

# Quantum Transport:

ATOM TO TRANSISTOR

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## Lecture 35: Radiative Lifetime

Ref. Chapter 10.1 & 10.2



*Network for Computational Nanotechnology*

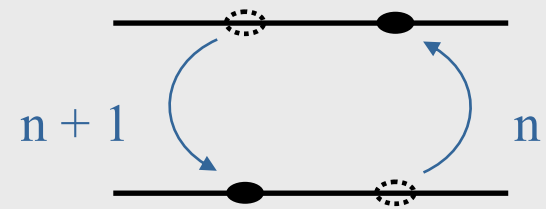
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# Introduction

00:00

• Ordinarily if we use the two levels for our basis functions, then the Hamiltonian will be diagonal. That would mean no transitions, because levels 1 and 2 would be completely decoupled from each other. For transition between levels, you need off diagonal elements such that there is coupling between levels. So the postulation is that because of the electromagnetic noise that is present, electron will be perturbed which is the scattering potential in  $[H]$ . The problem is that if you put any real potential, then its complex conjugate will be the other off-diagonal element; This means that the transitions from 1 to 2 and from 2 to 1 are equal. However what happens in equilibrium is that electrons relax at a much higher rate than they get excited.

## Emission and Absorption



$$i\hbar \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \epsilon_1 & [U_S]_{12} \\ [U_S]_{21} & \epsilon_2 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

• The number of upwards transitions is proportional to  $n$  and the number of downward transitions to  $n+1$ , where

$$n = \frac{1}{e^{\hbar\omega/k_B T} + 1} \quad \text{at } T=0, n=0$$

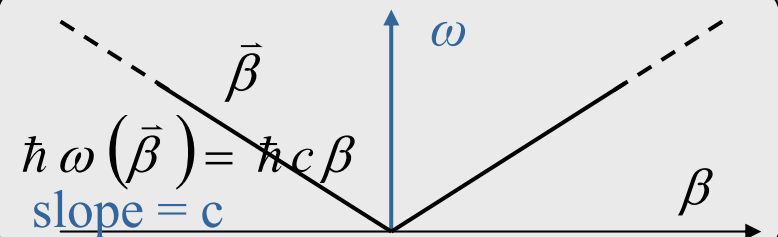
# Multi-Particle Picture

- That said, the emission/absorption process is much easier to understand in terms of a multi-particle electron-photon picture (as discussed in the previous lecture)

- If you think of the atom as being in one big box, then photons in the box can be described by plane waves:  $\cos(\vec{\beta} \cdot \vec{r} - \omega(\vec{\beta})t)$
- The relationship between  $\omega$  and  $\beta$  is linear. We have:

## Multi-Particle Levels

N-1 photon	N photon	N+1 photon
$\frac{\varepsilon_2 + (N-1)\hbar\omega}{\varepsilon_1 + (N-1)\hbar\omega}$	$\frac{\varepsilon_2 + (N)\hbar\omega}{\varepsilon_1 + (N)\hbar\omega}$	$\frac{\varepsilon_2 + (N+1)\hbar\omega}{\varepsilon_1 + (N+1)\hbar\omega}$



Note: With photons there is no exclusion principle

- One photon state means having one photon at a particular frequency. N photon state means having N photons at that frequency.

# Dissipation

09:20

- The continuous distribution of photons alters the 1-level picture from...

- Looking at the 0-photon state, when we put an electron in the upper level,  $\varepsilon_2$ , it likes to spread out (broaden) into the adjacent level and then fall back down to  $\varepsilon_1$  giving up a photon in the process

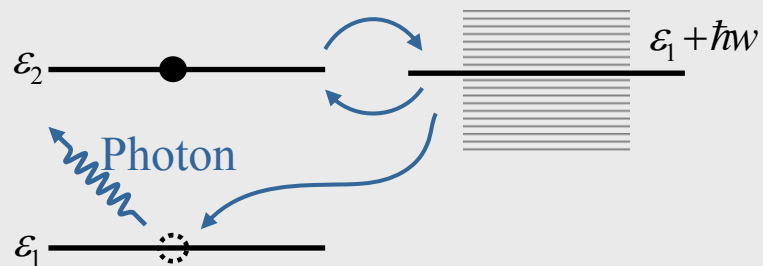
$$\varepsilon + N\hbar\omega$$

... to ...

