

ENERGY EIGEN VALUE OF ZINC OXIDE TRIANGULAR QUANTUM WELL AND ITS OPTICAL PROPERTIES

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To my family.

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Abstract

In this study we have developed the Hamiltonian and trial wave functions for the triangular quantum well. Then the schroendinger equation is solved analytically and numerically for determining the ground and excited state energy. This ground and excited state energy of triangular quantum well are calculated by using variational methods. The energy eigen value of states increase with an increment of applied field. By using the compact density matrix formalism and iterative procedure, the change in linear refractive index and absorptions coefficient is studied. The value of linear change in refractive index and absorption coefficient carried out for given value of transition energies and depending on the above calculated energy eigen value. As the transition energy or frequency increases, the peak of the spectra of the change in refractive index and change in linear absorption coefficient move toward the high energy region. Moreover, the magnitude of the absorption coefficient increases with an increment of transition energy.

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Chapter 1

Introduction

1.1 Back ground of the Study

In recent year, due to significant improvement in micro fabrication techniques like Molecular Beam Epitaxy and metal organic chemical vapor deposition, it is possible to fabricate quantum wells with varied potential profiles [1]. Quantum well, Quantum dot, Quantum wire heterostructure are classified as low- dimensional semiconductor quantum system become an important part with in semiconductor studies. Quantum well is a particular kind of heterostructure in which one thin "well" layer is surrounded by two "barriers". Quantum well have many interesting properties for electrical transport [2]. Quantum well are one example of heterostructure. In general heterostructure have many uses. They can be used for advanced electronic devices, optical component, optoelectronic devices and structures. (Mg, Zn) O are important for the potential applications in the fabrication of optical and electro- optical devices operating in the green- ultra violet region of the electron magnetic spectrum [3]. ZnO (Zn, Mg)O quantum wells have been successfully grown by different techniques such as Laser, assisted molecular beam epitaxy (LMBE), Metal In organic chemical vapor deposition and molecular beam epitaxy (MBE) [4]. ZnO/ZnMgO structure are

effective to obtain intense ultraviolet emission for laser and light emitted diode application. The principle of the Rayleigh - Ritz method is that we can adopt a trial wave function, which may have some parameters in it and then minimize the energy calculated with the wave function. This energy will be lowest energy level E_0 and gives a good approximation to the actual energy level. The next higher state can be developed by using a second parametrized basis function, which is made orthogonal to the first . The energy level of this wave function is then found by the same adjustment technique [5]. The calculation of the confinement energies and excitonic states requires a detailed knowledge of the band structure parameters.

The Piezoelectric field naturally modulated the quantum well energy states to create triangular potentials at opposite sides of the well[6]. Which causes separate confinement of the electron and holes, decrease of the wave function overlap effective in a plane (lateral) localization of the quantized electron-hole pair was found to play an important role.

The linear and nonlinear optical susceptibility can be determined by considering the symmetry properties of particular crystal [7]. In the process of two photon absorption an atom makes a transition from its ground state to an excited by the simultaneous absorption of two laser photons. Nonlinear optics is the study of phenomena that occur as a consequence of the modification of the optical properties of a material system by the presence of light. Typically, only laser light is sufficiently intense to modify the optical properties of a material system.

1.2 Statement of the Problem

A quantum well (QW) is a two dimensional system with discrete energy levels along one direction and continuous energy along the remaining two directions. Quantum wells (QW) have promised a lot of device applications such as modulation doped field effect transistors and Quantum well lasers. In addition to this QWs have been found to play a key role in optoelectronic applications. Understanding the peculiar optical properties of ZnO triangular quantum wells helps to use numerous application of modern technologies like high brightness, blue light emitting diodes and laser diodes. The triangular quantum well(s) is also important systems since the absorption coefficient value is reduced in the experimental measurement of the electro absorption when a triangular quantum well is used. In this study, we seek to determine the energy eigen value of ZnO triangular quantum well by using variational techniques.

Research questions are:

1. How can we determine the energy eigen value of ZnO triangular quantum well by using variational techniques?
2. What are the optical properties of ZnO triangular quantum wells?

1.3 Objectives

1.3.1 General Objective

The main objective of this study is:

- To determine the energy eigen value of ZnO triangular quantum wells and to describe its optical properties.

1.3.2 Specific Objectives

The specific objectives of the study are:

- To determine the energy eigen value of ZnO triangular quantum well by using Variation techniques.
- To describe the optical properties of ZnO Triangular quantum wells.

