The Time-dependent Perturbation Theory

→ A (very) brief recall of the time-independent perturbation theory:

perturbed Hamiltonian : $H = H_0 + \underbrace{\overset{\sim \epsilon H'}{H_1}}_{\text{perturbation.}}$

∵ Perturbations are assumed to be small, ~~eigen~~ we can consider terms upto $O(\epsilon)$ in the perturbation parameter for first order corrections:

→ Considering eigenstates:

$$|\psi\rangle = |\psi_0\rangle + \epsilon|\psi_1\rangle + O(\epsilon^2)$$

& eigenvalues:

$$E = E_0 + \epsilon E_1 + O(\epsilon^2).$$

upto $O(\epsilon)$:

$$\boxed{E_1 = \langle \psi_0 | H_1 | \psi_0 \rangle}$$

← The primary result of TIPT!!

&

$$\boxed{|\psi_1\rangle = \sum_{\phi} \frac{\langle \phi_0 | H_1 | \psi_0 \rangle}{\cancel{E_\phi} E_0^{(\psi)} - E_0^{(\phi)}} |\phi_0\rangle}$$

corrections to eigenvalue & eigenstates!

Now, when the perturbed Hamiltonian is time-dependent:

$$H(t) = H^0 + H'(t)$$

e.g.: A hydrogen atom with free Hamiltonian H^0 interacting with a weak external field (EM radiation) given by $H(t)$.

→ Such systems will be encountered in the AMP course!

→ We know, that the eigenkets $|n^0\rangle$ of H^0

i.e $\quad H^0|n^0\rangle = E_n^0|n^0\rangle$

must form a complete set given by the completeness relation:

$$\cancel{|\psi(t)\rangle = \sum_n c_n(t)|n^0\rangle}$$

$$\mathbb{1} = \sum_n |n^0\rangle\langle n^0|$$

$$\Rightarrow \quad \boxed{|\psi(t)\rangle = \sum_n c_n(t)|n^0\rangle}$$

→ The problem statement of TDPT:

"If at $t=0$ the system is in the eigenstate $|i^0\rangle$ of H^0, what is the amplitude for it to be in the eigenstate $|f^0\rangle$ $(f \neq i)$ at a later time $t=t$?"

→ First order TDPT :

Again, imagine the perturbed Hamiltonian $H'(t) \equiv \epsilon H'(t)$
s.t. $\epsilon \longrightarrow$ order of perturbation.

→ ∥er to the time-independent case,

$$\sum_n |n^\circ\rangle\langle n^\circ| = \mathbb{1}$$ ← Completeness theorem.

⇒ If $|\psi(t)\rangle$ is the eigenstate of the perturbed Hamiltonian, $H(t)$, then:

$$|\psi(t)\rangle = \sum_n \underbrace{c_n(t)}\, |n^\circ\rangle$$

↳ The time-dependence can only be incorporated in the coefficients of the eigenstates (basis).

→ Consider the unperturbed case ($H_1 \to 0$):

Then, $\cancel{c_n(t) =}\ |\psi(t)\rangle = e^{-iH_0 t}|\psi(0)\rangle$

$$\Longleftrightarrow \quad c_n(t) = e^{-iE_n^\circ t/\hbar}\ \cancel{|n^\circ\rangle}$$

→ Therefore, for the perturbed case let's assume:

$$\boxed{c_n(t) = d_n(t)\, e^{-iE_n^\circ t/\hbar}\ \cancel{|n^\circ\rangle}}$$

$$\Rightarrow \quad \boxed{|\psi(t)\rangle = \sum_n d_n(t)\, e^{-iE_n^\circ t/\hbar}\, |n^\circ\rangle} \equiv e^{-i(H_0+H_1)t}|\psi(0)\rangle$$

