

Explanation of Absorption and Conductivity Spectra of Some Nano $(ZnO)_x(Al_2O_3)_{1-x}$ Using String Schrodinger Quantum Model

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Abstract: In this work an electron that emits electromagnetic waves are considered as vibrating strings. Using ordinary Newton law of energy a useful expression for energy in a frictional media was found. Utilizing quantum oscillator model the electric potential was obtained as a function of frequency. This potential was used to find conductivity and absorption coefficient spectra. The spectrum of them resembles that of some nano metal oxides like $(ZnO)_x, (Al_2O_3)_{1-x}$.

Keywords: Strings, Newton Energy, Kinetic energy, Potential energy, conductivity, absorption coefficient, spectra, nano.

Introduction

Quantum mechanics is branch of science that used to describe the behavior of atoms [1, 2]. It's now widely used to describe the physical properties of matter. One of the most important properties are that concerned with energy. These include optical and electrical properties.

The ability of the convertor to covert solar radiation energy to a useful energy depends mainly on their optical properties. For instance, the efficient solar cell is the one convert most of solar radiation to electric energy. The solar heater efficiency is large when it convert large amount of radiation to useful energy [3].

Different attempts were made to study the optical and electrical properties of matter [4, 5]. The born of nano science raise a hope controlling the physical properties of matter by changing their nano structure, shape and size [6, 7]. This open new horizon so as to find new semiconductor and solar cell types that can hopefully increase efficiency and gives good performance [8, 9].

Therefore many researches were done to use nano science to change the physical Properties of matter [10, 11, and 12]. The ones that related to optical electrical properties are important for solar convertors [13, 14]. This is because they are used in solar cells [15, 16].

One of the most important parameters is the conductivity and absorption coefficient .This motivates to try to construct string semi classical model so as to find new expression for these coefficients that can explain some empirical relations. This is done in section (2). Section (3) and section (4) are devoted for discussion and conclusion.

String theory states that particle acts as vibrating strings having displacement and velocity:

$$\begin{aligned}
 x &= x_0 e^{i\omega t} \\
 v &= \frac{dx}{dt} = i\omega x = v_0 e^{i\omega t} \\
 x &= -\frac{iv}{\omega} \tag{1}
 \end{aligned}$$

The equation of motion of such string in the presence of potential (V) and friction relaxation time (t) is given by

$$m \frac{dv}{dt} = m \frac{dv}{dx} \frac{dx}{dt} = mv \frac{dv}{dx} = -\frac{dv}{dx} - \frac{m}{t} v$$

Where m represents the mass, integrating both sides gives:

$$\int mvdv = -\int dv - \frac{m}{t} \int vdx \tag{2}$$

$$\frac{1}{2}mv^2 + v = \frac{im}{\omega t} \int vdv = \frac{1}{2} \frac{i}{\omega t} mv^2 \tag{3}$$

Thee kinetic energy is given by

$$KE = \frac{1}{2}mv^2 \tag{4}$$

Thus equation (4) can be rewritten to be

$$\left(1 - \frac{i}{\omega t}\right) KE + V = constant \tag{5}$$

The constant of motion stands for the total energy E , which can be expressed in the form

$$E = \left(1 - \frac{i}{\omega t}\right) KE + V \quad (6)$$

$$V = E + \left(\frac{i}{\omega t} - 1\right) KE \quad (7)$$

When spectral was done electric magnetic field with varying electric and magnetic field is applied. Assume now that the electric potential (V) is applied such that the induced magnetic potential (V_m).in this case the expression of the energy and kinetic term for the new frequency (ω)for ($n=1$) are given by

$$E = \left(\frac{3}{2}\right)\hbar\omega \quad KE = \frac{1}{2}E \quad (8)$$

Thus equation (6) for oscillator, electric and magnetic potential, V_o, V, V_m is given

$$E = \frac{1}{2}\left(1 - \frac{i}{\omega t}\right)E + V_o + V - V_m$$

Thus

$$\frac{3}{2}\hbar\omega = \frac{3}{4}\left(1 - \frac{i}{\omega t}\right)\hbar\omega + V_o + V - V_m \quad (9)$$