1.4 Significance of the Study

Quantum well is a particular kind of heterostructure in which one thin "well" layer is surrounded by two "barriers". This work helps to understand peculiar optical properties of ZnO Triangular quantum well. In general this study have significant impact in the understanding of the physics of ZnO triangular quantum wells and its optical properties.

1.5 Limitation of the Study

Due to time constraint, the scope of the study is limited to the calculation of energy eigen value of ZnO triangular quantum well using variational techniques and description of its optical properties.

Chapter 2

Literature Review

2.1 Quantum Well

Semiconductor materials especially quantum wells and quantum dots are important for a number of recent demonstration of quantum optics effects[8]. Quantum wells (QW) are thin layered semiconductor structures in which we can observe and control many quantum mechanical effects[2, 9]. In Qw, charge carriers (electrons and holes) are free to move in two direction and quantized in one direction. The optical properties of semiconductor are therefore determine by transition between energy bands rather than between discrete levels[8]. They derive most of their special properties from the quantum confinement of charge carrier (” electron ” and ” holes ”) in thin layers of one semiconductor ” well ” material sandwiched between other semiconductor ” barrier ” layers. Many of the physical effects in QW structures can be seen at room temperature and can be exploited in real devices. QW semiconductors are very thin layer of smaller band gap material, E_{g1} , is sandwiched between two layers of larger band gap material, E_{g2} , technically this is done by the sophisticated techniques of Molecular Beam Epitaxy (MBE) or Metal Organic Chemical Vapor Deposition (MOCVD)[1, 9]. One-dimensional quantum wells are formed through epitaxial growth

of alternating layers of semiconductor materials with different band gaps. A single quantum well is formed from one semiconductor sandwiched between two layers of a second semiconductor having a larger band gap. The center of layer with the smaller band gap semiconductor forms the QW, while the two layers sandwiched the center layer create the potential barriers. QWs are one example of heterostructures made by joining different materials, in layers and with the materials joined directly at the atomic layer.

Among the fundamental QW properties of interest, the process of the carrier transfer from the bulk states[8]. In bulk semiconductor, conduction band electrons are free to move in all three directions forming a continuous energy spectrum but in QW conduction band electrons are confined in direction and are free to move in other two directions. The transition can take place over a continuous range of photon energies determine by the lower and the upper energy limit of the bands. An absorption band is therefore, with a threshold at the band gap energy E_g [8]. In contrast to bulk semiconductors excitonic effects are very clear in quantum well at room temperature have significant influence on device performance. For an emission, it is necessary that there should be an electron in the conduction band and an unoccupied level that means a hole in the valence band. These electrons and holes are typically injected into their respective bands either from an electrical current or previous optical excitation. The electrons that are injected relax very rapidly to the bottom of the conduction band by emission of phonons. Similarly the injected holes relax very rapidly to the top of the valence band. The radiative transitions therefore take place at energy very close to the band gap energy .The width of the emission line is determined by the thermal spread of the charge carriers with their bands or by inhomogeneous effects.

Strong inter band transitions can occur when the transitions are allowed by the electric dipole selection rule, and when semiconductor has a direct band gap. Indirect band gap, a phonon must be absorbed or emitted whenever the electron jumps between the bands, and this substantially reduces the transition probability [8]. In fact that the electrons and holes relax with their bands before emission occurs means that there is a qualitative difference between the emission and absorption spectra of a semiconductor. This contrasts with atomic spectral, where the absorption and emission lines both occur at the same energy.

2.2 Zinc Oxide (ZnO) and its Application in Technology

ZnO is a II-VI compound semiconductor whose ionicity resides at the borderline between the covalent and ionic semiconductor [10]. It is widely used in electro acoustic devices due to its large piezoelectricity. From the 1960s, synthesis of ZnO thin film has been an active field because of their application as sensors, transducers and catalyst[11]. ZnO is a key technological material. The lack of a center of symmetry, in Wurtzite, combined with large electromechanical coupling, result in strong piezoelectric and pyroelectric properties and consequent use of ZnO mechanical, actuators and piezoelectric sensors.

