5. Time-dependent Perturbation theory

SS 2024

AQM

[illegible]

[illegible]

In previous lecture we have started a study of time dependent problems in QM, and focused on few problems that can be solved EXACTLY

Such problems are indeed very RARE, so it will be useful to establish a way to deal with time-dependent problems PERTURBATIVELY

Remember in previous lecture we wrote for t-evolution

$$H(t) = H_0 + V(t) \qquad \text{with} \quad H_0|n\rangle = E_n|n\rangle$$

$$|\psi;t\rangle_S = \sum_n C_n(t)\, e^{-iE_nt/\hbar}\,|n\rangle \quad \Big\} \text{ Schrödinger}$$

$$|\psi;t\rangle_I = \sum_n C_n(t)\,|n\rangle \quad \Big\} \text{ Interaction picture}$$

We then found that the $c_n(t)$ fulfil a system of linear differential equations

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m V_{nm}(t)\, e^{i\omega_{nm} t}\, c_m(t)$$

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}$$

$$V_{nm}(t) = \langle n | V(t) | m \rangle$$

this is a good starting point to try & solve these equations perturbatively if $\underline{V(t) \sim \lambda \ll 1}$

Assume that @ $t=0$ system in $|i\rangle$

initial state

$$\Rightarrow \quad c_n(0) = \delta_{ni}$$

we ask ourselves what is the probability to find system in some final state $|f\rangle$

- since $V(t) \sim \lambda$, at zeroth order we can neglect its effect completely and write

$$i\hbar \frac{\partial}{\partial t} c_f(t) = 0 \Rightarrow c_f(t) = c_f(0) = \delta_{fi}$$

boundary constant

system REMAINS in $|i\rangle$

- to FIRST ORDER we can now say

$$V(t) = \lambda V(t)$$

$$c_f(t) = \delta_{fi} + \lambda c_f^{(1)}(t) + O(\lambda^2)$$

because $V \propto O(\lambda)$!

$$i\hbar \frac{\partial}{\partial t} c_f^{(1)}(t) = \sum_m V_{fm}(t) e^{i\omega_{fm} t} \delta_{mi}$$

$$= V_{fi}(t) e^{i\omega_{fi} t}$$

such that a solution can be written as

$$c_f^{(1)}(t) = -\frac{i}{\hbar}\int_0^t dt' \langle f|V(t')|i\rangle e^{i\omega_{fi}t'}$$

boundary condition

system starts in $|i\rangle$ @ $t=0$

δ_{fi} @ order zero !

this procedure could be iterated to any order.

We will do this in a more "elegant way"

using the INTERACTION PICTURE and working

with the EVOLUTION OPERATOR ("Propagator" $U(t,t_0)$)

$$|\psi;t\rangle_I = U_I(t,t_0)|\psi;t_0\rangle_I \qquad \text{INTER.}$$

evolves state from $t_0 \to t$

$$|\psi;t\rangle_S = \mathcal{U}_S(t,t_0)|\psi;t_0\rangle_S \qquad \text{SCHRÖDNG.}$$

remember $|\psi; t\rangle_S = e^{-iH_0 t/\hbar} \; |\psi; t\rangle_I$

As we know, in Schrödinger picture U_S satisfy its evolution equation

$$i\hbar \frac{\partial}{\partial t} U_S(t, t_0) = H_S(t)\, U_S(t, t_0)$$

where, if $H_S(t) = H_0$ (i.e. $V(t) = 0$)

we know how to write solution "formally"

$$\begin{cases} U_S^{(0)}(t, t_0) = e^{-iH_0(t-t_0)} \\ |\psi, t\rangle_S = e^{-iH_0(t-t_0)/\hbar}\, |\psi; t_0\rangle_S \end{cases}$$

<u>IMPORTANT</u> : we can get $\mathcal{U}_S$ from $\mathcal{U}_I$ simply

$$|\psi;t\rangle_I = e^{iH_0t/\hbar}\,|\psi;t\rangle_S$$

$$= e^{iH_0t/\hbar}\,\mathcal{U}_S(t,t_0)\,|\psi;t_0\rangle_S$$

$$= \underbrace{e^{iH_0t/\hbar}\,\mathcal{U}_S(t,t_0)\,e^{-iH_0t_0/\hbar}}_{\mathcal{U}_I(t,t_0)}\,|\psi;t_0\rangle_I$$

so $$\boxed{\mathcal{U}_I(t,t_0) = e^{iH_0t/\hbar}\,\mathcal{U}_S(t,t_0)\,e^{-iH_0t_0/\hbar}}$$

notice also that for $H_0|n\rangle = E_n|n\rangle$

$$\langle n|\mathcal{U}_I(t,t_0)|m\rangle = e^{i(E_nt-E_mt_0)/\hbar}\,\langle n|\mathcal{U}_S(t,t_0)|m\rangle$$

