Time dependent PT

(9.16)

Now let's consider perturbations that depend on time. Suppose we start in an eigenstate of H_0, the unperturbed Hamiltonian.

Then turn on perturbation $H'(t)$. What is prob. that a transition to another eigenstate of H_0 occurs?

Going back to our λ notation, total Hamiltonian is

$$H(\vec{r},t) = H_0(\vec{r}) + \lambda H'(\vec{r},t)$$

and now it's the time-dependent S.E. we solve, both for unperturbed eigenstates & the wave fn evolution of the full system.

For the unperturbed Hamiltonian, we have

$$H_0 \psi_n = E_n^{(0)} \psi_n = \hbar \omega_n \psi_n$$

and $$\psi_n(\vec{r},t) = \psi_n(\vec{r})\, e^{-i\omega_n t}$$

So since the ψ_n form a complete set, we expect the wave fn of the system to be a superposition of the ψ_n, but w/ coeff's that might depend on time:

$$\psi(\vec{r},t) = \sum_n c_n(t)\, \psi_n(\vec{r},t)$$

and we're interested in finding the $c_n(t)$. (9.17)

Note that $|c_n(t)|^2$ is prob of measuring system at time t + finding state ψ_n

To find the $c_n(t)$, use the time dep. Schr. eq'n.

we'll expand the c_n in powers of λ, as we did for time-indep PT, and collect powers of λ.

$$c_n(t) = c_n^{(0)} + \lambda c_n^{(1)}(t) + \lambda^2 c_n^{(2)}(t) + \cdots$$

no t dependence

Now, TDSE for $\Psi(\vec{r},t)$ is

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = (H_0 + \lambda H')\Psi(\vec{r},t)$$

Now subst $\Psi = \sum c_n(t)\psi_n(\vec{r})e^{-i\omega_n t}$, but without putting in the c_n expansion just yet:

$$\Rightarrow \sum_n \left[i\hbar \left(\frac{dc_n}{dt}\right) |\psi_n\rangle \right] + \cancel{\hbar\omega_n \Psi}$$

$$= \cancel{\hbar\omega_n \Psi} + \sum_n \lambda (H'|\psi_n\rangle)\, c_n(t)$$

and we can get rid of the summation on the LHS by taking the inner product w/ one of the ψ_n, say $\langle\psi_k|$

$$\Rightarrow \sum_n i\hbar\left(\frac{dc_n}{dt}\right)\underbrace{\langle \Psi_k | \Psi_n\rangle}_{e^{i(\omega_k-\omega_n)t}\underbrace{\langle \psi_k|\psi_n\rangle}_{\delta_{kn}}} = \sum_n \lambda \underbrace{\langle \Psi_k | H' | \Psi_n\rangle}_{H'_{kn}} c_n(t) \qquad \text{(9.18)}$$

H'_{kn} + note that it is w.r.t. Ψ_n, not ψ_n, ie, it contains $e^{i\omega t}$ factors

$$\Rightarrow i\hbar \frac{dc_k}{dt} = \lambda \sum_n H'_{kn} \underbrace{c_n(t)}_{c_n^{(0)} + \lambda c_n^{(1)} + \lambda^2 c_n^{(2)} + \cdots}$$

$c_k^{(0)} + \lambda c_k^{(1)} + \cdots$

So collecting powers of λ:

$$\lambda^0 : \quad i\hbar \frac{dc_k^{(0)}}{dt} = 0$$

$\Rightarrow$ 0^{th} order coeff's are const., as we noted above.

$$\lambda^1 : \quad i\hbar \frac{dc_k^{(1)}}{dt} = \sum_n H'_{kn} c_n^{(0)}$$

$$\vdots$$

$$\lambda^j : \quad i\hbar \frac{dc_k^{(j)}}{dt} = \sum_n H'_{kn} c_n^{(j-1)}$$

So again, we have a systematic method for finding each correction to c_n, based on result's for lower order corr's.

1^{st} order corr.:

Now Let's suppose the system is starting out in a definite eigenstate of H_0, $\psi_\ell(\vec{r},t)$. It is convential to take the initial time to be the distant past, i.e. $t \to -\infty$ (This is also used in scattering, and in QFT this initial state is sometimes referred to as the "in" state.)

