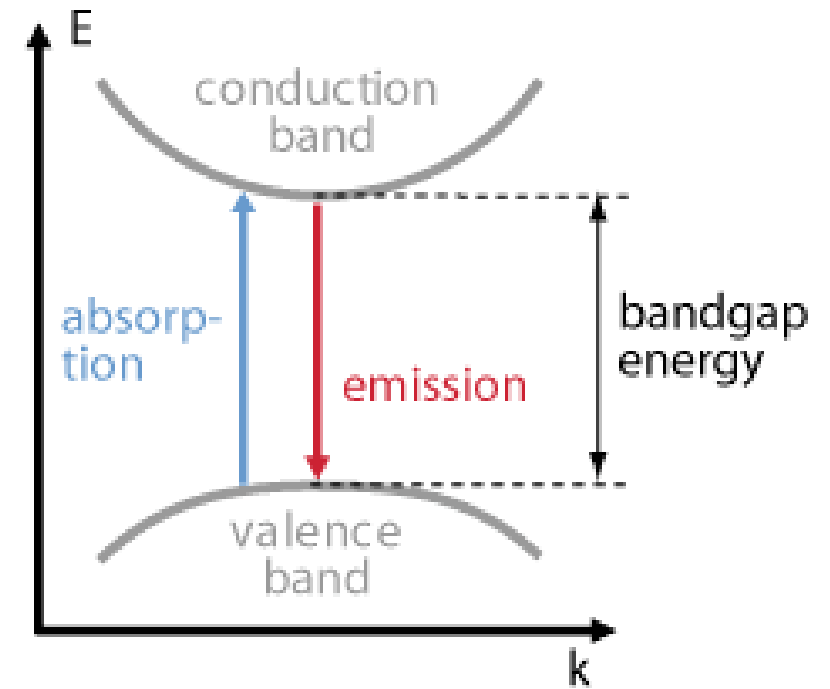# 21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Unit 3 : Session 1 : SLO 1

Concept of optical transitions in bulk Semiconductors

For the optical properties of semiconductors, the photons should interact with charge carriers. In the process of interaction three process occurs

- **Absorption**
- **Recombination**
- **Emission**

i.e., the photons are absorbed and emitted ; these processes are important in photonic devices using semiconductors. There are several type of transition possibilities can occur:
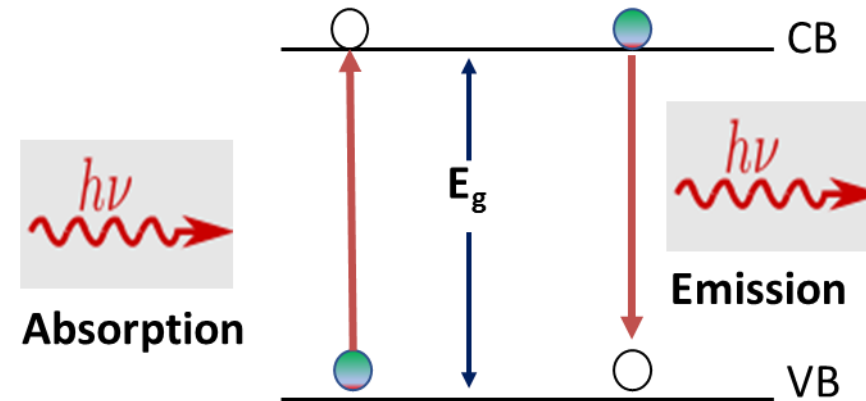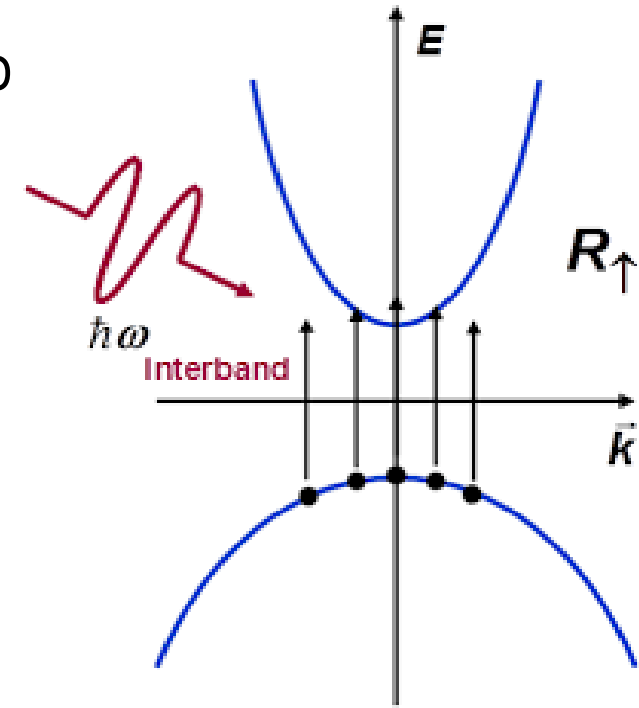
1. Band to band transition (Inter band transition)

2. Impurity level to band transition

3. Free carrier transition (Intra band transition)

In semiconductors electrons can make transitions between two energy states and create or destroy photons in the process.

- Band to band transition (Inter band transition)

An absorbed photon can result in an electron in the valence band making an upward transition to conduction band. This results electron-hole pair generation, followed by this electron-hole recombination takes place by the emission of Photon.

E.g.: Band to Band transition in GaAs can results absorption and emission of photons with wavelength of 0.087 μm or (corresponding to Eg = 1.42 eV)

- **Impurity level to band transition**

An absorbed photon results in a charge carriers transition between a donor (or) acceptor level to a band in semiconductor, mostly observed in doped semiconductors.

For example, if a p-type material is considered, the low energy photon absorbed by p-type semiconductor material leads transition of electron from valence band to acceptor level where it is trapped by acceptor atom. Thus, hole is created in Valence band and acceptor atom is ionized.

