Lecture #3

Time-dependent perturbation theory

Consider a physical system described by H_0 ⇒
$H_0 |n\rangle = E_n |n\rangle$ (assume for simplicity discrete and non-degenerate spectrum)
At $t=0$, a perturbation $\lambda V(t)$ is applied, so that
$\lambda \ll 1$
$H(t) = H_0 + \lambda V(t)$
If the system is initially in some stationary state $|i\rangle$, i.e. $|\psi(t=0)\rangle = |i\rangle$, what is the probability to find the system in the state $|f\rangle$ after time t? ⇒ i.e. find

$$P_{i\to f}(t) = |\langle f|\psi(t)\rangle|$$

Need to solve

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \left[H_0 + \lambda V(t)\right] |\psi(t)\rangle \quad (3.1)$$

with the initial condition $|\psi(t=0)\rangle = |i\rangle$
Problem: for most $V(t)$, Eq. (3.1) cannot be

solved exactly $\Rightarrow$ need approximation methods! (2)

Choose $\{|n\rangle\}$ basis and expand $|\Psi(t)\rangle$:

$$|\Psi(t)\rangle = \sum_n b_n(t)\,|n\rangle, \quad b_n(t) = \langle n|\Psi(t)\rangle \tag{3.2}$$

Also introduce

$$\langle n|V(t)|k\rangle = V_{nk}(t)\,;$$

$$\langle n|H_0|k\rangle = E_n\,\delta_{nk}$$

Multiply Eq. (3.1) by $\langle n|$:

$$i\hbar\frac{\partial}{\partial t}\langle n|\Psi(t)\rangle = \langle n|H_0|\Psi(t)\rangle +$$

$$+\lambda\langle n|V(t)|\Psi(t)\rangle \underset{\text{Eq.(3.2)}}{\Longrightarrow}$$

$$i\hbar\frac{db_n(t)}{dt} = E_n b_n(t) + \lambda\sum_k V_{nk}(t)\,b_k(t) \tag{3.3}$$

Present $b_n(t) = C_n(t)\,e^{-\frac{i}{\hbar}E_n t}$ and substitute $\Rightarrow$

$$i\hbar\frac{dC_n(t)}{dt} = \lambda\sum_k V_{nk}(t)\,C_k(t)\,e^{i\omega_{nk}t} \tag{3.4}$$

$$\omega_{nk} = \frac{E_n - E_k}{\hbar}$$

same as we got in Lecture #2 using interaction picture.

Unfortunately, the system of Eqs. (3.4) can be (3)
solved exactly only in the simplest cases $\Rightarrow$ need approx.
expand $C_n(t)$ in powers of λ:

$$C_n(t) = C_n^{(0)}(t) + \lambda C_n^{(1)}(t) + \lambda^2 C_n^{(2)}(t) + \dots$$

and plug into (3.4) $\Rightarrow$

$$i\hbar\left(\frac{dC_n^{(0)}(t)}{dt} + \lambda\frac{dC_n^{(1)}(t)}{dt} + \lambda^2\frac{dC_n^{(2)}(t)}{dt} + \dots\right) =$$

$$= \lambda\sum_k V_{nk}(t)\left(C_k^{(0)}(t) + \lambda C_k^{(1)}(t) + \lambda^2 C_k^{(2)}(t) + \dots\right) \cdot e^{i\omega_{nk}t};$$

Collect the terms with equal powers of λ:

$$\lambda^0: \quad \frac{dC_n^{(0)}}{dt} = 0 \Rightarrow C_n^{(0)} = \text{const} = \delta_{ni}$$

$$\lambda: \quad i\hbar\frac{dC_n^{(1)}}{dt} = \sum_k V_{nk}(t)\, C_k^{(0)}(t)\, e^{i\omega_{nk}t}$$

$$\vdots$$

$$\lambda^r: \quad i\hbar\frac{dC_n^{(r)}}{dt} = \sum_k V_{nk}(t)\, C_k^{(r-1)}(t)\, e^{i\omega_{nk}t}$$

$$i\hbar\frac{dC_n^{(1)}}{dt} = \sum_k V_{nk}(t)\,\delta_{ki}\, e^{i\omega_{nk}t} = V_{ni}(t)\, e^{i\omega_{ni}t}$$

