation goes like follows:

When $V(|\vec{r}|) = 0$, $ru \sim \sin kr$ (with k is given be $E = \hbar^2 k^2/2m$) no phase shift, and sine passes the origin. Now add a short range repulsive potential $V(|\vec{r}|) > 0$ near the origin. As if $E \downarrow$, so $k \downarrow$ so near the origin wavelength $\uparrow$, so sine still passes the origin but less steeper. However away from the origin wavelength should be still the same because we assume elastic collision E is still the same. Connecting these two sines, we get at far distance $ru \sim \sin k(r-a)$ shift to the right.

If we have an attractive potential $V(|\vec{r}|) < 0$ near the origin. $k \uparrow$ so near the origin wavelength $\uparrow$, so sine becomes steeper. Connecting with far field wave, we get $ru \sim \sin k(r+a)$ shift to the left.

3.5 Resonant Scattering

This discussion is very similar to Wigner-Weisskopf Approximation cf 1.7. We will define a quantity Γ. It will be both the decay rate and resonant width. The resonant can be seen from the cross section when (3.29) reaches maximum, i.e.

$$\delta_l = \frac{\pi}{2} \tag{3.31}$$

Let's imagine the target has one discrete energy eigenstate $|d\rangle$. The incident wave packet has continuous spectrum $|\psi_{\vec{p}}\rangle$ concentrated near the energy of $|d\rangle$ so $|d\rangle\langle d|$ is unity. We first find the transition amplitude which will give decay rate.

$$A_d(t) = \left\langle d \middle| e^{-iHt/\hbar} \middle| d \right\rangle$$

inserting $\int \frac{d^3p}{(2\pi\hbar)^3} \left|\psi^{in}_{\vec{p}}\right\rangle \left\langle\psi^{in}_{\vec{p}}\right|$,

$$A_d(t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{-iE_pt/\hbar} \left|\left\langle d\middle|\psi^{in}_{\vec{p}}\right\rangle\right|^2 \tag{3.32}$$

because

$$H\left|\psi^{in}_{\vec{p}}\right\rangle = E_p\left|\psi^{in}_{\vec{p}}\right\rangle \text{ where } E_p = \frac{p^2}{2m}$$

and using the ansatz (3.14)

$$\left|\psi^{in}_{\vec{p}}\right\rangle = \psi_{\vec{p}} + \frac{1}{E_p - H_0 + i\epsilon} V \left|\psi^{in}_{\vec{p}}\right\rangle \text{ where } \psi_{\vec{p}} = e^{i\vec{p}\cdot\vec{r}/\hbar} \tag{3.33}$$

In this way, clearly this setup is similar to our discussion of Decay of an Unstable State 1.5, i.e. cf (1.22) and follows

$$H = H_0 + V$$

$$H_0\left|d\right\rangle = E_d\left|d\right\rangle$$

$$H_0\left|\psi_{\vec{p}}\right\rangle = E_{\vec{p}}\left|\psi_{\vec{p}}\right\rangle$$

and

$$\begin{aligned} \langle d|d\rangle &= 1 \\ \langle\psi_{\vec{p}}|\psi_{\vec{p}'}\rangle &= (2\pi\hbar)^3\delta^{(3)}(\vec{p} - \vec{p}') \\ \langle d|\psi_{\vec{p}}\rangle &= 0 \end{aligned}$$

and cf (1.35), (1.36)

$$\begin{aligned} \langle\psi_{\vec{p}}|V|d\rangle &= V_{\vec{p}d} \\ \langle\psi_{\vec{p}}|V|\psi_{\vec{p}'}\rangle &= 0 \\ \langle d|V|d\rangle &= 0 \end{aligned}$$

Beck to (3.32), we need to evaluate $\langle d|\psi_{\vec{p}}^{in}\rangle$.

$$\langle d|\psi_{\vec{p}}^{in}\rangle = \frac{1}{E_p - E_d + i\epsilon}\int \frac{d^3p'}{(2\pi\hbar)^3} V_{d\vec{p}'} \langle \psi_{\vec{p}'}|\psi_{\vec{p}}^{in}\rangle$$

now we understand why we put $i\epsilon$ in the dominate in (3.33),

$$\langle \psi_{\vec{p}'}|\psi_{\vec{p}}^{in}\rangle = (2\pi\hbar)^3\delta^3(\vec{p}' - \vec{p}) + \frac{1}{E_p - E_{p'} + i\epsilon} V_{\vec{p}'d} \langle d|\psi_{\vec{p}}^{in}\rangle$$

so

$$\begin{aligned}
(E_p - E_d + i\epsilon)\langle d|\psi_{\vec{p}}^{in}\rangle &= \int \frac{d^3p'}{(2\pi\hbar)^3} V_{d\vec{p}'}\left((2\pi\hbar)^3\delta^3(\vec{p}' - \vec{p}) + \frac{1}{E_p - E_{p'} + i\epsilon} V_{\vec{p}'d}\langle d|\psi_{\vec{p}}^{in}\rangle\right) \\
&= V_{d\vec{p}} + \langle d|\psi_{\vec{p}}^{in}\rangle \underbrace{\int \frac{d^3p'}{(2\pi\hbar)^3}\frac{|V_{d\vec{p}'}|^2}{E_p - E_{p'} + i\epsilon}}_{\underbrace{P\int \frac{d^3p'}{(2\pi\hbar)^3}\frac{|V_{d\vec{p}'}|^2}{E_p - E_{p'}}}_{\equiv \Delta E_d(p)} - i\pi \underbrace{\int \frac{d^3p'}{(2\pi\hbar)^3}|V_{d\vec{p}'}|^2\delta(E_p - E_{p'})}_{\equiv \frac{\Gamma(p)}{2}}}
\end{aligned} \tag{3.34}$$

by principal value (1.40). Thus

$$\langle d|\psi_{\vec{p}}^{in}\rangle = \frac{V_{d\vec{p}}}{E_p - E_d - \Delta E_d(p) + \frac{i\Gamma(p)}{2}} \tag{3.35}$$

where we have taken out $i\epsilon$ because we have done with it. Back to (3.32)

$$A_d(t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{-iE_pt/\hbar}\frac{|V_{d\vec{p}}|^2}{(E_p - E_d - \Delta E_d(p) - \frac{i\Gamma(p)}{2})(E_p - E_d - \Delta E_d(p) + \frac{i\Gamma(p)}{2})}$$

think this as a complex integral of $\int_0^\infty dE$, because $d^3p = p^2dpd\Omega$, and $dp \to dE\frac{1}{v}$. We choose the contour: positive real axis+negative imaginary axis+the 1/4 circle, which encloses one pole

$$E_p = E_d + \Delta E_d(p) - \frac{i\Gamma(p)}{2} \tag{3.36}$$

The 1/4 circle gives 0 and the imaginary axis integral with $E_p \to iE$, gives

$$\int d\Omega \int_{-\infty}^{0} \frac{mpid(E)}{(2\pi\hbar)^3} e^{Et/\hbar} \frac{|V_{d\vec{p}}|^2}{(iE - E_d - \Delta E_d(p) - \frac{i\Gamma(p)}{2})(iE - E_d - \Delta E_d(p) + \frac{i\Gamma(p)}{2})}$$

which is roughly equal to

$$\int_{-\infty}^{\infty} d^3p e^{-\frac{p^2}{2m}t/\hbar} F(\vec{p})$$

such Gaussian like integral decays in time like

$$\sim t^{-3/2}$$

so we say this part is transient-like. It goes to 0. Just like mechanical driven oscillator problem: how the system starts off becomes irrelevant as time goes on. As we will see here it gives correction to the exponential decays.

So $A_d(t)$ is roughly equal to the contour integral

$$A_d(t) \sim (-2\pi i) \int \frac{p^2 d\Omega}{(2\pi\hbar)^3} e^{-i(E_d + \Delta E_d(p) - \frac{i\Gamma(p)}{2})t/\hbar} \frac{|V_{d\vec{p}}|^2}{-i\Gamma(p)}$$

where p satisfies (3.36). So we can rewrite it by assuming Γ and ΔE_d are very small

$$\left(\int \frac{p^2 d\Omega}{(2\pi\hbar)^3} e^{-i(E_d + \Delta E_d(p) - \frac{i\Gamma(p)}{2})t/\hbar} \frac{|V_{d\vec{p}}|^2}{\Gamma(p)} \right)_{p \text{ satisfies (3.36)}}$$

$$\begin{aligned} &= \int \frac{d^3p \delta(E_p - E_d)}{(2\pi\hbar)^3} e^{-i(E_d + \Delta E_d(p) - \frac{i\Gamma(p)}{2})t/\hbar} \frac{|V_{d\vec{p}}|^2}{\Gamma(p)} \\ &= e^{-i(E_d + \Delta E_d(p) - \frac{i\Gamma(p)}{2})t/\hbar} \frac{\Gamma(p)/2\pi}{\Gamma(p)} \quad (\because (3.34)) \\ &= e^{-i(E_d + \Delta E_d(p) - \frac{i\Gamma(p)}{2})t/\hbar} / 2\pi \end{aligned}$$

thus

$$A_d(t) = e^{-i(E_d + \Delta E_d(p))t/\hbar} e^{-\frac{\Gamma(p)}{2}t/\hbar} + t^{-3/2}$$

showing Γ is indeed the decay rate. To see it is also the decay width, we compute scattering amplitude $f(\theta,\phi)$

From (3.16)

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\left\langle\psi_{\vec{p}'}\middle|V\middle|\psi_{\vec{p}}^{in}\right\rangle$$

By (3.35)

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\frac{V_{\vec{p}'d}V_{d\vec{p}}}{E_p - E_d - \Delta E_d(p) + \frac{i\Gamma(p)}{2}} \tag{3.37}$$

thus

$$\frac{d\sigma}{d\Omega}(E_p) = |f(\theta,\phi)|^2 = \frac{m^2}{(2\pi\hbar^2)^2}\frac{|V_{\vec{p}'d}V_{d\vec{p}}|^2}{(E_p - E_d - \Delta E_d(p))^2 + \frac{(\Gamma(p))^2}{4}}$$

where $\vec{p}' = |\vec{p}|\,\hat{r}(\theta,\phi)$, showing the resonant happens at $E_p \sim E_d$ with width Γ.

Lecture 22 (4/16/14)

Finally we relate this resonant phenomena to the phase shift δ_0 discussion for low energy scattering.