4

→ Now, substituting $|\psi(t)\rangle$ into the TDSE:

$$(H^0 + H')|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle$$

$$\Rightarrow (H^0 + H')\sum_n d_n(t) e^{-iE_n^0 t/\hbar}|n^0\rangle = i\hbar\frac{\partial}{\partial t}\sum_n d_n(t) e^{-iE_n^0 t/\hbar}|n^0\rangle$$

$$\Rightarrow \sum_n \Big[\cancel{d_n(t) E_n^0 e^{-iE_n^0 t/\hbar}|n^0\rangle} + d_n(t) e^{-iE_n^0 t/\hbar} H'|n^0\rangle$$
$$- i\hbar \dot{d}_n(t) e^{-iE_n^0 t/\hbar}|n^0\rangle - \cancel{d_n(t) E_n^0 e^{-iE_n^0 t/\hbar}|n^0\rangle}\Big] = 0$$

$$\Rightarrow \sum_n \left[-i\hbar \dot{d}_n(t) + H'(t) d_n(t)\right] e^{-iE_n^0 t/\hbar}|n^0\rangle = 0$$

$$\Rightarrow \boxed{\sum_n \left[i\hbar \dot{d}_n(t) - H'(t) d_n(t)\right] e^{-iE_n^0 t/\hbar}|n^0\rangle = 0}$$

→ Consider another eigenstate $|f^0\rangle \neq |n^0\rangle$, s.t:

$$\underbrace{\langle f^0| e^{iE_f^0 t/\hbar}}_{\langle f^0(t)|} \sum_n \left[i\hbar \dot{d}_n - H' d_n\right] e^{-iE_n^0 t/\hbar}|n^0\rangle = 0$$

$$\Rightarrow \sum_n i\hbar \dot{d}_n e^{i(E_f^0 - E_n^0)t/\hbar} \underbrace{\langle f^0|n^0\rangle}_{\delta_{fn}} - \sum_n \langle f^0|H'(t)|n^0\rangle e^{i(E_f^0 - E_n^0)t/\hbar} d_n(t) = 0$$

$$\omega_{fn} = \frac{E_f^0 - E_n^0}{\hbar}$$

$$\Rightarrow \boxed{i\hbar \dot{d}_f = \sum_n \langle f^0|H'(t)|n^0\rangle e^{i\omega_{fn} t} d_n(t)}$$

Solving for $d_f(t)$:

→ Consider the case where $\underbrace{|\Psi(t=0)\rangle \equiv |i^0\rangle}_{H' \text{ is turned on at } t=0.}$

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

$$\Rightarrow \quad i\hbar\,\dot{d}_f(0) = \sum_n \langle f^0|\,H'(0)\,|n^0\rangle\, e^{i\omega_{fn}t}\,\delta_{ni} \to 0$$

$$\Rightarrow \quad \boxed{\dot{d}_f(0) = 0}$$

→ At t, upto first order $O(\epsilon)$:

$$i\hbar\,\dot{d}_f(t) = \sum_n \langle f^0|\,H'(t)\,|n^0\rangle\, e^{i\omega_{fn}t}\,\delta_{ni}$$

$$\Rightarrow \quad \boxed{\dot{d}_f(t) = -\frac{i}{\hbar}\langle f^0|\,H'(t)\,|i^0\rangle\, e^{i\omega_{fi}t}}$$

$$\Rightarrow \quad d_f(t) = -\frac{i}{\hbar}\int_0^t dt\,\langle f^0|\,H'(t)\,|i^0\rangle\, e^{i\omega_{fi}t} + C$$

→ To fix C:

$$d_f(t=0) = \begin{cases} 1, & f = i \\ 0, & f \neq i \end{cases}$$

$$\Rightarrow \quad C = \delta_{fi}$$

$$\Rightarrow \quad \boxed{d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_0^t dt'\,\langle f^0|\,H'(t')\,|i^0\rangle\, e^{i\omega_{fi}t'}}$$

valid approx. (first order) iff $|d_f(t)| \ll 1$ $(f \neq i)$

→ Application of the First-order TDPT:

"A Toy model"

↓

As usual, the 1D harmonic oscillator!

→ Consider a 1D H.O. in the ground state $|0\rangle$.

Unperturbed H: $H_0 = \dfrac{\hat{p}^2}{2m} + \dfrac{m\omega^2}{2}\hat{x}^2$

$$X \equiv \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^{\dagger})$$

perturbation : $\underbrace{H'(t) = -e\mathcal{E}X e^{-t^2/\tau^2}}_{\text{turned on at } t=-\infty}$

turned on at $\underline{\underline{t=-\infty}}$.

Q What is the probability that the oscillator is in the state $|n\rangle$ at $t \to \infty$?

