Quantum Transport:
Atom to Transistor

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Lecture 34: Why does an atom emit light?

Ref. Chapter 10.1

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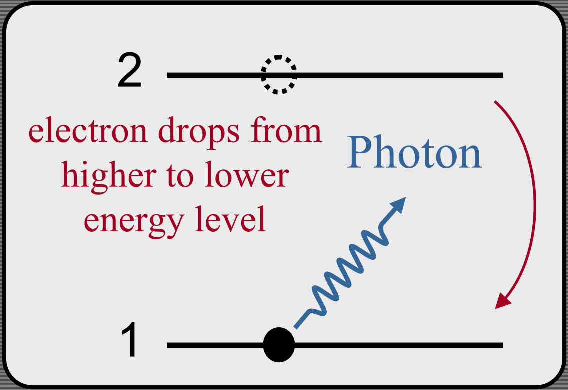
Introduction

• In the next few lectures we'll look at the interaction of electrons with the surrounding media, specifically photons and phonons

• To begin with, consider the following question: "Why does an atom emit light?"

• Recall, original motivation for the Schrödinger came from light emission (Hydrogen Gas Spectra)

Light Emission



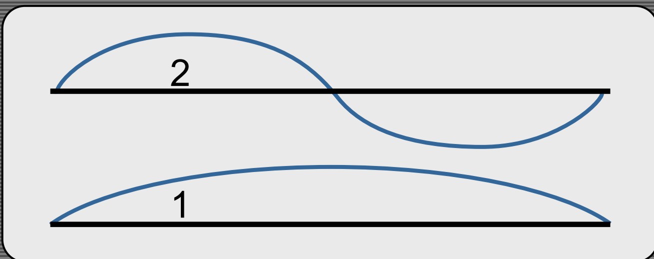
• So what makes the electron to emit light when it drops from a higher level of energy to a lower one?

• Notice that although the behavior of electrons is described by the Schrödinger equation, the equation as it stands does not predict the emission of light by an electron.

• To see this, let's look at the matrix version of Schrödinger equation describing our simple molecule with two levels (Next page):

Electron Excitaton and De-excitation

Basis Functions



- Suppose we only had these two levels, and we'd use these two states as our basis functions to describe the wave function, then the the Schrödinger equation would become a 2 2 matrix equation of the form:

$$i\hbar\begin{Bmatrix}\psi_1\\\psi_2\end{Bmatrix}=\begin{bmatrix}\varepsilon_1 & 0\\0 & \varepsilon_2\end{bmatrix}\begin{Bmatrix}\psi_1\\\psi_2\end{Bmatrix}$$

- This system evolves in time as

$$\psi_1(t)=\psi_1(0)e^{-(i\varepsilon_1 t)/\hbar}$$
$$\psi_2(t)=\psi_2(0)e^{-(i\varepsilon_2 t)/\hbar}$$

such that the probability remains unchanged.

$$P_1(t)=P_1(0)$$
$$P_2(t)=P_2(0)$$

- Therefore, following the Schrödinger equation in this form, an electron should not "fall" from a higher energy state to a lower energy state but it will remain there indefinitely. How ever all of us know that if we put an electron in a high state, it will emit light and go to a lower state. So what is happening?
- There are two ways to answer this. The first is simpler to understand, how ever it has some conceptual problems.

Electron Tickling

08:00

- What causes an electron to drop down even at absolute zero? People say that it is due to electromagnetic noise or zero-point fluctuations which effectively tickle an electron into a lower energy state. But this requires a Hamiltonian which is NON Hermition.

- Why Non-Hermition?

We must add off-diagonal terms $[U_S]_{12}$ and $[U_S]_{21}$ to the Schrödinger equation

$$i\hbar\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{bmatrix}\varepsilon_1 & [U_S]_{12}\\ [U_S]_{21} & \varepsilon_2\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

such that $[U_S]_{12} \neq 0$ and $[U_S]_{21} = 0$ at 0K and for T>0K, $[U_S]_{12} > [U_S]_{21}$

Note: At temperature greater than absolute zero other interactions beyond zero-point fluctuations also contribute to $[U_S]_{12}$ and $[U_S]_{21}$

Moving Up and Down

11:45

- *Why is it that* $[U_S]_{12} > [U_S]_{21}$ *at all temperatures?* A: This inequality guarantees that the number of downward transitions will always exceed the number of upward transitions which is a sound physical argument.