As before (3.20), we assume

$$[J,H] = 0 \qquad J^2\,|d\rangle = 0$$

i.e. $V_{\vec{p}d} = V_{\vec{p}'d}$ has no angular dependence. Then by (3.34)

$$\begin{aligned}
\Gamma(p) &= 2\pi\int\frac{d^3p'}{(2\pi\hbar)^3}\left|V_{d\vec{p}'}\right|^2\delta(E_p - E_{p'}) \\
&= 2\pi\frac{p^2}{(2\pi\hbar)^3}4\pi\frac{m}{p}\left|V_{d\vec{p}}\right|^2 = \frac{pm}{\pi\hbar^3}\left|V_{d\vec{p}}\right|^2
\end{aligned}$$

then by (3.37)

$$\begin{aligned}
f(\theta,\phi) &= -\frac{m}{2\pi\hbar^2}\frac{\frac{\pi\hbar^3}{pm}\Gamma(p)}{E_p - E_d - \Delta E_d(p) + \frac{i\Gamma(p)}{2}} \\
&= \frac{1}{k}\frac{\frac{\Gamma}{2}}{E_d + \Delta E_d - E_p - \frac{i\Gamma}{2}} \\
&= \frac{1}{k}\frac{1}{\frac{2(E_d+\Delta E_d - E_p)}{\Gamma} - i}
\end{aligned}$$

We want to equate this to (3.27) with δ_0 dominates

$$f(\theta,\phi) = \frac{1}{k}e^{-i(-\delta_0)}\sin\delta_0 = \frac{1}{k}\frac{\sin\delta_0}{\cos\delta_0 - i\sin\delta_0} = \frac{1}{k}\frac{1}{\cot\delta_0 - i}$$

so

$$\tan\delta_0 = \frac{\Gamma}{2(E_d + \Delta E_d - E_p)}$$

this shows precisely as E_p close to E_d with Γ ranges, δ_0 changes from 0 to π and passing $\pi/2$, which makes $\sigma_{l=0}$ reaches the maximum, cf (3.31). And by (3.30), the maximum value is $4\pi/k^2$ independent of Γ. Therefore if the scattering σ is very weak, we cannot change Γ small to make it stronger, however, we can control the adoptable detector to make Γ small so that the width is narrower to see resonance.

3.6 Identical Particles Scattering

The S matrix language is trivially simple to work with symmetrizing or antisymmetric state

$$\langle\vec{p}_1,...,\vec{p}_N|U_I(\infty,-\infty)|\vec{p}_b,\vec{p}_t\rangle$$

all we need to do is to write the interacting potential in second quantization language.

For stationary state method we need to do some work. This method works better if we study 2 identical particles head-on collision. We introduce center of mass and relative coordinate.

$$\begin{cases}\vec{R} & = \frac{m_1\vec{r}_1+m_2\vec{r}_2}{m_1+m_2} \\ \vec{r} & = \vec{r}_1-\vec{r}_2\end{cases} \iff \begin{cases}\vec{r}_1 = \vec{R}+\frac{\mu\vec{r}}{m_1} \\ \vec{r}_2 = \vec{R}-\frac{\mu\vec{r}}{m_2}\end{cases}$$

and

$$V(\vec{r}_1,\vec{r}_2) = V(\vec{r})$$

Then in the CM frame $\vec{R}=0$, $\vec{r}_{1,2}$ moves in the way as $\vec{r}$, so we reduce two-body problem to one-body problem. So

$$\psi(\vec{r}_1,\vec{r}_2) = \frac{e^{i\vec{R}\cdot\vec{P}/\hbar}}{(2\pi\hbar)^3}(e^{i\vec{p}\cdot\vec{r}/\hbar} + f(\theta,\phi)\frac{e^{ipr/\hbar}}{r})$$

where (θ, ϕ) is measured in the center of mass frame, and

$$\vec{P} = \frac{m_1\dot{\vec{r}}_1 + m_2\dot{\vec{r}}_2}{m_1 + m_2} \qquad \vec{p} = \vec{p}_1 - \vec{p}_2$$

the overall factor $\frac{e^{i\vec{R}\cdot\vec{P}/\hbar}}{(2\pi\hbar)^3}$ is the translation of the center of mass point, which we will ignore. Since they are indistinguishable. The correct wave function for bosons is

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[e^{i\vec{p}\cdot\vec{r}/\hbar} + e^{-i\vec{p}\cdot\vec{r}/\hbar} + (f(\theta,\phi) + f(\pi-\theta, \pi+\phi))\frac{e^{ipr/\hbar}}{r}\right]$$

$e^{i\vec{p}\cdot\vec{r}/\hbar}$ beam from the left and $e^{-i\vec{p}\cdot\vec{r}/\hbar}$ beam from the right. The $1/\sqrt{2}$ is to make the incoming wave probability to be consistent with what we did before. The differential cross for one of the two particles is

$$\frac{d\sigma}{d\Omega} = \underbrace{\frac{1}{2}}_{\text{from the } \frac{1}{\sqrt{2}}} |f(\theta,\phi) + f(\pi-\theta,\pi+\phi)|^2 \cdot \underbrace{2}_{\substack{\text{don't care which} \\ \text{one is coming out}}} \qquad \theta \in [0, \pi/2] \tag{3.38}$$

Another subtlety is that σ_{tot} is now 1/2 of before

$$\sigma_{tot} = \int_0^{2\pi} d\phi \int_0^1 d(\cos\theta)\frac{d\sigma}{d\Omega}$$

because we have taken care of the 2 in $\frac{d\sigma}{d\Omega}$

For fermions, we use

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[e^{i\vec{p}\cdot\vec{r}/\hbar} - e^{-i\vec{p}\cdot\vec{r}/\hbar} + (f(\theta,\phi) - f(\pi-\theta, \pi+\phi))\frac{e^{ipr/\hbar}}{r}\right]$$

E.g. in compute differential cross section for the scattering of two unpolarized deuterium nuclei (spin 1). For the total spin 2 (highest spin state is always symmetric, then next levels are always alternating), use (3.38). The next level total spin 1 must be antisymmetric, use

$$\frac{d\sigma}{d\Omega} = \frac{1}{2}|f(\theta,\phi) - f(\pi-\theta,\pi+\phi)|^2\, 2$$

The next level total spin 0 use (3.38).

4 Quantum Theory of Light & Path Integration

4.1 Quantization of Free EM fields

Although our treatment of quantization of EM doesn't care about covariance; in particular we choose Coulomb gauge, which is not covariant, as we will see this treatment is good enough for many applications. E.g. interaction light with matters gives decay of excited atoms (quantum electrodynamics); radiation of accelerating particles gives infrared catastrophe, classical Bremsstrahlung, and soft radiations (quantum field theory).

Recall free Maxwell equations

$$\nabla \cdot \vec{E} = 0 \tag{4.1}$$

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

$$\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t} \tag{4.2}$$

$$\nabla \times \vec{B} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} \tag{4.3}$$

Define potential $\vec{A}(\vec{r}, t)$

$$\vec{B} = \nabla \times \vec{A} \tag{4.4}$$

then by (4.2)

$$\nabla \times (\vec{E} + \frac{1}{c}\frac{\partial \vec{A}}{\partial t}) = 0 \implies \vec{E} + \frac{1}{c}\frac{\partial \vec{A}}{\partial t} = -\nabla \phi \tag{4.5}$$

Gauge freedom

$$\vec{A}, \phi \text{ and } \vec{A} + \nabla \Lambda, \phi + \frac{\partial \Lambda}{\partial t}$$

give the same $\vec{E}$ and $\vec{B}$ fields. We can impose a gauge condition: Coulomb gauge

$$\nabla \cdot \vec{A} = 0 \tag{4.6}$$

which is not Lorentz invariant, i.e. in moving frame this doesn't hold.

Take ∇ of (4.6), by (4.1) and (4.6)

$$\nabla \cdot (4.6) = -\nabla^2 \phi = 0 \implies \phi = 0$$

so

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} \tag{4.7}$$

write (4.3) in term of $\vec{A}$, by (4.7)

$$\underbrace{\nabla \times (\nabla \times \vec{A})}_{\nabla(\nabla\cdot\vec{A})-\nabla^2\vec{A}} = -\frac{1}{c}\frac{\partial \vec{E}}{\partial t}$$

so we obtain

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

wave equation for each component of $\vec{A}$. If we can diagonalize ∇^2, we get SHO.

Assume $\vec{E}, \vec{B}$ are in a box of volume $V = L^3$ and obey periodic boundary conditions. This assumption is not natural, but later we will let $L \to \infty$ anyway. Observe

$$\nabla^2 e^{i\vec{k}_{\vec{n}}\cdot\vec{r}} = -\vec{k}_{\vec{n}}^2 e^{i\vec{k}_{\vec{n}}\cdot\vec{r}}$$

where

$$\vec{k}_{\vec{n}} = \frac{2\pi}{L}(n_1, n_2, n_3) \quad n_i \in \mathbb{Z} \tag{4.8}$$

so

$$\vec{A}(\vec{r}, t) = \sum_{\vec{n}} \frac{e^{i\vec{k}_{\vec{n}}\cdot\vec{r}}}{\sqrt{V}} \sum_{i=1}^{3} \hat{\epsilon}_i(\vec{k}_{\vec{n}}) q_i(\vec{k}_{\vec{n}}, t) \tag{4.9}$$

q_i satisfies

$$\frac{d^2}{dt^2} q_i = -c^2 \vec{k}_{\vec{n}}^2 q_i = -w_k^2 q_i \tag{4.10}$$

where $w_k = c\left|\vec{k}_{\vec{n}}\right|$ the same w for $\vec{\epsilon}_i(\vec{k}_{\vec{n}})$ for all i.

$$\left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\right| = 1 \quad \forall i$$

is a unit real vector, it is called polarization. That is because by (4.7), the same

$\hat{\epsilon}_i(\vec{k}_{\vec{n}})$ will be in $\vec{E}$ since w is the same for each component. There are constraints for $\vec{\epsilon}_i$ and q_i.

$$\nabla \cdot \vec{A} = 0 \implies \vec{k}_{\vec{n}} \cdot \hat{\epsilon}_i(\vec{k}_{\vec{n}}) = 0$$

hence for each $\vec{k}_{\vec{n}}$ (i.e. for each mode $\vec{n}$), only two non-zero i, choose $i = \pm 1$, lie in a perpendicular plane to $\vec{k}$. So we can reasonably impose

$$\hat{\epsilon}_i(\vec{k}_{\vec{n}}) = \hat{\epsilon}_i(-\vec{k}_{\vec{n}}) \quad i = \pm 1$$

which is commonly seen in EM when light is reflected from a interface, polarization of $\vec{E}$ stays the same cf (4.15). Although knowing $\hat{\epsilon}_i$, $i = \pm 1$, are perpendicular to $\vec{k}$ does not automatically fix the directions of $\hat{\epsilon}_i$, but we will still insist that $\hat{\epsilon}_i$ is completely specified by $\vec{k}_{\vec{n}}$ for later convenience. And this amounts to have some rotational constants to be added to q_i. That is we impose

$$\hat{\epsilon}_i(\vec{k}_{\vec{n}}) \cdot \hat{\epsilon}_j(\vec{k}_{\vec{n}}) = \delta_{ij} \quad \text{for given } \vec{k}_{\vec{n}} \tag{4.11}$$

(with the convention that for linear polarization, we do not put $\hat{\epsilon}_{-1} = \hat{\epsilon}_1$, we put one of them to be $\vec{0}$.)