Metal oxide nanostructures have attracted considerable attention for their potential application in many technologies such as solar cells, electroluminescent devices, electro chromic windows and chemical sensors. To achieve high performance of these devices, the metal oxides used in these applications are required to possess high surface area as well as good electrical, electrochemical and structural properties. ZnO

is a direct band gap (3.37eV) semiconductor with a large exciton binding energy of 60meV at room temperature. It is widely exploited metal oxide material in photovoltaic application as a transparent conducting electrode[12]. Band gap engineering of ZnO be achieved by alloying with MgO or CdO. Adding Mg to ZnO increase the band gap, where as adding Cd to ZnO it decreases the band gap[13].

ZnO is an interesting material with application spanning from the simple and well-known to the highly advanced and sophisticated. Its wide band gap and high absorptivity have made it useful as ultraviolet- absorbing in everything from sun screens, advanced plastic, and rubber [14].

The availability of large single crystal is a big advantage of ZnO over GaN. For example, GaN is usually grown on sapphire, with a large lattice mismatch of 16percent that leads to an exceedingly high concentration of extended defects ($10^6 - 10^9\text{cm}^{-2}$). The epitaxy of ZnO films on native substrates can result in ZnO layers with reduced concentration of extended defects and consequently, better performance in electronic and photonic devices. Another big advantage over GaN is that ZnO is amenable to wet chemical etching [13]. In general a partial list of the properties of ZnO that distinguish it from other semiconductor or oxide it useful for applications includes: In Direct and wide band gap, large exciton binding energy, large piezoelectric constant, Strong luminescence, Thermal conductivity, and Radiation hardness.

The ZnO / (ZnMg) O material system holds several advantages for the fabrication of low defect type-I heterostructures[15]. ZnO and ZnMgO- layers can be used for fabricate highly reflective distributed Bragg's reflectors for applications in the ultraviolet and blue /green spectral range. ZnO has a large fundamental band gap of

3.37eV at room temperature [13]. Because ZnO has attracted more and more attention due to its interesting properties. The nature of high thermal conductivity, high luminous efficiency and mechanical and chemical robustness have made ZnO and its alloys the promising material system for light - emitting device operated at a ultra violet spectra region. When light sufficient energy is incident on to sample, absorbed photons impart excess energy to electrons within the material. This photon excitation causes electrons with the material to move into permissible excited states. This excited electrons eventually relax to their ground state with radiative and nonradiative relaxation the electrons, the emission of light called photo luminescence occurs. The most common radiative transition in semi conductors is between states in the conduction and valence band. Moreover, the excitons in ZnO- based quantum well (QW) heterostructure exhibit strong stability as compared to bulk semiconductors or III -V QWs due to the enhancement of the binding energy and reduction of the exciton - phonon coupling caused by quantum confinement[16]. An important step in order to design high performance ZnO based optoelectronic devices is the realization of band gap engineering to create barrier layers and quantum wells in heterostructure devices. An effect of built- in electric field inside QW layer might be taken into account for ZnO QWs having relatively high barrier height.

2.3 Density State of Quantum well

The application of the quantum wells are based mainly on the optical transitions around the high symmetry points in the two-dimensional Brillouin zone [17]. Macroscopic properties of any condensed matter system depend on the integral (total) density of state. The density of states is defined as the number of states per energy per unit

volume of real space.

$$\rho(E) = \frac{dN}{dE} = \frac{dN}{dK} \frac{dK}{dE} \quad (2.3.1)$$

In two dimensional electron or holes gas (2DEG), the total number of states per unit cross-sectional area is given by the spin degeneracy factor multiplied by the area of the circle of radius k , divided by the occupied by each state, i.e. [18].

$$N^{2D} = 2\pi k^2 \frac{1}{(2\pi)^2} \frac{1}{L^2}$$

$$N^{2D} = \frac{k^2}{2\pi} \quad (2.3.2)$$

The parabolic bands of effective mass theory is given by,

$$E = \frac{\hbar^2 k^2}{2m^*} \quad (2.3.3)$$

From equation (2.3.3) k (wave vector) becomes,

$$k = \left(\frac{2m^* E}{\hbar^2} \right)^{\frac{1}{2}} \quad (2.3.4)$$

Density of state in two dimension [18],

$$\rho^{2D}(E) = \frac{dN^{2D}}{dE} = \frac{dN^{2D}}{dK} \frac{dK}{dE} \quad (2.3.5)$$

