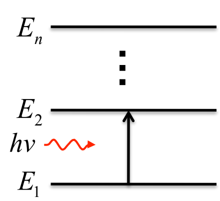
EE 232 Lightwave Devices
Lecture 5: Time-Dependent Perturbation Theory, Fermi's Golden Rule

Instructor: Ming C. Wu

University of California, Berkeley
Electrical Engineering and Computer Sciences Dept.

Time-Dependent Perturbation

Consider a quantum mechanical system:



$$H_0 \phi_n(\vec{r},t) = i\hbar \frac{\partial}{\partial t} \phi_n(\vec{r},t)$$

$$\phi_n(\vec{r},t) = \phi_n(\vec{r}) e^{-\frac{iE_n t}{\hbar}}$$

$\phi_n(\vec{r}) = |n\rangle$ an orthonormal set of eigenstates

$$\langle m|n\rangle = \int \phi_m^*(\vec{r})\phi_n(\vec{r})d\vec{r} = \delta_{mn}$$

Consider a single-frequency, time-varying stimulus

$$H'(\vec{r},t) = H'(\vec{r})e^{-iwt} + H'^{\dagger}(\vec{r})e^{iwt} \quad \text{for } t > 0$$

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

$$H\psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t)$$

Assuming $|H'| \ll |H_0|$

The new wavefunction can be expressed as a linear combination of original eigenstates with time-varying coefficients:

$$\psi(\vec{r},t) = \sum_n a_n(t)\phi_n(\vec{r})e^{-iE_n t/\hbar}$$

$|a_n(t)|^2$: probability of electron at state $|n\rangle$ at time t

Time-Dependent Perturbation (cont'd)

$$H\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

$$(H_0 + H')\sum_n a_n(t)\phi_n(\vec{r})e^{-iE_nt/\hbar} = i\hbar\sum_n \frac{da_n(t)}{dt}\phi_n(t)e^{-iE_nt/\hbar} + i\hbar\sum_n a_n(t)\phi_n(\vec{r})\left(\frac{-iE}{\hbar}\right)e^{-iE_nt/\hbar}$$

$$H'\sum_n a_n(t)\left|n\right\rangle e^{-iE_nt/\hbar} = i\hbar\sum_n \frac{da_n(t)}{dt}\left|n\right\rangle e^{-iE_nt/\hbar}$$

Multiply both sides by $\left\langle m\right|$ (i.e., multiply by $\phi_m^*(\vec{r})$ and integrate over $\vec{r}$)

$$\sum_n a_n(t)\left\langle m\right|H'\left|n\right\rangle e^{-iE_nt/\hbar} = i\hbar\sum_n \frac{da_n(t)}{dt}\left\langle m|n\right\rangle e^{-iE_nt/\hbar} = i\hbar\frac{da_m(t)}{dt}e^{-iE_mt/\hbar}$$

$$\frac{da_m(t)}{dt} = \frac{1}{i\hbar}\sum_n a_n(t)H'_{mn}(t)e^{i\omega_{mn}t}$$

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

First-Order Perturbation

To track the order of perturbation, let

$$H = H_0 + \lambda H'$$

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

Group terms with the same order of λ:

$$\frac{da_m^{(0)}(t)}{dt} = 0 \Rightarrow a_m^{(0)}(t) = \text{constant}$$

$$\frac{da_m^{(1)}(t)}{dt} = \frac{1}{i\text{h}}\sum_n a_n^{(0)}(t)H'_{mn}(t)e^{i\omega_{mn}t}$$

$$\frac{da_m^{(2)}(t)}{dt} = \frac{1}{i\text{h}}\sum_n a_n^{(1)}(t)H'_{mn}(t)e^{i\omega_{mn}t}$$

First-Order Perturbation (Cont'd)