↑

matrix elements are the same up to a phase

$$|\langle n|\mathcal{U}_I(t,t_0)|m\rangle|^2 = |\langle n|\mathcal{U}_S(t,t_0)|m\rangle|^2$$

Note that this is not true in general if we take matrix element between general states (no Energy Eigenstates)

$$|\langle \psi | \mathcal{U}_I(t,t_0) | \varphi \rangle|^2 \neq |\langle \psi | \mathcal{U}_S(t,t_0) | \varphi \rangle|^2$$

!

But is it simpler to compute $\mathcal{U}_I(t,t_0)$?

Using evolution equation for ket in Interaction pic.

$$i\hbar \frac{d}{dt} |\psi; t\rangle_I = V_I(t) |\psi; t\rangle_I$$

We see that

$$i\hbar \frac{\partial}{\partial t} |\psi; t\rangle_I = i\hbar \left[\frac{\partial}{\partial t} U_I(t,t_0)\right] |\psi; t_0\rangle$$

$$= V_I(t) |\psi; t\rangle_I$$

$$= V_I(t)\, U_I(t,t_0) |\psi; t_0\rangle$$

which gives

$$\Rightarrow \boxed{i\hbar \frac{\partial}{\partial t} U_I(t,t_0) = V_I(t)\, U_I(t,t_0)}$$

Same equation as for U_S, but ONLY with $\underline{\underline{V_I}}$

A formal solution is INTEGRAL EQUATION

$$U_I(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\, U_I(t',t_0)\, dt'$$

boundary condition @ $t=t_0$ (verify this by differentiation!)

This is particularly convenient to produce a perturbative expansion, since $V_I \ll H_0$ "small"

ITERATING "LHS into RHS" $\longrightarrow$

$$\mathcal{U}_I(t,t_0) = \mathcal{U}_I^{(0)}(t,t_0) + \mathcal{U}_I^{(1)}(t,t_0) + \dots$$

ZEROTH ORDER : Drop $V_I(t)$

$$U_I^{(0)}(t,t_0) = \mathbb{1} + O(V_I)$$

nothing happens !

FIRST ORDER : keep only one power of V_I

$\Rightarrow$ substitute $\mathcal{U}_I = \mathcal{U}_I^{(0)}$ in RHS

$$\mathcal{U}_I^{(1)}(t,t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\,dt'$$

SECOND ORDER : keep terms $\propto O(V_I^2)$

$$\mathcal{U}_I^{(2)}(t,t_0) = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, V_I(t')\,V_I(t'')$$

etc ... $\Rightarrow$ DYSON SERIES !

How do we derive now diff. Eq. for $c_n(t)$?

remember $|\psi_i, t\rangle_I = \sum_n c_n(t) |n\rangle$

such that $c_f(t) = \langle f | \psi_i, t\rangle_I$ which becomes

$$c_f(t) = \langle f | \mathcal{U}_I(t, t_0) | \psi_i, t_0\rangle_I$$

and expanding $\mathcal{U}_I$ assuming $|\psi_i, t_0\rangle_I = |i\rangle$

energy eigenstate

- AT ZEROTH ORDER

$$c_f^{(0)}(t) = \langle f | \mathbb{1} | \psi_i, t_0\rangle_I$$

$$= \langle f | i\rangle = \delta_{fi} \quad \text{as before}$$

- At FIRST ORDER we need non-trivial contribution from $U_I(t, t_0)$

$$c_f^{(1)}(t) = \langle f| \left(-\frac{i}{\hbar}\right) \int_{t_0}^{t} dt' \, V_I(t') \underbrace{|\psi_i, t_0\rangle_I}_{|i\rangle}$$

$$= -\frac{i}{\hbar} \int_{t_0}^{t} dt' \, \langle f| V_I(t') |i\rangle$$

$$\left(V_I(t) = e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar} \right) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' \, e^{\frac{i(E_f - E_i)t}{\hbar}} \langle f| V(t) |i\rangle$$

which is what we found already:

$$c_f(t) = \delta_{fi} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, e^{i\omega_{fi} t} \langle f| V(t) |i\rangle$$

From here, easier to derive expression for $c_f^{(2)}(t)$

$\Uparrow$ EXERCISE

TRANSITION PROBABILITY

$$P(i \to f) = | c_f^{(1)}(t) + c_f^{(2)}(t) + \dots |^2$$

Assuming $|f\rangle \neq |i\rangle$!