Ans: We know from our derivation:

$$\cancel{d_n(\infty) =}$$
$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_{t_i}^{t} \langle f^0|H'|i^0\rangle e^{i\omega_{fi}(t'-t_i)}dt'$$

$$\Rightarrow \boxed{d_n(\infty) \doteq -\frac{i}{\hbar}\int_{-\infty}^{\infty} (-e\mathcal{E})\langle n|X|0\rangle e^{-t^2/\tau^2} e^{i\underbrace{\boxed{n\omega}}_{=\omega_{n0}}t}dt}$$

→ Calculating $\langle n|x|0\rangle$:

$$\langle n|x|0\rangle = \langle n|a+a^{\dagger}|0\rangle\left(\frac{\hbar}{2m\omega}\right)^{1/2}$$

$$= \left(\cancelto{0}{\langle n|a|0\rangle} + \langle n|a^{\dagger}|0\rangle\right)\left(\cdots\right)$$

$$= \langle n|1\rangle\left(\cdots\right)$$

$$= \delta_{n1}\left(\frac{\hbar}{2m\omega}\right)^{1/2}$$

⇒ Only possible state under the perturbation $H'(t)$ is $|n\rangle = |1\rangle$!!

$$\therefore \quad d_1(\infty) = \frac{ie\mathcal{E}}{\hbar}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\int_{-\infty}^{\infty} e^{-t^2/\tau^2} e^{i\omega t}\, dt$$

$$= \frac{ie\mathcal{E}}{\hbar}\left(\frac{\hbar}{2m\omega}\right)^{1/2}(\pi\tau^2)^{1/2} e^{-\omega^2\tau^2/4}$$

⇒ Probability of transition $|0\rangle \longrightarrow |1\rangle$:

$$\boxed{P_{0\to1} = |d_1|^2 = \frac{e^2\mathcal{E}^2\pi\tau^2}{2m\omega\hbar} e^{-\omega^2\tau^2/2}} = |c_1|^2$$

$$\because |c_1|^2 = \left|e^{-iE_1 t/\hbar}\right|^2 |d_1|^2$$

→ Another example : The Periodic perturbation.

"e.g : An atom placed b/w plates of a condenser connected to AC source."

As a toy model, let's consider

$$H^1(t) = H^1 e^{-i\omega t}$$

→ Again, let's assume $H^1(t=0) \lneq 0$.

$$\Rightarrow \quad d_f(t) = -\frac{i}{\hbar}\int_0^t \langle f^0 | H^1(t') | i^0 \rangle e^{i\omega_{fi} t'} dt'$$

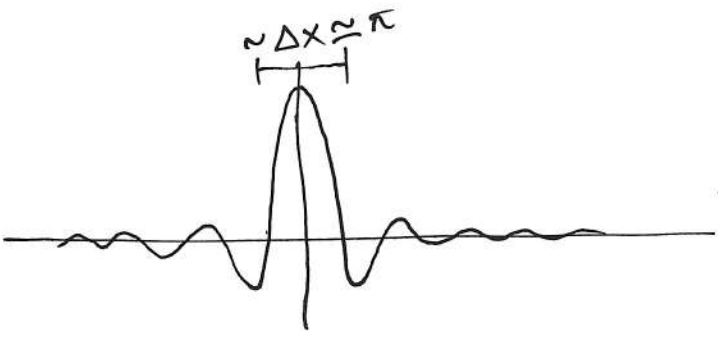
$$= -\frac{i}{\hbar}\int_0^t \langle f^0 | H^1 | i^0 \rangle e^{i(\omega_{fi} - \omega)t'} dt'$$

$$\Rightarrow \quad \boxed{d_f(t) = -\frac{i}{\hbar}\langle f^0 | H^1 | i^0 \rangle \frac{e^{i(\omega_{fi}-\omega)t} - 1}{i(\omega_{fi} - \omega)}}$$