- To formalize, let the rate at which electrons go from level 2 to level 1, $S_{2\rightarrow 1}$, be some constant, $K_{2\rightarrow 1}$, times a product of the Fermi functions

$$S_{2\rightarrow 1} = K_{2\rightarrow 1}\, f_2\,(1 - f_1)$$

- Similarly, the rate from level 1 to level 2 may be represented as

$$S_{1\rightarrow 2} = K_{1\rightarrow 2}\, f_1\,(1 - f_2)$$

- At equilibrium these two rates must be equal, hence

$$\frac{K_{1\rightarrow 2}}{K_{2\rightarrow 1}} = \frac{f_2(1-f_1)}{f_1(1-f_2)} = \frac{(1-f_1)/f_1}{(1-f_2)/f_2}$$

Rate Analysis

15:40

- Continuing our derivation of $K_{1\to2} / K_{2\to1}$ …

$$f_{1,2} = \frac{1}{e^{(\varepsilon_{1,2}-\mu)/k_B T} + 1}$$

and

$$1/f_{1,2} = 1 + e^{(\varepsilon_{1,2}-\mu)/k_B T}$$

$$(1 - f_{1,2}) = \frac{e^{(\varepsilon_{1,2}-\mu)/k_B T}}{e^{(\varepsilon_{1,2}-\mu)/k_B T}}$$

$$\therefore \frac{K_{1\to2}}{K_{2\to1}} = e^{(\varepsilon_1-\varepsilon_2)/k_B T}$$

and at $T=0$ this expression equals 0 so the electron wants to jump from 1 to 2 but not from 2 to 1.

- Main point: At any temperature the rate at which electrons move from 2 to 1 is much greater than the rate from 1 to 2

- At the beginning of the last century, Einstein successfully argued that if the number of photons present is n then the number of downward transitions is proportional to $(n+1)$ and the number of upward transitions to n:

$K_{2\to1} = K(n+1)$ and
$K_{1\to2} = Kn$

Bose-Einstein Factor

20:15

- Where for the transition rates

$K_{2\to1} = K(n+1)$ and

$K_{1\to2} = Kn$

n is given by the Bose-Einstein factor

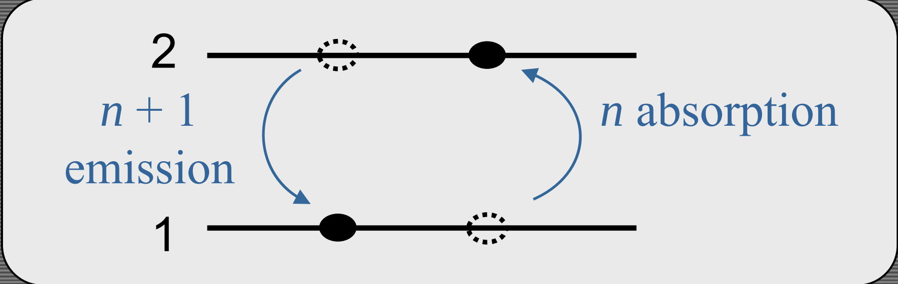
$$n = \frac{1}{e^{\hbar\omega/k_BT} - 1}$$

Note that $\dfrac{K_{2\to1}}{K_{1\to2}} = 1 + 1/n = e^{\hbar\omega/k_BT}$

$$\therefore (1+n)/n = e^{\hbar\omega/k_BT} = e^{(\varepsilon_2-\varepsilon_1)/K_BT}$$

showing that the Bose-Einstein factors demonstrate the same proportionality as the Fermi functions of levels 1 and 2

Absorption and Emission Transition Rates



- Of course we expect the rate of downward transitions to exceed that of upward transitions such that at equilibrium lower energy states are more likely to be occupied than higher energy states. Perhaps the most satisfactory explanation of this fact lies in what is known as the **many-particle** viewpoint

