Tuesday, March 12, 2013

Time-dependent perturbation theory

Previously, we showed that a time-dependent perturbation $W(t)$ applied at time $t \geq 0$ will produce a transition from an initial state $|\varphi_i\rangle$ (eigenstate of unperturbed Hamiltonian H_0) to another eigenstate $|\varphi_j\rangle$ $(j \neq i)$ with probability

to 1st order:

$$P_{ij}(t) = |\langle \varphi_j | \psi(t) \rangle|^2 \qquad (|\psi(t\leq 0)\rangle = |\varphi_i\rangle)$$

$$= |c_j(t)|^2$$

$$\Leftrightarrow \boxed{P_{ij}(t)\Big|_{t\geq 0} = \frac{1}{\hbar^2}\left|\int_0^t \langle \varphi_j | W(t') | \varphi_i \rangle e^{i\omega_{ji}t'} dt'\right|^2}$$

with $\omega_{ji} = \dfrac{E_j - E_i}{\hbar}$

$$c_j(t) = \lambda c_j^{(1)}(t)\Big|_{1^{st}\text{ order}} = \boxed{\frac{1}{i\hbar}\int_0^t \langle \varphi_j | W(t') | \varphi_i \rangle e^{i\omega_{ji}t'} dt'}$$

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-i\frac{E_n}{\hbar}t} |\varphi_n\rangle$$

$c_j^{(1)}(t) \sim$ Fourier component of $\underbrace{W(t) \text{ seen by } |\varphi_j\rangle}_{\langle \varphi_j | W(t) | \varphi_i \rangle}$

at frequency $= \omega_{ji}$

(i.e. you should be thinking about excitation in Fourier space)
↳ the different "photons" that can contribute to transitions

note1: the transition from $|\varphi_i\rangle$ to $|\varphi_j\rangle$ corresponds to the absorption of one quantum of energy $\Delta E = \hbar\omega_{ji}$

note 2: $$c_i(t) \simeq 1 + \lambda c_i^{(1)}(t) = 1 + \frac{1}{i\hbar}\int_0^t \langle\varphi_i|W(t')|\varphi_i\rangle dt'$$

$$\Rightarrow P_{ii}(t) = \left|1 + \frac{1}{i\hbar}\int_0^t \langle\varphi_i|W(t')|\varphi_i\rangle dt'\right|^2$$

alternatively, use the normalization condition: $P_{ii}(t) = 1 - \sum_n P_{ni}(t)$

note 3: 1^{st} order approximation is valid only for $P_{jk} \ll 1 \Leftrightarrow c_j(t) \simeq c_j^{(0)}(t) \simeq 0$

as soon as $c_j^{(1)}(t)$ becomes appreciable 2^{nd} and 3^{rd} order correction can become important. (etc. ...)

2nd order (briefly)

$\underline{\underline{r=2}}$ $$i\hbar\frac{d}{dt}c_k^{(2)}(t) = \sum_n \hat{W}_{kn}(t)\, c_n^{(1)}(t)\, e^{i\omega_{kn}t}$$

$$\Rightarrow c_k^{(2)}(t) = \frac{1}{i\hbar}\int_0^t \sum_n W_{kn}(t'')\, c_n^{(1)}(t'')\, e^{i\omega_{kn}t''} dt''$$

$$= -\frac{1}{\hbar^2}\sum_n \int_0^t \hat{W}_{kn}(t'')e^{i\omega_{kn}t''}\left[\int_0^{t''} \hat{W}_{ni}(t')e^{i\omega_{ni}t'} dt'\right]dt''$$

$$\lambda^2 c_k^{(2)}(t) = -\frac{1}{\hbar^2}\sum_n \int_0^t W_{kn}(t'')e^{i\omega_{kn}t''}\left[\int_0^{t''} W_{ni}(t')e^{i\omega_{ni}t'} dt'\right]dt''$$

absorption and emission of multiple quanta

(virtual transitions to intermediate $|\varphi_n\rangle$ states)

$$C_k(t) \simeq \lambda C_k^{(1)}(t) + \lambda^2 C_k^{(2)}(t) \Rightarrow P_{ik}(t) \simeq \left| \lambda C_k^{(1)}(t) + \lambda^2 C_k^{(2)}(t) \right|^2$$