Similarly, a hole may be trapped by an ionized acceptor atom. This results may be in the electron decay from its acceptor level to recombine with hole. The energy may be released radiatively (photons) or non-radiatively (phonons)

E.g.: In Hg doped Ge the wavelength of absorption and emission between valence and conduction band is 14 μm.
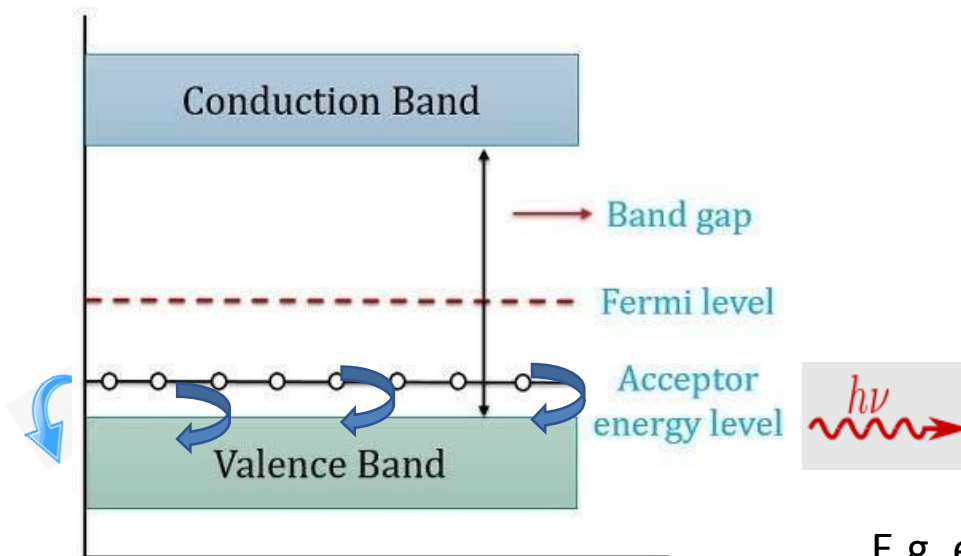

E.g. emission

E.g. Absorption
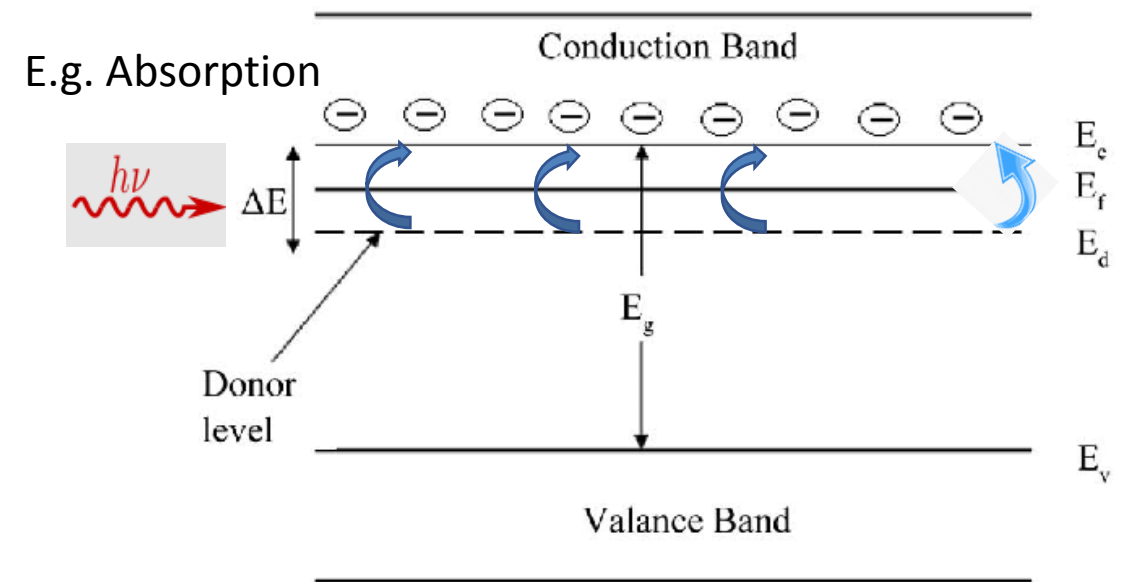
- **Free carrier transition (Intra band transition):**

An absorbed photon can impart its energy to an electron in a given band, causing it to move higher level in that band. If a lower-level conduction band is considered, by absorbing photon energy the electron moves to next higher energy level in the same conduction band.

Similarly due to thermalization, electron relaxes down to the bottom of the conduction band while releasing its energy in the form of phonons.
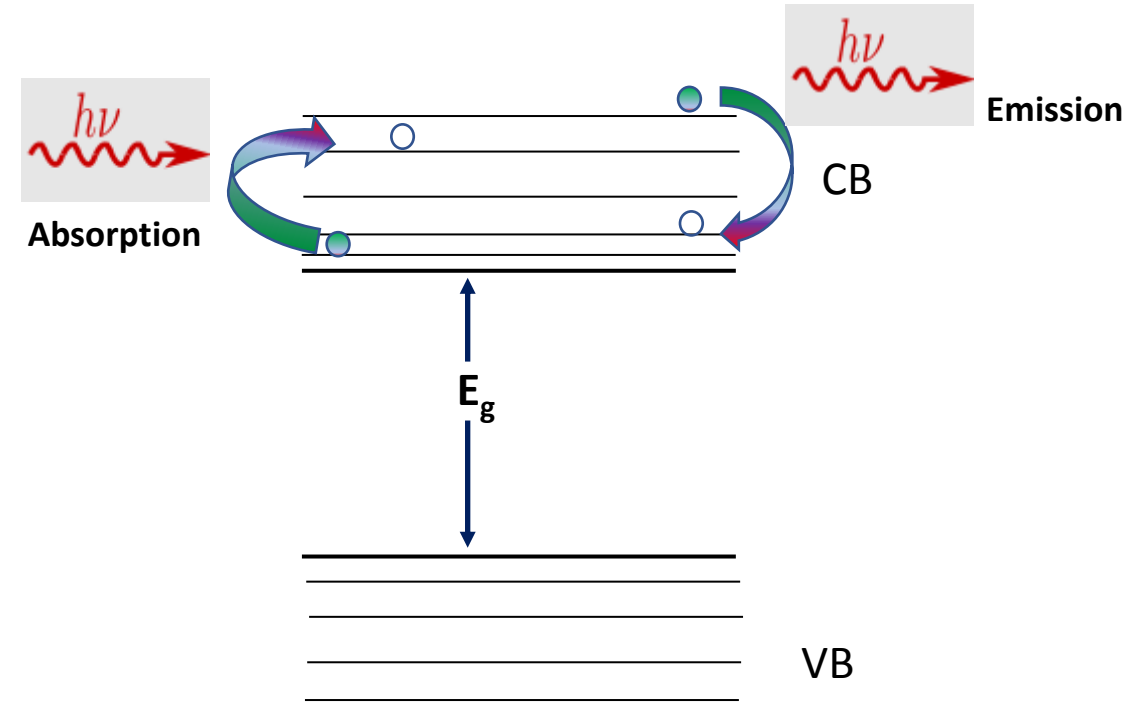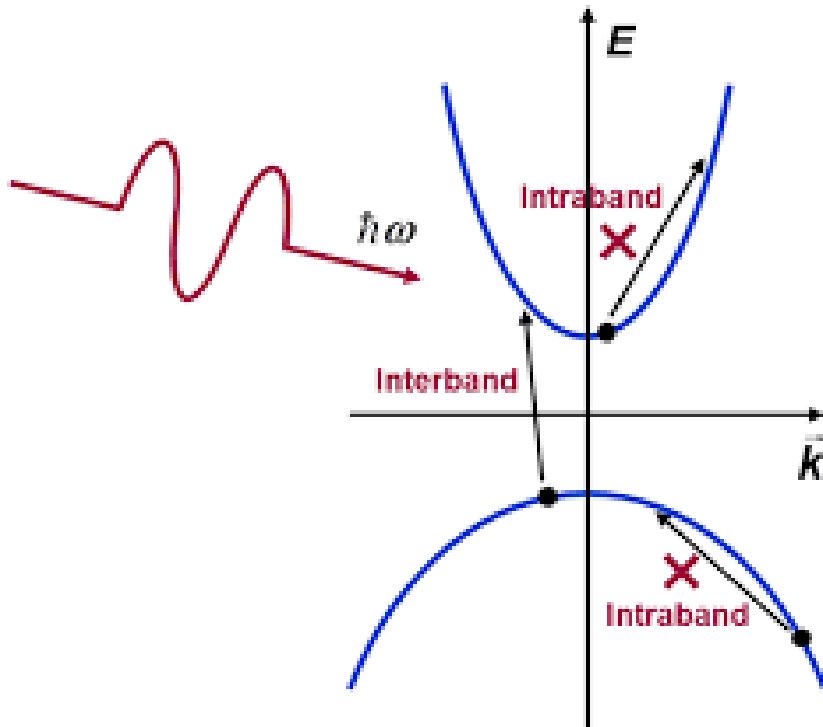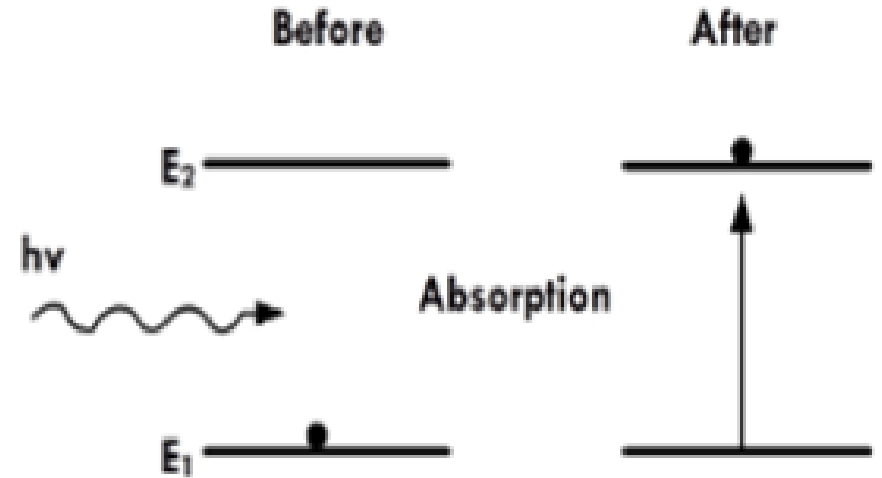
21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Unit 3 : Session 1 : SLO 2