Furthermore we impose $\vec{A}$ to be real,

$$\vec{A} = \sum_{\vec{n}} \frac{e^{i\vec{k}_{\vec{n}} \cdot \vec{r}}}{\sqrt{V}} \sum_{i=\pm 1} \hat{\epsilon}_i(\vec{k}_{\vec{n}}) q_i(\vec{k}_{\vec{n}})$$

and

$$\vec{A}^* = \sum_{\vec{n}} \frac{e^{i\vec{k}_{\vec{n}} \cdot \vec{r}}}{\sqrt{V}} \sum_{i=\pm 1} \hat{\epsilon}_i(\vec{k}_{\vec{n}}) q_i^*(\vec{k}_{\vec{n}})$$

since the sum is taken over all $\vec{n}$, we can re-index $\vec{n} \to -\vec{n}$,

$$\vec{A}^* = \sum_{\vec{n}} \frac{e^{i\vec{k}_{\vec{n}} \cdot \vec{r}}}{\sqrt{V}} \sum_{i=\pm 1} \hat{\epsilon}_i(\vec{k}_{\vec{n}}) q_i^*(-\vec{k}_{\vec{n}})$$

so

$$\vec{A} = \vec{A}^* \iff q_i(\vec{k}_{\vec{n}}) = q_i^*(-\vec{k}_{\vec{n}}) \iff \begin{cases} q_i^{re}(\vec{k}_{\vec{n}}) = q_i^{re}(-\vec{k}_{\vec{n}}) \\ q_i^{im}(\vec{k}_{\vec{n}}) = -q_i^{im}(-\vec{k}_{\vec{n}}) \end{cases} \tag{4.12}$$

what kind of solutions of ode (4.10) look like: e.g. it could look like

$$q_i = Ce^{i\mathrm{sgn}(\vec{k}_{\vec{n}}\cdot\hat{x})(w_k t+\phi_i)} \tag{4.13}$$

the phase ϕ_i is to determined whether it is linear, circular or mix polarization.

$$q_i^{re} = C\cos(\mathrm{sgn}(\vec{k}_{\vec{n}}\cdot\hat{x})(w_k t+\phi_i)) \qquad q_i^{im} = C\sin(\mathrm{sgn}(\vec{k}_{\vec{n}}\cdot\hat{x})(w_k t+\phi_i))$$

so

$$p_i = Cm(i\mathrm{sgn}(\vec{k}_{\vec{n}}\cdot\hat{x})w_k)e^{i\mathrm{sgn}(\vec{k}_{\vec{n}}\cdot\hat{x})(w_k t+\phi_i)}$$

so we too have

$$p_i(\vec{k}_{\vec{n}}) = p_i^*(-\vec{k}_{\vec{n}}) \tag{4.14}$$

Notice the actual forms of p_i, q_i in position space are not important, because eventually we will express them in terms of $a_i(\vec{k}_{\vec{n}})$, and $a_i^+(\vec{k}_{\vec{n}})$ in Fock space.

Recall EM energy

$$H = \frac{1}{8\pi}\int d^3r(\vec{E}^2 + \vec{B}^2)$$

By (4.7), (4.11)

$$\begin{aligned} \int d^3r\vec{E}^2 &= \sum_{\vec{n}\vec{n}'} \frac{1}{c^2} \underbrace{\int d^3r \frac{e^{-i\vec{k}_{\vec{n}'}\cdot\vec{r}} e^{i\vec{k}_{\vec{n}}\cdot\vec{r}}}{V}}_{\delta(\vec{k}_{\vec{n}'}-\vec{k}_{\vec{n}})} \sum_{i,j} \underbrace{\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\hat{\epsilon}_j(\vec{k}_{\vec{n}'})}_{=\delta_{ij}} \dot{q}_i^*(\vec{k}_{\vec{n}'})\dot{q}_j(\vec{k}_{\vec{n}}) \\ &= \sum_{\vec{n}}\sum_{i=\pm1} \frac{1}{c^2}\left|\dot{q}_i(\vec{k}_{\vec{n}})\right|^2 \end{aligned}$$

Likewise by (4.4), (4.11)

$$\begin{aligned}
\int d^3r\vec{B}^2 &= \sum_{\vec{n}\vec{n}'}\frac{1}{c^2}\underbrace{\int d^3r\frac{e^{-i\vec{k}_{\vec{n}'}\cdot\vec{r}}e^{i\vec{k}_{\vec{n}}\cdot\vec{r}}}{V}}_{\delta(\vec{k}_{\vec{n}'}-\vec{k}_{\vec{n}})}\sum_{i,j}\underbrace{\left(i\vec{k}_{\vec{n}}\times\hat{\epsilon}_i(\vec{k}_{\vec{n}})\right)\cdot\left(i\vec{k}_{\vec{n}'}\times\hat{\epsilon}_j(\vec{k}_{\vec{n}'})\right)}_{=\delta_{ij}\vec{k}_{\vec{n}}^2}q_i^*(\vec{k}_{\vec{n}'})q_j(\vec{k}_{\vec{n}}) \\
&= \sum_{\vec{n}}\sum_{i=\pm1}\vec{k}_{\vec{n}}^2\left|q_i(\vec{k}_{\vec{n}})\right|^2
\end{aligned}$$

thus

$$H = \frac{1}{4\pi c^2}\sum_{\vec{n}}\sum_{i=\pm1}\frac{1}{2}\left(\left|\dot{q}_i(\vec{k}_{\vec{n}})\right|^2 + w_k^2\left|q_i(\vec{k}_{\vec{n}})\right|^2\right)$$

Lecture 23 (4/21/14)

This reminds us of SHO

$$H = \frac{1}{2}m\dot{q}^2 + \frac{1}{2}mw^2q^2$$

so we say the effective mass for each mode $\vec{n}$ is

$$m = \frac{1}{2\pi c^2}$$

not $\frac{1}{4\pi c^2}$ because $1/2$ is used to cancel $\sum_{i=\pm1}$ so that each mode looks like a SHO not two SHO's.

Now we are going to push the analogy all the way.

Put

$$p_i = m\dot{q}_i$$

Recall Ladder operator for SHO

$$a = \sqrt{\frac{mw}{2\hbar}}q + i\frac{1}{\sqrt{2mw\hbar}}p$$

For us, now q, p consist two different functions (odd and even), see remark follows (4.12), we define ladder operator for EM

$$
\begin{aligned}
a_i(\vec{k}_{\vec{n}}) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{mw}{2\hbar}}q_i(\vec{k}_{\vec{n}}) + i\frac{1}{\sqrt{2mw\hbar}}p_i(\vec{k}_{\vec{n}})\right) &= \frac{1}{\sqrt{2}}(\underbrace{\sim q_i^{re} + i \sim p_i^{re}}_{a_i^{even}} + i\underbrace{\sim q_i^{im} + i \sim p_i^{im}}_{a_i^{odd}}) \\
a_i^+(\vec{k}_{\vec{n}}) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{mw}{2\hbar}}q_i^+(\vec{k}_{\vec{n}}) - i\frac{1}{\sqrt{2mw\hbar}}p_i^+(\vec{k}_{\vec{n}})\right) &= \frac{1}{\sqrt{2}}(\underbrace{\sim q_i^{+re} - i \sim p_i^{+re}}_{a_i^{+even}} - i\underbrace{\sim q_i^{+im} - i \sim p_i^{+im}}_{a_i^{+odd}}) \\
&= \frac{1}{\sqrt{2}}(\underbrace{\sim q_i^{re} - i \sim p_i^{re}}_{a_i^{+even}} - i\underbrace{\sim q_i^{im} - i \sim p_i^{im}}_{a_i^{+odd}})
\end{aligned}
$$

Unlike the + on right side of equations, +on a is no long just the hermitian conjugate, it is also the symbol for creation. the $1/\sqrt{2}$ factor is conventional so that the following commutator expressions will be simpler. After we separate a^{even} and a^{odd}, (by the way a^{even} and a^{odd} commute, because they are different functions), we can apply (2.19) and (2.21).

We get

$$
\begin{aligned}
[a_i(\vec{k}_{\vec{n}}), a_j^+(\vec{k}_{\vec{m}})] &= \frac{1}{2}\left([a_i^{even}, a_j^{+even}] + [a_i^{odd}, a_j^{+odd}]\right) \\
&= \frac{1}{2}\left(\delta_{ij}\delta_{nm} + \delta_{ij}\delta_{nm}\right) = \delta_{ij}\delta_{nm}
\end{aligned}
$$

$$
[a(\vec{k}_{\vec{n}}), a(\vec{k}_{\vec{m}})] = [a^+(\vec{k}_{\vec{n}}), a^+(\vec{k}_{\vec{m}})] = 0
$$

so it is clear that EM fields are Bosons-photons.