So as $t \to -\infty$ $\psi(\vec{r},t) = \psi_\ell(\vec{r},t) \Rightarrow \boxed{c_n^{(0)} = \delta_{n\ell}}$ There's only one!

Now subst. into eq'n for $c_k^{(1)}$:

$$i\hbar \frac{dc_k^{(1)}}{dt} = \sum_n H'_{kn} c_n^{(0)} = H'_{k\ell}$$

And we can integrate this to find $c_k^{(1)}$:

$$c_k^{(1)}(t) = \frac{-i}{\hbar} \int_{-\infty}^{t} H'_{k\ell}(\vec{r},t')\,dt'$$

$\langle \psi_k | H' | \psi_\ell \rangle$

Now suppose in the perturbation Hamiltonian H' the space + time dependence factorize, so

$$H'(\vec{r},t) = \mathcal{H}'(\vec{r})f(t)$$

Then for the H' matrix elements we get

$\rightarrow$

(9.20)

$$H'_{k\ell} = \langle \varphi_k e^{i\omega_k t} | \mathcal{H}(\vec{r}) \, f(t) \, | e^{-i\omega_\ell t} \varphi_\ell \rangle$$ & let $\omega_{k\ell} \equiv \omega_k - \omega_\ell$

$$= \langle \varphi_k | \mathcal{H}' | \varphi_\ell \rangle e^{i(\omega_k - \omega_\ell)t} f(t)$$

$$= \mathcal{H}'_{k\ell} e^{i\omega_{k\ell} t} f(t) \qquad \omega_{k\ell} = \omega_k - \omega_\ell = \frac{E_k^{(0)} - E_\ell^{(0)}}{\hbar}$$

So plugging in to the integral for $c_k(t)$, we get

$$c_k^{(1)}(t) = -\frac{i}{\hbar} \mathcal{H}'_{k\ell} \int_{-\infty}^{t} e^{i\omega_{k\ell} t'} f(t') dt'$$

So this tells you how the perturbation populates all the states at 1st order.

[Aside: What happens if H' has t dependence only, i.e. no $\vec{r}$ dependence? Then $\mathcal{H}' = 1$ and

$$\mathcal{H}'_{k\ell} = \langle \varphi_k | 1 | \varphi_\ell \rangle = \delta_{k\ell}$$

$\Rightarrow$ no other states besides ℓ get populated at 2nd order!]

Then the transition probability fr/ state ℓ to state k is, at 1st order

$$\boxed{P_{\ell \to k} = |c_k^{(1)}|^2 = \left| \frac{\mathcal{H}'_{k\ell}}{\hbar} \right|^2 \left| \int_{-\infty}^{\infty} e^{i\omega_{k\ell} t'} f(t') dt' \right|^2}$$

Ex Gaussian time dep.

Take $H' = \mathcal{H}'(\vec{r})\,\dfrac{e^{-t^2/\tau^2}}{\tau\sqrt{\pi}}$ + assume

system starts in ground state. Pert. turns on at $t = -\infty$, slowly increases, is max at $t = 0$, + then decreases symmetrically in t.

From p. 9.20, will need

$$I = \int_{-\infty}^{\infty} e^{i\omega_{k0}t'} f(t')\,dt'$$

$$= \frac{1}{\tau\sqrt{\pi}} \int_{-\infty}^{\infty} e^{i\omega_{k0}t'} e^{-t'^2/\tau^2}\,dt'$$

$$= e^{-(\omega_{k0}\tau)^2/4} = e^{-(E_0 - E_k)^2\tau^2/4\hbar^2}$$

$\Rightarrow$ Transition prob is

$$P_{0\to k} = \left|\frac{\mathcal{H}'_{k0}}{\hbar}\right|^2 e^{-(E_0 - E_k)^2\tau^2/2\hbar^2}$$

Let's apply TDPT to the case where the perturbing Hamiltonian H' has a harmonic (i.e. sin or cos) time dependence w/ a single frequency, e.g from an E-M field (aka light). (9.22)

Take $H'(\vec{r},t) = \begin{cases} 0 & t<0 \\ 2\mathcal{H}'(\vec{r})\cos\omega t & t\geq 0 \end{cases}$

freq. of applied pert.

