Lecture 19

Time dependent perturbation theory

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

$$|\Psi_I(t)\rangle = e^{iH_0 t} |\Psi_S(t)\rangle$$

$$O_I(t) = e^{iH_0 t} O_S e^{-iH_0 t}$$

equation:

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

$$|\Psi_I(0)\rangle = |\Psi_S(0)\rangle = |\Psi_H\rangle$$

Integral formulation

$$|\Psi_I(t)\rangle = |\Psi_I(0)\rangle - i \int_0^t V_I(t') |\Psi_I(t')\rangle \, dt'$$

solution by iteration

$$|\Psi_I(t)\rangle = |\Psi_I(0)\rangle +$$

$$\sum_{n=1}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \times$$

$$V_I(t_1) \cdots V_I(t_n) |\Psi_I(0)\rangle$$

The iterative solution satisfies the integral equation provided it converges

HW

$$\| |\psi\rangle \| = \langle \psi | \psi \rangle^{1/2}$$

$$||| O ||| = \sup_{\| |\psi\rangle \| \neq 0} \frac{\| O |\psi\rangle \|}{\| |\psi\rangle \|}$$

properties – show HW

$$\| O |\psi_I\rangle \| \leq ||| O ||| \, \| |\psi\rangle \|$$

$$||| O_2 O_1 ||| \leq ||| O_2 ||| \, ||| O_1 |||$$

$$||| O_1 + O_2 ||| \leq ||| O_1 ||| + ||| O_2 |||$$

Consider the 3^{rd} order term

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \, V_I(t_1) V_I(t_2) V_I(t_3)$$

$$t_1 \geq t_2 \geq t_3$$

We can relabel the t_i's in six different ways with 3 times $t_1 \; t_2 \; t_3$

there are $3!$ possible orderings

$t_1 \geq t_2 \geq t_3$	$V_I(t_1) V_I(t_2) V_I(t_3)$
$t_1 \geq t_3 \geq t_2$	$V_I(t_1) V_I(t_3) V_I(t_2)$
$t_2 \geq t_1 \geq t_3$	$V_I(t_2) V_I(t_1) V_I(t_3)$
$t_2 \geq t_3 \geq t_1$	$V_I(t_2) V_I(t_3) V_I(t_1)$
$t_3 \geq t_1 \geq t_2$	$V_I(t_3) V_I(t_1) V_I(t_2)$
$t_3 \geq t_2 \geq t_1$	$V_I(t_3) V_I(t_2) V_I(t_1)$

all 6 integrals give the same answer. This suggests defining the time ordered product

$$T\left(V_I(t_1) V_I(t_2) V_I(t_3) \right) =$$

$$\theta(t_1-t_2)\,\theta(t_2-t_3)\, V_I(t_1) V_I(t_2) V_I(t_3) +$$

$$\theta(t_1-t_3)\,\theta(t_3-t_2)\, V_I(t_1) V_I(t_3) V_I(t_2) +$$

$$\theta(t_2-t_1)\,\theta(t_1-t_3)\, V_I(t_2) V_I(t_1) V_I(t_3)$$

$$\theta(t_2-t_3)\,\theta(t_3-t_1)\, V_I(t_2) V_I(t_3) V_I(t_1)$$

$$\theta(t_3-t_1)\,\theta(t_1-t_2)\, V_I(t_3) V_I(t_1) V_I(t_2)$$

$$\theta(t_3-t_2)\,\theta(t_2-t_1)\, V_I(t_3) V_I(t_2) V_I(t_1)$$

with this definition the iterative solution can be expressed as

$$|\Psi_I(t)\rangle = |\Psi_I(0)\rangle + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \times T\left(V_I(t_1) \cdots V_I(t_n)\right)$$