Optical absorption process

Optical absorption process :

Absorption is the process in which the photons are absorbed by the semiconductor materials causes transition of electron from valence band to conduction band.

Consider direct band to band absorption
The condition for absorption to happen, the incident photon energy must be equal or grater than the bandgap i.e., $h\nu \geq E_g$, corresponding wavelength $\lambda = hc/E_g$.

The electron-hole pairs are generated due to absorption of photon having energy grater or equal to bandgap.

This leads to the increase of concentration of mobile charge carriers and increase the conductivity of the material. So, the material behaves as a photoconductor with a conductivity proportional to photon flux, the effect is used to detect light.

Emission process: Generally, the emission process takes place in two types in optical devices

1.Spontaneous emission
2.Stimulated emission

Spontaneous emission:

spontaneous emission, this process requires a conduction band energy state occupied by an electron and an empty valence band energy state. The electron itself transit from conduction band to valence band spontaneously by releasing a photon.

This photon has a random direction and phase.

E_2 ——————— •

E_1 ———————

Spontaneous emission

(a)
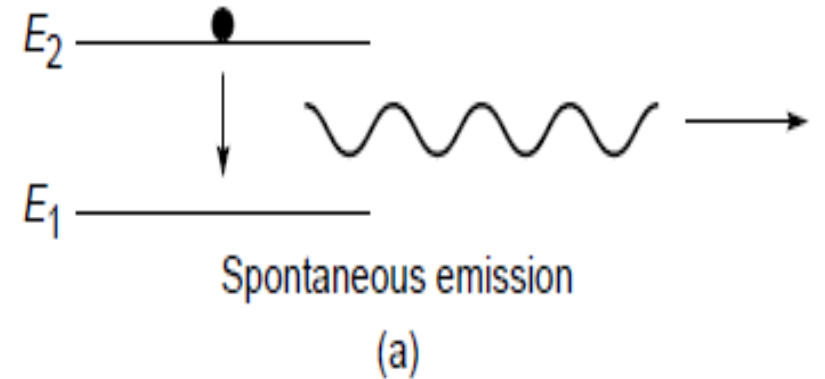
This is the opposite of the common situation in equilibrium, but at a finite temperature there will be a small number of full states in the conduction band and empty states in the valence band. Also, electrons and holes can be created via optical absorption and other pumping mechanisms.
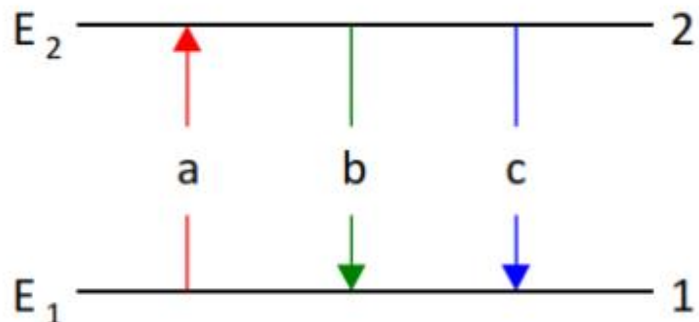
Stimulated emission:

An incident photon causes an upper-level atom to decay, emitting a "stimulated" photon whose properties are identical to those of the incident photon.