Finally we want to express everything in terms of a and a^+. We can forget about the spatial and temporal dependence in q, p, a, a^+, once we write everything in second quantization language, it is true in all time. First we write

$$
a_i^+(\vec{k}_{\vec{n}}) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{mw}{2\hbar}}q_i(-\vec{k}_{\vec{n}}) - i\frac{1}{\sqrt{2mw\hbar}}p_i(-\vec{k}_{\vec{n}})\right)
$$

or

$$
a_i^+(-\vec{k}_{\vec{n}}) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{mw}{2\hbar}}q_i(\vec{k}_{\vec{n}}) - i\frac{1}{\sqrt{2mw\hbar}}p_i(\vec{k}_{\vec{n}})\right)
$$

so

$$q_i(\vec{k}_{\vec{n}}) = \sqrt{\frac{\hbar}{mw}}\left(a_i(\vec{k}_{\vec{n}}) + a_i^+(-\vec{k}_{\vec{n}})\right) = \sqrt{\frac{2\pi\hbar c}{\left|\vec{k}_{\vec{n}}\right|}}\left(a_i(\vec{k}_{\vec{n}}) + a_i^+(-\vec{k}_{\vec{n}})\right)$$

and

$$p_i(\vec{k}_{\vec{n}}) = -i\sqrt{mw\hbar}\left(a_i(\vec{k}_{\vec{n}}) - a_i^+(-\vec{k}_{\vec{n}})\right) = -i\sqrt{\frac{\hbar\left|\vec{k}_{\vec{n}}\right|}{2\pi c}}\left(a_i(\vec{k}_{\vec{n}}) - a_i^+(-\vec{k}_{\vec{n}})\right)$$

Therefore (4.9) becomes

$$\vec{A}(\vec{r}) = \sum_{\vec{n}}\sqrt{\frac{2\pi\hbar c}{\left|\vec{k}_{\vec{n}}\right|}}\frac{e^{i\vec{k}_{\vec{n}}\cdot\vec{r}}}{\sqrt{V}}\sum_{i=\pm1}\hat{\epsilon}_i(\vec{k}_{\vec{n}})\left(a_i(\vec{k}_{\vec{n}}) + a_i^+(-\vec{k}_{\vec{n}})\right)$$

Likewise we can show

$$\vec{E}(\vec{r}) = i\sum_{i,\vec{n}}\sqrt{\frac{2\pi\hbar c\left|\vec{k}_{\vec{n}}\right|}{V}}\hat{\epsilon}_i(\vec{k}_{\vec{n}})\left(a_i(\vec{k}_{\vec{n}})e^{i\vec{k}_{\vec{n}}\cdot\vec{r}} - a_i^+(\vec{k}_{\vec{n}})e^{-i\vec{k}_{\vec{n}}\cdot\vec{r}}\right) \tag{4.15}$$

$$\vec{B}(\vec{r}) = i\sum_{i,\vec{n}}\sqrt{\frac{2\pi\hbar c}{V\left|\vec{k}_{\vec{n}}\right|}}\vec{k}_{\vec{n}}\times\hat{\epsilon}_i(\vec{k}_{\vec{n}})\left(a_i(\vec{k}_{\vec{n}})e^{i\vec{k}_{\vec{n}}\cdot\vec{r}} - a_i^+(\vec{k}_{\vec{n}})e^{-i\vec{k}_{\vec{n}}\cdot\vec{r}}\right) \tag{4.16}$$

$$H = \frac{1}{8\pi}\int_{V\to\infty} d^3r(E^2+B^2) = \sum_{\vec{n}}\hbar w_k\sum_i\left(a_i^+(\vec{k}_{\vec{n}})a_i(\vec{k}_{\vec{n}}) + \frac{1}{2}\right) \tag{4.17}$$

$$\vec{P} = \frac{1}{4\pi c}\int_{V\to\infty} d^3r\vec{E}\times\vec{B} = \sum_{\vec{n}}\hbar\vec{k}_{\vec{n}}\sum_i a_i^+(\vec{k}_{\vec{n}})a_i(\vec{k}_{\vec{n}}) \tag{4.18}$$

$\vec{A}$,$\vec{E}$,$\vec{B}$ are indeed real. (4.17) and (4.18) show each photon carries energy $\hbar w$ and momenta $\hbar\vec{k}$. The polarization contributes nothing to the energy nor momenta, so it is like an internal degree of freedom, e.g. like spin. Notice a_i^+ alone does not create a photon. It is $\sum_i a_i^+$ who creates photon with energy, momenta, and what kind of polarization, i.e. in what directions of $i = \pm1$, and phase difference cf (4.13). So

$$a_i^+(\vec{k}_{\vec{n}}) \text{ knows not only } \vec{k}_{\vec{n}} \text{ but also polarization} \tag{4.19}$$

Likewise in (4.17) don't count 2 polarizations as two particles. When we study hydrogen decay, we will see how photon is produced. One can also study how hyperfine splitting produce photons, using

$$H^{hfs} = -\underbrace{\frac{g_e e}{2mc}\vec{S}_e}_{\vec{\mu}_e} \cdot \vec{B}(r_e)$$

where $\vec{B}$ is given by (4.16). See practice final problem 2.

a_i^+ acts on Fock space. An element of the Fock space looks like

$$\left| ...., n_{\vec{k}_{\vec{n}},\hat{\epsilon}_i}, ... \right\rangle \tag{4.20}$$

each $n_{\vec{k}_{\vec{n}},\hat{\epsilon}_i}$ represents a photon state with specified wave number $\vec{k}_{\vec{n}}$ and polarization $\hat{\epsilon}_i$, and n itself is the occupation number.

1/2 in (4.17) is the vacuum energy for the nth mode, because

$$_{\vec{n}}\langle 0|H|0\rangle_{\vec{n}} = \hbar w/2$$

It has some real measurable effects, e.g. Casimir forces. 2 parallel metallic plates are separated by some distance. The fluctuation of vacuum energy will produce an attractive force. The ∞ sum of vacuum energy is still an open question. It gives 10^6 times more energy than the expanding universe can tolerate.

4.2 Spontaneous Decay

Suppose a Hydrogen in its excited state $|n\rangle$, we show in the present of EM field it decays to $|n'\rangle$ and produce a photon.

$$\begin{aligned} H &= \frac{[\vec{p}_{op} + \frac{e}{c}\vec{A}_{op}]^2}{2m} - \frac{e^2}{|\vec{r}|} + H_{EM} \\ &= \underbrace{\frac{\vec{p}}{2m} - \frac{e^2}{|\vec{r}|} + \sum_{i,\vec{n}} \hbar w_k \left(a_i^+(\vec{k}_{\vec{n}}) a_i(\vec{k}_{\vec{n}}) + \frac{1}{2} \right)}_{H_0} + \underbrace{\frac{e\vec{p}\cdot\vec{A}}{mc}}_{V} + \underbrace{\frac{e^2}{2mc^2}\vec{A}^2}_{\text{very small}} \end{aligned} \tag{4.21}$$

We ignore the last term just like before cf Quantum mechanics I note equation (3.4). Otherwise it will contain $(a^+)^2$, producing 2 photons.

By Fermi Golden rule

$$R_{n\to n'+\gamma} \;=\; \frac{2\pi}{\hbar}\sum_{i,\vec{k}_{\vec{n}}}\left|\left\langle \gamma(\vec{k}_{\vec{n}},\hat{\epsilon}_i),n'\left|\frac{e\vec{p}\cdot\vec{A}}{mc}\right|0,n\right\rangle\right|^2\delta(E_{n'}+\hbar w_{\vec{n}}-E_n)$$

the 0 in the initial state $|0,n\rangle$ means 0 photon. Since $\vec{p}$ acts only on $|n\rangle$ and a^+ acts only on $|0\rangle$, we separate them

$$R_{n\to n'+\gamma} \;=\; \frac{2\pi}{\hbar}\sum_{i,\vec{n}}\left|\sum_{\vec{m},j}\left\langle \gamma(\vec{k}_{\vec{n}},\hat{\epsilon}_i)\left|\sqrt{\frac{2\pi\hbar c}{V\left|\vec{k}_{\vec{m}}\right|}}a_j^+(-\vec{k}_{\vec{m}})\frac{e}{mc}\right|0\right\rangle\hat{\epsilon}(\vec{k}_{\vec{m}})\left\langle n'\left|p_{op}e^{i\vec{k}_{\vec{m}}\cdot\vec{r}}\right|n\right\rangle\right|^2 \delta(E_{n'}+\hbar w_{\vec{n}}-E_n)$$

It is non-zero only when

$$j=i \qquad \vec{m}=-\vec{n} \text{ or } \vec{k}_{\vec{m}}=-\vec{k}_{\vec{n}}$$

$$R_{n\to n'+\gamma}=\frac{2\pi}{\hbar}\sum_{i,\vec{n}}\frac{2\pi\hbar c}{Vk_{\vec{n}}}\frac{e^2}{m^2c^2}\left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\left\langle n'\left|p_{op}e^{-i\vec{k}_{\vec{n}}\cdot\vec{r}}\right|n\right\rangle\right|^2\delta(E_{n'}+\hbar w_{\vec{n}}-E_n)$$

set $e^{-i\vec{k}_{\vec{n}}\cdot\vec{r}}=1$ for dipole approximation for the same reason we discussed before cf (1.32) and follows. By (4.8), the space

$$\Delta\vec{k}=\frac{2\pi}{L}$$

let $L\to\infty$, we can turn $\sum$ into $\int$

$$\sum_{\vec{n}}\left(\frac{2\pi}{L}\right)^3=\int d^3k \tag{4.22}$$

so

$$\begin{aligned}
R_{n\to n'+\gamma} &= \frac{1}{2\pi}\int d^3k \frac{e^2}{km^2c}\sum_i \left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\langle n'|p_{op}|n\rangle\right|^2 \delta(E_{n'}+\hbar ck - E_n) \\
&= \frac{1}{2\pi}k\frac{1}{\hbar c}\frac{e^2}{m^2c}\int d\Omega \sum_i \left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\langle n'|p_{op}|n\rangle\right|^2 \qquad (4.23)
\end{aligned}$$

where k is fixed by the energy conservation $k = (E_n - E_{n'})/\hbar c$. $d\Omega$ is the solid angle of $\vec{k}$ over all angles.

In the expression above it makes no difference whether the two polarization have phase difference, so we have get that information from another means, e.g. conservation of angular momentum.

Suppose choose

$$\langle n'|p_{op}|n\rangle \propto \hat{z} \qquad (4.24)$$

to the $\hat{z}$ direction (why is $\langle n'|p_{op}|n\rangle$ as vector? justify later). Then we know how to define the integral $\int d\Omega$. In particular θ is the angle between $\vec{k}$ and $\langle n'|\vec{p}|n\rangle$. To evaluate $\sum_i \left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\langle n'|\vec{p}|n\rangle\right|^2$ for each Ω, we put Cartesian coordinate $\hat{x} = \hat{\epsilon}_{-1}$, $\hat{y} = \hat{\epsilon}_1$, and $\hat{z} = \hat{k}$, then

$$\begin{aligned}
\sum_{i=\pm}\left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\langle n'|p_{op}|n\rangle\right|^2 &= |\langle n'|p_{op}|n\rangle|^2 - \hat{k}\cdot\langle n'|p_{op}|n\rangle \\
&= \sin^2\theta\,|\langle n'|p_{op}|n\rangle|^2
\end{aligned}$$

thus

$$\begin{aligned}
\int d\Omega\sum_i\left|\hat{\epsilon}_i(\vec{k}_{\vec{n}})\cdot\langle n'|p_{op}|n\rangle\right|^2 &= \int d\Omega\sin^2\theta\,|\langle n'|p_{op}|n\rangle|^2 \\
&= \frac{8\pi}{3}|\langle n'|p_{op}|n\rangle|^2
\end{aligned}$$

so

$$R_{n\to n'+\gamma} = \frac{4}{3}\frac{k}{\hbar c}\frac{e^2}{m^2c}|\langle n'|p_{op}|n\rangle|^2$$

Lecture 24 (4/23/14)

Later we want to use selection rules:

$$\langle n'|r_{op}|n\rangle = 0 \text{ unless } \begin{cases} \Delta l = \pm 1 \\ \Delta m = \pm 1, 0 \end{cases}$$

so now we use a trick to write $\langle n'|p_{op}|n\rangle$ in terms of $\langle n'|r_{op}|n\rangle$. Since $H_0 = \frac{p^2}{2m} - \frac{e^2}{r}$ and $p = \frac{\hbar}{i}\nabla$

$$[H_0, \vec{r}] = -\frac{\hbar^2}{2m}2\nabla = -\frac{\hbar}{m}ip \tag{4.25}$$

thus

$$\langle n'|p_{op}|n\rangle = -i\frac{m}{\hbar}\langle n'|[H_0, r_{op}]|n\rangle = i\frac{m}{\hbar}\hbar(w_n - w_{n'})\langle n'|r_{op}|n\rangle$$

where w_n was the same atomic frequency defined in (1.60). Typically for hydrogen $w_n - w_{n'} \approx 10^{15}\text{sec}^{-1}$.