Many-Particle Viewpoint

25:31

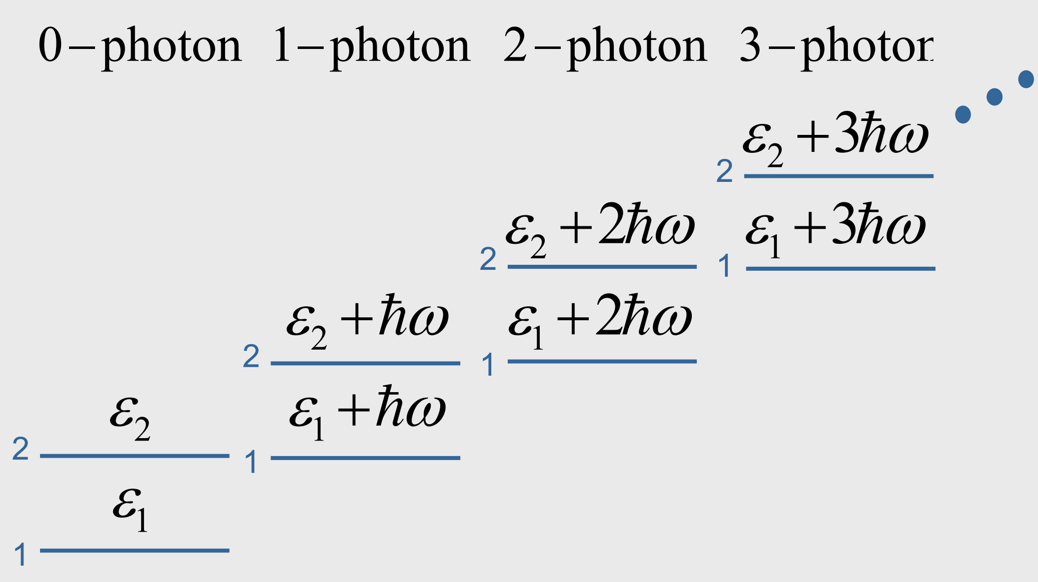
- An electron interacting with multiple photons may be viewed as one big many-particle system with a single wave function:

$$\Psi = \psi \otimes \Phi$$

where ψ is the electron wavefunction convolved with photon wavefunction Φ

- This system has an infinite number of electron-photon states. The first four are shown in the following diagram

First Four Electron-Photon States

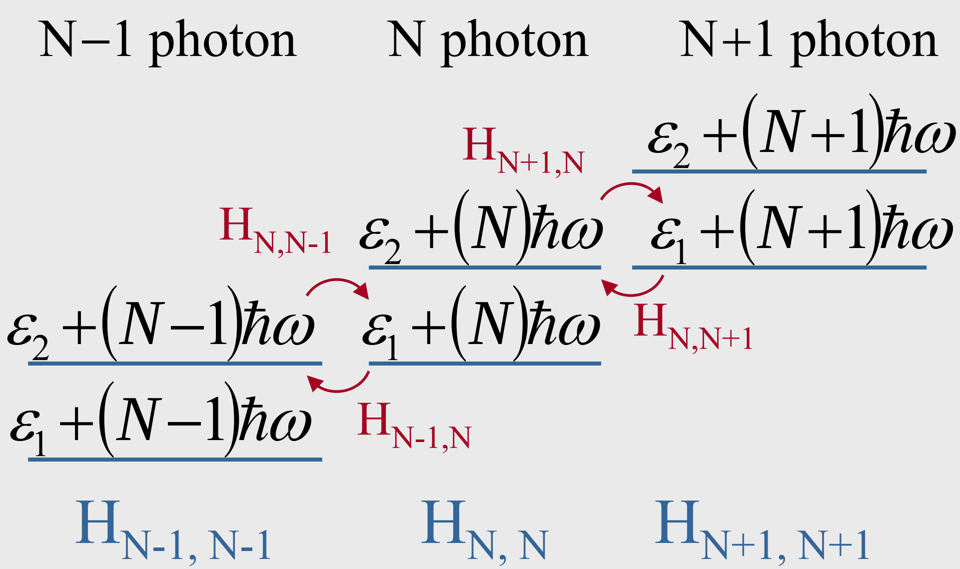


Many-Particle Schrödinger Equation

30:28

• In general we can right a Schrödinger Equation including both electrons and photons