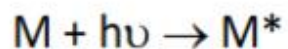The term "stimulated" underlines the fact that this kind of radiation only occurs if an incident photon is present.
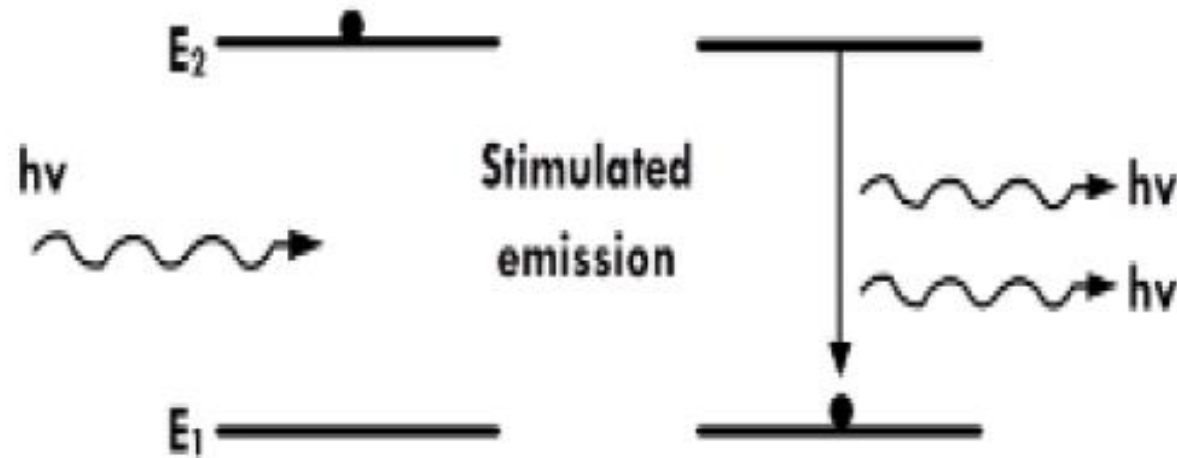
a absorption

b spontaneous emission

c stimulated emission

Absorption

Molecule absorbs a quantum of radiation (a photon) and is excited from 1 to 2.

$$M + h\upsilon \rightarrow M*$$

(state 1)   (state 2)

Spontaneous emission

M* (in state 2) spontaneously emits a photon of radiation.

$$M* \rightarrow M + h\upsilon$$
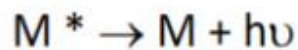
Stimulated emission

A quantum of radiation is required to stimulate M* to go from 2 to 1.

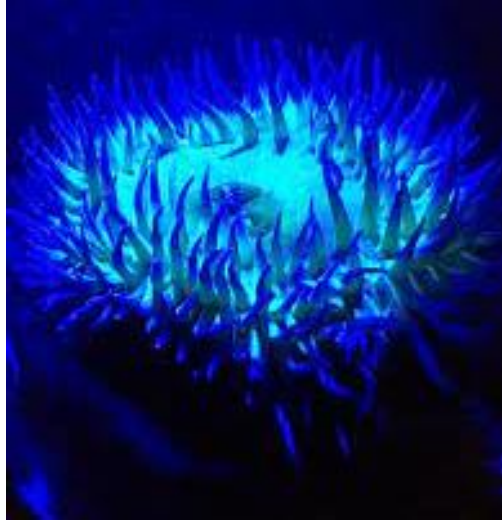$$M* + h\upsilon \rightarrow M + 2h\upsilon$$
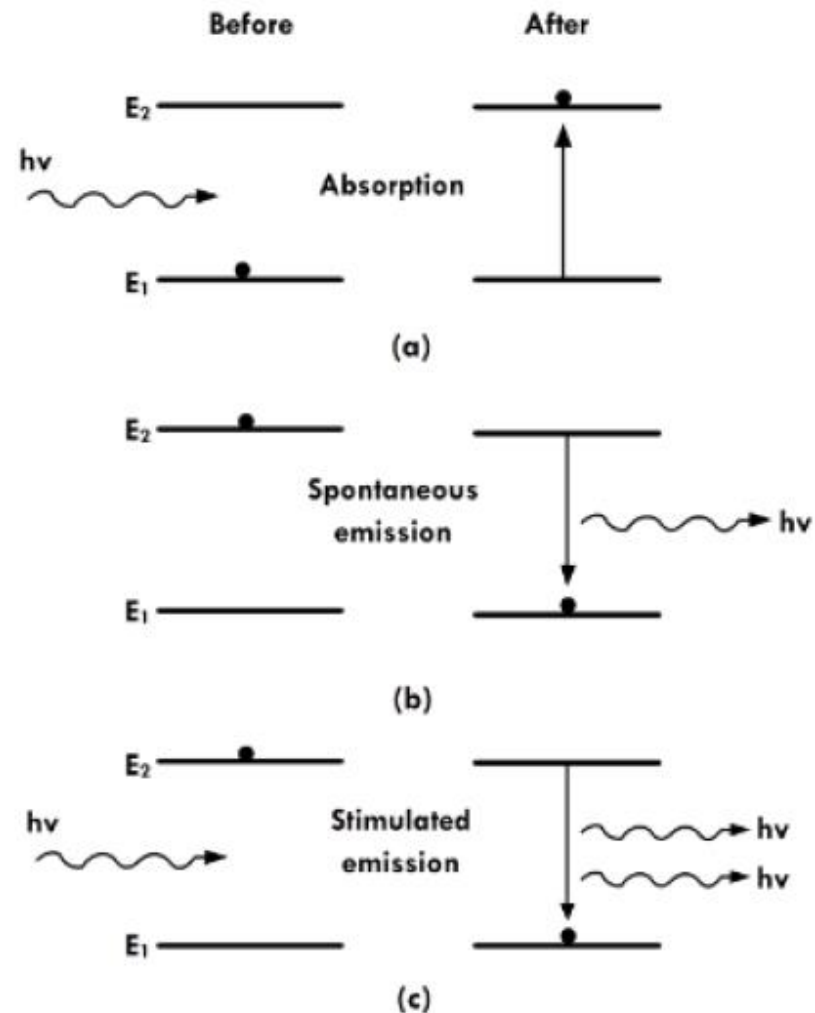
21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Unit 3 : Session 2 : SLO 1

Concept of recombination process

- When a semiconductor is illuminated with light an electron in the valence band making an upward transition to conduction band.

- This results electron-hole pair generated, the reverse process of electron-hole annihilation is called recombination.