Thus the electric potential takes the form

$$V = \frac{3}{4}\hbar(\omega - \omega_o) + V_m \quad (10)$$

Following langev in the larmer frequency is given by

$$\omega_L = \omega - \omega_0 \quad (11)$$

Thus

$$V = \frac{3}{4}\hbar\omega_L + V_m = E_\omega + V_m \quad (12)$$

This relation holds for a single frequency. However when the frequency is continuous the energy which results from the whole frequency range is given by

$$E_L = \sum_i E_{\omega_i} = \int E_\omega d\omega_L = \frac{3\hbar}{4} \int \omega_L d\omega_L = \frac{3\hbar}{8} \omega_L^2 \quad (13)$$

Thus

$$V = E_L + V_m$$

$$V = \frac{3\hbar}{8} \omega_L^2 + V_m = \frac{3\hbar}{8} (\omega - \omega_0)^2 + V_m \quad (14)$$

But the resistance (R) is define to be

$$R = \frac{\rho L V}{A I} \quad (15)$$

Where ρ, L, A, V and I is standing for the resistivity, length, area, electric potential and current respectively.

There fore

$$\rho = \frac{AV}{LI} = \frac{A}{8LI} [3\hbar(\omega - \omega_o)^2 + 8V_m] \quad (16)$$

$$\rho = \rho_o [\hbar(\omega - \omega_o)^2 + 4V_m] \quad (17)$$

Where:

$$\rho_o = \frac{A}{8LI} \quad (18)$$

Thus the conductivity is

$$\sigma = \frac{8LI}{A} \frac{1}{[\hbar(\omega - \omega_o) + 2V_m]} \quad (19)$$

$$\sigma = \frac{\sigma_o}{3\hbar(\omega - \omega_o)^2 + 2V_m} \quad (20)$$

The absorption coefficient is given by

$$\alpha = \frac{\sigma}{cn} = \frac{\alpha_o}{3\hbar(\omega - \omega_o)^2 + 8V_m} \quad (21)$$

Where

$$\alpha_o = \frac{\sigma_o}{cn} \quad (22)$$

The plot of α and α versus λ can be done with the aid of the equations [let $\omega_o = \frac{c}{\lambda_o}$]

$$\sigma = \frac{\sigma_o}{3\hbar c^2 \left[\frac{\lambda_o - \lambda}{\lambda_o \lambda}\right]^2 + 8V_m} \quad (23)$$

Since the spectrum is narrow, thus

$$\lambda \approx \lambda_0 \quad \lambda \lambda_0 = \lambda_0^2 \quad (24)$$

$$\sigma = \frac{\sigma_0 \lambda_0^4}{3hc^2[\lambda_0 - \lambda]^2 + 8 \lambda_0^2 V_m} \quad (25)$$

Similarly

$$\alpha = \frac{\alpha_0 \lambda_0^4}{3hc^2[\lambda_0 - \lambda]^2 + 8 \lambda_0^2 V_m} \quad (26)$$

$$\sigma = \frac{\sigma_0}{[(\lambda_0 - \lambda)^2 + 10^{-3}] \times 10^{-18}}$$