Derivate equation (2.3.2) by dk then we get,

$$\frac{dN^{2D}}{dK} = \frac{k}{\pi} \quad (2.3.6)$$

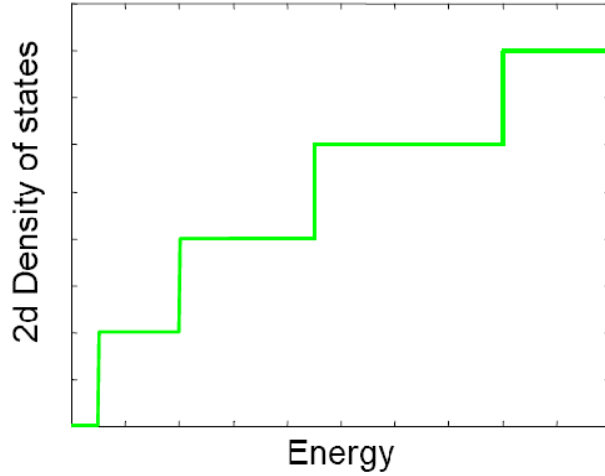


Figure 2.1: The density of states for quantum well(2D)[18].

And Derivate equation (2.3.4)by dE it gives,

$$\frac{dK}{dE} = \frac{1}{2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{1}{2}} E^{-\frac{1}{2}} \quad (2.3.7)$$

Using equation (2.3.6)and (2.3.7) in to equation (2.3.5) then the density state of two dimension is becomes,

$$\rho^{2D}(E) = \frac{m^*}{\pi\hbar^2} \quad (2.3.8)$$

Generally the density state of quantum well (2 dimensional) is given by,

$$\rho^{2D}(E) = \frac{A}{2\pi} \left(\frac{2m^*}{\hbar^2} \right) \quad (2.3.9)$$

where A is surface area

2.4 Optical Property in Quantum well

The unique properties of low dimensional semiconductor materials are originated from the quantum confinement of the motion of electrons [19]. Depending on dimensionality, in the two dimensional structure quantum well, the quantization of the particle motion occurs in one dimension, while the particle is free to move in other two directions. In the case of quantum well structures, the conduction band will be quantized to several subbands along the growth direction due to quantum confinement. In quantum well, the electron and the holes are free to move in the direction parallel to the layers [2]. Hence, we do not really have discrete energy states for electrons and holes in quantum well: we have instead "subbands" that start at the energies calculated for the confined states. Optical measurement constitutes the most important means of determining the band structures of semiconductors[20]. photon induced electronic transitions can occur between different bands, which lead to the determination of the energy band gap, or with in a single band such as a free - carrier absorbtion.

The quantum well looks like artificial model, which has an application in the real world. Although an infinitely deep well cannot be made it is simple now days to grow structures that are close to an ideal infinite well. A heterostructure consisting of a thin sandwiched of ZnO between two thick layers of ZnMgO provides a simple quantum well. Free electrons have energy,

$$E_0 = \frac{\hbar^2 k^2}{2m_0 m_e} \quad (2.4.1)$$

Electrons in the semiconductor live in the conduction band which changes their energy in two ways. First energy must be measured from the bottom of the band E_c rather than from zero, second electrons behave as though their effective mass $m_0 m_e$ or (m^*) .

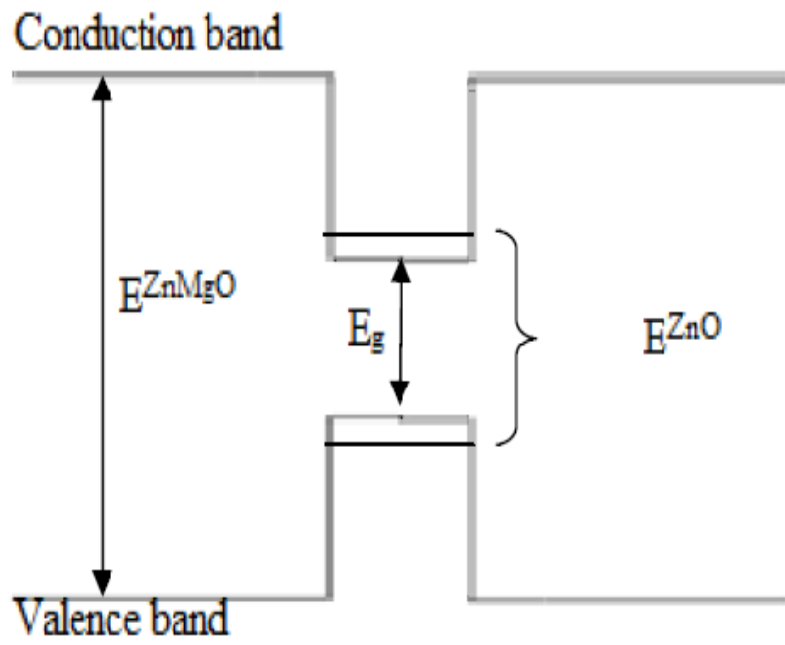


Figure 2.2: The schematic diagram of optical properties of quantum well

Thus energy is given by

$$E_c(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m_0 m_e} \quad (2.4.2)$$