Generally, one tends to go only to 1st order

Special case : Sinusoidal perturbation (1st order)

We consider a perturbation $W(t) = W\cos(\omega t)$

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

In this case $c_j(t)\Big|_{1^{st}\text{ order}} \simeq \dfrac{1}{i\hbar}\displaystyle\int_0^t \langle \varphi_j | W\cos(\omega t') | \varphi_i \rangle e^{i\omega_{ji} t'} dt'$

$$= \frac{\langle \varphi_j | W | \varphi_i \rangle}{2i\hbar} \int_0^t \left[e^{i(\omega + \omega_{ji})t'} + e^{-i(\omega - \omega_{ji})t'} \right] dt'$$

$$= \frac{\langle \varphi_j | W | \varphi_i \rangle}{2i\hbar} \left[\frac{e^{i(\omega+\omega_{ji})t'}}{i(\omega+\omega_{ji})}\Bigg|_0^t + \frac{e^{-i(\omega-\omega_{ji})t'}}{i(\omega-\omega_{ji})}\Bigg|_0^t \right]$$

$$= \frac{\langle \varphi_j | W | \varphi_i \rangle}{2\hbar} \Bigg[\underbrace{\frac{1 - e^{i(\omega+\omega_{ji})t}}{\omega + \omega_{ji}}}_{\substack{\text{"anti-resonant" term} \\ (\text{for } E_j > E_i \\ \text{i.e. } \omega_{ji} > 0)}} + \underbrace{\frac{1 - e^{-i(\omega-\omega_{ji})t}}{\omega - \omega_{ji}}}_{\substack{\text{resonant term} \\ (\text{for } E_j > E_i \\ \text{i.e. } \omega_{ji} > 0)}} \Bigg]$$

If we place ourselves in the limit $|\omega - \omega_{ji}| \ll |\omega_{ji}|$ (i.e. $\omega \sim \omega_{ji}$), then we can neglect the anti-resonant term with respect to the resonant term.

$$c_j(t)\Big|_{1^{st}\ order} \simeq \frac{\langle\varphi_j|W|\varphi_i\rangle}{2\hbar}\, e^{-i\frac{(\omega-\omega_{ji})t}{2}} \left(\frac{e^{+i\frac{(\omega-\omega_{ji})t}{2}} - e^{-i\frac{(\omega-\omega_{ji})t}{2}}}{\omega-\omega_{ji}}\right)$$

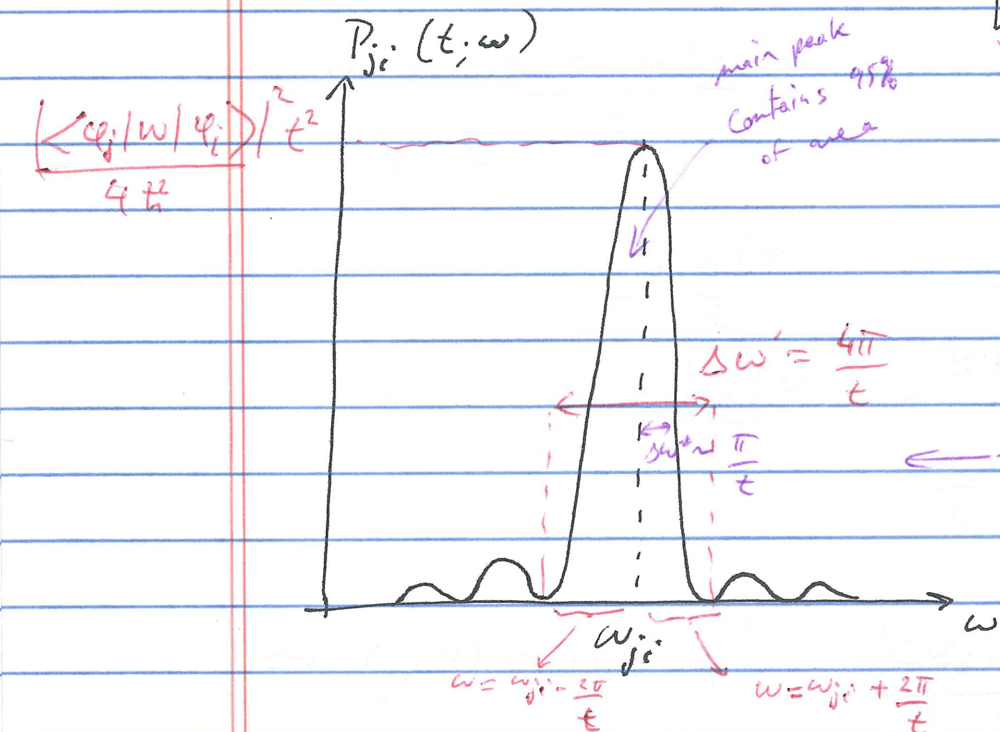
$$\simeq +i\frac{\langle\varphi_j|W|\varphi_i\rangle}{2\hbar}\, \frac{e^{-i\frac{(\omega-\omega_{ji})t}{2}}}{\left(\frac{\omega-\omega_{ji}}{2}\right)}\, \sin\left[\frac{(\omega-\omega_{ji})}{2}t\right]$$