$$\varepsilon + N\hbar\omega$$

$$\varepsilon + \hbar c\beta$$

## Dissipation into Photon Reservoir

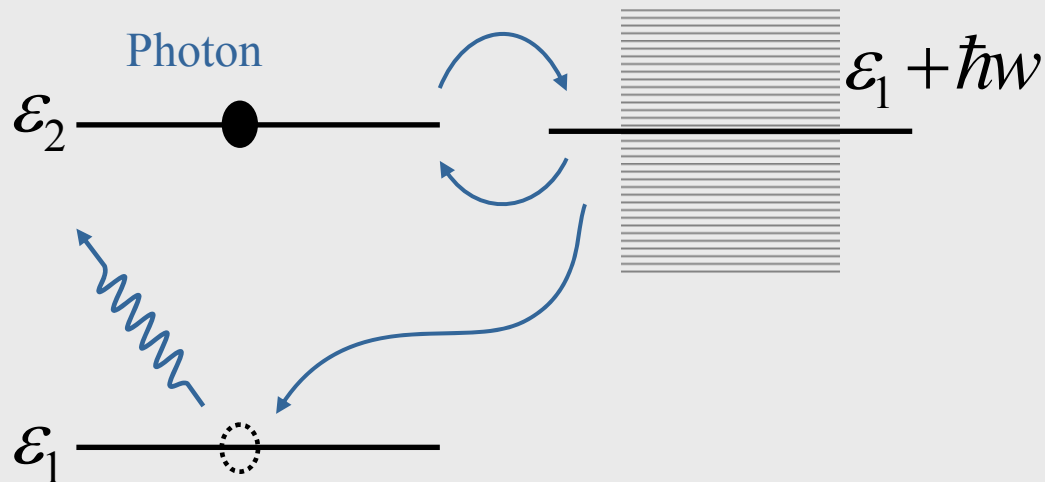


- This has important implications for photon emission from excited states

- Importantly, this behavior can be viewed much the same as dissipation into a contact
- So the question is how one calculates the rate at which the electron goes away when it's put in a state.

- Because adjacent levels act as photon reservoirs we may use the Green's function formalism to derive the radiative lifetime of an electron

## Dissipation into Photon Reservoir



- So we can use the self-energy expression

$$\Sigma = \tau g \tau^+$$

and to get an estimate of the lifetime take

$$\hbar/\tau_r = \Gamma_1 = \tau a \tau^+$$

The process may be viewed as  $|2,0\text{ph}\rangle \rightarrow |1,1\text{ph}\rangle$  where radiative lifetime is like another self-energy



• Note:  $\tau$  is a physical quantity which constitutes the coupling between levels and  $\tau_\gamma$  is the escape rate of electron from one state to another.

• Formally, therefore the broadening of the 0-photon state is given as:

$$\Gamma_1 = \tau a \tau^+ = \sum_{\vec{\beta}} |\tau(\vec{\beta})|^2 2\pi\delta(E - \varepsilon_1 - \hbar\omega(\vec{\beta}))$$

- Where  $2\pi\delta(E - \varepsilon_1 - \hbar\omega(\vec{\beta}))$  is the photon reservoir spectral function a.
- Imposing periodic boundary this summation may be transformed into an integral

$$\begin{aligned} \hbar/\tau_r &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \left[ \frac{\beta^2 d\beta \sin\theta d\theta d\phi}{8\pi^3} V |\tau(\vec{\beta})|^2 \times 2\pi\delta(\varepsilon_2 - \varepsilon_1 - \hbar\omega(\vec{\beta})) \right] \\ &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \left[ \frac{\omega^2 d\omega \sin\theta d\theta d\phi}{8\pi^3 c^3} V |\tau(\vec{\beta})|^2 \times 2\pi\delta(\varepsilon_2 - \varepsilon_1 - \hbar\omega(\vec{\beta})) \right] \\ &= \int_0^\pi \int_0^{2\pi} \frac{\sin\theta d\theta d\phi}{8\pi^3 c^3} |\tau(\vec{\beta})|^2 \left( \frac{\varepsilon_2 - \varepsilon_1}{\hbar} \right)^2 \times \frac{2\pi}{\hbar} V \quad (\text{V is the volume}) \end{aligned}$$