$\Rightarrow$

$$\Rightarrow \quad C_n^{(1)}(t) = \frac{1}{i\hbar}\int_0^t V_{ni}(t')\, e^{i\omega_{ni}t'}\, dt'$$

Then substitude $C_n^{(1)}(t)$ into the equation for $\frac{dC_n^{(2)}}{dt}$, etc. to find higher-order terms.

The transition probability

$$P_{if}(t) = |\langle f|\Psi(t)\rangle|^2 = |\langle f|\sum_n b_n(t)|n\rangle|^2$$

$$= |\sum_n b_n(t)\delta_{nf}|^2 = |b_f(t)|^2 = |C_f(t)|^2 =$$

$$= |C_f^{(0)}(t) + \lambda C_f^{(1)}(t) + \ldots|^2$$

Assuming that $i \neq f \Rightarrow C_f^{(0)} = 0$

To the first-order,

$$P_{if}(t) = |\lambda C_f^{(1)}(t)|^2 = \frac{\lambda^2}{\hbar^2}\left|\int_0^t V_{fi}(t')\, e^{i\omega_{fi}t'}\, dt'\right|^2$$

(3.5)

Alternative approach to derivation of (3,5) $\Rightarrow$

Consider time evolution of a state ket in the interaction picture $\Rightarrow$ $|\alpha, t_0; t\rangle_I = U_I(t, t_0) \cdot |\alpha, t_0; t_0\rangle_I$;

To find $U_I(t, t_0) \Rightarrow$

U_I ↑ propagator in the interaction picture

$\Rightarrow$ solve $i\hbar \frac{d}{dt} U_I(t, t_0) = V_I(t)\, U_I(t, t_0)$

(Recall $A_I = e^{\frac{i}{\hbar}H_0 t} A_S\, e^{-\frac{i}{\hbar}H_0 t}$, $A = V$)

with the initial condition $U_I(t_0, t_0) = 1 \Rightarrow$

$$U_I(t, t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\, U_I(t', t_0)\, dt' = \quad (3.6)$$

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

$$= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, V_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, V_I(t')\, V_I(t'') \, +$$

$$+ \dots \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \dots \int_{t_0}^{t^{(n-1)}} dt^{(n)}\, V_I(t')\, V_I(t'') \dots V_I(t^{(n)}) + \dots$$

Dyson series $\Rightarrow$ can compute to any order (finite)

Let's say we know $U_I(t, t_0)$.

Then, if the system is at $t = t_0$ in the state $|i\rangle$, which is an eigenstate of H_0 $\Rightarrow$

$$\underbrace{|i, t_0; t\rangle_I}_{\substack{\| \\ \sum_n c_n(t)\underbrace{|n\rangle}_{\leftarrow \text{ eigenstates of } H_0}}} = U_I(t, t_0) \underbrace{|i\rangle_I}_{\substack{\| \\ |i, t_0; t_0\rangle_I}}$$

Then, $c_n(t) = \langle n | U_I(t, t_0) | i \rangle$

the probability of transition from $|i\rangle$ to $|n\rangle$ is

$$\mathcal{P}_{i \to n} = |c_n(t)|^2 = |\langle n | U_I(t, t_0) | i \rangle|^2 \underset{\substack{\uparrow \\ \text{Eq. (3.6)} \\ \text{(Dyson series)}}}{=}$$

$$= \left| \delta_{ni} + \left(-\frac{i}{\hbar}\right) \int_{t_0}^{t} \underbrace{e^{i\omega_{ni}t'} V_{ni}(t')}_{\langle n | V_I | i \rangle = e^{i\omega_{ni}t} V_{ni}(t)} dt' + \ldots \right|^2 ,$$

which is the same as Eq. (3.5) !