So for this case,

$$f(t) = 2\cos\omega t$$

& plugging into the expansion coeff. (& using $\cos\omega t = \dfrac{e^{i\omega t}+e^{-i\omega t}}{2}$)

[where recall l = initial state, k = final state for which we're finding transition prob]

$$\Rightarrow c_k(t) = \frac{-i\mathcal{H}'_{kl}}{\hbar}\int_0^t e^{i\omega_{kl}t'}\left(e^{-i\omega t'}+e^{+i\omega t'}\right)dt'$$

pert. turned on at $t=0$

$$= -i\frac{\mathcal{H}'_{kl}}{\hbar}\left[\frac{e^{i(\omega_{kl}-\omega)t'}}{i(\omega_{kl}-\omega)} + \frac{e^{i(\omega_{kl}+\omega)t'}}{i(\omega_{kl}+\omega)}\right]_0^t$$

$$= -\frac{\mathcal{H}'_{kl}}{\hbar}\left[\frac{e^{i(\omega_{kl}-\omega)t}-1}{\omega_{kl}-\omega} + \frac{e^{i(\omega_{kl}+\omega)t}-1}{\omega_{kl}+\omega}\right]$$

& then note $e^{i\theta/2}\sin\frac{\theta}{2} = e^{i\theta/2}\dfrac{\left(e^{i\theta/2}-e^{-i\theta/2}\right)}{2i} = \dfrac{e^{i\theta}-1}{2i}$

so the numerators can get replaced...

and we have (9.23)

$$c_k(t) = -\frac{i 2 \mathcal{H}'_{k\ell}}{\hbar}\left[e^{i(\omega_{k\ell}-\omega)t/2} \frac{\sin[(\omega_{k\ell}-\omega)t/2]}{\omega_{k\ell}-\omega} + e^{i(\omega_{k\ell}+\omega)t/2} \frac{\sin(\omega_{k\ell}+\omega)t/2}{\omega_{k\ell}+\omega} \right]$$

Now, we've seen forms like $\frac{\sin kx}{k}$ before,

and we know that they're peaked at $k \to 0$.

So our coefficient, and hence our transition prob, will be biggest for $\underset{\substack{\uparrow \\ \text{applied}}}{\omega} \simeq \pm \omega_{k\ell}$.

But remember what $\omega_{k\ell}$ is: $\hbar(E_k - E_\ell) = \omega_{k\ell}$

So these two prob. maxima correspond to

$E_k = E_\ell + \hbar\omega$ system absorbs energy $\hbar\omega$ (corresp to energy of a photon)

and, perhaps more surprisingly,

$E_k = E_\ell - \hbar\omega$ system radiates away energy $\hbar\omega$ corresp. to applied field

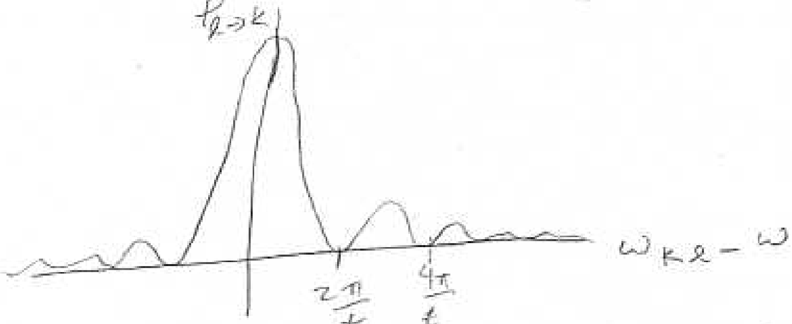
$\Rightarrow$ "stimulated emission"

<u>Aside</u>: This is how lasers work. Start w/ system of atoms in excited state k. 1st photon stimulates emission of 1st atom, which stimulates more, etc. (Trick is to make sure you always have more excited atoms than not so emission dominates absorption...)

