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The Quantum Expression of the Role of Relaxation Time on Optical Absorption in Semi Conductors

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Abstract

In this work theoretical method based on classical mechanics, Maxwell equations and quantum mechanics is utilized to find the mathematical expression for relaxation time, this expression play an important role in the simulation of quantum semiconductor devices .One has studied the relaxation time in the semi classical approximation, the optical potential, perturbation method and generalized Schrödinger Equation for relaxation time. Theoretical relation between the relaxation time and absorption coefficient is obtained. At last one has studied the quantum mechanical absorption coefficient, absorption coefficient for Maxwell's equations and quantum mechanics, and parameters affecting absorption coefficient.

Keywords: Semiconductors (sc), optical absorption , electromagnetic waves (e.m.w) relaxation time, perturbation method.

Introduction

Semi conductors (sc) play an important role in our day life. They are widely used in electronic devices like computers, mobiles, televisions, solar cells and sensors. The physics of semi conductors are presented in many standard texts [1,2]. The optical properties of (sc) are an important factor in understanding the performance of optical sensors and solar cells. These properties are based on the interaction of electromagnetic waves (e.m.w) with matter. The optical properties of semiconductors provide an important tool for studying energy band structure, impurity levels, excitations, localized defects, lattice vibrations, and certain magnetic excitations.

The efficiency of a solar cell is dependent on the optical absorption of the semiconductor used to fabricate the solar cell. In bulk crystalline materials and even in thin films, the bulk absorption coefficient is the most important parameter that determines the optical absorption. Classical models such as Drude model or Drude-Lorentz model describe the optical absorption based on the complex dielectric function [5,9]. This approach works very well for the absorption of photons by the electrons inside a band, for example, conduction band. However, from band to band excitation of electrons, a detailed understanding of the band structure of the material is essential. To calculate optical absorption in

semiconductors, one has to invoke quantum mechanical models using Schrodinger's wave equation [2, 6].

When a radiation beam or particle beam enters a medium its intensity decreases due to the decrease in its energy per particle and due to decrease of the number of particles. This indicates the existence of a resistive force which causes these changes. The time taken by a particle on the beam to stop is called relaxation time $(τ)$. The relaxation time is defined as a time between two successive collisions. This relaxation time can be obtained by different quantum methods.

The relaxation time is an important parameter of obtaining the electrical optical properties of semiconductors. There some techniques, such as optical potential, for the determination of the relaxation time, but it is important to simply determine the relaxation time by a different methods. These methods are presented by expectation value, perturbation method, optical potential, and Schrödinger Equation. These methods generate a new mathematical formula for relaxation time.

Generalized schrödinger equation for relaxation time

Recently same attempts are made to modify and generalize Schrödinger equation to start from the wave function inside matter instead of free space. This model is utilized to construct a new energy band theory. The inclusion of the effect of matter in this theory gives a motivation to try to see the form of energy and effective mass inside matter. According to this model the upper conduction energy band edge is given by: [69]

$$
E = \frac{\hbar^2}{2mn^4} |C_1|\sigma^2
$$
 (2.1)

Where
$$
|C_1| = 1 - \frac{\chi}{2\varepsilon}
$$
 $\qquad \sigma = \frac{\text{ne}^2 \tau}{\text{m}}$ (2.2)

Thus

$$
E = \frac{\hbar}{2mn_{\perp}^4} \left| C_1 \right|^2 \frac{e^4 \tau^2}{m^2} n^2
$$
 (2.3)

Utilizing equation (3.17) and (3) one gets

$$
E = \frac{\hbar}{2mn^4} |C_1|^2 \frac{e^4 \tau^2}{m^2} (4\pi N_D)^2 \left(\frac{\beta}{4\pi m}\right)^3 \hbar^4 K^4
$$
 (2.4)

Hence

$$
\nabla_{K} E = \text{sc} \frac{2\hbar}{mn^{4}{}_{1}} |C_{1}|^{2} \frac{e^{4} \tau^{2}}{m^{2}} (4\pi N_{D})^{2} \left(\frac{\beta}{4\pi m}\right)^{3} \hbar^{4} K^{3}
$$

$$
\nabla^{2}{}_{K} E = \frac{4\hbar}{mn^{4}{}_{1}} |C_{1}|^{2} \frac{e^{4} \tau^{2}}{m^{2}} (4\pi N_{D})^{2} \left(\frac{\beta}{4\pi m}\right)^{3} \hbar^{4} K^{2}
$$
(2.5)