- Recombination process may be radiative or non- radiative

1. If electron annihilated with hole energy is released equal to E ≥ E_g called radiative recombination, in this process a photon of energy E= $h\nu$ is released

2. If electron annihilated with hole energy is released equal to E < E_g called non radiative recombination, in this process phonons are released

Recombination of electron – hole pairs observed in different optical processes

Luminescence: Process where electron hole pairs created and recombined radiatively

Photoluminescence: electron- hole pairs are generated due to absorption of light and recombination occurs radiatively

Cathodoluminescence: electron – hole pairs are generated by the electron bombardment, and radiative recombination occurs
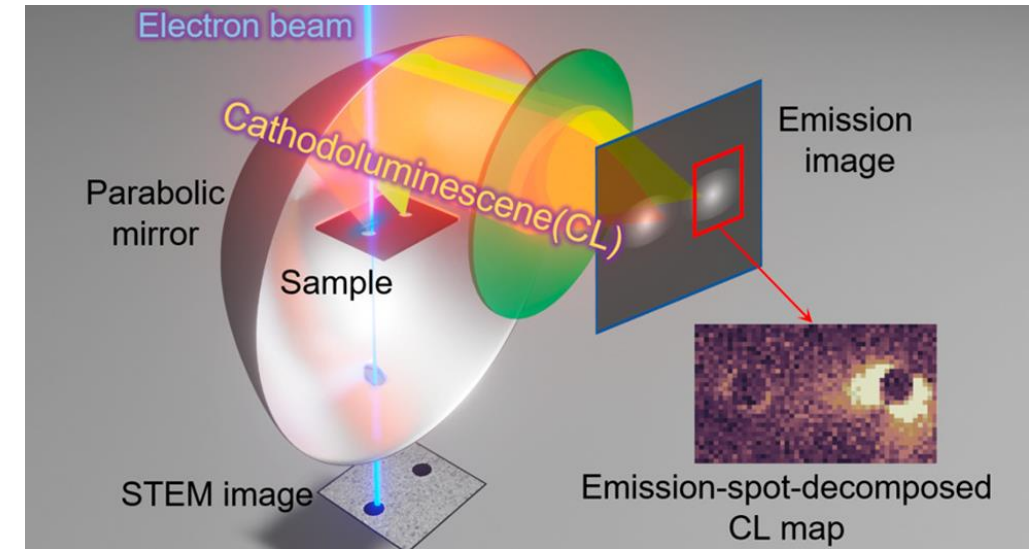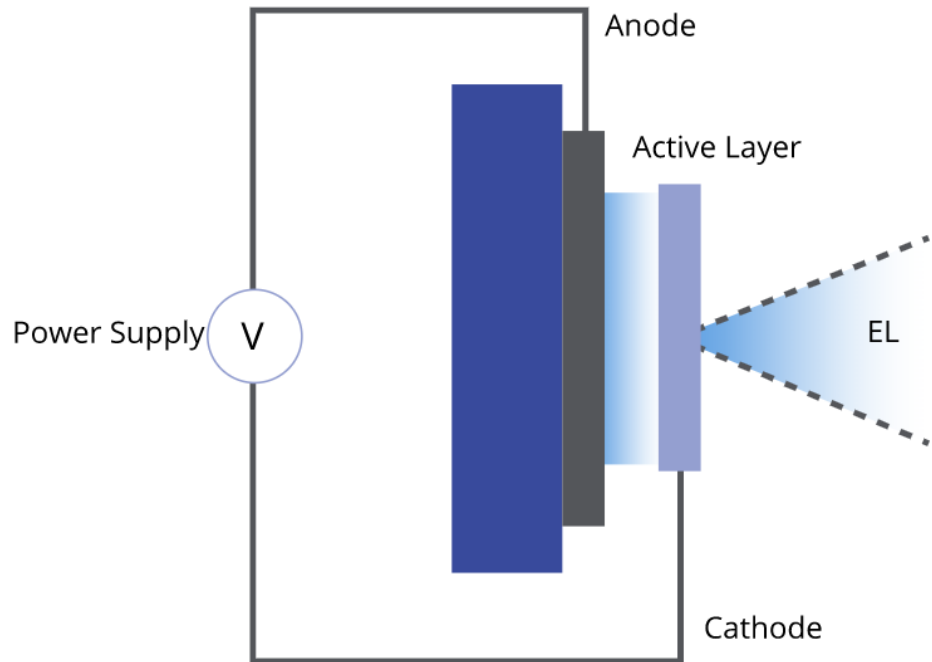
Electroluminescence: process of radiative recombination following injection of electrons and holes, with p-n junction or similar device.

21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

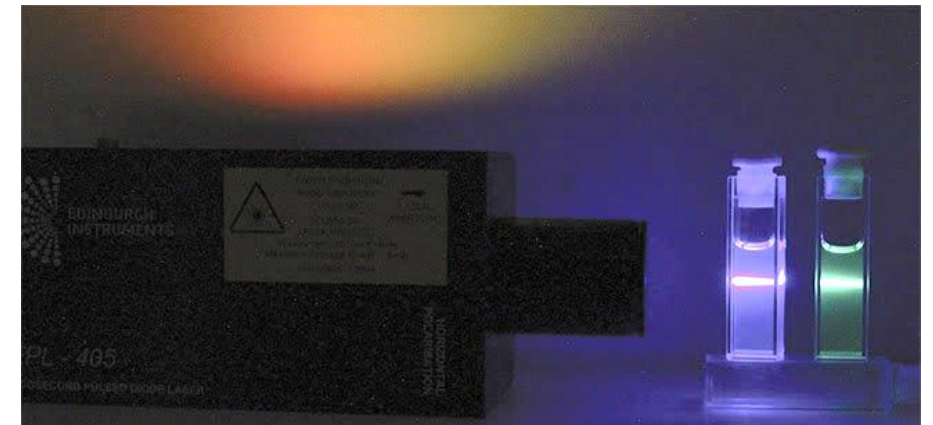## Unit 3 : Session 2 : SLO 2

Optical recombination process

When a semiconductor is under equilibrium without any incident photon (or) injection of electron the carrier density can be calculated from an equilibrium Fermi level using Fermi Dirac statistics

$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

But when light is illuminated non equilibrium carrier concentration is created and above relation is not valid, hence Fermi Dirac distribution for electrons and holes in non equilibrium condition are

The Fermi function for electrons:

Fermi level split into two, if the intrinsic carrier concentration is lower than the generated/injected carriers.

$$f(E)_n \approx \exp\left(\frac{E_{Fn} - E_C}{kT}\right)$$

E_{Fn} – electron quasi fermi level
E_{Fp} – hole quasi fermi level

The Fermi function for holes:

$$f(E)_p \approx \exp\left(\frac{E_V - E_{Fp}}{kT}\right)$$

Further, carrier concentration is calculated as

$$n = N_C \exp\left[\frac{E_{Fn} - E_C}{kT}\right] \qquad \text{and} \qquad p = N_V \exp\left[\frac{E_V - E_{Fp}}{kT}\right]$$

The excess carriers generated in semiconductor at non equilibrium condition must eventually recombine :

Generation rate (G) = recombination rate (R)

- The generation-recombination process involves transition of charge carriers across the energy bandgap and is different for direct & indirect bandgap semiconductor materials.

- The probability of radiative recombination is very high in direct bandgap semiconductors due to momentum & energy conservation.

- Recombination rate of charge carriers is depending upon the lifetime of charge carriers.