## Deriving the Coupling

- To arrive at an expression for coupling between the 0-photon and 1-photon state we must consider the potential that an electron feels due to one photon
- The electric field of a single photon with wave vector  $\vec{\beta}$  is

$$\vec{\mathcal{E}} = \hat{v} \varepsilon_0 \sin(\vec{\beta} \cdot \vec{r} - \omega(\vec{\beta})t)$$

We want to know if the box had just one photon, then what electric field would be present. One way to do this is to look at the total energy in the EM wave:

$$\mathcal{E}_{Total} = \mathcal{E}_E^2 + \mathcal{E}_M^2 = \frac{V}{2} \varepsilon \varepsilon_0^2 = \hbar \omega$$

where  $V$  is the volume of the box containing the photon

- Thus, 
$$|\varepsilon_0| = \sqrt{\frac{2\hbar\omega}{\varepsilon V}}$$

- Now, to write the potential we use the well known relationship

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t}$$

$$\therefore \vec{A} = \hat{v} A_0 \cos(\vec{\beta} \cdot \vec{r} - \omega(\vec{\beta})t)$$

$$|A_0| = \sqrt{\frac{2\hbar}{\omega \varepsilon V}}$$

- Note, however, that the potential created by a photon is a vector potential and may not be simply added to the Schrödinger equation as the typical electro-static scalar potential we are familiar with.

- General Approach:  
→ A scalar potential,  $U$ , is included in the Hamiltonian as

$$H = \frac{p^2}{2m} + U$$

- and the EM vector potential,  $\vec{A}$ , as

$$H = \frac{(\vec{p} + q\vec{A})^2}{2m} \quad (1)$$

- To find the coupling term we need to know how much the Hamiltonian changed due to addition of one photon. Expanding 1:

$$H = \frac{q}{2m} (\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) + \frac{q^2}{2m} \vec{A} \cdot \vec{A}$$

$$\vec{A} \cdot \vec{A} \approx 0 \quad \text{Negligible}$$

$$\vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p} \quad \text{if} \quad \vec{\nabla} \cdot \vec{A} = 0$$

- So the Hamiltonian becomes:

$$H = \frac{q}{m} (\vec{A} \cdot \vec{p})$$



# Coupling Element

- As done earlier, we adopt

$$\vec{A} = \hat{v} A_0 \cos(\vec{\beta} \cdot \vec{r} - \omega(\vec{\beta})t)$$

thus the addition to Hamiltonian is

$$H = \frac{q}{m} (\vec{A} \cdot \vec{p}) = qA_0/2m (\vec{p} \cdot \hat{v}) \left( e^{+i\vec{\beta} \cdot \vec{r}} e^{-i\omega(\beta)t} + e^{-i\vec{\beta} \cdot \vec{r}} e^{i\omega(\beta)t} \right)$$

- Furthermore we denote  $e^{+i\vec{\beta} \cdot \vec{r}} e^{-i\omega(\beta)t}$  as the absorption term and  $e^{-i\vec{\beta} \cdot \vec{r}} e^{i\omega(\beta)t}$  as the emission term.

$$i\hbar \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \underbrace{\begin{bmatrix} \epsilon_1 & [U_S]_{12} \\ [U_S]_{21} & \epsilon_2 \end{bmatrix}}_{[H]} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

- So for the coupling element we have:  $H_{12} = \frac{qA_0}{2m} \int dr^3 \phi_1^* (\vec{p} \cdot \hat{v} e^{+i\vec{\beta} \cdot \vec{r}}) \phi_2$