Thus the relaxation time can be given by (2.5) to be

$$
\nabla^{2}{}_{K}E = \sqrt{-\frac{4\hbar}{mn^{4}_{1}}|C_{1}|^{2}}\frac{e^{4}\tau^{2}}{m^{2}}(4\pi N_{D})^{2}(\frac{\beta}{4\pi n})^{3}\hbar^{4}K^{2}
$$

\n
$$
\tau = [(\nabla_{K}^{2}E)/(\frac{4\hbar}{mn_{1}^{4}})|C_{1}|^{2}(\frac{e^{4}}{m^{2}})(4\pi N_{D})^{2}(\frac{\beta}{4\pi n})^{3}\hbar^{4}k^{2}]^{\frac{1}{2}}
$$
(2.6)
\nOr the relaxation time can given by equation below :-
\n
$$
\tau = \sqrt{[(\nabla_{K}^{2}E)/(\frac{4\hbar}{mn_{1}^{4}})|C_{1}|^{2}(\frac{e^{4}}{m^{2}})(4\pi N_{D})^{2}(\frac{\beta}{4\pi n})^{3}\hbar^{4}k^{2}]}
$$
(2.7)

Quantum relaxation time and absorption coefficient

When a radiation beam or particle beam enters a medium its intensity decreases due to the decrease in its energy per particle and due to decrease of the number of particles. This indicates the existence of a resistive force which causes these changes. The time taken by a particle on the beam to stop is called relaxation time (τ) . τ is defined as a time between two successive collisions. This relaxation time can be obtained by different quantum methods. For instance one can use perturbation method to find the change in particle energy due to a resistive potential. For simplicity assume the perturbing part of Hamiltonian \hat{H}_1 to be a constant i.e.:

$$
\hat{H}_1 = -V_0 \tag{3.1}
$$

In this case the perturbation, i.e. change in energy is given by:

$$
E_1 = (\hat{H}_1)_{kk} = \int \overline{U}_k (-V_0) U_k dr = -V_0 \int \overline{U}_k U_k dr = -V_0 \quad (3.2)
$$

Where the total energy E is given by:

$$
E = E_k + E_1 \tag{3.3}
$$

The energy change is given by:

$$
\Delta E = |E_1| = V_0 \tag{3.4}
$$

According to uncertainty principle the relaxation time is given by:

$$
\tau = \Delta t = \frac{\hbar}{\Delta E} = \frac{\hbar}{V_0} \tag{3.5}
$$

Here relaxation time means the time taken by the particle in the perturbed excited state. This equation indicates that the strong resistive force $V_0 \to \infty$, causes the relaxation time to be short $\tau \to 0$ which is in conformity with commonsense.

Relaxation time can also be obtained by utilizing the optical potential V_I which is introduced to account for particle energy losses in inelastic scattering where the wave function of the free particle takes the form:

$$
\psi = Ae^{\frac{-V_{t}}{\hbar}}e^{-i\frac{Et}{\hbar}}
$$
\n(3.6)

For constant optical potential:

$$
V_I = constant \tag{3.7}
$$

The current density \hat{j} and hence the bam intensity I are given by:

$$
I = nevX\hbar w \tag{3.8}
$$

Thus using (3.6) and (3.7) yields:

$$
I = hf |\psi|^2 \nu = A^2 \nu e^{-\frac{2V_l}{\hbar}thf} = I_0 e^{-\frac{2V_l}{\hbar}t}
$$
 (3.9)

The time τ taken by the beam to decrease can be defined to be:

$$
\frac{I}{I_0} = e^{-2\frac{V_I}{\hbar}\tau} = e^{-1}
$$
\n
$$
\frac{2V_I}{\hbar}\tau = 1
$$
\n
$$
\tau = \frac{\hbar}{2V_I}
$$
\n(3.10)

Again the expression for the relaxation time τ resembles that obtained perturbation method. The two expressions coincide if one sets:

 $2^{\degree 0}$ $V_I = \frac{1}{2}V_I$

In this case:

$$
\tau = \frac{\hbar}{V_0} \tag{3.11}
$$

The relaxation time can also be obtained quantum mechanically, if one treats atoms and electrons as harmonic oscillators subjected to resistive force μv beside the restoring force $-k_0 x$ in this case the total force is given by:

$$
ma = -mv^2x = -k_0x + \mu v \tag{3.12}
$$

But:

$$
x = x_0 e^{iwt} \dots \dots \dots \dots \nu = v_0 e^{iwt} = \frac{v_0}{x_0} x_0 e^{iwt} \dots \dots \nu = \frac{v_0}{x_0} x \tag{3.13}
$$

Thus:

$$
ma = -mw^2x = -k_0x + \mu \frac{v_0}{x_0} x = \left(\mu \frac{x_0}{v_0} - k_0\right)x
$$
 (3.14)

$$
-mw^{2}x = (\mu_{0} - k_{0})x
$$
........where.... $\mu_{0} = \frac{\mu x_{0}}{v_{0}}$

Hence:

$$
w^{2} = \left(\frac{k_{0} - \mu_{0}}{m}\right)
$$

$$
\therefore w = \pm \frac{\sqrt{k_{0} - \mu_{0}}}{\sqrt{m}}
$$
 (3.15)

Treating atoms as harmonic oscillators, the force is given by:

$$
F = -kx = -(k_0 - \mu_0)x
$$
\n(3.16)

And utilizing Schrödinger equation for harmonic oscillator the energy is given by:

$$
E_n = n + \frac{1}{2} \hbar \frac{\sqrt{k_0 - \mu_0}}{\sqrt{m}}
$$
 (3.18)

When the resistive force $F_r = \mu_0 x$ dominate i.e:

⁰ ⁰ ⁰ ⁰ *^F ^F*.............. *^x k ^x*............... *k ^r*

Thus the energy can be written as:

$$
E_n = \pm \left(n + \frac{1}{2} \right) \hbar \frac{\sqrt{\mu_0 - k_0}}{\sqrt{m}} i \dots \dots \dots \dots f \text{or} \dots n = 0 \tag{3.19}
$$

$$
w_0 = \frac{\sqrt{\mu_0 - k_0}}{\sqrt{m}} \dots \dots \dots \dots \dots E_n = \pm \frac{1}{2} \hbar w_0 i \tag{3.20}
$$

In this case the time dependent part of Schrödinger equation becomes:

$$
\psi = Ae^{-i\frac{E_n}{\hbar}t} = Ae^{-\frac{i}{\hbar}(\pm\hbar w_0 t)t} = Ae^{\pm w_0 t}
$$
 (3.21)

For decaying one chooses the minus sign to get: $w = Ae^{-w_0 t}$ (3.23)

$$
(3.2
$$

Thus the intensity of the beam becomes:

$$
I = n\nu \hbar w = |\psi|^2 \nu \hbar w
$$

\n
$$
I = A^2 v e^{-2w_0 t} \hbar w = I_0 e^{-2w_0 t}
$$
\n(3.24)

The relaxation time is given by:

$$
\frac{I}{I_0} = e^{-2w_0 \tau} = e^{-1} \dots \dots \dots Hence \dots 2w_0 \tau = 1
$$

$$
\therefore \tau = \frac{1}{2w_0}
$$
 (3.25)

$$
\tau = \frac{2\sqrt{m}}{\sqrt{\mu_0 - k_0}}\tag{3.26}
$$

For very strong resistive force:

$$
\tau = \frac{2\sqrt{m}}{\sqrt{\mu_0}}\tag{3.27}
$$

Thus:

$$
\tau \approx \frac{1}{\mu_0^{1/2}} \approx \frac{1}{F_r^{1/2}}
$$
\n(3.28)

Again strong resistive force causes relaxation time to be short. Relaxation time can also be found by using semi classical approximation. For electrons subjected to only coulomb electric force of the nucleus F_e the equation of motion of the electron becomes:

$$
\frac{mv_0^2}{r} = mw_0^2 r = F_e
$$
\n(3.29)