- In general, both radiative and non-radiative recombinations are considered, the total lifetime is given as

$$\frac{1}{\tau} = \frac{1}{\tau_r} + \frac{1}{\tau_{nr}}$$

$$R = \frac{\Delta n}{\tau}$$

Here, τ represents resultant lifetime of the electron-hole pairs,
R – recombination rate, Δn – change in the number of carriers.
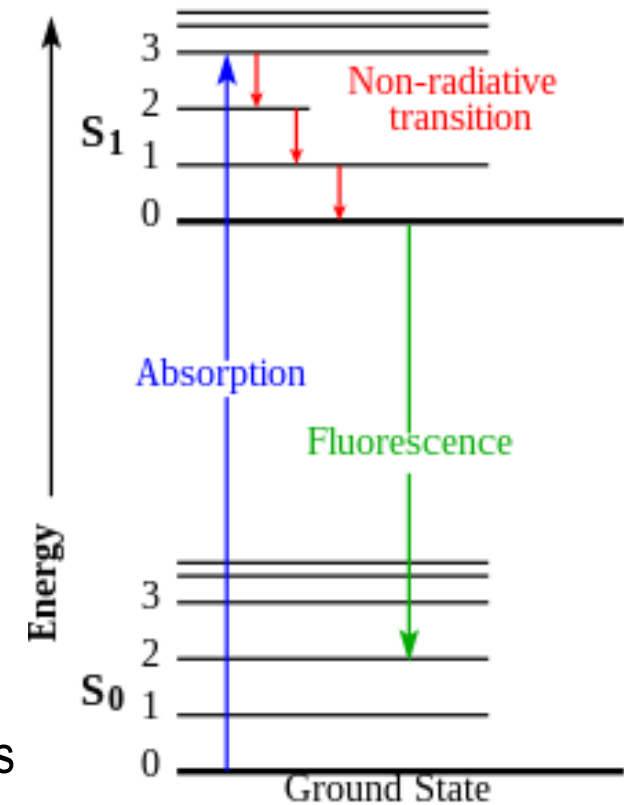
Simple Jablonski's diagram, The naming of the electronic states is based on the spin angular momentum configuration of each state.

R can be written as,

$$R = R_r + R_{nr}$$

Here, R_r – radiative recombination rate, R_{nr} – non-radiative recombination rate

We can write the internal quantum efficiency of the molecule as,

$$\eta_r = \cfrac{1}{1 + \left[\cfrac{\tau_r}{\tau_{nr}} \right]}$$

η_r should be higher for high radiative recombination in semiconductors, for example in LEDs.

From the equation, it is derived that the lifetime of non-radiative electron-hole pairs should be as high as possible to get maximum η_r.

# 21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Unit 3 : Session 3 : SLO 1

Explanation for spontaneous emission

To understand Spontaneous Emission and Stimulated Emission,
Let us consider a system containing two energy levels namely the ground state and the excited state.

For an atom (particle) to move from the ground state to the excited state it should absorb energy at least equal to the difference between the two energy levels.

Let E_1 is the energy of atoms in the ground state and E_2 the energy of atoms in the excited state then the energy required for excitation should be greater than or equal to $E_2 - E_1$
When atom deexcite energy equivalent to E_2-E_1 is released.
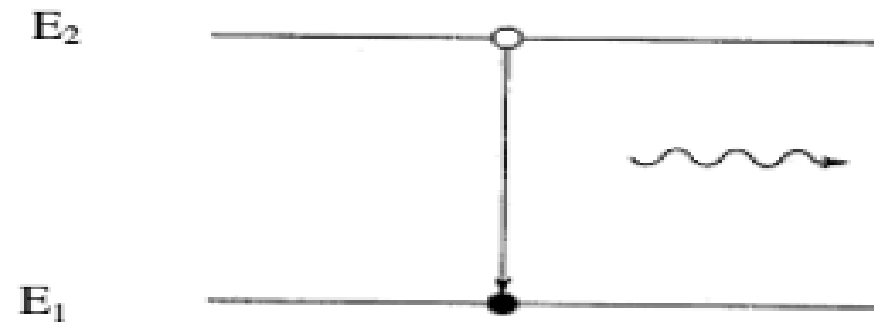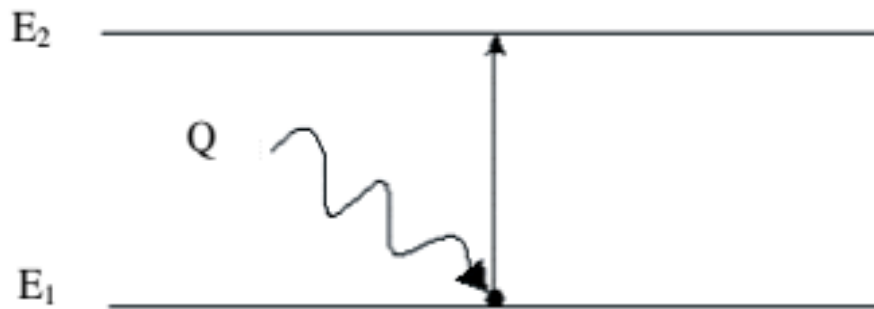
Spontaneous Emission

Any process which occurs without involvement of external factor is called a spontaneous process

Consider a particle in excited state and after spending its life time it decays automatically to ground state releasing energy. It will be called a spontaneous emission process

E_2

E_1
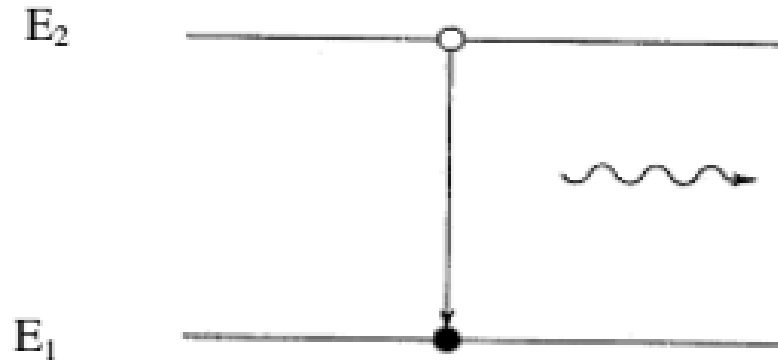
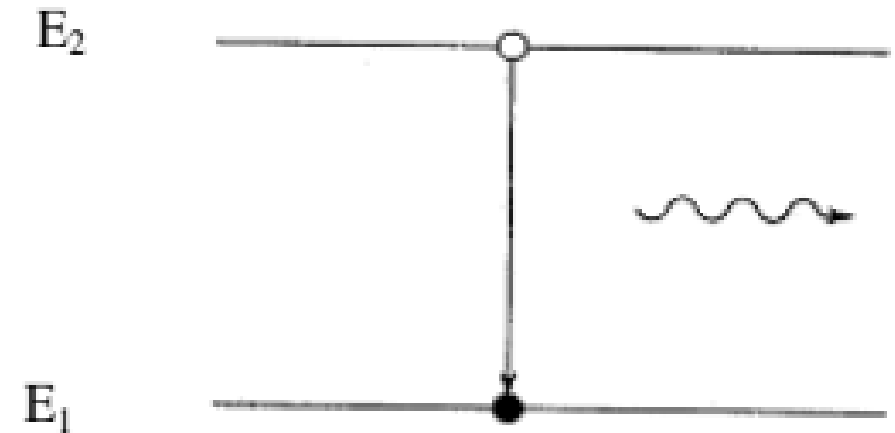Now the system in excited state. It can go to ground state by

i) spontaneous emission or ii) stimulated emission

Let system goes to ground state by spontaneous emission after spending it life time. Then Number of atoms deexcite to ground state is