EXAMPLE

Consider a particle of mass m, charge q, in potential of 1-dim oscillator on x-axis

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

perturbed by $V(t) = qE\,x\, e^{-t^2/\tau^2}$

@ $t = -\infty$; $V(t=-\infty) = 0$; $\underline{H_0 |n\rangle = \overbrace{\hbar\omega(n+\tfrac{1}{2})}^{E_n} |n\rangle}$

assume particle in ground state of H_0 ; $|0\rangle$

We would like the probability to find it in $|n\rangle$ after some long time $t \gg \tau$

$$C_n^{(1)}(t) = -\frac{i}{\hbar} qE \int_{-\infty}^{t} dt'\, e^{i\omega_{n0} t'} \langle n|x|0\rangle e^{-t'^2/\tau^2}$$

if $t \gg \tau$ $\quad \hookrightarrow \sim \int_{-\infty}^{+\infty}$ and we get

$$C_n(\infty) = -\frac{i}{\hbar} qE \langle n|x|0\rangle \int_{-\infty}^{+\infty} dt' \, e^{-in\omega t'} e^{-t'^2/\tau^2}$$

$$= -\frac{i}{\hbar} qE \langle n|x|0\rangle \left[\sqrt{\pi}\, \tau \, e^{-\frac{n^2\omega^2\tau^2}{4}} \right]$$

for matrix element use $x = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^{+} \right)$

creation & annihilation operators

$$\langle n|x|0\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n|a^{+}|0\rangle$$ since $\underline{a|0\rangle = 0}$

$$= \sqrt{\frac{\hbar}{2m\omega}} \delta_{n1}$$ $\neq 0$ only if $n = 1$

$$C_n(\infty) = -\frac{i}{\hbar} qE\tau \sqrt{\frac{\hbar\pi}{2m\omega}} \, e^{-\frac{n^2\omega^2\tau^2}{4}} \delta_{n1}$$

$\Rightarrow$ probability to find system in $|1\rangle$ is

$$|c_1(\infty)|^2 = \frac{\pi}{2}\left(\frac{q^2E^2\tau^2}{m\hbar\omega}\right)e^{-\frac{\omega^2\tau^2}{2}}$$

NOTICE • $|c_1(\infty)|^2 \to 0$ if $\tau \to \infty$

which means potential $V(t)$ is turned on very slowly

$\Rightarrow$ ADIABATIC PERTURBATION gives no transition! } more later!

• $V(t) \propto x$ implies a "selection rule"

$\Rightarrow$ only transition $n \to n+1$

$n \to n-1$

are possible!

if $V(t) \propto x^2$, also $n \to n \pm 2$ would be possible!

We consider now some special CLASSES of perturbations and try to make general statements from first order perturbation theory

SUDDEN PERTURBATION

We imagine a perturbation that acts on a very short time compared to typical time-scale of evolution of the system

Case just studied

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 + qE x e^{-t^2/\tau^2}$$

period oscillator $T = \frac{2\pi}{\omega}$

typical time perturbation $\left\{ \begin{array}{l} \tau \ll T = \frac{2\pi}{\omega} \\ \\ \tau\omega \ll 2\pi \end{array} \right.$

Transition probability

$|C_1(\infty)|^2 \propto \tau^2 \longrightarrow 0$ as $\underline{\underline{\tau \to 0}}$

there is no transition !

this is expected on general grounds.