thus

$$P_{ji}(t;\omega)\ \cancel{P_{ji}(t)} = \frac{|\langle\varphi_j|W|\varphi_i\rangle|^2}{4\hbar^2}\underbrace{\left[\frac{\sin\left[\frac{(\omega-\omega_{ji})t}{2}\right]}{\left(\frac{\omega-\omega_{ji}}{2}\right)}\right]^2}$$

$$\simeq \left|\frac{\frac{(\omega-\omega_{ji})t}{2}}{\left(\frac{\omega-\omega_{ji}}{2}\right)}\right|^2 \text{ for } \omega\to\omega_{ji}$$

$$\simeq t^2$$



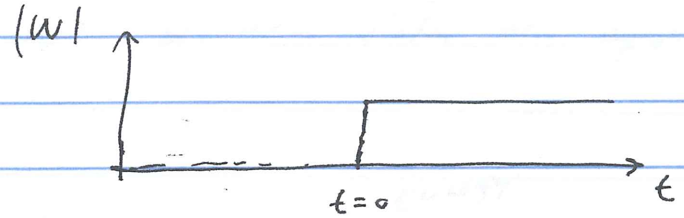
$\leftarrow \Delta E = \hbar\Delta\omega = \frac{\hbar\pi}{t}$

$\Rightarrow \Delta E\,\Delta t \sim \hbar(\pi)$ general form of Heisenberg uncertainty relation.

this treatment is only valid for $|\omega_{ji}| \gg \frac{\Delta\omega}{t}$

~~note: one can calculate the response to a step function $W(t)$, by setting $\omega = 0$ (however, you must keep the anti-resonant term)~~

Special case: Constant perturbation (step function)



we can treat this case by choosing a cosine perturbation with $\omega = 0$!

in this case, (1^{st} order)

$$c_j(t)\Big|_{1^{st}\text{order}} = \frac{\langle \varphi_j | W | \varphi_i \rangle}{2\hbar} \, \frac{2 - e^{i\omega_{ji}t} + e^{+i\omega_{ji}t}}{\omega_{ji}}$$

$$= \frac{\langle \varphi_j | W | \varphi_i \rangle}{\hbar} \, \frac{1 - e^{i\omega_{ji}t}}{\omega_{ji}}$$