When a magnetic field of the flux density B and a resistive force $F_r = \mu v$ are taken into account the equation of motion of the electron becomes:

$$
\frac{mv^2}{r} = mw^2r = F_e + F_m - F_r = mw_0^2r - Bev - \mu v \tag{3.30}
$$

$$
m(w^2 - w_0^2)r = (-Be - \mu)wr
$$
\n(3.31)
\n
$$
m(w + w_0)(w - w_0) = (-Be - \mu)w
$$
\n(3.32)

For small change in $(w)[w \approx w_0]$

 $\Delta w = w_L = w_0 - w$

Since F_r decreases $w \langle w_0 \rangle$

$$
m(2w)\Delta w = (Be \quad \mu)w
$$

$$
\Delta w = w_L = \frac{\mu + Be}{m}
$$
 (3.33)

Using uncertainty relation and treating the electron and the atom as harmonic oscillators, the energy change, thus takes the form:

$$
\Delta E = \hbar \Delta w = \left(\frac{\mu + Be}{m}\right) \tag{3.34}
$$

And the relaxation time reads:

$$
\tau = \Delta t = \frac{\hbar}{\Delta E} = \frac{m}{\mu + Be}
$$
\n
$$
\therefore \tau \approx \frac{1}{\mu + Be}
$$
\n(3.35)\n(3.36)

Quantum mechanical absorption coefficient

The absorption coefficient can also be obtained by using the wave function of the photon which takes from [36]

$$
\psi = Ae^{i(kx-wt)} \tag{4.1}
$$

The density of photons is given by:

$$
n = |\psi|^2 = \overline{\psi}\psi \tag{4.2}
$$

Thus the radiation intensity is given by:

$$
I = hfnv = |\psi|^2 chf = \overline{\psi}\psi chf = \hbar w c |\psi|^2
$$
\n(4.3)

When photons enter matter k is replaced by k . As a result the wave function is given by:

$$
\psi = Ae^{i(\tilde{k}x - wt)} \tag{4.4}
$$

The wave vector inside matter can be found with the aid of (3.22) to be:

$$
\widetilde{k} = k \left(1 + \frac{1}{2} x \right) = k \left(1 + \frac{1}{2} x_1 + \frac{1}{2} x_2 i \right)
$$
\nUsing the sum function takes the form:

\n
$$
k = k \left(1 + \frac{1}{2} x_1 + \frac{1}{2} x_2 i \right)
$$
\n(4.5)

Hence the wave function takes the form:

$$
\psi = Ae^{i[k(1+x_1)x-wt]}e^{-\frac{-kx_2}{2}x}
$$
\n(4.6)

$$
\overline{\psi} = Ae^{-\frac{kx_2}{2}x}e^{-i[k(1+x_1)x-wt]}
$$
\n(4.7)

Therefore the intensity is given by:

$$
I = A^2 C e^{-kx_2 x} = I_0 e^{-kx_2 x}
$$
\n(4.8)

But since:

 $I = I_0 e^{-\alpha x}$

It follows that the absorption coefficient is given by:

$$
\alpha = kx_2 \tag{4.9}
$$

In view of relations (3.9) and (3.11) one gets:

$$
x_2 = -\frac{be^2 N}{a^2 + b^2} = \frac{e^2 N (Be - \mu r) w}{\left(\frac{F_0}{x_0} - w^2 m\right)^2 + w^2 (\mu_r - Be)^2}
$$
(4.10)

In view of (3.18) the above equation reads:

$$
x_2 = \frac{CC_2 e^2 k^4 (Be - \mu r)}{\left(\frac{F_0}{x_0} - C^2 k^2 m\right)^2 + C^2 k^2 (Be - \mu_r)^2}
$$
\n(4.11)

Where:

$$
C_2 = \frac{4\pi N_0}{3} \left(\frac{\beta}{2\pi n}\right)^{3/2} \hbar^2
$$
 (4.12)

Thus the absorption coefficient is given by:

$$
\alpha = \frac{CC_2 e^2 (Be - \mu r) k^5}{\left(F_0 / x_0 - C^2 k^2 m\right)^2 + C^2 k^2 (Be - \mu r)}
$$
\n(4.13)