Imagine $V(t)$ acts for $t \in [-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}]$

with $\varepsilon \to 0$

Schrödinger Equation

$$|\psi; \tfrac{\varepsilon}{2}\rangle - |\psi; -\tfrac{\varepsilon}{2}\rangle = -\frac{i}{\hbar}\int_{-\frac{\varepsilon}{2}}^{\frac{\varepsilon}{2}} dt\, V(t)\,|\psi; t\rangle$$

if $\varepsilon \to 0$ $\quad \int_{-\frac{\varepsilon}{2}}^{\frac{\varepsilon}{2}} dt\, V(t)|\psi; t\rangle \sim O(\varepsilon)$ if

$V(t)$ FINITE !

For finite $V(t)$ then

$$\lim_{\varepsilon \to 0} \left[\quad \right] \Rightarrow |\psi_i, -\tfrac{\varepsilon}{2}\rangle = |\psi_i, +\tfrac{\varepsilon}{2}\rangle$$

no change in state :

More realistic problem, ATOM with atomic number Z

electron in 1s

Imagine now nucleus undergoes β decay

$\Rightarrow$ it emits an electron and $Z \to Z+1$

(a neutron becomes a proton)

Electron is relativistic, so we can "classically" estimate time-scale of interaction through time taken by electron to "leave" the $n=1$ shell

$$\tau \sim \frac{a_0}{Z} \cdot \frac{1}{c} \sim \frac{\text{radius}}{\text{velocity}}$$

What is instead the characteristic time-scale of the system $\Rightarrow$ how much time the electron takes to go around the 1s state ?

$$T' \sim \left(\frac{a_0}{Z}\right) \cdot \frac{1}{\underbrace{Z \alpha c}_{\text{electron velocity}}} = \frac{a_0}{Z^2 \alpha c}$$

$\uparrow$ size shell

$$v \sim \frac{e^2}{4\pi\varepsilon_0 \hbar c} \cdot c \quad \text{for } \frac{mv^2}{2} \sim \frac{e^2}{4\pi\varepsilon_0 r}$$

so $\frac{\tau}{T'} = Z\alpha$ remember $\alpha = \frac{1}{137}$

so as long as $Z \ll 137$, we expect the interaction to be "sudden"

$\Rightarrow$ after β-decay, e^- in 1s shell will have stayed there ! just now, this is a superposition of eigenstates of "new" Atom with $\underline{Z^* = Z+1}$

$\Rightarrow$ clearly this is NOT TRUE if $V(t) \sim \delta(t)$

in that case $\displaystyle\int_{-\varepsilon}^{+\varepsilon} \delta(t)\, dt = 1$!

perturbation not negligible, see exercises !

HARMONIC PERTURBATION

A very large number of perturbation potentials of importance for physics can be parametrized by Harmonic functions of time

$$V(t) = M\, e^{\pm i\omega t} \, ; \quad M \text{ time independent}$$

(and if $V(t)$ not Harmonic, one could decompose it into its Fourier modes !)

$$C_f(t) = \delta_{fi} - \frac{i}{\hbar} \int_{t_0}^{t} dt'\, e^{i\omega_{fi} t} \langle f | V(t) | i \rangle$$

Specializing our general formula once more to system in state $|i\rangle$ @ $t=0$, we get

$$c_f^{(1)}(t) = -\frac{i}{\hbar}\langle f|M|i\rangle \int_0^t dt'\, e^{i\omega_{fi}t'}\, e^{\pm i\omega t'}$$

the integral over the exponentials can be done easily giving

$$\int_0^t dt'\, e^{i[\omega_{fi}\pm\omega]t'} = \frac{e^{i[\omega_{fi}\pm\omega]t} - 1}{i[\omega_{fi}\pm\omega]}$$

$$= e^{i\frac{[\omega_{fi}\pm\omega]}{2}t}\,\frac{\sin\left(\frac{\omega_{fi}\pm\omega}{2}t\right)}{\left[\frac{\omega_{fi}\pm\omega}{2}\right]}$$

such that the probability can be computed as

$$P_{i\to f} \propto |c_f^{(1)}(t)|^2$$

$$|c_f^{(1)}(t)|^2 = \frac{|\langle f|H|i\rangle|^2}{\hbar^2}\left[\frac{\sin\left(\frac{\omega_{fi}\pm\omega}{2}t\right)}{\frac{\omega_{fi}\pm\omega}{2}}\right]^2$$