The sandwiched acts like a quantum well, because E_c is higher in ZnMgO than ZnO and difference ΔE_c provides the barrier that confines the electrons. We could measure the energy levels by shining light on the sample and determining which frequencies were absorbed. A photon is absorbed by exciting an electron from low level to higher one, and the energy of the photons matches the difference in electric energy level. It is given by,

$$\hbar\omega = E_{e2} - E_{e1} \quad (2.4.3)$$

Semiconductors have energy levels in other bands. The most important of this is valence band, E_v below the conduction band. The band curve is down ward, in a function of K, E_v is giving by,

$$E_v(\vec{k}) = E_v - \frac{\hbar^2 k^2}{m_0 m_e} \quad (2.4.4)$$

The conduction bands and valence bands are separated by an energy called band gap energy, E_g is given by,

$$E_g = E_c - E_v \quad (2.4.5)$$

The valence band is completely full and the conduction band is completely empty in a pure semiconductor at zero temperature. Optical absorption must therefore list an electron from the valence to the conduction band. In a bulk sample of ZnO this can occur, provided that $\hbar\omega > E_g^{ZnO}$ similarly we need $\hbar\omega > E_g^{ZnMgO}$ in ZnMgO. The

process level behind the empty state or hole in the valence band so the subscript h is used to identify parameters of the valence band. Quantum well ZnO, absorption cannot start at $\hbar\omega = E_g^{ZnO}$, because the states in the well are quantized. The lowest energy at which absorption can occur is given by difference in energy, $E_{e1} - E_{h1}$, between the lowest state in the well on the conduction band and the lowest in the well in the valence band. Absorption can occur at higher energy. The strongest quantization occurs between corresponding states in two bands, so that $n_e = n_h = n$. The strong absorption occurs at the frequency given by,

$$\hbar\omega_n = E_{en} - E_{hn} \quad (2.4.6)$$

The energy levels (E_{en}) in a well of width a is given by,

$$E_{en} = E_c + \frac{\hbar^2 \pi^2 n_e^2}{2m_0 m_e a^2} \quad (2.4.7)$$

where k is wave vector and given by, $k^2 = \frac{\pi^2 n^2}{a^2}$ and a is well width

Energy of the bound states (E_{hn}) are given by,

$$E_{hn} = E_v - \frac{\hbar^2 \pi^2 n^2}{2m_0 m_h a^2} \quad (2.4.8)$$

where $k^2 = \frac{\pi^2 n^2}{a^2}$

Using equation (2.4.7) and (2.4.8) into equation (2.4.6) then we get,

$$\begin{aligned} \hbar\omega_n &= \left(E_c + \frac{\hbar^2 \pi^2 n^2}{2m_0 m_e a^2} \right) - \left(E_v - \frac{\hbar^2 \pi^2 n^2}{2m_0 m_h a^2} \right) \\ \hbar\omega_n &= (E_c - E_v) + \frac{\hbar^2 \pi^2 n^2}{2m_0 m_e a^2} + \frac{\hbar^2 \pi^2 n^2}{2m_0 m_h a^2} \end{aligned} \quad (2.4.9)$$

Using equation (2.4.5) in to equation (2.4.9) then the energy in quantum well is given by,

$$\hbar\omega_n = E_g + \frac{\hbar^2\pi^2n^2}{2m_0a^2} \left[\frac{1}{m_e} + \frac{1}{m_h} \right] \quad (2.4.10)$$

where the effective mass is given by, $\frac{1}{m_{eh}} = \frac{1}{m_e} + \frac{1}{m_h}$

The barrier in a semiconductor are finite and absorption occurs in the ZnMgO barriers for all frequencies where $\hbar\omega > E_g^{ZnMgO}$, no absorption is possible for $\hbar\omega < E_g^{ZnO}$ and there is a continuous band of absorption for $\hbar\omega > E_g^{ZnMgO}$, between these frequencies discrete lines are produced by transition between states in the quantum well with energies given by equation (2.4.10). The width of the well can be inferred from the energy of this lines, if the effective masses are known. In practice slightly different experiment is usually performed called photoluminescence light with $\hbar\omega > E_g^{ZnMgO}$ is shown on the sample which excites many electrons from the valence to the conduction band every where. Some of the electrons trapped in the quantum well and the same thing happen to the hole in the valence band. It is then possible for the electron to fall from the conduction band in to the hole in the valence band and released the difference in energy a light. This luminescence in the reverse process to the absorption and occur at the same energies.