$N_{sp} = A_{21}N_2$

N_2-Number atoms in the Excited state
A_{21}- Proportionality constant, Einstein coefficient

E_2

E_1

21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

## Unit 3 : Session 3 : SLO 2

Explanation for stimulated emission

Stimulated Emission

Any process which occurs with involvement of external factor is called a stimulated process.
Consider a particle in excited state and it stimulated to decay before its lifetime by external factor (electromagnetic radiation, etc.) to ground state releasing energy. It will be called a stimulated emission process.
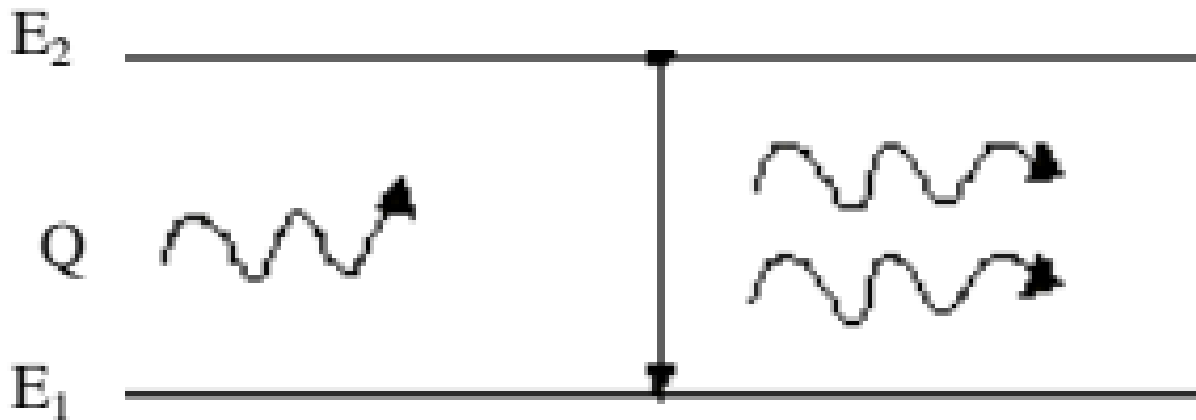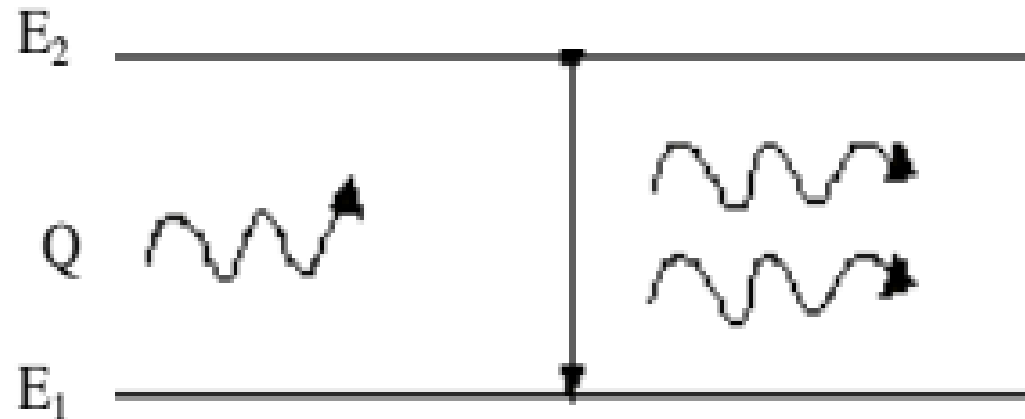
Let system goes to ground state by stimulated emission by external energy and forcing it to deexcite. Then Number of atoms deexcite to ground state by stimulated emission is

$N_{st} = B_{21}N_2Q$

N_2-Number atoms in the Excited state
B_{21}- Proportionality constant, Einstein coefficient
Q – Energy density

Absorption: When energy is gained by a system, and it goes to higher energy level from lower energy level it is called absorption. Since External energy is involved, it is stimulated process.

When a transition takes place from initial state to final state, The number of transitions depend on the number of particles in the initial state.

The number of atoms, per unit volume excited due to absorption will be proportional to N, the number of atoms per unit volume in the ground state and Q, the energy density of the incident radiation.

Hence, the number of atoms undergoing excitation per unit volume per unit time can be expressed as

$N_{ab} = QB_{12}N_1$

N_1-Number atoms in the ground state
B_{12}- Proportionality constant called
Einstein coefficient
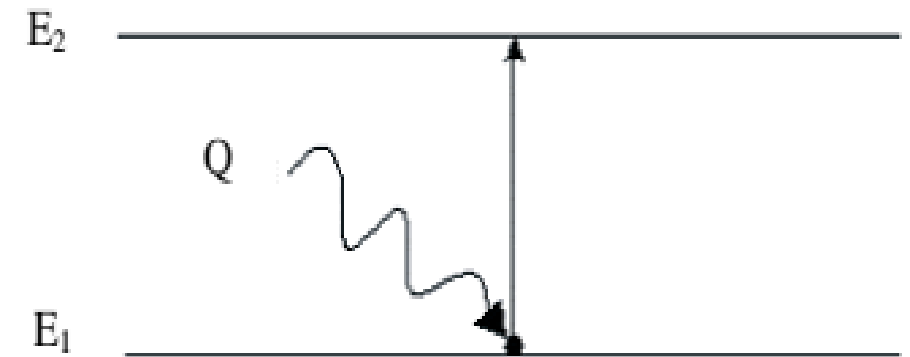
Einstein Relation for stimulated emission

Under steady state the total number of absorption is equal to total number of emission. Therefore