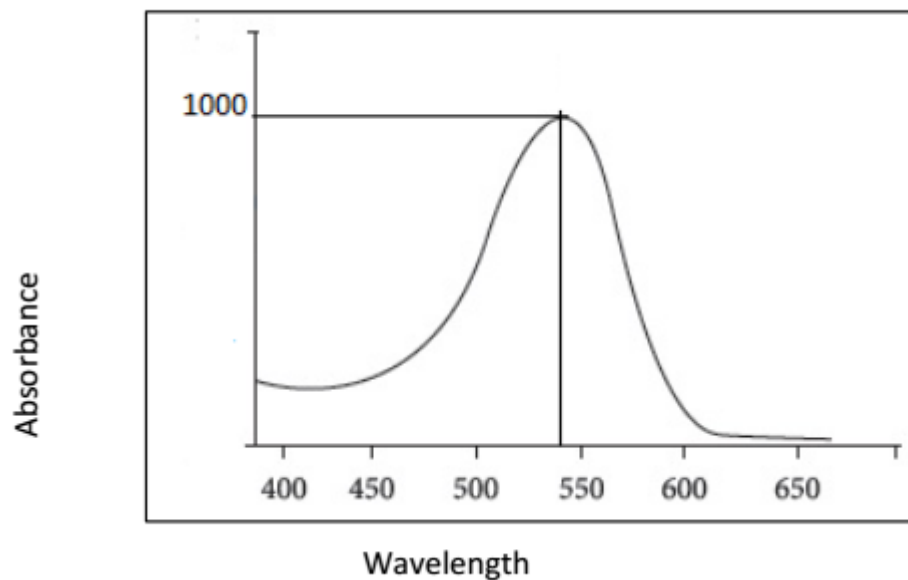


Figure (1) Absorbance (α) against wave length (λ)

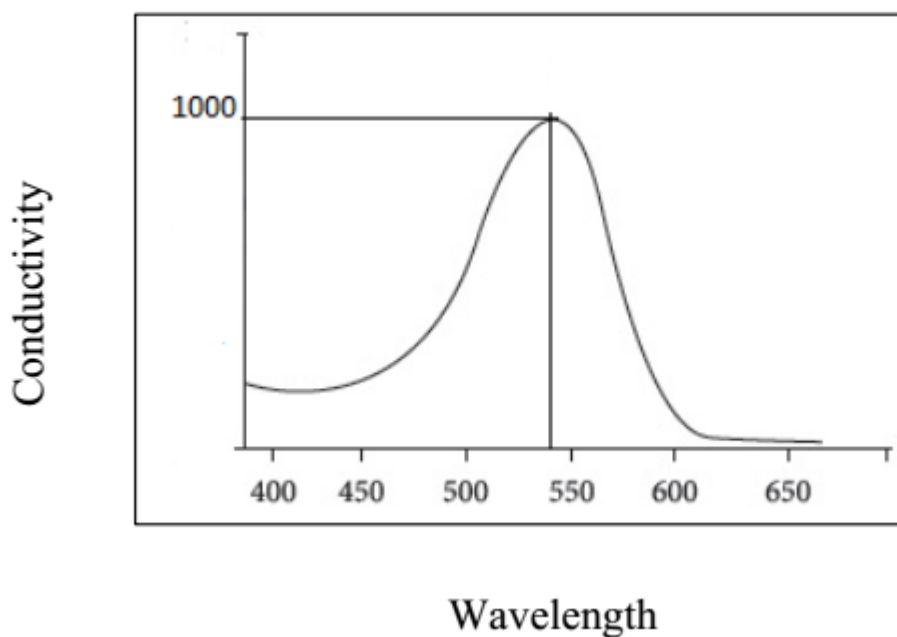


Figure (2) Conductivity (σ) against wave length(λ)

$$\alpha = \frac{1}{(\lambda_0 - \lambda)^2 + 10^{-3}}$$

$$\sigma = \frac{1}{(\lambda_0 - \lambda)^2 + 10^{-3}}$$

The energy of classic osillator can be obtained also by using the concept of wffetive value.

The effective displacement and velocity, are thus ginen by

$$x_e = \frac{x_0}{\sqrt{2}} v_e = \frac{v_0}{\sqrt{2}} \tag{27}$$

Hence the kinetic energy and effective kinetic energy are given by

$$K = \frac{1}{2} m v_2 = \frac{1}{2} m v_0^2 e^{i\omega t} \tag{28}$$

$$K_e = \frac{1}{2} m v_e^2 = \frac{1}{4} m v_0^2 \tag{29}$$

Simallarly potential energy and effective potential are given by

$$V_e = \frac{1}{2} k x_e^2 = \frac{1}{2} m \omega^2 \frac{x_0^2}{2} \tag{30}$$

$$V_e = \frac{1}{4} m \omega^2 x_0^2 \tag{31}$$

But from (1)

$$x_0 = -\frac{i v_0}{\omega}$$

Numirically

$$x_0^2 = \frac{v_0^2}{\omega^2} \tag{32}$$

Therefore equation (29)