Initial state i at t=0 and final state f

$$\begin{cases} a_i^{(0)}(t) = 1 \\ a_m^{(0)}(t) = 0 \text{ if } m \neq i \end{cases}$$

$$\frac{da_f^{(1)}(t)}{dt} = \frac{1}{i\hbar} H'_{fi}(t) e^{i\omega_{mi}t} = \frac{1}{i\hbar}\left(H'_{fi} e^{-i\omega t} + H'^{\dagger}_{fi} e^{i\omega t} \right) e^{i\omega_{mi} t}$$

$$= \frac{1}{i\hbar}\left(H'_{fi} e^{i(\omega_{mi}-\omega)t} + H'^{\dagger}_{fi} e^{i(\omega_{mi}+\omega)t} \right)$$

$$a_f^{(1)}(t) = \frac{-1}{\hbar}\left(H'_{fi} \frac{e^{i(\omega_{mi}-\omega)t}-1}{\omega_{mi}-\omega} + H'^{\dagger}_{fi} \frac{e^{i(\omega_{mi}+\omega)t}-1}{\omega_{mi}+\omega} \right)$$

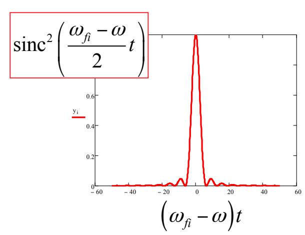
We are only interested at frequencies near resonance:

$$\left|a_f^{(1)}(t)\right|^2 = \frac{4\left|H'_{fi}\right|^2}{\hbar^2} \frac{\sin^2\left(\frac{\omega_{mi}-\omega}{2}t\right)}{\left(\omega_{mi}-\omega\right)^2} + \frac{4\left|H'^{\dagger}_{fi}\right|^2}{\hbar^2} \frac{\sin^2\left(\frac{\omega_{mi}+\omega}{2}t\right)}{\left(\omega_{mi}+\omega\right)^2}$$

Fermi's Golden Rule

$$\frac{\sin^2\left(\frac{\omega_{fi}-\omega}{2}t\right)}{\left(\omega_{fi}-\omega\right)^2} = \frac{t^2}{4}\text{sinc}^2\left(\frac{\omega_{fi}-\omega}{2}t\right)$$

$$\rightarrow \frac{\pi t}{2}\delta(\omega_{fi}-\omega) \quad \text{as } t \rightarrow \infty$$



$$\left|a_f^{(1)}(t)\right|^2 = \frac{2\pi t\left|H'_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}-\omega) + \frac{2\pi t\left|H'^{\dagger}_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}+\omega)$$

Transition Rate:

$$W_{i\rightarrow f} = \frac{d}{dt}\left|a_f^{(1)}(t)\right|^2 = \frac{2\pi\left|H'_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}-\omega) + \frac{2\pi\left|H'^{\dagger}_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}+\omega)$$

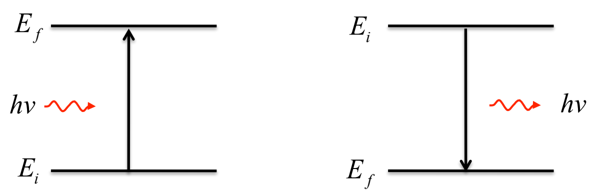
Note: $\delta(E_f - E_i - \hbar\omega) = \frac{1}{\hbar}\delta(\omega_f - \omega_i - \omega)$

$$W_{i\rightarrow f} = \frac{2\pi\left|H'_{fi}\right|^2}{\hbar}\delta(E_f - E_i - \hbar\omega) + \frac{2\pi\left|H'^{\dagger}_{fi}\right|^2}{\hbar}\delta(E_f - E_i + \hbar\omega)$$

Physical Interpretation

$$W_{i\to f} = \frac{2\pi |H'_{fi}|^2}{\hbar}\delta(E_f - E_i - \hbar\omega) + \frac{2\pi |H'^{\dagger}_{fi}|^2}{\hbar}\delta(E_f - E_i + \hbar\omega)$$

$E_f = E_i + \hbar\omega$ Absorption of a photon	$E_f = E_i - \hbar\omega$ Emission of a photon



- **Conservation of energy**
- **Transition rate is proportional to the square of the "matrix element"**

Distributed Final States

- **If the final state is a distribution of states, the transition rate is proportional to the density of states of the final state:**

$$W_{i\to f} = \frac{2\pi |H'_{fi}|^2}{\hbar}\rho_f\delta(E_f - E_i - \hbar\omega) + \frac{2\pi |H'^{\dagger}_{fi}|^2}{\hbar}\rho_f\delta(E_f - E_i + \hbar\omega)$$

$E_f = E_i + \hbar\omega$ Absorption of a photon	$E_f = E_i - \hbar\omega$ Emission of a photon