Lecture 20

Time dependent perturbation theory

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

$$V_I(t) = e^{iH_0 t/\hbar} V_S(t) e^{-iH_0 t/\hbar}$$

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

$$|\Psi_I(t)\rangle = |\Psi_I(0)\rangle - \frac{i}{\hbar}\int_0^t V_I(t')|\Psi_I(t')\rangle dt'$$

equation can be solved by iteration for finite t and

$$\| V_S(t) \| \leq V < \infty$$

$$H_0|n\rangle = E_n|n\rangle$$

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

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

$|c_n(t)|^2$ = probability of finding $|\Psi_S(t)\rangle$ in n^{th} eigenstate of H_0 at time t

$$c_n(t) = c_n(0) - \frac{i}{\hbar}\sum_{m=1}^{\infty}\int_0^t e^{i(E_n-E_m)t'/\hbar}\langle n|V_s(t')|m\rangle$$
$$c_m(t')\,dt'$$

This is an infinite set of coupled integral equations for the coefficients $c_n(t)$

When
(1) VT is small
(2) $c_n(0) = \delta_{nk}$
(3) $n \neq k$

we have

$$c_n(t) \simeq -\frac{i}{\hbar}\int_0^t e^{i(E_n-E_m)\frac{t'}{\hbar}}\langle n|V_s(t')|k\rangle\,dt'$$

This assumes that the first order expansion in VT is a good approximation

Last time we considered

Case 1: V_s is independent of time

Then

$$c_n(t) = -\frac{i}{\hbar}\langle n|V_s|k\rangle \int_0^t e^{i(E_n-E_k)t'/\hbar}\, dt' =$$

$$-\frac{i}{\hbar}\langle n|V_s|k\rangle\, e^{i(E_n-E_k)\frac{t}{2\hbar}} \frac{2i\sin\left(\frac{(E_n-E_k)t}{2\hbar}\right)}{i(E_n-E_k)/\hbar}$$

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

This give the transition probability at time t as

$$\boxed{|c_n(t)|^2 = P_{k\to n}(t) \simeq \frac{1}{\hbar^2}|\langle n|V_s|k\rangle|^2 \frac{\sin^2\left(\frac{E_n-E_k}{2\hbar}t\right)}{\left(\frac{(E_n-E_k)}{2\hbar}\right)^2}}$$

where this probability is sharply peaked when $E_n = E_k$

case 2

Assume $V_s(t) = \theta(t) e^{i\omega t} V$

then the only change is that

$$e^{i(E_n - E_k)\frac{t}{\hbar}} \to e^{i(E_n - E_k + \omega\hbar)\frac{t}{\hbar}}$$

then to get the desired probability we need to replace $E_n - E_k$ by $E_n - E_k + \hbar\omega$

$$\boxed{|C_n(t)|^2 = P_n(t) \simeq \frac{1}{\hbar^2} |\langle n | V_s | k \rangle|^2 \frac{\sin^2\left(\frac{E_n - E_k + \hbar\omega}{2} \frac{t}{\hbar}\right)}{\left(\frac{E_n - E_k + \hbar\omega}{2\hbar}\right)^2}}$$

This peaks when

$$\boxed{\omega \simeq \frac{E_k - E_n}{\hbar}}$$

case 3

$$V_I(t) = \theta(t) V_s \cos(\omega t)$$

$$= \frac{1}{2} \theta(t) V_s \left(e^{i\omega t} + e^{-i\omega t} \right)$$

we can directly use the results from case 2 to get

$$c_n(t) \simeq -\frac{i}{2\hbar} \langle n | V_s | k \rangle \times \Bigg[e^{i\left(\frac{E_n - E_k + \hbar\omega}{2} \frac{t}{\hbar}\right)} \frac{\sin\left(\frac{E_n - E_k + \hbar\omega}{2} \frac{t}{\hbar}\right)}{\frac{E_n - E_k + \hbar\omega}{2\hbar}} + e^{i\left(\frac{E_n - E_k - \hbar\omega}{2} \frac{t}{\hbar}\right)} \frac{\sin\left(\frac{E_n - E_k - \hbar\omega}{2} \frac{t}{\hbar}\right)}{\frac{(E_n - E_k - \hbar\omega)}{2\hbar}} \Bigg]$$

in this case we <u>can't</u> add the squares of the probability amplitudes because there are interference terms. Normally one of these 2 terms is dominant