N-Photon System



…with coupling $H_{N+1,N}$, $H_{N,N+1}$, $H_{N,N-1}$, $H_{N-1,N}$ between adjacent levels

• This gives an overall Schrödinger Equation:

$$i\hbar \begin{Bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \vdots \end{Bmatrix} = \begin{bmatrix} H_{00} & H_{01} & & \\ H_{10} & H_{11} & H_{12} & \\ & H_{21} & H_{22} & \\ & & & \ddots \end{bmatrix} \begin{Bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \vdots \end{Bmatrix}$$

Note: Each of Ψ_0, Ψ_1, Ψ_2, etc. has two components (one for level 1 and one for level 2)

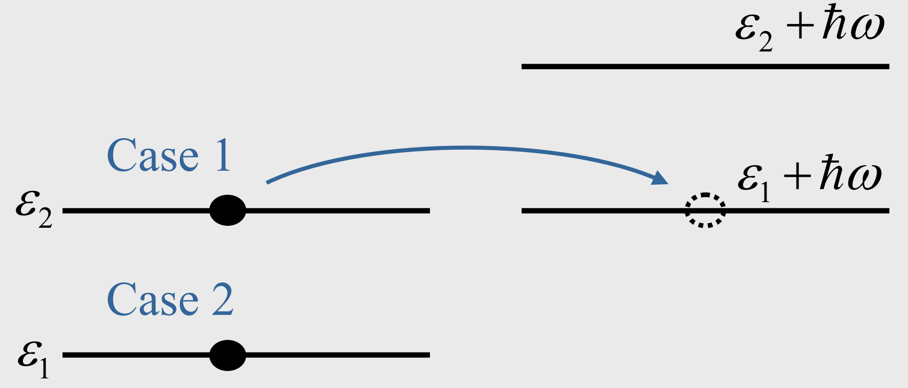
• Solving this equation we can get the basis functions of the electron-photon Hilbert space

Transitions

34:54

- So what happens when we put an electron in a state at T=0?
- *Case 1*: Put an electron in the ε_2 level. Due to electron-photon coupling it wants to make the transition over to the 1-photon subspace, that is the degenerate adjacent level $\varepsilon_1 + \hbar\omega$. So the whole process of emission becomes a transfer between two states with the same energy.

Electrons at T=0 in ε_2 and ε_1 states



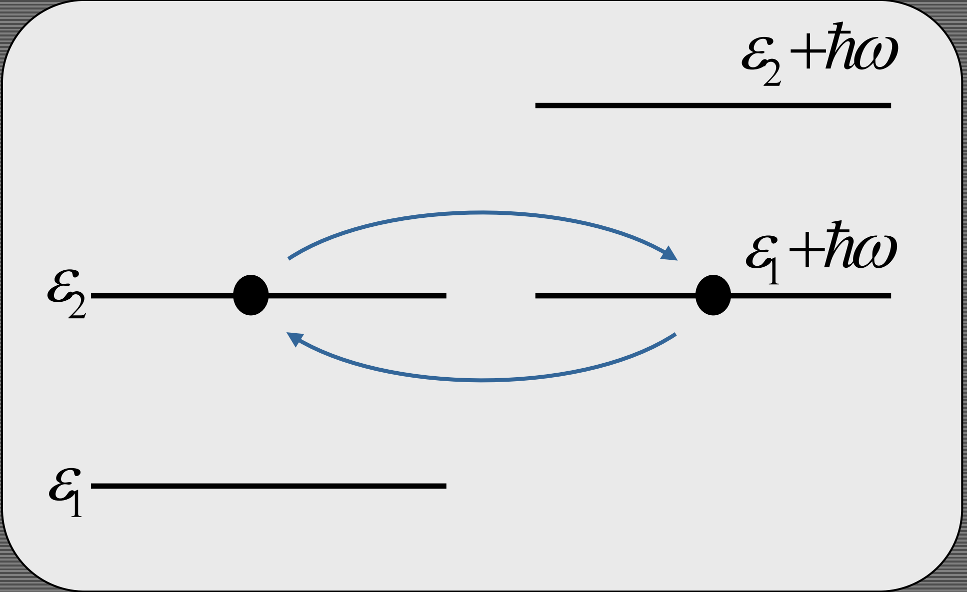
- *Case 2*: Put an electron in the ε_1 level. Here the electron can't move because it has no degenerate or lower states to go to. At T=0 it will stay there forever.