We use this to check convergence

* $|||V_I(t)||| = |||e^{iH_0 t} V e^{-iH_0 t}||| \leq$

$|||e^{iH_0 t}|||\ |||V_S|||\ |||e^{-iH_0 t}||| =$

$|||V_S|||$

* If $V_S = V_S(t)$ let

$$V = \max_{0 \leq t' \leq t} |||V_S(t')|||$$

* $\| T(V_I(t_1) \cdots V_I(t_n)) |\Psi_I(0)\rangle \| \leq$

$||| T(V_I(t_1) \cdots V_I(t_n)) |||\ \| \Psi_I(0)\rangle \| =$

$$||| \Theta(t_{\sigma(1)} - t_{\sigma(2)}) \cdots \Theta(t_{\sigma(n-1)} - t_{\sigma(n)})$$

$$V_I(t_{\sigma(1)}) \cdots V_I(t_{\sigma(n)}) ||| \; || \Psi_I(0)\rangle || \leq$$

$$||| V_s(t_{\sigma(1)}) ||| \cdots ||| V_s(t_{\sigma(n)}) ||| \; || \Psi_I(0)\rangle || \leq$$

$$V^n \, || \Psi_I(0)\rangle$$

Since $\int_0^t = t$ combining everything

$$||| \, |\Psi_I(t)\rangle \, ||| =$$

$$||| \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \, dt_n \, T(V_I(t_1) \, V_I(t_n)) \, |\Psi_I(0)\rangle ||$$

$$\leq \sum_{n=0}^{\infty} \frac{1}{n!} || \int_0^t dt_1 \, dt_n \, T(V_I(t_1) \cdots V_I(t_n)) \, |\Psi_I(0)\rangle ||$$

$$\leq \sum_{n=0}^{\infty} \frac{t^n}{n!} V^n \, || \Psi_I(0)\rangle || = e^{tV} \, || \, |\Psi_I(0)\rangle ||$$

This shows that the series generated by iteration converges

assuming

$$\max_{0 \le t' \le t} \| V_S(t') \| < \infty$$

$$t < \infty$$

This converges even if V is not small

Application:

Assume $H_0 |n\rangle = E_n |n\rangle$ has been solved for all n

* expand $|\Psi_I(t)\rangle$ in the complete set of eigenstate of H_0

$$|\Psi_I(t)\rangle = \sum_{n=1}^{\infty} |n\rangle\langle n|\Psi_I(t)\rangle$$

$$= \sum_{n=1}^{\infty} |n\rangle C_n(t)$$

Interpretation of $C_n(t)$

$$C_n(t) = \langle n | \Psi_I(t) \rangle =$$

$$= \langle n | e^{iH_0 t} | \Psi_s(t) \rangle =$$

$$= e^{iE_n t} \langle n | \Psi_s(t) \rangle$$

$$\boxed{|C_n(t)|^2 = |\langle n | \Psi_s(t) \rangle|^2 =}$$

probability of finding $|\Psi_s(t)\rangle$ in the n^{th} eigenstate of H_0

Equations for $C_n(t)$

$$\langle n | \Psi_I(t) \rangle = \langle n | \Psi_I(0) \rangle - i \int_0^t \sum_m \langle n | V_I(t') | m \rangle \langle m | \Psi_I(t') \rangle dt'$$

$$= C_n(0) - i \int_0^t \sum_m e^{i(E_n - E_m)t'} \langle n | V_s(t') | m \rangle C_m(t') \, dt'$$

normally the assumption is that the system is initially in the state k

$C_n(0) = \delta_{nk}$ - Then

$$C_n(t) = \delta_{nk} - i \sum_m \int_0^t e^{i(E_n - E_m)t'} \langle n | V_s(t') | m \rangle C_m(t') dt'$$

case

(1) V is small

(2) $n \neq k$ - what probability of transition to a different state

(3) $V_s(t) = \theta(t) V$

Then to first order in V

$$C_n(t) \simeq \delta_{nk} - i \int_0^t e^{i(E_n - E_k)t'} \langle n | V | k \rangle dt'$$