(9.24)

Let's consider <u>absorption</u>, so $E_k > E_\ell$, and look at how the transition prob depends on the applied freq. ω. Plug $c_k(t)$, 1^{st} term only (if $E_k > E_\ell$, then $\omega_{k\ell} > 0$ and 2^{nd} term is always small)

$$\Rightarrow P_{\ell\to k} = |c_k(t)|^2 = 4 \frac{|\mathcal{H}'_{k\ell}|^2}{\hbar^2} \frac{\sin^2\left[\frac{1}{2}(\omega_{k\ell}-\omega)t\right]}{(\omega_{k\ell}-\omega)^2}$$



+ notice spread in freq. depends on how long pert. is turned on.

But this spread in freq. is (think of ω fixed) really a spread in energies E_k that get excited by the perturbation; the most likely ones are those falling in an interval $\sim \frac{2\pi}{t}$

$$\text{or} \quad \omega_{k\ell} - \omega \sim \frac{2\pi}{t} \Rightarrow \underbrace{|E_k - (E_\ell + \hbar\omega)|}_{\Delta E} \lesssim \frac{2\pi\hbar}{t}$$

So if we have a lot of identical systems, this ΔE corresponds to energy spread in the ensemble, + it is consistent w/ the uncertainty principle.

Now let's look at what happens to the prob. in the limit of very long times (or v. high frequencies) + consider either emission or absorption $\longrightarrow$ to be possible.

The $\dfrac{\sin^2 (\omega_{k\ell} \pm \omega)t/2}{(\omega_{k\ell} \pm \omega)^2}$ terms can be rewritten (9.23)

$$\frac{\sin^2 (\;)t/2}{t(\;)^2}$$ which looks like the rep. of a δ-fn! See plot on prev page; it gets narrower as $t \to \infty$

w/an extra overall factor of t

So the transition prob becomes

$$P_{\ell \to k} \to \frac{2\pi t}{\hbar^2} |\mathcal{H}'_{k\ell}|^2 \delta(\omega_{k\ell} \pm \omega)$$

and the transition rate, or prob/unit time, is

doubleu, not omega! $\longrightarrow$ $$W_{\ell k} = \frac{2\pi}{\hbar^2} |\mathcal{H}'_{k\ell}|^2 \delta(\omega_{k\ell} \pm \omega)$$

$\Rightarrow$ in the long time limit, the perturbation only affects a single energy diff., or if you like, the system only sees a single frequency.

(end of long time limit discussion

Finally, we can generalize to the common case where the final state energies lie in a continuum; think ionization of an atom or free particle scattering. Then the final states are described by some density, viz

we're back to absorption

no. of states in interval E_k to E_k+dE_k is $dN = g(E_k)\,dE_k$

↑ density of final states

Let the prob for a transition into an interval 2Δ abt E_k be $\overline{P}_{\ell \to k}$

(9.26)

Then

$$\overline{P_{l\to k}} = \int_{E_k-\Delta}^{E_k+\Delta} P_{l\to k}\, g(E_k')\, dE_k'$$

$$= \int_{E_k-\Delta}^{E_k+\Delta} \frac{4|\mathcal{H}'_{kl}|^2}{\hbar^2(\omega_{kl}-\omega)^2} \sin^2\left[\tfrac{1}{2}(\omega_{kl}-\omega)t\right] g(E_k')\, dE_k'$$

where there is also E_k' dependence in $\mathcal{H}'$ and ω_{kl}

Now, let's take Δ small, and assume $\mathcal{H}'$ and $g(E_k')$ are slowly varying fns of E_k, so we can take them to be const over the range of integration.

Then

$$\overline{P_{l\to k}} \simeq |\mathcal{H}'_{kl}|^2 g(E_k) \int_{E_k-\Delta}^{E_k+\Delta} \frac{4\sin^2[\ ]}{\hbar^2(\omega_{kl}-\omega)^2}\, dE_k'$$

and since we know $\dfrac{\sin^2[\ ]}{(\omega_{kl}-\omega)^2}$

falls off fast, we may as well extend the limits of integration to $\pm\infty$

and we get

$$\overline{P_{l\to k}} = t\left[\frac{2\pi}{\hbar} g(E_k)|\mathcal{H}'_{kl}|^2\right]$$

so the rate is (=prob/unit time)

$$\boxed{\overline{w_{lk}} = \frac{2\pi}{\hbar} g(E_k)|\mathcal{H}'_{kl}|^2}$$

Fermi's golden rule

applies e.g. to interaction of radiation w/ atoms & to scattering