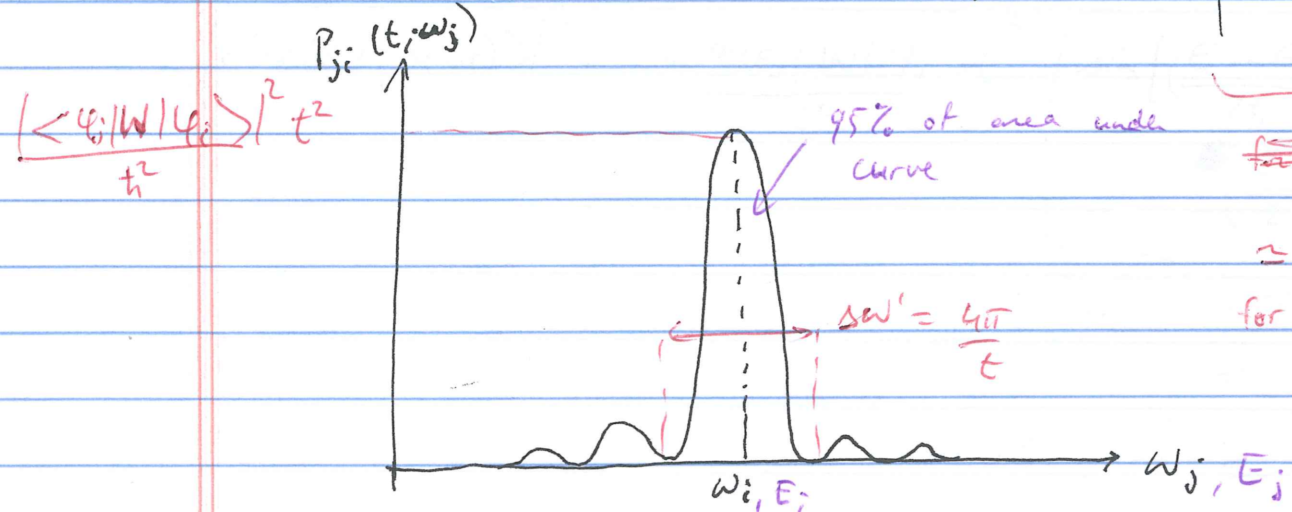
$$= \frac{i\langle \varphi_j | W | \varphi_i \rangle}{\hbar} \, \frac{e^{\frac{i\omega_{ji}t}{2}}}{\frac{\omega_{ji}}{2}} \, \underbrace{\frac{e^{-\frac{i\omega_{ji}t}{2}} - e^{\frac{i\omega_{ji}t}{2}}}{2i}}_{\sin\left(\frac{\omega_{ji}}{2}t\right)}$$

$$\Rightarrow P_{ji}(t) = |c_j(t)|^2 = \frac{|\langle \varphi_j | W | \varphi_i \rangle|^2}{\hbar^2} \underbrace{\left| \frac{\sin\left(\frac{\omega_{ji}t}{2}\right)}{\frac{\omega_{ji}}{2}} \right|^2}$$

~~for t~~ $\simeq \pi t \, \delta\left(\frac{\omega_j - \omega_i}{2}\right)$

$\simeq 2\pi\hbar t \, \delta(E_j - E_i)$

for $t \to$ ~~∞~~ large $\left(t \gg \frac{1}{\omega_{ji}}\right)$



Conclusion: Thus a step function perturbation tends to drive transitions only between states of equal energy (for $t \to$ large)

Stopped here

Coupling to a continuous energy spectrum

If instead of a final state $|\varphi_j\rangle, E_j$ there is continuum of final states $|\varphi(\alpha)\rangle, E(\alpha)$ with a density of states $\rho(E)\,dE$, then we are interested in calculating

$|\varphi(\alpha)\rangle$ are all orthogonal

$$\delta P_{ji} \to \delta P_{\delta\alpha,i} = \int_{\substack{\alpha \in \delta\alpha \\ \text{interval}}} d\alpha \, |\langle \varphi(\alpha) | \psi(t) \rangle|^2$$

if we can associate the continuous index α with an energy, then we have

$$\delta P_{\delta\alpha,i} \to \delta P_{\delta E,i} = \int_{E \in \delta E} dE \, \rho(E) |\langle \varphi(E) | \psi(t) \rangle|^2$$

for a step function perturbation $W(t)$, we have

$$|\langle \varphi(E) | \psi(t) \rangle|^2 = \left(\frac{|\langle \varphi(E) | W | \varphi_i \rangle|^2}{\hbar^2}\right) \underbrace{\left(\frac{\sin\left[\left(\frac{E - E_i}{2\hbar}\right)t\right]}{\left(\frac{E-E_i}{2\hbar}\right)} \right)^2}_{\simeq 2\pi\hbar t\,\delta(E_j - E_i)}$$

$\delta P_{\delta E,i}$ integral is easy!