In this case the integral can be computed analytically

$$C_n(t) \simeq \delta_{nk} - i \langle n | V_s | k \rangle \frac{e^{i(E_n - E_k)t} - 1}{i(E_n - E_k)}$$

$$= \delta_{nk} - i \langle n | V_s | k \rangle e^{i \frac{E_n - E_k}{2} t} \times 2 \frac{\sin\left(\frac{E_n - E_k}{2} t\right)}{(E_n - E_k)}$$

For $n \neq k$ this becomes

$$\boxed{|C_n(t)|^2 = |\langle n | V_s | k \rangle|^2 \left(\frac{\sin\left(\frac{E_n - E_k}{2} t\right)}{\left(\frac{E_n - E_k}{2}\right)} \right)^2}$$

remark

This is strongly peaked near $E_n \approx E_k$

Case of an explicit time dependent potential

example 1

$$V_S = \Theta(t) V \cos(\omega t)$$

for a system initially in state $|k\rangle$ the first order approximation for making a transition to $|n\rangle$ for $n \neq k$ is

$$c_n(t) \simeq \delta_{nk} - i \int_0^t e^{i(E_n - E_k)t'} \langle n|V|k\rangle \cos(\omega t') dt'$$

we write $\cos(\omega t) = \frac{1}{2}(e^{i\omega t} + e^{-i\omega t})$

for $n \neq k$ this becomes

$$c_n(t) = -\frac{i}{2} \langle n|V|k\rangle \int_0^t \left(e^{i(E_n - E_k + \omega)t'} + e^{i(E_n - E_k - \omega)t'} \right) dt'$$

integrating gives

$$-\frac{i}{2}\langle n|V|k\rangle\left\{e^{i(E_n-E_k+\omega)t/2}\frac{\sin\left(\frac{E_n-E_k+\omega}{2}t\right)}{\frac{E_n-E_k+\omega}{2}}+\right.$$

$$\left.e^{i(E_n-E_k-\omega)t/2}\frac{\sin\left(\frac{E_n-E_k-\omega}{2}t\right)}{\frac{E_n-E_k-\omega}{2}}\right\}$$

when this is squared there are 3 terms — the square of the one with $E_n-E_k\pm\omega$ closest to 0 will be the largest — ignoring the other 2 terms

$|c_n(t)|^2 =$ probability of making a transition from $|k\rangle$ to $|n\rangle$ after time t is

$$\simeq\frac{1}{4}|\langle n|V|k\rangle|^2\frac{\sin^2\left(\frac{E_n-E_k\pm\omega}{2}t\right)}{\left(\frac{E_n-E_k\pm\omega}{2}\right)^2}$$

Note – I have been using $\hbar = 1$

If I include the factors of $\hbar$ this becomes

$$P_n = \frac{1}{4} |\langle n|V|k\rangle|^2 \frac{\sin^2\left(\frac{E_n - E_k \pm \hbar\omega}{2\hbar} t\right)}{\left(\frac{E_n - E_k \pm \hbar\omega}{2}\right)^2}$$

(note you can see this is dimensionless)

More general time dependence

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

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

In this case the dominant contribution is for $\hbar\omega \simeq E_n - E_k$

$$P_n \to |\langle n|\tilde{V}(\omega)|k\rangle|^2 \frac{\sin^2\left(\frac{E_n - E_k \pm \hbar\omega}{2\hbar} t\right)}{\left(\frac{E_n - E_k \pm \hbar\omega}{2}\right)^2}$$

example

Hydrogen atom in an electromagnetic field

$$\phi = 0 \qquad \bar{A} = A\hat{x}e^{i(\omega t - \frac{\omega}{c}z)}$$

$$\bar{E} = -\frac{\partial A}{\partial t} = -i\omega A\hat{x}e^{i(\omega t - \frac{\omega}{c}z)}$$

$$\bar{B} = \bar{\nabla}\times\bar{A} = -i\frac{\omega A}{c}\hat{y}e^{i(\omega t - \frac{\omega}{c}z)}$$