2.5 Triangular Quantum Well

Quantum wells (QWs) are grown with various shapes as rectangular quantum wells (RQW) (Greene and Bajaj, 1983; Miller et al., 1984), parabolic quantum wells (PQW) (Merlin, 1987; Brey et al., 1989-II), triangular quantum wells(TQW) (Jiang and Wen, 1994-II) etc[21]. Calculation of electron and hole energy levels and hence the transition energies in such quantum wells will be useful for many advanced studies on them.

The intersubband transitions and impurity binding energy in differently shaped semiconductor quantum wells under magnetic field are calculated by Yesilgul et al., (2011) using a variational method with in the effective mass approximation. The triangular well is a type of potential well which is quite common in every day semiconductor devices, such as the common metal oxide semiconductor(MOS) transistor. The Piezoelectric field naturally modulated the QW energy states to create triangular potentials at opposite sides of the well [6], which causes separate confinement of the electron and holes, decrease of the wave function overlap effective in a plane (lateral) localization of the quantized e-h pair was found to play an important role .For the quantum wells especially for a well thickness smaller than the three dimension(3D) free exciton Bohr radius a_B [6]. The optical inter-subband transition between the states of two triangular QWs, one for the electrons in conduction band and another one for the holes in valence band[22]. The triangular well is useful because it is a simple description of the potential well at a doped heterojunction. The triangular quantum well is important systems science the absorption coefficient value is reduced in the experimental measurement of the electro absorption.

The countered potential is the triangular quantum well for which the potential $V(z)$ is linear for $z > 0$ and has infinite barrier at $z = 0$ [23]. In this case of triangular potential well, as $V(z) = eFz$, the Schrödinger equation for the envelope wave function is given by,

$$\frac{-\hbar^2}{2m^*} \left[\frac{d^2}{dz^2} + eFz \right] \psi(z) = E\psi(z) \quad (2.5.1)$$

Where F is the electric field.

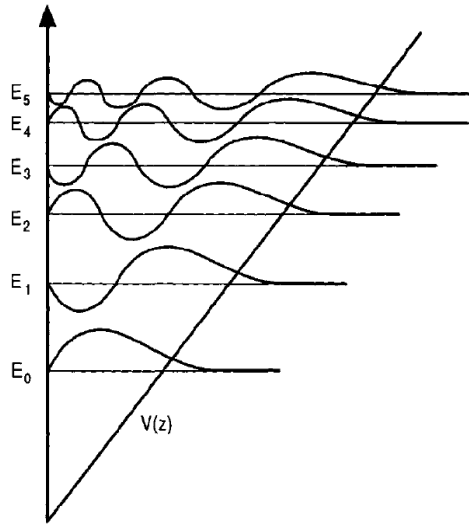


Figure 2.3: Wave functions and subband energies in a triangular quantum well[23].

2.6 Variational Techniques/Method/

The variational method can give a good estimate of the lowest order mode by choosing an appropriate trial function and carrying out an optimization; the method becomes quite cumbersome when applied to higher order modes[24]. The exact analytical solution of the Schrodinger equation is possible only in a few cases. Even the direct numerical solution by integration is often not feasible in practice, especially in systems with more than one particle. There are, however extremely useful approximated methods that can in many cases reduce the complete problem to a much simpler one. The energies of the ground state and the first excited state are determined by minimizing the expectation value of Hamiltonian[25].

$$E = \frac{\langle \psi | H^* \psi \rangle}{\langle \psi | \psi \rangle} \quad (2.6.1)$$

Hamiltonian equation is given by,

$$\frac{-\hbar^2}{2m} \left[\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right] + \hat{V} = \hat{H} \quad (2.6.2)$$

The variational methods provide an estimate of the energy of the lowest state of the system. Although this might seem a rather specialized task, the method is important for its accuracy, for its applicability to complicated problems, and because many numerical methods are available to minimize a function.