$$K_e = \frac{1}{4} m \omega^2 x_0^2 \tag{33}$$

Adirict comparision of (31) and (33) yields

$$K_e = V_e \tag{34}$$

For classical string the total energy is given by

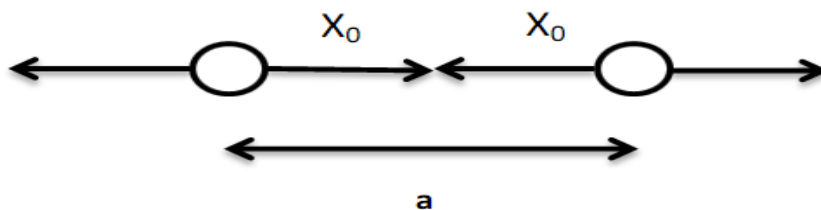
$$E = K + V = -2K \tag{35}$$

Then the kinetic energy is given by

$$K = \frac{1}{2} E \tag{36}$$

The string energy can be found in terms of the distance between successive atoms.

If the distance between two successive atoms or particels is a . Thus one can assume the maximum vibration displacement to be



$$x_0 = \frac{1}{2} a \tag{37}$$

$$K_e = \frac{1}{16} m \omega^2 a^2 \tag{38}$$

$$E = 2K_e = \frac{1}{8} m \omega^2 a^2 \tag{39}$$

Using equation (6), one gets the total energy of the osillator is given by

$$E_0 = \left(1 - \frac{i}{\omega_0 t}\right) K_0 + V_0 = \frac{1}{2} \left(1 - \frac{i}{\omega_0 t}\right) E_0 + V_0$$

$$V_0 = \frac{1}{2} \left(1 - \frac{i}{\omega_0 t}\right) E_0 \tag{40}$$

But

$$E = \left(1 - \frac{i}{\omega t}\right) K + V_o + V - V_m = \frac{1}{2} \left(1 - \frac{i}{\omega t}\right) E + V_o + V - V_m$$

$$\frac{1}{2} \left(1 + \frac{i}{\omega t}\right) E = V_o + V - V_m = \frac{1}{2} \left(1 + \frac{i}{\omega t}\right) E_0 + V - V_m \quad (41)$$

In view of equation ()

$$V = \frac{1}{2} (E - E_0) + \frac{1}{2t} \left(\frac{E}{\omega} - \frac{E_0}{\omega}\right) + V_m \quad (42)$$

with the aid the equation (39)

$$E = \frac{1}{8} m \omega^2 a^2 E_0 = \frac{1}{8} m \omega_0^2 a^2 \quad (43)$$

Thus equation(41) gives

$$V = \frac{m}{16} a^2 (\omega - \omega_0^2) + \frac{i m a^2}{16t} \left[\frac{\omega^2}{\omega} - \frac{\omega_0^2}{\omega}\right] + V_m \quad (44)$$

For narrow range spectrum

$$\omega \approx \omega_0 \quad (45)$$

Therefore

$$V = \frac{m a^2}{16} a^2 (\omega - \omega_0^2) + \frac{i m a^2}{16t \omega_0} (\omega - \omega_0^2) + V_m$$

$$= \frac{m a^2}{16} \left(1 + \frac{i}{t \omega_0}\right) (\omega - \omega_0^2) + V_m$$

$$= \frac{m a^2}{16} \left(1 + \frac{i}{t \omega_0}\right) (\omega - \omega_0^2) (\omega + \omega_0) (\omega - \omega_0) + V_m$$

$$V = \frac{m a^2}{16} \left(1 + \frac{i}{t \omega_0}\right) (2 \omega_0) \omega_L + V_m$$

$$= (c_1 + i c_2) \omega_L + V_m = E_{1\omega} + i E_{2\omega} + V_m \quad (46)$$

Where

$$c_1 = \frac{8 a^2 \omega_0}{8} c_2 = \frac{m a^2}{8t} \quad (47)$$

ω_L is the larmer frequency.