Notice $\langle n'|r_{op}|n\rangle$ is a vector

$$\langle n'|r_{op}|n\rangle = \langle n'|x|n\rangle\,\hat{x} + \langle n'|y|n\rangle\,\hat{y} + \langle n'|r_{op}|n\rangle\,\hat{z} \tag{4.26}$$

so $\langle n'|p_{op}|n\rangle$ is too a vector and we define it to be the $\hat{z}$ direction, see (4.24).

Similar to oscillator strength defined in (1.59), we define

$$f_{nn'} = \frac{2m}{\hbar}(w_n - w_{n'})\frac{1}{3}\left|\langle n'|r_{op}|n\rangle\right|^2$$

and we have Thomas–Reiche–Kuhn sum rule

$$\sum_n f_{nn'} = Z = 1$$

Pf.

$$\begin{aligned} \sum_n f_{nn'} &= \sum_n \frac{2m}{\hbar^2}(E_n - E_{n'})\frac{1}{3}\langle n'|r_{op}|n\rangle\langle n|r_{op}|n'\rangle \\ &= \sum_n \frac{m}{3\hbar^2}\left(\langle n'|r|n\rangle\langle n|[H,r]|n'\rangle - \langle n'|[H,r]|n\rangle\langle n|r|n'\rangle\right) \end{aligned}$$

Then use something similar to (4.25)

$$H = \underbrace{\frac{p_1^2}{2m} + ... + \frac{p_Z^2}{2m}}_{H_0} + \sum_i^Z \frac{Ze^2}{|r_i|} + \frac{1}{2}\sum_{i \neq j}^Z \frac{e^2}{|r_i - r_j|} \tag{4.27}$$

so

$$[H, r] = [H_0, r] = -Z\frac{\hbar^2}{2m}2\nabla = -Z\frac{\hbar}{m}ip$$

so

$$\begin{aligned} \sum_n f_{nn'} &= \sum_n \frac{-iZ}{3\hbar}\left(\langle n'|r|n\rangle \langle n|p|n'\rangle - \langle n'|p|n\rangle \langle n|r|n'\rangle\right) \\ &= \frac{-iZ}{3\hbar}\langle n'|[r,p]|n'\rangle = Z \end{aligned}$$

notice in this proof H (4.27) can be any atom, not just hydrogen like atoms. QED.

We find

$$R_{n\to n'+\gamma} \approx 10^9 \mathrm{sec}^{-1}$$

We now want to know at the what direction photon is coming out and with what polarization. So we are back to (4.23)

$$\frac{dR_{n\to n'+\gamma}}{d\Omega}(\theta,\phi) \sim \sum_i \left|\hat{\epsilon}_i(\vec{k}_{\vec{n}}) \cdot \langle n'|r_{op}|n\rangle\right|^2 \tag{4.28}$$

before integrating over all $\vec{k}$ directions. Whatever direction of $\vec{k}$ in terms of (θ, ϕ), and whatever $\hat{\epsilon}_i$ give the maximum rate is the most likely direction of photon emission and polarization.

See Undergraduate quantum mechanics II notes section 5.5 Selection Rule

$$\langle n'l'm'|z|nlm\rangle = 0 \text{ unless } m = m'$$

$$\langle n'l'm'|x|nlm\rangle = 0 \quad \langle n'l'm'|y|nlm\rangle = 0 \text{ unless } m' - m = \pm 1$$

Therefore if

$$\Delta m = 0$$

(4.28) is maximal when

$$\hat{\epsilon}_i \parallel \hat{z} \text{ for } i = \pm 1$$

so two $\hat{\epsilon}_i$ are the same or by convention one of them is $\vec{0}$, it reduces $\vec{E}$ to plane wave, linear polarized. And $\vec{k}$ lie on xy plane. Hence detected photon coming from the xy plane are mostly linear polarized. If we put detect along $\hat{z}$, then $\hat{\epsilon}_i$ has to $\perp$ to $\hat{z}$, see no radiation.

If

$$\Delta m = m' - m = -1$$

i.e. the angular momentum of the atom in $\hat{z}$ decreases by $-\hbar$. (4.28) is maximal when

$$\hat{\epsilon}_i \perp \hat{z} \text{ for } i = \pm 1$$

we can have two possibilities:

1) If $\vec{k} \perp \hat{z}$, then

$$\hat{\epsilon}_{-1} = \hat{\epsilon}_1$$

or by convention one of them is $\vec{0}$, hence we get mostly linear polarized light.

2) If $\vec{k} \parallel \hat{z}$, choose $\hat{\epsilon}_{\pm 1}$ to be orthogonal to each other and to conserve angular momentum, it must be circular polarized.

4.3 Bloch-Nordsieck Radiation

We want to compute the radiation of an accelerating electron. We will get the same answer in Jackson equation (15.6)

$$I(w) = \frac{2}{3\pi}\frac{e^2}{c}\,|\Delta\beta|^2 \qquad w\tau \ll 1(\text{low freq limit})$$

The only difference is that Jackson uses classical EM, while as we do QED.

First we consider no acceleration. We approximates electron classically, with definite trajectory, $\vec{r} = \vec{v}t$, and constant velocity. That is because, like Jackson, we ignore high energy photons, only consider soft photons, $\hbar k \ll p = mv$, so no recoil to the electrons. We drop the A^2 term in the expansion of H.

We can think the free electron is an unbound electron from a hydrogen atom, so we can borrow (4.21) with little modification

$$
\begin{aligned}
H &= \sum_{i,\vec{n}} \hbar w_k \left(a_i^+(\vec{k}_{\vec{n}}) a_i(\vec{k}_{\vec{n}}) + \frac{1}{2} \right) + \frac{e\vec{p}\cdot\vec{A}}{mc} \\
&= \sum_{i,\vec{n}} \hbar w_k \left(a_i^+(\vec{k}_{\vec{n}}) a_i(\vec{k}_{\vec{n}}) + \frac{1}{2} \right) + \frac{e}{mc} \sum_{\vec{n}} \sqrt{\frac{2\pi\hbar c}{k_{\vec{n}}}} \frac{e^{i\vec{k}_{\vec{n}}\cdot\vec{r}}}{\sqrt{V}} \sum_{i=\pm1} \vec{p}\cdot\hat{\epsilon}_i(\vec{k}_{\vec{n}}) \left(a_i(\vec{k}_{\vec{n}}) + a_i^+(-\vec{k}_{\vec{n}}) \right) \\
&\approx \sum_{i,\vec{n}} h w_{k_{\vec{n}}} \Bigg[\left(a_i^+(\vec{k}_{\vec{n}}) + \sqrt{\frac{2\pi\hbar c}{k_{\vec{n}}V}} \vec{p}\cdot\hat{\epsilon}_i(\vec{k}_{\vec{n}}) \frac{e}{mc} \frac{1}{\hbar w_k} e^{i\vec{k}_{\vec{n}}\cdot\vec{r}} \right) \\
&\qquad \cdot \left(a_i(\vec{k}_{\vec{n}}) + \sqrt{\frac{2\pi\hbar c}{k_{\vec{n}}V}} \vec{p}\cdot\hat{\epsilon}_i(\vec{k}_{\vec{n}}) \frac{e}{mc} \frac{1}{\hbar w_k} e^{-i\vec{k}_{\vec{n}}\cdot\vec{r}} \right) + \frac{1}{2} \Bigg]
\end{aligned}
\tag{4.29}
$$

where $\vec{r}$, the position of the electron, in the exponent is equal to

$$\vec{r} = \vec{v}t$$

Such time-dependent H is good candidate for adiabatic approximation: groundstate moves with $H(t)$, because the frequency in H

$$\vec{k}_{\vec{n}} \cdot \vec{v} \ll kc = w_k$$

If we multiply out (4.29), we will get extra

$$\left(\sqrt{\frac{2\pi\hbar c}{k_{\vec{n}}V}} \vec{p}\cdot\hat{\epsilon}_i(\vec{k}_{\vec{n}}) \frac{e}{mc} \frac{1}{\hbar w_k} \right)^2 \sim O(A^2)$$

but we can ignore it by one of the assumptions.

Now H (4.29) looks like free quantized EM field with new creation/annihilation operators

$$a_i^{\vec{p}}(k_{\vec{n}}) = a_i(\vec{k}_{\vec{n}}) + \vec{p}\cdot \underbrace{\sqrt{\frac{2\pi\hbar c}{k_{\vec{n}}V}} \hat{\epsilon}_i(\vec{k}_{\vec{n}}) \frac{e}{mc} \frac{1}{\hbar w_{k_{\vec{n}}}} e^{-i\vec{k}_{\vec{n}}\cdot\vec{v}t}}_{:=\vec{A}_{i\vec{n}}} \tag{4.30}$$

which has explicitly time dependence. Clearly the groundstate of $a_i^{\vec{p}}(k_{\vec{n}})$,

$$|0\rangle_{\vec{p}} \text{ s.t. } a_i^{\vec{p}}(k_{\vec{n}})\,|0\rangle_{\vec{p}} = 0 \tag{4.31}$$

is not the groundstate of $a_i(k_{\vec{n}})$, so the groundstate is not 0 photon, so as the electron moves, it carries some photon cloud. But as we will see, it doesn't produce radiation, so no physical observable effect.