2.7 Linear Optics

Linear optics is a subfield of optics, consisting of linear systems and is the opposite of nonlinear optics. Linear optics includes most applications of lenses, mirrors, wave plates, diffraction gratings and many other common optical components and systems. In linear optics, the induced polarization depends linearly on the electric field strength in a manner that can often be described by the relationship [7]

$$\vec{P}(t) = \epsilon_0 \chi^{(1)} \vec{E}(t) \quad (2.7.1)$$

where the constant of the proportionality $\chi^{(1)}$ is known as the linear susceptibility and ϵ_0 the permittivity of free space.

According to the rules of quantum mechanics, the expectation value of the electric dipole moment is given by,

$$\langle \tilde{P} \rangle = \langle \psi | \hat{\mu} | \psi \rangle \quad (2.7.2)$$

The contribution linear in the applied field amplitude is given by

$$\langle \tilde{P}^{(1)} \rangle = \langle \psi^{(0)} | \mu | \psi^{(1)} \rangle + \langle \psi^{(1)} | \mu | \psi^{(0)} \rangle \quad (2.7.3)$$

$$\langle \tilde{P}^{(1)} \rangle = \frac{1}{\hbar} \sum_p \sum_m \left(\frac{\mu_{mg} [\mu_{mg} \cdot E(\omega)]}{\omega_{mg} - \omega_p} + \frac{[\mu_{mg} \cdot E(\omega_p)] \mu_{mg}}{\omega_{mg}^* + \omega_p} \right) \exp(-i\omega_p t) \quad (2.7.4)$$

Finally we introduce the linear susceptibility defined through the relation,

$$P_i^1(\omega_p) = \epsilon_0 \sum_j \chi_{ij}^{(1)} E_j(\omega_p) \quad (2.7.5)$$

then $\chi_{ij}^{(1)}(\omega_p)$ becomes

$$\chi_{ij}^{(1)} = \frac{N}{\epsilon_0 \hbar} \sum_m \left(\frac{\mu_{mg}^i \mu_{mg}^j}{\omega_{mg} - \omega_p} + \frac{\mu_{mg}^j \mu_{mg}^i}{\omega_{mg}^* + \omega_p} \right) \quad (2.7.6)$$

Nonlinear optical phenomena are "nonlinear" in the sense that they occur when the response of a material system to an applied optical field. For example, second order harmonic generation occur as a result of the atomic response that scales quadratically with the strength of the applied optical field [7]. In order to describe more precisely what we mean by an optical non linearity, let us consider how the dipole moment per unit volume, or polarization $\vec{P}(t)$, of a material system depends on the strength $\vec{E}(t)$ of an applied optical field.

In nonlinear optics, the optical response can often be described by generalizing equation (2.7.1) by expressing the polarization $\vec{P}(t)$ as a power series in the field strength $\vec{E}(t)$ as

$$\vec{P}(t) = \epsilon_0 [\chi^{(1)} \vec{E}^{(1)}(t) + \chi^{(2)} \vec{E}^{(2)}(t) + \chi^{(3)} \vec{E}^{(3)}(t) + \dots] \quad (2.7.7)$$

The quantities $\chi^{(2)}$ and $\chi^{(3)}$ are known as the second and third order nonlinear optical susceptibility respectively.

2.8 Density Matrix Formalism

We calculate the nonlinear optical susceptibility through the use of the density matrix formulation of quantum mechanics [7]. We use this formalism because of it is capable of treating effects, such as collision broadening of the atomic resonances. That cannot be treated by the simple- theoretical formalism based on the atomic wave function. The density matrix formalism follows from the basic laws of the quantum mechanics. We can describe all of the physical properties of the system in terms of the wave function $\psi_s(\vec{r}, t)$ appropriate to the state. This function obeys the Schrödinger equation.

$$i\hbar \frac{\partial \psi_s(\vec{r}, t)}{\partial t} = \hat{H} \psi_s(\vec{r}, t) \quad (2.8.1)$$

where \hat{H} denotes the Hamiltonian operator of the system. It is represent as

$$\hat{H} = \hat{H}_0 + \hat{V}(t) \quad (2.8.2)$$

where \hat{H}_0 is the Hamiltonian for a free atom and $\hat{V}(t)$ represents the interaction of energy, and Wave function of state as

$$\psi_s(\vec{r}, t) = \sum_n C_n^s(t) U_n(\vec{r}) \quad (2.8.3)$$

The functions $U_n(\vec{r})$ are the energy eigen solutions to the time independent Schrödinger equation. Using equation (2.8.3) in (2.8.1), Schrödinger equation obtain,

$$i\hbar \sum_n \frac{dC_n^s(t)}{dt} U_n(t) = \sum_n U_n^s(t) \hat{H} U_n(\vec{r}) \quad (2.8.4)$$