Cycle

- We can now see why an electron in an upper state emits light. The process of emission may be viewed as a transition between two states of the same energy, the electron goes from ε_2 to ε_1 and the photon subspace increases by one

- But if this was all there was to it, the Schrödinger equation would dictate a cycle such that the electron continuously emits and absorbs photons

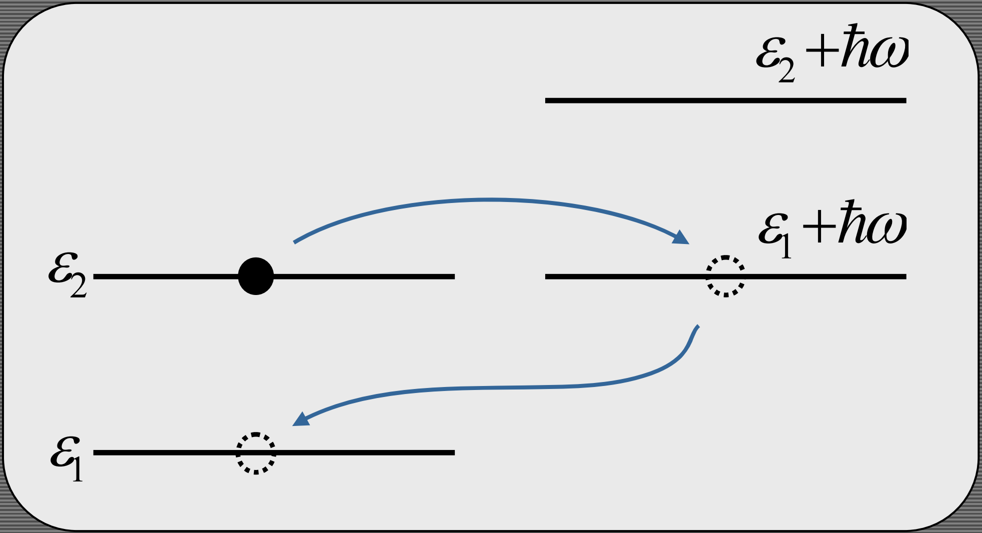
Continuous Emission and Absorption Cycle



Real World

• But because adjacent levels function much like a contact, in the real world our photon is released and dissipated. End result: the electron-photon multi-particle falls down from $\varepsilon_1 + \hbar w$ to ε_1