$$|E| = A\omega \qquad |B| = \frac{A\omega}{c} \qquad |B|c = |E|$$

The Hamiltonian becomes

$$H = \underbrace{\frac{(\bar{P} - \frac{e}{c}\bar{A})^2}{2m}}_{\text{Covariant Derivative}} - \underbrace{e\phi}_{0} - \frac{e^2}{r}$$

$$= \underbrace{\frac{P^2}{2m} - \frac{e^2}{r}}_{H_0} - \frac{e}{2mc}(\bar{P}\cdot\bar{A} + \bar{A}\cdot\bar{P}) + \frac{e^2A^2}{2mc^2}$$

ignore in the weak field limit

here

$$V = -\frac{e}{2mc}\left(AP_x e^{-i\frac{\omega}{c}z} + P_z \cdot A e^{-i\frac{\omega}{c}z}\right)e^{i\omega t}$$

in this case

$$V = -\frac{eA}{mc} P_x e^{-\frac{i\omega}{c}z} e^{i\omega t}$$

In this case for states $|n\ell m\rangle$

$$\boxed{P_{n\ell m \to n'\ell' m'} \simeq \left(\frac{eA}{mc}\right)^2 |\langle n'\ell' m'| P_x e^{-\frac{i\omega}{c}z} |n\ell m\rangle|^2 \frac{\sin^2\left(\frac{E-E'+\omega}{2}t\right)}{\left(\frac{E-E'+\omega}{2}\right)^2}}$$

example 2

In some case the potential can cause a transition to a state with a continuous energy spectrum — for instance if the potential causes an atom to ionize then the energy of the final state is continuum

$\langle n | V | m \rangle \rightarrow$

$\rho(E)\, dE \, \langle E | V | m \rangle$

where $\rho(E)$ is called the density of final states

The probability of getting a transition between

$E_n \pm \frac{\Delta E}{2}$ is

$$P = \int_{E_n - \frac{\Delta E}{2}}^{E_n + \frac{\Delta E}{2}} \langle n | V | E \rangle \rho(E) \langle E | V | n \rangle \frac{\sin^2\left(\frac{E_n - E}{2\hbar} t\right)}{\left(\frac{E - E_n}{2}\right)^2}$$

Let $u = \frac{(E_n - E)t}{2\hbar}$ $\qquad \frac{du}{dE} = -\frac{t}{2\hbar}$

$\frac{2\hbar u}{t} = E_n - E \qquad E = E_n - \frac{2\hbar u}{t}$

$u : -\frac{\Delta E\, t}{2\hbar} \quad \frac{\Delta E\, t}{2\hbar}$

as $t \to \infty$ the limits of integra get large.

$$P \to \int |\langle E_n - \tfrac{2\hbar u}{t} | V | n\rangle|^2 \rho(E_n - \tfrac{2\hbar u}{t})(-\tfrac{2\hbar}{t})$$

$$du \quad \frac{\sin^2 u}{(\omega/t)^2}$$

$$\int |\langle E_n - \tfrac{2\hbar u}{t} |V| n\rangle|^2 \rho(E_n - \tfrac{2\hbar u}{t})(-\tfrac{2\hbar}{t}) t^2$$

$$\frac{\sin^2 u}{\hbar^2 u^2}$$

$\frac{\sin^2 u}{u^2}$ falls off for large $u \Rightarrow$

for large t $\quad E_n - \frac{2\hbar u}{t} \to E_n$

$$\langle E_n | V | n\rangle^2 \rho(E_n)(-2\hbar)$$

The integral $\int_{-\infty}^{\infty} \frac{\sin^2 u}{u^2}\, du = \pi$

$$\frac{2\pi}{\hbar} |\langle E_n | V | n\rangle|^2 \rho(E_n)\, t$$

This means that for large t the transition probability grows $\propto$ to t

$$\boxed{\frac{dP}{dt} \to (\text{const}) = \frac{2\pi}{\hbar}|\langle E_n|V|E_n\rangle|^2 \rho(E_n)}$$

This result is called Fermi golden rule.