We want to express $|0\rangle_{\vec{p}}$ in terms of $|0\rangle$. Observe (4.31)

$$a_i(k_{\vec{n}})\,|0\rangle_{\vec{p}} = -\vec{p}\cdot\vec{A}_{i\vec{n}}\,|0\rangle_{\vec{p}} \quad \forall i,\vec{n} \tag{4.32}$$

so $|0\rangle_{\vec{p}}$ is eigenvector of $a_i(k_{\vec{n}})$ with eigenvalue $-\vec{p}\cdot\vec{A}_{i\vec{n}}$. This reminds us of coherence states, see quantum mechanics notes I section 2.2 coherence state. Therefore

$$|0\rangle_{\vec{p}} = \prod_{i,\vec{n}}\sum_{j=0}^{\infty}\frac{(-a_i^+(k_{\vec{n}})\vec{p}\cdot\vec{A}_{i\vec{n}})^j}{j!}\,|0\rangle\,e^{-\frac{1}{2}\left|\vec{p}\cdot\vec{A}_{i\vec{n}}\right|^2}$$

why is $\prod_{i,\vec{n}}$ product? because only product can satisfy (4.32). e.g. then $i=-1$; $\vec{n}_1=(1,0,0), \vec{n}_2=(1,1,0)$; $j=0,1,2$, ignoring $\vec{p}\cdot\vec{A}_{i\vec{n}}$

$$\begin{aligned}
\prod_{i,\vec{n}}\sum_{j=0}^{\infty}\frac{(-a_i^+(k_{\vec{n}}))^j}{j!}\,|0\rangle &= \left(1-a_i^+(k_{n_1})+\frac{(a_i^+(k_{n_1}))^2}{2!}\right)\left(1-a_i^+(k_{n_2})+\frac{(a_i^+(k_{n_2}))^2}{2!}\right)|0\rangle \\
&= \left(1-a_i^+(k_{n_1})+\frac{(a_i^+(k_{n_1}))^2}{2!}\right)\left(|0\rangle-|1_{i,n_2}\rangle+\frac{1}{2}\sqrt{2}\,|2_{i,n_2}\rangle\right) \\
&= |0\rangle-|1_{i,n_2}\rangle+\frac{\sqrt{2}}{2}\,|2_{i,n_2}\rangle-|1_{i,n_1}\rangle+\frac{\sqrt{2}}{2}\,|2_{i,n_1}\rangle+|1_{i,n_1},1_{i,n_2}\rangle \\
&\quad -\frac{\sqrt{2}}{2}\,|1_{i,n_1},2_{i,n_2}\rangle-\frac{\sqrt{2}}{2}\,|2_{i,n_1},1_{i,n_2}\rangle+\frac{1}{2}\,|2_{i,n_1},2_{i,n_2}\rangle
\end{aligned} \tag{4.33}$$

Now we want to consider a rapid change

$$\vec{p}\to\vec{p}'$$

at $t=0$. Sudden acceleration, but the states do change. So $|0\rangle_{\vec{p}}$ is still $|0\rangle_{\vec{p}}$, but it is not the groundstate $|0\rangle_{\vec{p}'}$.

From (4.30)

$$a_i^{\vec{p}}(k_{\vec{n}}) = a_i^{\vec{p}'}(\vec{k}_{\vec{n}})+(\vec{p}-\vec{p}')\cdot\vec{A}_{i\vec{n}}$$

so $|0\rangle_{\vec{p}}$ is eigenvector of $a_i^{\vec{p}'}(k_{\vec{n}})$ with eigenvalue $(\vec{p}'-\vec{p})\cdot\vec{A}_{i\vec{n}}$. Thus

$$|0\rangle_{\vec{p}} = \prod_{i,\vec{n}} \sum_{j=0}^{\infty} \frac{[a_i^{+\vec{p}'}(k_{\vec{n}})(\vec{p}-\vec{p}')\cdot\vec{A}_{i\vec{n}}]^j}{j!} |0\rangle_{\vec{p}'} e^{-\frac{1}{2}\left|(\vec{p}-\vec{p}')\cdot\vec{A}_{i\vec{n}}\right|^2} \tag{4.34}$$

Let us show now we are getting some physical effect, by computing radiated energy. (of course not to include 1/2, the vacuum energy)

$$\begin{aligned} \text{radiated energy} &= \sum_{i,\vec{n}} {}_{\vec{p}}\left\langle 0\middle| a_i^{+\vec{p}'}(k_{\vec{n}}) a_i^{\vec{p}'}(\vec{k}_{\vec{n}}) \middle| 0\right\rangle_{\vec{p}} \hbar w_k \\ &= \sum_{i,\vec{n}} \left|(\vec{p}-\vec{p}')\cdot\vec{A}_{i\vec{n}}\right|^2 \hbar w_{k_{\vec{n}}} \qquad (4.35) \\ &= \sum_{i,\vec{n}} \frac{2\pi\hbar c}{k_{\vec{n}} V}[(\vec{p}-\vec{p}')\cdot\hat{\epsilon}_i]^2 \frac{e^2}{m^2c^2}\frac{1}{\hbar w_{k_{\vec{n}}}} \end{aligned}$$

let $V\to\infty$, use (4.22), choose $\vec{p}-\vec{p}'$ to be $\hat{z}$

$$\begin{aligned} \text{radiated energy} &= 2\pi \int d\cos\theta \int_0^{\infty} k^2 dk \frac{1}{(2\pi)^3}\frac{2\pi\hbar c}{k}\cos^2\theta(\vec{p}-\vec{p}')^2 \frac{e^2}{m^2c^2}\frac{1}{\hbar c k} \times 2 \\ &= \frac{2}{3}\frac{e^2}{\pi c^3}\left(\frac{\vec{p}-\vec{p}'}{m}\right)^2 \int_0^{\infty} dw \qquad (4.36) \end{aligned}$$

$\times 2$ for polarization.

The reason we don't get any radiation in the constant velocity case before because

$$\sum_{i,\vec{n}} {}_{\vec{p}}\left\langle 0\middle| a_i^{+\vec{p}}(k_{\vec{n}}) a_i^{\vec{p}}(\vec{k}_{\vec{n}}) \middle| 0\right\rangle_{\vec{p}} \hbar w_k = 0$$

Let's contemplate (4.36). It looks like divergent. But since we only consider soft photons, the integral should really be

$$\int_0^{w_{max}} dw$$

where

$$w_{max} \ll cp/\hbar$$

Lecture 25 (4/28/14)

The more serious issue is called "infrared catastrophe", when one wants to count the number of emitted photons from the radiated energy

$$\# = \frac{\text{radiated energy}}{\hbar w} \sim \int_0^{w_{max}} \frac{1}{\hbar w} dw \to \infty$$

"infrared" means it is these small w photons causing the problem. The qft philosophy is that there must be some other ∞ to cancel it. Indeed we find that when $w \to 0$, see (4.30)

$$A_{i\vec{n}}(w=0) \to \infty$$

Since we cannot detect arbitrary soft photon anyway, we don't care there are ∞ many of them. But we can find the upper cutoff. Pick an arbitrary $\tilde{w} \leq w_{max}$ and we ask : what is the probability that no photons with $> \tilde{w}$ emitted? which is equal to the probability of getting frequency all photons$\leq \tilde{w}$

$$P = \sum_{l_{\vec{n}},\ldots,m_{\vec{n},i},n_{\vec{n},i}=0}^{\infty} \left| {}_{\vec{p}'} \langle \ldots, l_{\vec{n},i}, \ldots, m_{\vec{n},i}, n_{\vec{n},i}, 0, 0\ldots, 0, \ldots |0\rangle_{\vec{p}} \right|^2 \text{ with 0 occupancy for } w_{\vec{n}} > \tilde{w}$$

the notation is defined in (4.20). Plugging in $|0\rangle_{\vec{p}}$ by (4.34), and cf (4.33), we infer from the normalization factor

$$\prod_{i,\vec{n}} e^{-\frac{1}{2}\left|(\vec{p}-\vec{p}')\cdot \vec{A}_{i\vec{n}}\right|^2}$$

that if we had computed the probability of getting frequency all photons without a threshold $\tilde{w}$, we would've get 1, i.e. the normalization canceled. Now we don't have completely cancellation,

$$P = \prod_{\substack{\vec{n} \text{ s.t. } w_{\vec{n}} > \tilde{w} \\ i}} e^{-\frac{1}{2}\left|(\vec{p}-\vec{p}')\cdot \vec{A}_{i\vec{n}}\right|^2} = e^{\sum_{i,\vec{n} \text{ s.t. } w_{\vec{n}} > \tilde{w}} -\frac{1}{2}\left|(\vec{p}-\vec{p}')\cdot \vec{A}_{i\vec{n}}\right|^2}$$

so we can use similar calculation in (4.35) without hw term,

$$P = e^{\frac{2}{3}\frac{e^2}{\pi c^3}\left(\frac{\vec{p}-\vec{p}'}{m}\right)^2 \ln \frac{w_{max}}{\tilde{w}}}$$

which is indeed 1 as $\tilde{w} \to w_{max}^{-}$.

What we have done here is a baby version of renormalization from qft. E.g. when one computes $e^{-}+Ze$ scattering. The 2nd order vertex, with virtual photons, is a divergent vertex. To get finite answer, one will add soft photons, i.e. off shell-radiation. So one will likely define a threshold whose photons are coming out, not too parallel to the motion of the electron.

4.4 One Particle Path Integrals

Recall in the beginning of this semester we mentioned that to solve (1.1), we may be attempting to write down (1.2), which was not well-defined unless we meant it as Riemann sum, cf (1.8). Now we want to explore this idea further. We are interested in computing transition amplitude

$$\left\langle q' \middle| e^{-iHt/\hbar} \middle| q \right\rangle \tag{4.37}$$

the notation $|q\rangle$ is borrowed from classical mechanics, what we really mean is that a Schrodinger state $|\psi(q)\rangle$ that depends on $q(0) = q$ and similarly $|q'\rangle$ means some state $|\psi(q')\rangle$ that depends $q(t) = q'$.

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

we write $e^{-iHt/\hbar}$ as

$$e^{-iHt/\hbar} = \left[e^{-\frac{i}{\hbar}(\frac{p^2}{2m}+V(q))\epsilon} \right]^N = \left[e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(q)\epsilon} \right]^N \tag{4.38}$$

where

$$\epsilon = \frac{t}{N}$$

Why can we separate q and p? They don't commute. Recall

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

so $[A,B]\sim\epsilon^2$, so ignore it. A more careful treatment will recognize that A,B contain i, so we may first forget i in H, put

$$(4.38)\to e^{-Ht/\hbar}$$

so no i in A,B, then clearly $[A,B]\ll A,B$, then do analytic continuation, let $t\to it$.

