DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

18PYB103J –Semiconduuctor Physics

Optical Transitions Using Fermi's Golden Rule

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Introduction

Fermi's golden rule is a simple expression for the transition probabilities between states of a quantum system, which are subjected to a perturbation. It is used for a large variety of physical systems covering, e.g., nuclear reactions, optical transitions, or scattering of electrons in solids.

Consider a semiconductor illuminated by electromagnetic radiations (light). The interaction between photons and the electrons in the semiconductor can be described by the Hamiltonian operator.

$$\vec{H} = \frac{1}{2m_0}(\vec{p} - e\vec{A})^2 + \overrightarrow{V}(r)$$

Where ,

m_0 *is the free electron mass,* $\vec{A}$ *is the vector potential accounting part of electromagnetic field.*

$\overrightarrow{V}(r)$ *is the periodic potential and* $e = -|e|$

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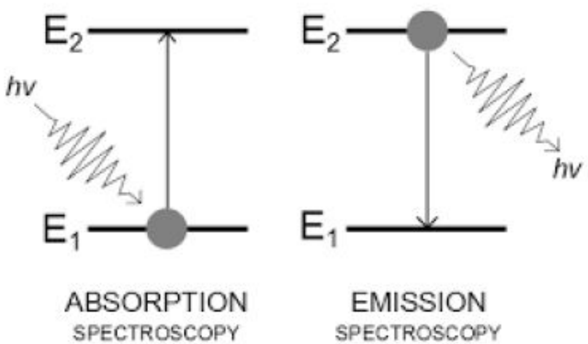

Using the time dependent perturbation theory, the transition rate for the absorption of a photon can be derived, assuming an electron is initially at state E_1 is given by Fermi’s Golden rule

$$W_{abs} = \frac{2\pi}{\hbar}\left|< b\left|H'(r)\right|a >\right|^2 \delta\left(E_b - E_a - \hbar\omega\right)$$

Where $E_b > E_a$ is assumed.

The total upward transition rate per unit volume

Where $E_b > E_a$ has been assumed. The total upward transition rate per unit volume(S^{-1}, cm^{-3}) in the crystal taking into account the probability that state a is occupied and state b is empty is

$$R_{a-b} = \frac{2}{V}\sum_{K_a}\sum_{K_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^2 \delta\left(E_b - E_a - \hbar\omega\right) f_a\left(1 - f_b\right)$$

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Where we sum over the initial and final states and assume that the Fermi-Dirac distribution f_a is the probability that the state a is occupied. A similar expression holds for f_b with E_a replaced by E_b, and $(1 - f_b)$ is probability that the state b is empty. The prefactor 2 takes into account the sum over spins, and the matrix element H'_{ba} is given by

$$H'_{ba} = |< b|H'(r)|a >|^2 = \int \psi^*(r)H'(r)\psi_a(r)d^3r$$

Similarly, The transition rate for the emission of a photon (fig.2) if an electron is initially at state b is.

$$W_{ems} = \frac{2\pi}{\hbar}|< a|H'^{+}(r)|b >|^2\,\delta(E_a - E_b + \hbar\omega)$$

The downward transition rate per unit volume (S^{-1} cm^{-3}) is

$$R_{b-a} = \frac{2}{V}\sum_{K_a}\sum_{K_b}\frac{2\pi}{\hbar}|H'^{+}{}_{ab}|^2\,\delta(E_a - E_b + \hbar\omega)f_b(1 - f_a)$$

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Using the even property of the delta function, $\delta\left(-x\right) = \delta\,(x) and\ \left|H'_{ba}\right| = \left|H'^{+}_{ab}\right|$.

The net upward transition rate per unit volume can be written as,

$$R\ = R_{a\to b} - R_{b\to a}$$

$$R = \frac{2}{V}\sum_{K_a}\sum_{K_b}\frac{2\pi}{\hbar}\left|H'_{ba}\right|^{2}\delta\,(E_b - E_a - \hbar\omega)(f_a - f_b)$$

An Optical absorption coefficient

The absorption coefficient $\alpha_0\,(\frac{1}{Cm})$ in the crystal is the fraction of photons absorbed per unit distance

$$\alpha_0\ = \frac{Number\ or\ Photons\ absorbed\ per\ second\ per\ unit\ volume}{Number\ of\ injected\ photons\ per\ second\ per\ unit\ area}$$

The injected number of photons per second per unit area of the optical intensity ρ (W/Cm^2) divided by the energy of a photon ($\hbar\omega$). Therefore,

$$\alpha\,(\hbar\omega) = \frac{R}{\frac{p}{\hbar\omega}} = \frac{\hbar\omega R}{\left(\frac{n_r C \varepsilon_0 \omega^2 A_0{}^2}{2}\right)}$$

Where, R is the net upward transition rate per unit volume

ω - $\frac{2\pi}{\lambda}$, wave number / angular velocity

C- Velocity of light

n_r – Refractive index of the medium.

A – Vector potential for electromagnetic field.

ε_0- Permittivity of the free space.

Thank you