Then we can ignore the other one

$$\boxed{|E_n - E_k \pm \hbar\omega| \gg |E_n - E_k \mp \hbar\omega|}$$

in this case

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

case 4 – arbitrary time dependence

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

then we get

$$\boxed{c_n(t) = P_n(t) \simeq -\frac{i}{\hbar} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \langle n|\tilde{V}(\omega)|k\rangle e^{i\frac{E_n - E_k + \hbar\omega}{2\hbar} t} \times \frac{\sin\left(\frac{E_n - E_k + \hbar\omega}{2\hbar} t\right)}{\left(\frac{E_n - E_k + \hbar\omega}{2\hbar}\right)}}$$

case 5 - continuous energy

(Fermi's golden rule)

$$|n\rangle \to \gamma, \; |n'\rangle$$

relative kinetic energy

γ = photon

$$I = \int |E\rangle \, dE \, \rho(E) \langle E|$$

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

example - moving electron,

$$E = \frac{p^2}{2m} \qquad \frac{dE}{dp} = \frac{|\vec{p}|}{m}$$

$$I = \int |\uparrow p\rangle \, d^3p \, \langle \uparrow p| + \int |\downarrow p\rangle \, d^3p \, \langle \downarrow p|$$

$$= \int |\uparrow p\rangle \, d\Omega \, p^2 \frac{dp}{dE} \langle p \uparrow| \, dE + \int |\downarrow p\rangle \, d\Omega \, p^2 \frac{dp}{dE} \langle p \downarrow| \, dE$$

$$\rho(E) = d\Omega \, p^2 \frac{m}{p} \, 2$$

consider

$$\int_{E_0-\frac{\Delta E}{2}}^{E_0+\frac{\Delta E}{2}} \frac{dP}{dE}\, dE$$

probability of transition to a state with energy E between $E_0-\frac{\Delta}{2} \le E \le E_0+\frac{\Delta}{2}$

$$\frac{dP}{dE}\Delta E = \frac{1}{\hbar^2}\int_{E_0+\frac{\Delta E}{2}}^{E_0-\frac{\Delta E}{2}} \langle R|V_s|E\rangle \rho(E)\, dE\, \langle E|V_s|k\rangle$$

$$\left[e^{i\frac{E_k-E}{2\hbar}t} \frac{\sin\left(\frac{E_k-E}{2\hbar}t\right)}{\left(\frac{E_k-E}{2}\right)} \times e^{\frac{i(E-E_k)t}{2\hbar}} \frac{\sin\left(\frac{E-E_k}{2\hbar}t\right)}{\left(\frac{E-E_k}{2}\right)} \right]$$

since $\frac{\sin x}{x} = \frac{\sin(-x)}{(-x)}$ this

becomes

$$\frac{dP}{dE}\Delta E = \frac{1}{\hbar^2}\int_{E_0-\frac{\Delta E}{2}}^{E_0+\frac{\Delta E}{2}} |\langle R|V_s|E\rangle|^2 \rho(E)\, dE$$

$$\frac{\sin^2\left(\frac{E_k-E}{2\hbar}t\right)}{\left(\frac{E_k-E}{2\hbar}\right)^2}$$

It is useful to look at the large time limit of this expression (note – large but not so large that first order perturbation theory breaks down)

Let $u = \frac{E - E_k}{2} \frac{t}{\hbar}$ $\quad E - E_k = \frac{2\hbar u}{t}$

$du = \frac{1}{2}\frac{t}{\hbar} dE \qquad dE = \frac{2\hbar}{t} du$

$E_0 \pm \frac{\Delta E}{2} = \frac{2\hbar u}{t} + E_k \pm$

$u = \frac{t}{2\hbar}(E \pm \Delta E - E_k)$

changing variables

$$\frac{dP}{dE}\Delta E = \frac{1}{\hbar^2}\int \frac{2\hbar}{t} du \left|\langle E_k + \frac{2u\hbar}{t} | V | k\rangle\right|^2$$

$$p\left(E_k + \frac{2u\hbar}{t}\right) \frac{\sin^2(u)}{u^2/t^2}$$

for $E_0 = E_k \quad u = \pm \frac{\Delta E\, t}{2\hbar}$

$\frac{\sin^2 u}{u^2}$ is sharply peaked

while for large t $\pm \frac{\Delta E t}{2\hbar}$

can be extended to $\pm \infty$

$$P = \frac{2t}{\hbar} \int_{-a}^{a} \rho\left(E_a + \frac{2u\hbar}{t}\right) \frac{\sin^2 u}{u^2}$$

$$\left|\left\langle E + \frac{2u\hbar}{t} \middle| V_s \middle| E_a \right\rangle\right|^2 du$$

for $t \gg 2u_{max}\hbar$ we can

ignore the $\frac{2u\hbar}{t}$ in the

density of states and the

potential matrix element

to get

$$P \simeq \frac{2t}{\hbar} \rho(E_a) \left|\langle E | V_s | E_a \rangle\right|^2 \times$$

$$\underbrace{\int_{-\infty}^{\infty} \frac{\sin^2 u}{u^2}}_{= \pi}$$

$$\boxed{P \simeq t \times \frac{2\pi}{\hbar} \rho(E) \left|\langle E | V_s | E_a \rangle\right|^2}$$

This means that for small V and large times

$$\boxed{\frac{dP}{dt} = \text{transition rate approaches the constant value } \frac{2\pi}{\hbar}\rho(E)|\langle E|V|E_0\rangle|^2}$$

this result is called Fermi's golden rule.