When ω_L is the continuous by integration, where

$$E_1 = \sum_i E_{1\omega_i} = c_1 \int \omega_L d\omega_L = \frac{1}{2} c_1 \omega_L^2$$

$$E_2 = \sum_i E_{2\omega_i} = c_2 \int \omega_L d\omega_L = \frac{1}{2} c_2 \omega_L^2 \quad (48)$$

Inserting equation (48) in equation (46) gives the potential energy related to electrons emitting continuous radiation spectra, in the form

$$V = E_1 + i E_2 + V_m$$

$$V = \frac{1}{2} (c_1 + i c_2) \omega_L^2 + V_m \quad (49)$$

For simplicity, asume that the friction exists. In this case

$$c_L = \frac{m a^2}{8t} = \frac{a^2}{8} \gamma = 0 \quad (50)$$

In view of equation (16) the resistivity and conductivity are given by

$$\rho = \frac{AV}{LI} = \frac{A}{LI} (c_1 \omega_L^2 + V_m) = \rho_0 (c_1 \omega_L^2 + V_m)$$

$$\sigma = \frac{1}{\rho} = \frac{\sigma_0}{c_1 (\omega - \omega_0) + V_m} \quad (51)$$

Using the fact that

$$\omega = \frac{c}{\lambda} \omega_0 = \frac{c}{\lambda_0} \sigma_0 \quad (52)$$

$$\sigma = \frac{c_1 c^2}{\lambda^2 \lambda_0^2} (\lambda_0 - \lambda)^2 + V_m \quad (53)$$

Since

$$\lambda \approx \lambda_0 \quad (54)$$

It following that the conductivity is given by

$$\sigma = \frac{\sigma_0 \lambda_0^4}{(c_1 c^2 (\lambda_0 - \lambda)^2 + \lambda_0^4 V_m)} \quad (55)$$

Similarly the absorption coefficient can be given according to equation (21) to be

$$\alpha = \frac{\sigma}{nc}$$

$$\alpha = \frac{\alpha_0}{(c_1 c^2 (\lambda_0 - \lambda)^2 + \lambda_0^4 V_m)} \quad (56)$$

Discussion

String theory is the one of the most promising physical theories that can be utilized to be explain physical phenomena. This motivates to consider electrons as vibrating strings subjected to fields as well as friction as shown by equation (1) and (2). The energy for this system in equation (6) shows that it consists of imaginary part standing for energy lost due to the friction beside the ordinary kinetic and potential term. The frictional energy depends on the kinetic energy, relaxation time as well as the frequency. Its dependence on speed and kinetic energy is compatible with common sense and experiment.

Using the expression for the average potential energy for harmonic oscillator of the quantum system in equation (8) together with the Newtonian total energy relation, the kinetic and potential energy of the free oscillating are found in terms of the total energy as indicated in equations (12) and (13). It was shown that the kinetic and potential energies are equal to each other and equals half of the total energy. Utilizing the expression of energy (7) for the frictional mediums, a useful expression for the potential of string in the absence of external field in equation (14).

In spectral techniques an electromagnetic field having electric and magnetic field is applied. Equation (16) shows that the applying external electric field beside the magnetic field, two additional terms were added to energy E , one standing for the electric field, potential which is denoted by V , the other V_m stands for the magnetic potential.

According to equation (17) the electric potential is frequency dependent, where it is proportional directly to the larger frequency as equation (18) indicates. If the accelerated electrons emit continuous spectrum the potential is given by equation (21).

Using the definition of resistivity, conductivity and absorption coefficient, for narrow spectrum, equation (30) and equation (33) shows their dependence on the wavelength of emitted radiation due to the vibration. The emitted photon frequency is assumed to be that of the electron.

It is very interesting to note that the shape of the theoretical relations of the conductivity and absorption coefficient against the wavelength resembles Lorentzian and Gaussian shape. These theoretical relations fortunately are compatible with empirical ones that describes the same relations for some nano metal oxide like $(ZnO)_x$, $(Al_2O_3)_{1-x}$.

Conclusion

Using string model in addition to quantum and Newton laws a useful expression of energy in resistive medium was found. This relation was used to obtain a conductivity and absorption coefficient. The spectra of conductivity and absorption coefficient resembles Lorentzian and Gaussian one, and resembles empirical one for some nano metal oxides.

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