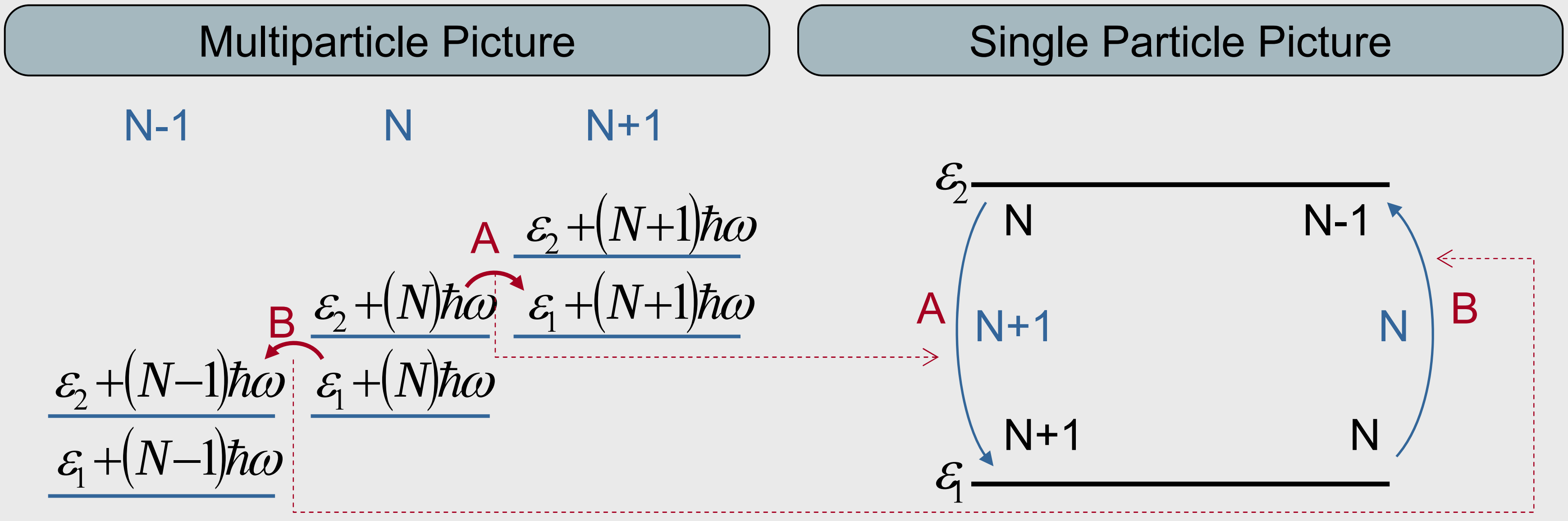
Real World Emission



• This effect is just like the dissipation of an electron into an infinite reservoir. And again in numerical simulation recurrence is limited by $i0^+$

N-Photon Subspace

• The general multiparticle picture around the N-photon subspace relates to the single particle picture as…



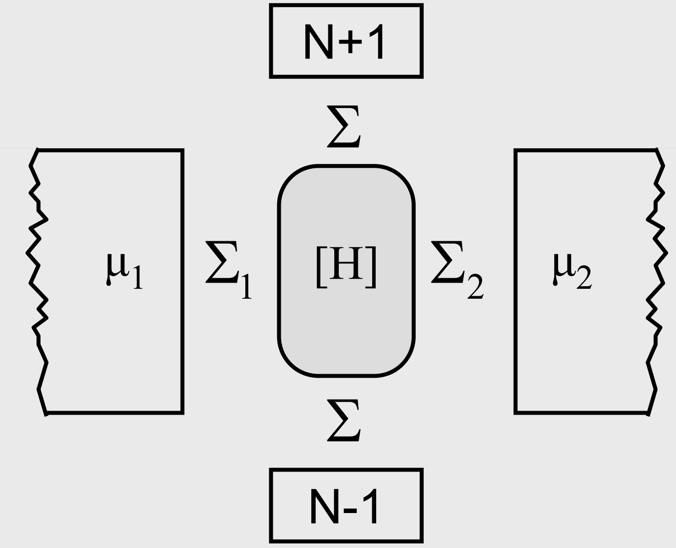
• Where the dotted arrows in the above diagram show the equivalent level couplings in both representations.

Photon Contacts

- Note: At zero temperature all the action happens in the 0-photon subspace and at higher temperatures it occurs in some positive integer n-photon subspace found by the proper Bose-Einstein Factor

- *How does this formalism relate to the original device picture?* A: Typically the device lies some N-photon subspace, the adjacent N-1 and N+1 subspaces are treated as contacts with their own self-energy and coupling

Device Coupled to N+1 and N-1 Photon Subspaces



Closing Comments

46:00

• *Next Lecture*: Look at the coupling constants K_{nm} between levels

• *Final Comment*: As we have seen, not everything in quantum mechanics follows from Schrödinger's equation – take for example the Fermi function. One might imagine that the Schrödinger equation is incomplete, but in fact it is not. To reach the same results as those given by the Fermi function and other such approximations we must solve a gigantic multiparticle Schrödinger equation. This, for most practical problems, is almost, if not completely, impossible.