<u>example</u>

Hydrogen - Like atom in a time varying electromagnetic field

$$H = \frac{1}{2m}\left(\bar{p} - \frac{e}{c}\bar{A}\right)^2 - \frac{ze^2}{r} - e\phi$$

we choose a field

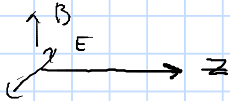
$$\bar{A} = A\hat{x}e^{i(\omega t - \frac{\omega}{c}z)}, \quad \phi = 0$$

This corresponds to fields

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

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

$$|\bar{B}| c = |\bar{E}|$$



for a weak field we can ignore the A^2 term in the potential

$$H \simeq \frac{p^2}{2m} - \frac{Ze^2}{r} - \frac{e}{2mc}(\bar{p}\cdot\bar{A} + \bar{A}\cdot\bar{p})$$

$$\frac{p^2}{2m} - \frac{Ze^2}{r} - \frac{e}{mc} A P_x e^{i(\omega t - \frac{\omega}{c} z)}$$

In this case

$$V_s(t) = \left(-\frac{e}{mc} A P_x e^{-i\frac{\omega}{c} z}\right) \times e^{i\omega t}$$

for this electromagnetic wave to cause a transition from $|n\ell m\rangle$ to $|n'\ell' m'\rangle$

$$|C_{nem \to n'e'm'}|^2 \simeq$$

$$\frac{1}{\hbar^2} \left| \langle n'e'm' | -\frac{eA}{mc} P_x e^{i\frac{\omega}{c} z} | nem \rangle \right|^2 \times \frac{\sin^2\left(\frac{E-E'+\hbar\omega}{2\hbar} t\right)}{\left(\frac{E-E'+\hbar\omega}{2\hbar}\right)^2}$$

$$\frac{e^2A^2}{\hbar^2 m^2 c^2} \left| \langle n'e'm' | -\frac{eA}{mc} P_x e^{i\frac{\omega}{c} z} | nem \rangle \right|^2$$

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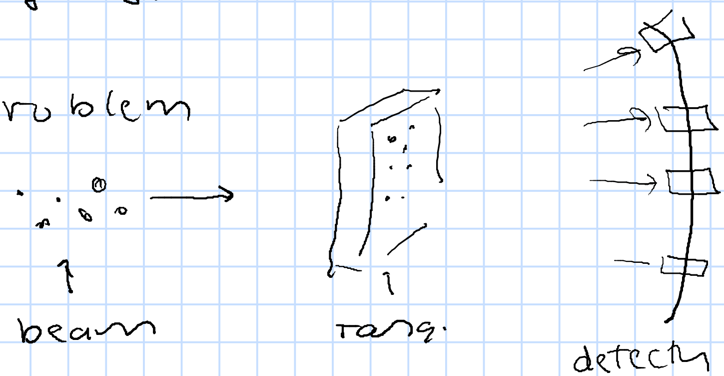
scattering theory — see my typed notes.

problem



question - what can we learn about the interaction by looking at what comes out in the detector?

① beam is given by a classical stastical ensemble of particle moving with mean velocity $\bar{v}$

$$\rho_B = \sum P_{bn} \, |\psi_{B_n}\rangle\langle\psi_{B_n}|$$

② the target is described by another ensemble with mean velocity 0 in the

$$\rho_T = \sum P_{Tn} \, |\psi_{T_n}\rangle\langle\psi_{T_n}|$$

We assume that the target is sufficiently thin or dilute so typically a beam particle collides with at most 1 target particle

After these particles collide they head towards detectors. A given detector will respond when one of the particle state overlaps with a state of the detector

We begin by considering a specific particle - beam state $|\Psi_{-}(t)\rangle$

We consider another state that could be detected by detectors $|\Psi_{+}(t)\rangle$

We assume both states satisfy the Schrodinger equation

$$i\hbar \frac{|\Psi_\pm(t)\rangle}{dt} = H|\Psi_\pm(t)\rangle$$

It follow that the probability from a $-$ state to a $+$ state is

$$P_{+-} = |\langle\Psi_+(t)|\Psi_-(t)\rangle|^2$$

since $|\Psi_\pm(t)\rangle = e^{-iHt/\hbar}|\Psi_\pm(0)\rangle$

the probability P_{+-} is independent of time. If $t \simeq 0$ is approximately the time of collision, we do not know much about the structure of these states however if the interaction between the 2 particles is short range long before the collision $|\psi_-\rangle$ looks like 2 free particle; similarly long after the collisions $|\psi_+\rangle$ also looks like a pair of particles heading towards a detector