$N_{ab} = N_{sp} + N_{st}$

$N_1 B_{12} Q = N_2 A_{21} + N_2 B_{21} Q$

Rearranging we get,

$$Q = \frac{A_{21}}{\left(\dfrac{N_1}{N_2}\right) B_{12} - B_{21}}$$

Maxwell Boltzmann Distribution

Boltzmann distribution law specifies what fraction of atoms are found in any particular energy state for any given equilibrium temperature.
If N_0 is Number of particles in ground level and N_i is number of particles in the ith level, then

$$\frac{N_i}{N_o} = \exp\left(\frac{-E_i}{kT}\right)$$

$$N_i = N_o \exp(-E_i/kT)$$
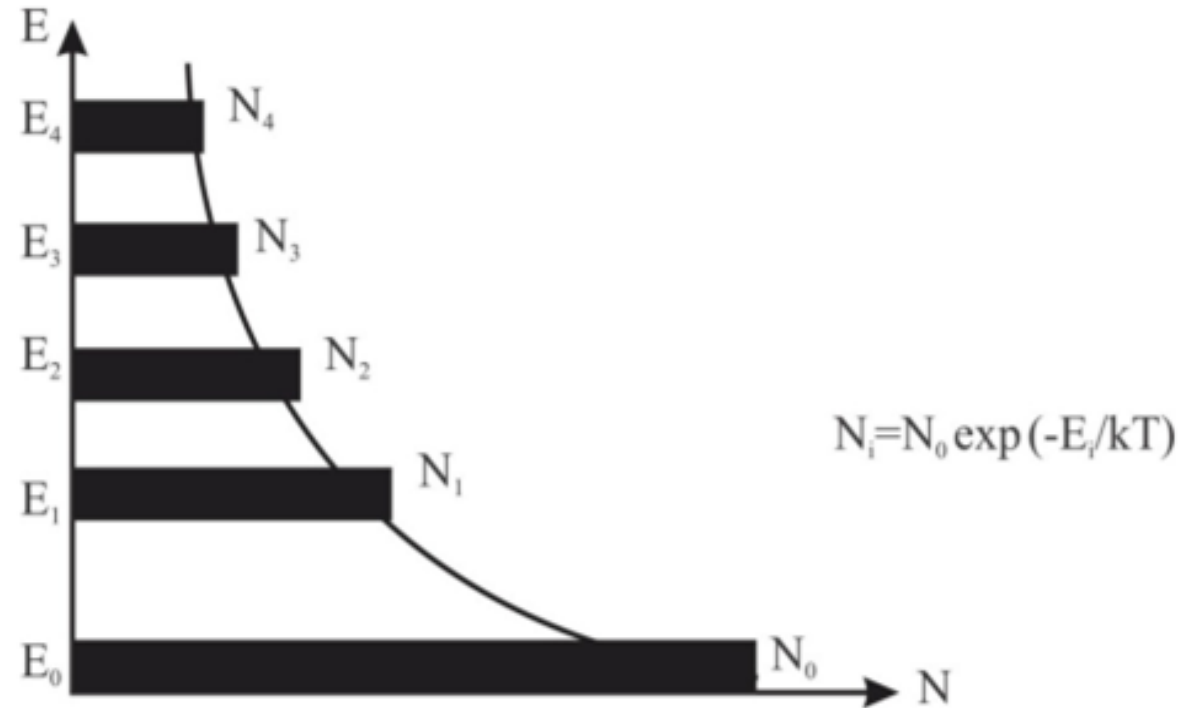
Therefore, we can write

$$\frac{N_1}{N_2} = e^{(E_2 - E_1)/kT}$$

Or

$$\frac{N_1}{N_2} = e^{h\nu/kT}$$

Using Boltzmann distribution

$$Q = \frac{A_{21}}{\left(\dfrac{N_1}{N_2}\right)B_{12} - B_{21}}$$

which can be written as

$$Q = \frac{A_{21}}{B_{12}e^{h\nu/kT} - B_{21}}$$

Since $B_{12} = B_{21}$, we can write

$$Q = \frac{A_{21}}{B_{21}(e^{h\nu/kT} - 1)}$$

From Planck's relation for the blackbody the energy density is

$$Q = \frac{8\pi hc}{\lambda^5} \frac{1}{(e^{hv/kT} - 1)}$$

But,

$$Q = \frac{A_{21}}{B_{21}(e^{hv/kT} - 1)}$$

Equating both, we get

$$\boxed{\frac{A_{21}}{B_{21}} = \frac{8\pi hc}{\lambda^5}}$$

This is ratio of Einstein co-coefficient for spontaneous emission and stimulated emission. This shows that stimulated emission is finite. This is also known as Einstein relation for stimulated emission.

21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Unit 3 : Session 4 : SLO 1

Solving Problems

1.   A semiconductor diode laser has a peak emission wavelength of 1.55 µm. Find its band gap in eV.

Sol: Energy gap of semiconductor, Eg = energy of emitted photon, hv

images where c = velocity of light = 3 × 108 m/s

Wavelength, λ = 1.55 µm = 1.55 × 16⁻⁶ m

Energy gap, Eg = ?

$$E_g = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.55 \times 10^{-6}} J$$

$$= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.55 \times 10^{-6} \times 1.6 \times 10^{-19}} eV = 0.8 \, eV$$

A He-Ne laser emits light at a wavelength of 632.8nm and has an output power of 3.2 mw. How many photons are emitted in each minute by this laser when operating?

$$\lambda = 6328 \text{ x } 10^{-10}\text{m} \qquad P = 3.2 \text{ mw} = 3.2 \text{ x } 10^{-3} \text{ w}$$

$$v = c/\lambda = 4.74 \text{ x } 10^{14} \text{ Hz}$$

$$E = hv = 3.14 \text{ x } 10^{-19} \text{ J}$$
$$P = nE$$
$$n = P/E = 1.019 \text{ X } 10^{16}$$

Photons /minute $= n$ x 60

$$= 6.11 \text{ x } 10^{17} \text{ photons / minute.}$$

21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Unit 3 : Session 4 : SLO 2

Solving Problems

Find the relative population of the two states in Nd:YAG laser that produces a light beam of wavelength 1.06µm at 300K.

Given Data: $\lambda = 1.06 \times 10^{-6}$ m and T = 300 K

$$\frac{N_2}{N_1} = e^{-(E_2 - E_1)/kT} = e^{-h\nu/kT}$$

$$= e^{-hC/\lambda KT}$$

$$= 2.13 \times 10^{-20}$$

What fraction of sodium atom is in the first excited state in a sodium vapour lamp at a temperature of 250°C.

$$T = 250 + 273 = 523 \ K$$

$$K = 1.38 \ x \ 10\text{-}23 \ J/K$$

$$\lambda = 5900 \ x \ 10^{-10}m$$

$$N_2/N_1 = e^{-(E_2 - E_1)/kT} = e^{-h\nu/kT}$$

$$\nu = C/\lambda$$

$$= e^{-hC/\lambda KT}$$

$$= 5.414 \ x \ 10^{-21}$$