∴ The probability of transition $i \to f$:

$$P_{i\to f} = |d_f|^2 = \frac{1}{\hbar^2}\left|\langle f^0 | H^1 | i^0 \rangle\right|^2 \frac{\left|e^{i(\omega_{fi}-\omega)t} - 1\right|^2}{(\omega_{fi} - \omega)^2} \quad \text{H/W}$$

$$= \frac{1}{\hbar^2}\left|\langle f^0 | H^1 | i^0 \rangle\right|^2 \underbrace{\left[\frac{\sin^2[(\omega_{fi}-\omega)t/2]}{(\omega_{fi}-\omega)^2 t^2}\right]}_{\downarrow} \cdot t^2$$



$\longrightarrow P \sim \dfrac{\sin^2 x}{x^2}$

→ Due to the nature of $\frac{\sin^2 x}{x^2}$ term in $P_{i \to f}$,

& since the width of the peak $\sim \boxed{\Delta x \simeq \pi}$

$\Rightarrow$ The phase : $\underbrace{|(\omega_{fi} - \omega)t/2| \lesssim \pi}$ → $P_{i \to f}$ is dominant for this phase.

$$\Rightarrow \left| \left(\frac{E_f^\circ - E_i^\circ}{\hbar} t - \omega t \right) \frac{1}{2} \right| \lesssim \pi$$

$$\Rightarrow \left| (E_f^\circ - E_i^\circ) t - \hbar \omega t \right| \lesssim 2 \hbar \pi$$

$$\Rightarrow \boxed{E_f^\circ t = (E_i^\circ t + \hbar \omega t) \pm 2\pi\hbar}$$

Or, $\boxed{E_f^\circ - E_i^\circ = \hbar\omega \pm \frac{2\hbar\pi}{t}}$

$$\Rightarrow \boxed{E_f^\circ - E_i^\circ = \hbar\omega \left(1 \pm \frac{2\pi}{\omega t} \right)}, \quad t \neq 0 \ (>0)$$

→ Note: for small t E_f° may not necessarily be $E_i^\circ + \hbar\omega$ — the system has no preferred energy level!!

→ For large t : $E_f^\circ - E_i^\circ \approx \hbar\omega$

$\Rightarrow \boxed{E_f^\circ \approx E_i^\circ + \hbar\omega}$ ← sys. starts to behave like a driven H.O.!!

H/W: Why? Think!!

→ It's as if, the perturbed system realizes the periodicity after considerable cycles have passed (i.e $\omega t \gg 2\pi$)!

→ A curious question: What about $t \to \infty$?

→ Consider a periodic case w/ pert. b/w $-T/2$ to $T/2$:

$$\Rightarrow \quad d_f = \lim_{T\to\infty} \frac{-i}{\hbar} \int_{-T/2}^{T/2} H^1_{fi}\, e^{i(\omega_{fi}-\omega)t'}\, dt'$$

$$\approx -\frac{i}{\hbar} H^1_{fi} \boxed{\int_{-\infty}^{\infty} e^{i(\omega_{fi}-\omega)t'}\, dt'} \Rightarrow 2\pi\, \delta(\omega_{fi}-\omega)!$$

$$\Rightarrow \quad P_{i\to f} = \frac{4\pi^2}{\hbar^2} |H^1_{fi}|^2\, \delta(\omega_{fi}-\omega)\, \delta(\omega_{fi}-\omega)$$

$$= \frac{4\pi^2}{\hbar^2} |H^1_{fi}|^2\, \delta(\omega_{fi}-\omega) \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega_{fi}-\omega)t}\, dt$$

$$= \frac{2\pi}{\hbar^2} |H^1_{fi}|^2\, \delta(\omega_{fi}-\omega) \lim_{T\to\infty}(T) \qquad [\because \omega_{fi}=\omega]$$

∴ The average transition rate:

$$R_{i\to f} \equiv \frac{P_{i\to f}}{T} = \frac{2\pi}{\hbar} |H^1_{fi}|^2\, \hbar\, \delta(\omega_{fi}-\omega)$$

$$\Rightarrow \boxed{R_{i\to f} = \cancel{\frac{2\pi}{\hbar} |H^1_{fi}|^2 \delta}\; \frac{2\pi}{\hbar} |\langle f^0 | H^1 | i^0 \rangle|^2\, \underbrace{\delta(E_f^0 - E_i^0 - \hbar\omega)}_{\text{Contribution iff } \Delta E = \hbar\omega!!}}$$

$\boxed{\text{Fermi's golden rule}}$

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