* There is no common time when both states are simple - however to calculate $|\psi_\pm(t)\rangle$ we need an initial condition

The simplest thing is to choose the initial condition for $|\psi_-(t)\rangle$ at a time before the collision when

The particles are not interacting ($t = -T_i$) while for the final state it is convenient to choose an initial time T_f after the particles have separate beyond the range of the interaction

$$|\Psi_-(-T_i)\rangle = |\Psi_-^0(-T_i)\rangle$$

$$|\Psi_+(T_F)\rangle = |\Psi_+^0(T_F)\rangle$$

where the states on the right are free particle states

$-T_I$ can be the time at beam preparation while T_F can be the time of detection. Making T_I or T_F larger changes nothing since the minimum values of T_I & T_F depend on the choice of wave packet,

To remove this dependence consider $T_{F,I} \rightarrow \infty$

The initial conditions can then be expressed using the scattering asymptotic condition

$$\lim_{t \to -\infty} \| e^{-iHt/\hbar} |\Psi_-(0)\rangle - e^{-iH_0t/\hbar} |\Psi_-^0(0)\rangle \| = 0$$

$$\lim_{t \to +\infty} \| e^{-iHt/\hbar} |\Psi_+(0)\rangle - e^{-iH_0t/\hbar} |\Psi_+^0(0)\rangle \| = 0$$

since $e^{-iHt} = U(t)$ is unitary

we can express these as

$$\lim_{t \to -\infty} \| |\Psi_-(0)\rangle - e^{i\frac{H}{\hbar}t} e^{-i\frac{H_0}{\hbar}t} |\Psi_-^0(0)\rangle \| = 0$$

$$\lim_{t \to +\infty} \| |\Psi_+(0)\rangle - e^{i\frac{H}{\hbar}t} e^{-i\frac{H_0}{\hbar}t} |\Psi_+^0(0)\rangle \| = 0$$

We express these equations

as

$$|\Psi_\pm(0)\rangle = \lim_{t\to\pm\infty} e^{iHt} e^{-iH_0 t} |\Psi_\pm^0(0)\rangle$$

where $|\Psi_-^0(0)\rangle$ is the state

of a non interacting beam

particle system at time 0

while $|\Psi_+^0(0)\rangle$ is the state

of free detected particles at

time 0.

The scattering probability is

$$P = |\langle\Psi_+(0)|\Psi_-(0)\rangle|^2$$

where

$$\langle\Psi_+(0)|\Psi_-(0)\rangle =$$

$$\lim_{\substack{t\to\infty \\ s\to-\infty}} \langle\Psi_+^0(0)| e^{itH_0/\hbar} e^{-i(t-s)H/\hbar} e^{-isH_0/\hbar} |\Psi_-^0(0)\rangle$$

definitions

$$\boxed{\begin{aligned} \Omega_+ &= \lim_{t\to\infty} e^{iHt} e^{-iH_0 t} \\ \Omega_- &= \lim_{t\to-\infty} e^{iHt} e^{-iH_0 t} \end{aligned}}$$

These are called Moller wave operators. It follows that

$$\langle \Psi_+(0) | \Psi_-(0) \rangle =$$

$$\langle \Psi_+^0(0) \Omega_+^\dagger \Omega_- | \Psi_-^0(0) \rangle$$

definition: scattering operator

$$S = \Omega_+^\dagger \Omega_-$$

$$P = |\langle \Psi_+^0(0) | S | \Psi_-^0(0) \rangle|^2$$

properties

$$\boxed{\begin{aligned} H \Omega_\pm &= \Omega_\pm H_0 \\ H_0 S &= S H_0 \end{aligned}}$$

proof

$$\lim_{t\to\infty} e^{isH/\hbar} e^{iHt/\hbar} e^{-iH_0t/\hbar} =$$

$$\lim_{t\to\infty} e^{i(s+t)H/\hbar} e^{-i(s+t)H_0t/\hbar} e^{isH_0/\hbar}$$

let $t' = t+s$ s fixed

$$\lim_{t'\to\infty} e^{iHt'/\hbar} e^{-iH_0t'/\hbar} e^{isH_0/\hbar}$$

$$= \Omega_+ e^{isH_0/\hbar}$$

$$\therefore \quad e^{isH/\hbar} \Omega_+ = \Omega_+ e^{isH_0/\hbar}$$

$\frac{\partial}{\partial s}\Big|_{s=0}$ gives

$$H\Omega_+ = \Omega_+ H_0$$

the same proof for $t \to -\infty$ gives

$$H\Omega_- = \Omega_- H_0$$

$$H_0 S = H_0 \Omega_+^\dagger \Omega_- = \Omega_+^\dagger H \Omega_-$$

$$= \Omega_+^\dagger \Omega_- H_0 = S H_0$$