After separating q,p, we insert complete $\int dq_i\,|q_i\rangle\langle q_i|$ into (4.37), then insert complete $\int dp_i\,|p_i\rangle\langle p_i|$,

$$\langle q'|e^{-iHt/\hbar}|q\rangle = \prod_{i=0}^{N-1}\left\{\int_{-\infty}^{\infty}dq_i\left\langle q_{i+1}\left|e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon}e^{-\frac{i}{\hbar}V(q)\epsilon}\right|q_i\right\rangle\right\}_{q_N=q'}\delta(q_0=q) \quad (4.39)$$

$$= \prod_{i=0}^{N-1}\{\int_{-\infty}^{\infty}dq_i dp_i\underbrace{\left\langle q_{i+1}\left|e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon}\right|p_i\right\rangle}_{\frac{e^{ip_iq_{i+1}/\hbar}}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}\frac{p_i^2}{2m}\epsilon}}\underbrace{\left\langle p_i\left|e^{-\frac{i}{\hbar}V(q)\epsilon}\right|q_i\right\rangle}_{\frac{e^{-ip_iq_i/\hbar}}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}V(q_i)\epsilon}}\}_{q_N=q'}\delta(q_0=q)$$

$$= \prod_{i=0}^{N-1}\{\int_{-\infty}^{\infty}\frac{dq_i dp_i}{2\pi\hbar}e^{\frac{i\epsilon}{\hbar}[\overbrace{p_i\frac{q_{i+1}-q_i}{\epsilon}}^{p\dot{q}}\overbrace{-\frac{p_i^2}{2m}-V(q_i)}^{-H}]}\}_{q_N=q'}\delta(q_0=q) \quad (4.40)$$

In this way we convert operators, like

$$\text{operators }\frac{p^2}{2m}\to\text{functions of real numbers }\frac{p^2}{2m}$$

so it becomes easier to manipulate. Another advantage is that these functions and the measures are scalar, so they are Lorentz invariant. In (4.40), since q_i and q_{i+1} are independent integral variables, it seems that it can change abruptly. But actually the path is very smooth, because for the exponent not to vanish we have

$$p(q_{i+1}-q_i)\sim\hbar$$

and from (4.39)

$$p^2\sim 2m\hbar/\epsilon$$

so

$$(q_{i+1} - q_i) \sim \sqrt{\epsilon\hbar/2m} \ll 1$$

Take $N \to \infty$, we get continuous smooth deformation of paths and absorb constants like $\sqrt{2\pi\hbar}$ into the measures, we write in a mnemonic friendly form, called canonical expansion

$$\langle q'|e^{-iHt/\hbar}|q\rangle = \int d[p(t')]d[q(t')]e^{\frac{i}{\hbar}\int_0^t dt'[\overbrace{p\dot{q} - H(p,q)}^{L}]} \tag{4.41}$$

To real evaluate it, one should return to the discrete (lattice) version, (4.40). The exponential is called the action, which is path dependent. To compute action, one first fixes a path by picking a set of values for (q_i, p_i) $\forall i$ which gives a path (parametrized by t') in the configuration space obeying $q(t) = q'$, $q(0) = q$.

Since the p_i integral is a Gaussian, we can simplify (4.40).

$$\begin{aligned}
\text{In } (4.40) \quad \to \quad & \int_{-\infty}^{\infty} dp_i e^{-\frac{i}{\hbar}\epsilon\frac{p_i^2}{2m} + \frac{i}{\hbar}p_i(q_{i+1}-q_i)} \\
= \quad & \int_{-\infty}^{\infty} dp_i e^{-\frac{i\epsilon}{2m\hbar}[p_i - \frac{q_{i+1}-q_i}{\epsilon}m]^2 + i\frac{(q_{i+1}-q_i)^2}{2\epsilon}\frac{m}{\hbar}} = \sqrt{\pi}\sqrt{\frac{2m\hbar}{i\epsilon}}e^{i\frac{(q_{i+1}-q_i)^2}{2\epsilon}\frac{m}{\hbar}}
\end{aligned}$$

so

$$\begin{aligned}
(4.40) \quad = \quad & \prod_{i=0}^{N-1}\{\int_{-\infty}^{\infty} dq_i\sqrt{\frac{m}{2\pi\hbar i\epsilon}}e^{\frac{i\epsilon}{\hbar}[\left(\frac{q_{i+1}-q_i}{\epsilon}\right)^2\frac{m}{2} - V(q_i)]}\}_{q_N=q'}\delta(q_0 = q) \\
= \quad & \int d[q(t')]e^{\frac{i}{\hbar}\int_0^t dt'[\overbrace{\frac{1}{2}m\dot{q}(t')^2 - V(q(t'))}^{L}]}
\end{aligned} \tag{4.42}$$

absorbing constants like $\sqrt{\frac{m}{2\pi\hbar i\epsilon}}$ into the measure and fix the 2 end points. When $\hbar \to 0$, by method of stationary phase, we get classical result. Beside (4.42) is simpler than (4.41), it is also cleaner, for L is now function of $q, \dot{q}$.

Lecture 26 (4/30/14)

There aren't many exact solvable path integral problems. As an academic exercise, let's evaluate the integral (4.42) for $V = 0$. Actually we already know the answer for

$$\langle q'|e^{-iHt/\hbar}|q\rangle = \sqrt{\frac{m}{2\pi\hbar it}}e^{\frac{i(q'-q)^2}{2\hbar t}m} \tag{4.43}$$

That is because $\langle q'|e^{-iHt/\hbar}|q\rangle$ satisfies the Green's function

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q'^2} - i\hbar\frac{\partial}{\partial t}\right)\langle q'|e^{-iHt/\hbar}|q\rangle = 0$$

with the initial condition

$$\langle q'|e^{-iHt/\hbar}|q\rangle_{t=0} = \delta(q'-q)$$

We want to get the same answer from (4.42).

$$(4.42) = \lim_{N\to\infty}\left(\frac{mN}{2\pi\hbar it}\right)^{N/2}\prod_{i=0}^{N-1}\{\int_{-\infty}^{\infty}dq_i\}e^{\frac{i}{\hbar}\sum_{i=0}^{N-1}(q_{i+1}-q_i)^2\frac{m}{2t}N}{}_{q_N=q',q_0=q}$$

The classical solution for $q(t')$ should be a constant motion

$$q(t') = q + \frac{q'-q}{t}t'$$

The classical action (ignoring i and $\hbar$)

$$\text{action} = \int_0^t dt'\frac{1}{2}m\left(\frac{dq}{dt'}\right)^2 = \frac{1}{2}m\left(\frac{q'-q}{t}\right)^2 t \tag{4.44}$$

Quantum mechanically we allow fluctuation δq_i

$$q_i = q(t' = \frac{t}{N}i) = q + \frac{q'-q}{t}\left(\frac{t}{N}i\right) + \delta q_i \tag{4.45}$$

with $\delta q_0 = \delta q_N = 0$. As we will see, this gives the correct answer. This is kind of

WKB on steroids. Thus the quantum action (ignoring i and $\hbar$)

$$\begin{aligned}\sum_{i=0}^{N-1}(q_{i+1}-q_i)^2\frac{m}{2t}N &= \frac{m}{2t}N\sum_{i=0}^{N-1}\left(\frac{q'-q}{N}+\delta q_{i+1}-\delta q_i\right)^2\\ &= \frac{m}{2t}N\sum_{i=0}^{N-1}\left(\frac{q'-q}{N}\right)^2+2(\frac{q'-q}{N})(\delta q_{i+1}-\delta q_i)+(\delta q_{i+1}-\delta q_i)^2\\ &= \frac{(q'-q)^2}{2t}m+\frac{m}{t}(q'-q)(\delta q_N-\delta q_0)+\frac{mN}{2t}\sum_{i=0}^{N-1}(\delta q_{i+1}-\delta q_i)^2\end{aligned}$$

So the first term on the right agrees the classical action (4.44), and it gives the half of the answer (4.43), so we only need to show

$$\lim_{N\to\infty}\left(\frac{mN}{2\pi\hbar it}\right)^{N/2}\prod_{i=1}^{N-1}\{\int_{-\infty}^{\infty}dq_i\}e^{\frac{i}{\hbar}\frac{mN}{2t}\sum_{i=0}^{N-1}(\delta q_{i+1}-\delta q_i)^2}=\sqrt{\frac{m}{2\pi\hbar it}} \tag{4.46}$$

This is an example of a general $N-1$ dimensional Gaussian integral. To be rigorous and have (4.46) well-defined like a Gaussian, we really have to put $t\to -it$, and at the end put back $t\to it$. Otherwise (4.46) is not positive definite.

$$\prod_{i=1}^{N-1}\int_{-\infty}^{\infty}dx_i e^{\sum_{i,j=1}^{N-1}-x_iM_{ij}x_j} \tag{4.47}$$

where M_{ij} is symmetric, so $x_iM_{ij}x_j$ is positive definite. Find an orthogonal matrix O (i.e. $O^{-1}=O^t$ and $\det O=\pm 1$) which diagonalizes M

$$O^tMO=\begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_{N-1}\end{pmatrix} \tag{4.48}$$

change of variable

$$x=Oy$$

then

$$
\begin{aligned}
(4.47) \quad &= \prod_{i=1}^{N-1} \int_{-\infty}^{\infty} dy_i \underbrace{\left| \det\left(\frac{\partial x_i}{\partial y_j}\right) \right|}_{1} e^{-y^t D y} \\
&= \prod_{i=1}^{N-1} \int_{-\infty}^{\infty} dy_i e^{-\lambda_i y_i^2} = \prod_{i=1}^{N-1} \sqrt{\frac{\pi}{\lambda_i}} = \frac{\pi^{\frac{N-1}{2}}}{\sqrt{\det M}}
\end{aligned}
$$

So the work remains to find $\det M$ of (4.46).

$$
\sum_{i=0}^{N-1} (\delta q_{i+1} - \delta q_i)^2 = \sum_{i,j=0}^{N-1} \delta q_i M_{ij} \delta q_j
$$

Observe that

$$
\begin{aligned}
\sum_{i=0}^{N-1} (\delta q_{i+1} - \delta q_i)^2 &= \sum_{i=0}^{N-1} (\delta q_{i+1})(\delta q_{i+1} - \delta q_i) - \sum_{i=0}^{N-1} (\delta q_i)(\delta q_{i+1} - \delta q_i) \\
&= \sum_{i=1}^{N} \delta q_i (\delta q_i - \delta q_{i-1}) - \sum_{i=1}^{N-1} (\delta q_i)(\delta q_{i+1} - \delta q_i) \\
&= \sum_{i=1}^{N-1} \delta q_i (\underbrace{-\delta q_{i+1} + 2\delta q_i - \delta q_{i-1}}_{\approx -\frac{d^2 \delta q}{d\epsilon^2} \epsilon^2})
\end{aligned}
$$

Effectively what we have done is the discrete version of integration by parts

$$
\int_0^t dt' \left(\frac{d\delta q}{dt'}\right)^2 = -\int_0^t \delta q \frac{d^2 \delta q}{dt^2} dt'
$$

We claim if we write

$$
-\delta q_{i+1} + 2\delta q_i - \delta q_{i-1} = \sum_{j=1}^{N-1} M_{ij} \delta q_j
$$

with $\delta q_0 = \delta q_N = 0$, so e.g. when $i = N$, we only have

$$
2\delta q_i - \delta q_{i-1}
$$

so the matrix form is the following

$$M = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & 2 & \\ & & & & \ddots \end{pmatrix}$$

then M will be diagonal in the Fourier basis, i.e. with eigenvectors

$$v^{(l)} = \begin{pmatrix} \sqrt{\frac{2}{N}} \sin \frac{\pi l}{N} \\ \sqrt{\frac{2}{N}} \sin \frac{\pi 2 l}{N} \\ \vdots \\ \sqrt{\frac{2}{N}} \sin \frac{\pi k l}{N} \\ \vdots \end{pmatrix} \qquad l = 1, ..., N-1$$

This is very similar to solve N coupled 1D oscillator problem from mechanics. The Fourier basis is orthogonal

$$\sum_{k=1}^{N-1} \sqrt{\frac{2}{N}} \sin \frac{\pi k l}{N} \sqrt{\frac{2}{N}} \sin \frac{\pi k l'}{N} = \delta_{ll'}$$

so they make up the orthogonal transform matrix O in (4.48).