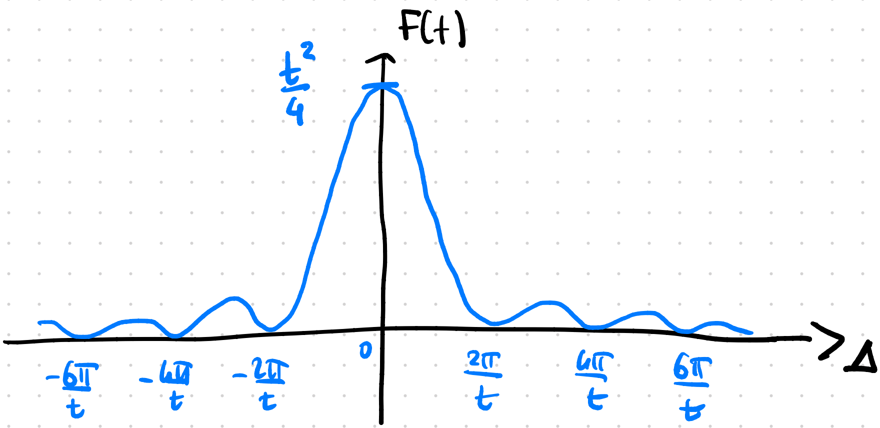
now let's call:

$$\omega_{fi}\pm\omega = \frac{E_f - E_i \pm \hbar\omega}{\hbar} = \Delta$$

and consider the behavior of the function

$$F(t) = \frac{4}{\Delta^2}\sin^2\left[\frac{t\Delta}{2}\right]$$

modulo $\frac{\langle f|H|i\rangle}{\hbar^2}$



as $t \to \infty$, the function becomes increasingly peaked at $\Delta = 0$, while far from $\Delta = 0$ it oscillates very rapidly.

take some regular function $f(\Delta)$, then

$$\lim_{t\to\infty} \int_{-\infty}^{+\infty} d\Delta \; f(\Delta) \, \frac{4}{\Delta^2} \sin^2\left[\frac{t\Delta}{2}\right]$$

$$= \int_{-\infty}^{+\infty} d\Delta \left[f(\Delta) - f(0)\right] \frac{4}{\Delta^2} \sin^2\left[\frac{t\Delta}{2}\right] \Rightarrow 0$$

peaked on zero!

$$+ f(0) \underbrace{\int_{-\infty}^{+\infty} d\Delta \, \frac{4}{\Delta^2} \sin^2\left[\frac{t\Delta}{2}\right]}_{2\pi t}$$

$$= 2\pi t \, f(0)$$

which is a possible representation of the Dirac δ- function

$$\frac{4}{\Delta^2} \sin^2\left(\frac{t\Delta}{2}\right) \xrightarrow{t\to\infty} 2\pi t \, \delta(\Delta)$$

$$= 2\pi \hbar \, t \, \delta(E_f - E_i \pm \hbar\omega)$$

so after a "long time" T we find for the transition probability PER UNIT TIME

$$\Gamma_{i\to f} = \frac{|C_f(t)|^2}{T} = \frac{2\pi}{\hbar} |\langle f | M | i \rangle|^2 \, \delta(E_f - E_i \pm \hbar\omega)$$

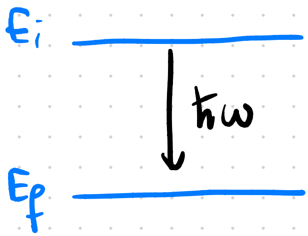
$\Rightarrow$ transitions require $\hbar\omega = |E_f - E_i|$

this is called FERMI GOLDEN RULE (F.G.R.)

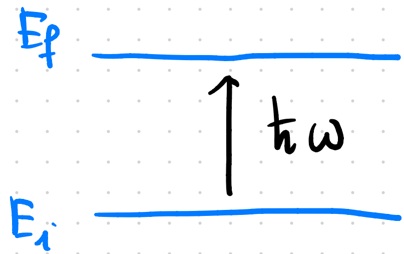
the formula is extremely important and we will use it A LOT in next lectures

NOTICE:

A system can go through a transition if potential supplies correct energy $\begin{cases} \hbar\omega = E_f - E_i \\ \hbar\omega = E_i - E_f \end{cases}$



stimulated EMISSION $e^{+i\omega t}$!



stimulated ABSORPION $e^{-i\omega t}$!

Quantum system alone does NOT conserve energy, or $E_f = E_i \mp \hbar\omega$

In first case, system "emits" energy into the potential and falls to lower state

In second case it absorbs it and gets to excited state