In the case when B , F_0 and μ _r are small, equation (4.13) becomes:

$$
\alpha = \frac{C_2 e^2 (Be - \mu r)}{C^3 m^2} k \tag{4.14}
$$

But if B and μ_r are extremely large, the absorption coefficient can thus given by:

$$
\alpha = \frac{C_2 e^2 k^3}{(Be - \mu r)}
$$
\n(4.15)

Absorption coefficient from maxwell's equations and quantum mechanics

Maxwell's equations can be utilities to find the electric susceptibility. According to these equations the electric field satisfies:

$$
\nabla^2 E - \mu E \frac{\partial^2 E}{\partial t^2} - \sigma \mu \frac{\partial E}{\partial t} = 0
$$
\n(5.1)

Let the solution be in the form:

$$
E = E_0 e^{i(wt - kx)} \dots \dots \dots \dots \dots P = xE
$$
 (5.2)

Substituting (5.2) in (5.1) yields:

$$
-k^{2} + \mu \varepsilon w^{2} - \sigma \mu w i = 0
$$

$$
\varepsilon = \frac{k^{2} + \sigma \mu w i}{\mu w^{2}}
$$
(5.3)

But

 ψ

$$
\varepsilon = \varepsilon_0 (1 + x) \tag{5.4}
$$

As a result the electric susceptibility is given by:

$$
x = \frac{k^2 - 1}{\varepsilon_0 \mu_0 \mu_r w^2} + \frac{\sigma}{\varepsilon_0 w} i = \frac{1}{C^2 \mu_0 \varepsilon_0 \mu r} - 1 + \frac{\sigma i}{w \varepsilon_0} = x_1 + ix_2
$$
 (5.5)

The real and complex parts can take the form:

w w x C ^r ^w ^r x 0 0 2 2 0 1 2 1...........,........ 1 1 1 (5.6)

Where the relative magnetic permittivity satisfies the relation:

$$
\mu = \mu r \mu_0 \tag{5.7}
$$

According to equation (3.22) the wave number is given by:

$$
\widetilde{k} = k \left(1 + \frac{1}{2} x \right) = k + \frac{1}{2} x k = k + \frac{1}{2} \left(\frac{1}{\mu r} - 1 - \frac{\sigma}{\varepsilon_0 w} i \right) k = \left(\frac{1}{2} + \frac{1}{2\mu r} \right) k + \frac{\sigma}{\varepsilon_0 w} i \tag{5.8}
$$

The conductivity σ is also given by:

$$
\sigma = \frac{ne^2}{m}\tau\tag{5.9}
$$

As a result the wave function in the medium takes the form:

$$
= Ae^{i(\tilde{k}x-wt)}
$$

$$
\psi = Ae^{-\frac{\sigma}{\varepsilon_0 w}x}e^{i[\frac{1+\mu r}{2\mu x}]kx-wt]}
$$
(5.10)

The intensity can thus be given to be:

$$
I = chf |\psi|^2 = I_0 e^{-2\frac{\sigma}{\varepsilon_0 w}x} = I_0 e^{\frac{-2ne^2\tau}{me_0 w}x} = I_0 e^{-\alpha x}
$$
 (5.11)

Therefore the absorption coefficient with the aid of (3.18) can be given by:

$$
\alpha = \frac{2ne^2\tau}{m\varepsilon_0 w} = \frac{8\pi}{3} N_0 \left(\frac{\beta}{2\pi m}\right)^{3/2} \hbar^2 k^2
$$
 (5.12)

It is clear that the absorption coefficient depends on the wave number k.

Parameters affecting absorption coefficient

The conductivity and absorption coefficient γ are related, according to the relation[48]

$$
\alpha = \frac{C\mu\sigma}{n_1} \tag{6.1}
$$

$$
\sigma = \frac{ne^2\tau}{m^*}
$$
\n(6.2)

Where μ stands for the magnetic permeability, σ represents the conductivity while n_1 is the refractive index. The photo conductivity is thus expressed in terms of the relaxation time and effective mass, according to the relation (6.2). The absorption coefficient is thus given by

$$
\alpha = \frac{c\mu ne^2 \tau}{m^* n_1} \tag{6.3}
$$

According to equations (3.26) the absorption coefficient is k dependent through m^* and it goes like

$$
\alpha \approx (2k - 6C_1k + 4C_1^2k^3)
$$
 (6.4)
Equation (4.15) shows that the effective mass affects α to go like:

 $\alpha \approx k^4$ (6.5)

The absorption coefficient is also dependent on the K via the effective mass where equation (5.9) yields:

$$
\alpha \approx k^5 \tag{6.6}
$$

The relaxation time is dependent on the magnetic flux density as shown by equations (3.36) In view of equations (6.1) , (6.2) and (6.3)

$$
\alpha \approx \frac{1}{\mu + Be} \tag{6.7}
$$

With the aid of (6.3) the absorption coefficient is directly related to K as shown by equations (3.26) [beside (4.14)], (3.15)), (5,10) and (5.6) respectively:

The absorption coefficient is also proportional to the concentration of impurities N since it is proportional to free carries concentration n as shown by equation (6.3)

The effect of the magnetic properties on the a absorption coefficient can also be obtained with the aid of equations (3.22) and (3.23) to get

$$
\alpha = \frac{2\pi\mu c \chi_2 \omega}{n_1} \tag{6.15}
$$

Bearing in mind Langven expression for Larmer frequency [67]

$$
\omega_L = \omega = \frac{Be}{2m} \tag{6.16}
$$

The absorption coefficient takes the form

$$
\alpha = \frac{2\mu c \chi_2}{n_1} \frac{Be}{2m} \tag{6.17}
$$

The effect of spin and orbital angular momention can be incorporated via the atomic magnetic moment beside the magnetization vector (M) which is given according to quantum paramagnetic theory as $[59]$

$$
M = \frac{ng^2 m_s^2 \mu_o^2}{kT} \quad H = \chi H \tag{6.18}
$$

Thus the absorption coefficient is related to the spin quantum number m_s via the magnetic susceptibility. Where g is the splitting factor and μ_B is called Bohr agnation.

Discussion

Equation (2.7) , show the quantum expression of relaxation time as a function of the photon energy , this expression play an important role in the simulation of quantum semiconductor devices .

From equation (6.3), we find that (when $(\tau = 0$, then $\alpha = 0$), and $\alpha s \tau = \infty$, $\alpha = \infty$), this means, when the relaxation time increases , the optical absorption coefficient increases .

Equation (3.5) indicates that the strong resistive force $V_0 \rightarrow \infty$, causes the relaxation time to be short

 $\tau \rightarrow 0$ which is in conformity with commonsense.

Equation (3.36), show that, the relaxation time is dependent on the magnetic flux density.

From the expression $\left[\tau = \sqrt{\frac{\left(\nabla_k^2 E\right)}{\pi n}}\right]$ $\left(\frac{4\hbar}{mn_1^4}\right)|C_1|^2\left(\frac{e^4}{m^2}\right)$ $\sqrt{\frac{4\hbar}{mn_1^4}}$ | C_1 | $2\left(\frac{e^4}{m^2}\right)$ $(4\pi N_D)^2 \left(\frac{\beta}{4\pi n}\right)^3$ ħ⁴ k^2], and

equation (6.3), we find that ,[when $E \to 0$, $\tau \to 0$, $\alpha \to 0$, means no absorption], the light travels through the semiconductor material, [when $E \gg 0$, $\tau \gg 0$, $\alpha \gg 0$, means absorption.

The relaxation time is dependent on the magnetic flux density as shown by equations (3.36) .

Equation (6.9) shows that the absorption coefficient dependent on the wave vector (K) .

Conclusion

The mathematical model for the relaxation time expressed in terms of quantum mechanics expectation value , this model play an important role in the simulation of quantum semiconductor devices . From our result it is clear that the relaxation time affects on the absorption coefficient of semiconductors, also the relaxation time is dependent on the magnetic flux density. Also our results indicate that the optical absorption coefficient depends on the wave vector (K) . The coefficient (K) is an optical property of the semiconductor material , and is related to the index of refraction (n) , which merely determines how much light is absorbed by the semiconductor material, if k > 0 means absorption, $k = 0$, no absorption

(The light travels through semiconductor material) .

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