Lecture 27 -Last Lec- (5/5/14)

Indeed compute

$$\begin{aligned} \left(M v^{(l)}\right)_j &= -\sqrt{\frac{2}{N}} \sin \frac{\pi (j+1) l}{N} + 2\sqrt{\frac{2}{N}} \sin \frac{\pi j l}{N} - \sqrt{\frac{2}{N}} \sin \frac{\pi (j-1) l}{N} \\ &= \left(2 - 2\cos \frac{\pi l}{N}\right) \sqrt{\frac{2}{N}} \sin \frac{\pi j l}{N} \\ &= \left(2 - 2\cos \frac{\pi l}{N}\right) \left(v^{(l)}\right)_j \end{aligned}$$

or

$$M \begin{pmatrix} \sqrt{\frac{2}{N}} \sin \frac{\pi l}{N} \\ \sqrt{\frac{2}{N}} \sin \frac{\pi 2l}{N} \\ \vdots \\ \sqrt{\frac{2}{N}} \sin \frac{\pi k l}{N} \\ \vdots \end{pmatrix} = \left(2 - 2\cos\frac{\pi l}{N}\right) \begin{pmatrix} \sqrt{\frac{2}{N}} \sin \frac{\pi l}{N} \\ \sqrt{\frac{2}{N}} \sin \frac{\pi 2l}{N} \\ \vdots \\ \sqrt{\frac{2}{N}} \sin \frac{\pi k l}{N} \\ \vdots \end{pmatrix}$$

By (4.45), q, q' are constant, so replace $dq_i \to d\delta q_i$, therefore

$$\begin{aligned} \text{LHS (4.46)} &= \lim_{N\to\infty} \left(\frac{mN}{2\pi\hbar it}\right)^{N/2} \prod_{i=1}^{N-1} \{\int_{-\infty}^{\infty} d\delta q_i\} e^{\frac{i}{\hbar}\frac{mN}{2t}\sum_{i,j=0}^{N-1}\delta q_i M_{ij}\delta q_j} \\ &= \lim_{N\to\infty} \left(\frac{mN}{2\pi\hbar it}\right)^{N/2} \left(\frac{2\pi\hbar it}{mN}\right)^{(N-1)/2} \prod_{l=1}^{N-1} \frac{1}{\sqrt{2-2\cos\frac{\pi l}{N}}} \\ &= \sqrt{\frac{m}{2\pi\hbar it}} \underbrace{\lim_{N\to\infty} \sqrt{N} \prod_{l=1}^{N-1} \frac{1}{\sqrt{2-2\cos\frac{\pi l}{N}}}}_{=1} \end{aligned}$$

In fact it is equal to 1 for all $N > 1$. Since $1 - \cos\frac{\pi l}{N} = 2\sin^2\frac{\pi l}{2N}$, we prove (courtesy of Rafael Krichevsky)

$$\prod_{l=1}^{N-1} \sin\frac{\pi l}{2N} = \frac{\sqrt{N}}{2^{N-1}}$$

Indeed we consider

$$\begin{aligned} \prod_{l=1}^{N-1} \sin\frac{\pi l}{2N} &= \sqrt{\prod_{l=1}^{2N-1} \sin\frac{\pi l}{2N}} \\ &= \sqrt{\prod_{l=1}^{2N-1} \frac{e^{i\frac{\pi l}{2N}}}{2i}\left(1 - e^{-i\frac{\pi l}{N}}\right)} \\ &= \sqrt{\frac{e^{i\frac{\pi}{2N}(2N-1)N}}{(2i)^{2N-1}} \prod_{l=1}^{2N-1}\left(1 - e^{-i\frac{\pi l}{N}}\right)} \end{aligned} \tag{4.49}$$

We want to apply a well-known result from complex variable: the product of the distance from 1 to the other Nth roots of unity is N. That is

$$\prod_{l=1}^{N-1}\left(1-e^{-i\frac{2\pi l}{N}}\right)=N \tag{4.50}$$

That is because let $\xi = e^{-i\frac{2\pi}{N}}$

$$(z-\xi)(z-\xi^2)\cdot ... \cdot(z-\xi^{N-1})(z-1)=z^N-1$$

that is because z^N-1 has at most N distinct roots, and the left hand side has exact N distinct roots, and the coefficient of the highest powers are both 1.

On the other hand

$$z^N-1=(z-1)(z^{N-1}+z^{N-2}+...+1)$$

cancel $z-1$, so

$$(z-\xi)(z-\xi^2)\cdot ... \cdot(z-\xi^{N-1})=z^{N-1}+z^{N-2}+...+1$$

now putting $z=1$, we obtain (4.50).

Now change $N\to 2N$ in (4.50), we get what we want in (4.49), thus

$$\prod_{l=1}^{N-1}\sin\frac{\pi l}{2N}=\sqrt{\frac{e^{i\frac{\pi}{2N}(2N-1)}}{(2i)^{2N-1}}2N}=\frac{\sqrt{N}}{2^{N-1}}$$

Dyson Wick Expansion

In general $V\neq 0$, but we can still follow the idea in (4.45). Find the classical solution, and adding fluctuation, we will get something similar to (4.46)

$$\prod_{i=1}^{N-1}\int_{-\infty}^{\infty} d\delta q_i e^{\sum_{i,j=1}^{N-1}-\delta q_i M_{ij}\delta q_j+O(\delta q^3)}$$

which may not have analytic solutions. But if we assume the classical solution is dominated solution, so fluctuation is small, we Taylor expand and bring down the

$O(\delta q^3)$ so we get some kind of moments, so it can be solved analytically.

4.5 Bosonic Path Integrals

For a system of bosons we would start with a classical field theory which when quantized has as quanta, the bosons of interest, looking like mulit-SHO. For example, to treat photons, we would start with the classical field $\vec{A}(\vec{r}, t)$ and Lagrangian

$$L = \frac{1}{8\pi^2} \int d^3 r [\vec{E}^2(\vec{r}) - \vec{B}^2(\vec{r})]$$

Similar to (4.42)

$$\begin{aligned}
\left\langle [\vec{A}'(\vec{r})] \middle| e^{-iHt/\hbar} \middle| [\vec{A}(\vec{r})] \right\rangle &= \prod_{i=0}^{N-1} \prod_{\vec{r}} \left\{ \int d\vec{A}^{(i)}(\vec{r}) \right\} e^{\frac{i}{\hbar} \frac{1}{8\pi} \int_0^t dt' [\vec{E}^2(\vec{r}, t') - \vec{B}^2(\vec{r}, t')]} \\
&= \prod_{i=0}^{N-1} \prod_{\vec{r}} \left\{ \int d\vec{A}^{(i)}(\vec{r}) \right\} e^{\frac{i}{\hbar} \frac{1}{8\pi} \epsilon \sum_n [\frac{1}{c} \frac{(\vec{A}^{(n+1)}(\vec{r}) - \vec{A}^{(n)}(\vec{r}))}{\epsilon^2} - (\nabla \times \vec{A}^{(i)}(\vec{r}))^2]}
\end{aligned}$$

where $[\vec{A}(\vec{r})]$ too means some state $|\psi\rangle$ that depends on $\vec{A}(\vec{r})$, and the infinite integral $\left\{ \int d\vec{A}^{(i)}(\vec{r}) \right\}$ can be too made well-defined by going to discrete grid (lattice in space).

4.6 Fermionic Path Integrals

Use the Grassmann variables we studied before (2.42), we can write

$$\begin{aligned}
H &= \sum_{i=1}^{K} H(p_i, q_i) \\
&= \sum_{k,k'} a_k^+ a_{k'} \langle \psi_k | H | \psi_{k'} \rangle
\end{aligned}$$

here ψ_k, $1 \leq k \leq K$ are the single particle states which a_k, a_k^+, q_k, $\frac{d}{dq_k}$ are empty or fill. One can show by using

$$\int dq = 0 \qquad \int q dq = 1$$

that

$$\begin{aligned}
\left\langle q_1^\dagger, ..., q_k^\dagger \middle| T\left\{ e^{-\frac{i}{\hbar}\int_0^t H(t')dt'} \right\} \middle| \psi \right\rangle &= \left\langle q_1^\dagger, ..., q_k^\dagger \middle| T\left\{ e^{-\frac{i}{\hbar}\sum_{i,j=1}^{N}\int_0^t \frac{\partial}{\partial q_i} H_{ij} q_j dt'} \right\} \middle| \psi \right\rangle \\
&= \lim_{N\to\infty} \prod_{n=0}^{N-1} \left\{ \prod_{i=1}^{K} \int dq_i^{(n)} \int d\bar{q}_i^{(n)} e^{\frac{i}{\hbar}\epsilon \sum_{i=1}^{K} \bar{q}_i^{(n)} (q_i^{(n+1)} - q_i^{(n)})} \right. \\
&\quad \left. e^{-\frac{i}{\hbar}\epsilon \sum_{i,j=1}^{K} \bar{q}_j^{(n)} H_{ij} q_j^{(n)}} \right\}_{q_i^{(n+1)} = q_i^f} \psi(q_1^{(0)}, ..., q_K^{(0)})
\end{aligned}$$