Multiply equation (2.8.4) from left by U_m^* and integrate over all space.

$$\hat{H}_{mn} = \int U_m^*(\vec{r}) \hat{H} U_n(\vec{r}) d^3\vec{r} \quad (2.8.5)$$

Then we obtain result,

$$i\hbar \frac{dC_m^s(t)}{dt} = \sum_n H_{mn} \hat{C}_n^s(t) \quad (2.8.6)$$

The expectation value of any observable quantity can be calculated in terms of the wave function of the system. The expectation value of $\langle A \rangle$ can be expressed in terms of the probability amplitude $C_n^s(t)$

$$\langle A \rangle = \sum_{mn} C_m^{*s} C_n^s A_{mn} \quad (2.8.7)$$

We define the elements of density matrix of the system by

$$\rho_{nm} = \sum_s \rho(s) C_m^{*s} C_n^s \quad (2.8.8)$$

The density matrix is useful because it can be used to calculate the expectation value of any observable quantity. The expectation value overall possible states of the system to yield,

$$\langle \bar{A} \rangle = \sum_s \rho(s) \sum_{nm} C_m^{*s} C_n^s A_{mn} \quad (2.8.9)$$

Using equation (2.8.8) and (2.8.9) the ensemble average of the quantum mechanical expectation value of the observable quantity A^* becomes,

$$\langle \bar{A} \rangle = \sum_{nm} \rho_{nm} A_{mn} \quad (2.8.10)$$

The double summation in the equation can be simplified as follows:

$$\sum_{nm} \rho_{nm} A_{mn} = \sum_n \left(\sum_m \rho_{nm} A_{mn} \right) = \sum_n (\hat{\rho} \hat{A})_{nn} = \text{tr}(\hat{\rho} \hat{A}) \quad (2.8.11)$$

In order to determine how any expectation value evolves in time, it is thus necessary only to determine how the density matrix itself evolves in time. By direct time differentiation of equation (2.8.8), we obtain that,

$$\dot{\rho}_{nm} = \frac{d\rho_{nm}}{dt} = \sum_s \frac{d\rho(s)}{dt} C_m^{*s} C_n^s + \sum_s \rho(s) \left(C_m^{*s} \frac{dC_n^s}{dt} + \frac{dC_m^{*s}}{dt} C_n^s \right) \quad (2.8.12)$$

For $\rho(s)$ does not vary in time so that the first term in this expression vanishes. We can then evaluate the second term straight forward by using Schrdinger equation. Therefore we obtain,

$$\dot{\rho}_{nm} = \frac{d\rho_{nm}}{dt} = \frac{i}{\hbar} \sum_v (\rho_{nm} H_{vm} - H_{nv} \rho_{vm}) \quad (2.8.13)$$

Finally the summation over v can be performed formally to write this result as commutation relation,

$$\dot{\rho}_{nm} = \frac{d\rho_{nm}}{dt} = \frac{i}{\hbar} (\hat{\rho} \hat{H} - \hat{H} \hat{\rho})_{nm} = \frac{-i}{\hbar} [\hat{H}, \hat{\rho}]_{nm} \quad (2.8.14)$$

when there are certain interactions (such as resulting from collisions between atoms) that cannot conveniently be included in Hamiltonian description, such interaction lead to a change in the state of the system, and hence of no vanishing of $\frac{d\rho(s)}{dt}$. We include such effects in the formalism by adding phenomenological damping terms to the equation of motion (2.8.14) The density matrix equation to have the form

$$\dot{\rho}_{nm} = \frac{d\rho_{nm}}{dt} = \frac{-i}{\hbar} [\hat{H}, \hat{\rho}]_{nm} - \gamma_{nm} (\rho_{nm} - \rho_{nm}^{eq}) \quad (2.8.15)$$

The second term on the right hand side is a phenomenological damping term, which indicates that ρ_{nm} relaxes to its equilibrium value ρ_{nm}^{eq} at rate of γ_{nm} .

Chapter 3

Materials and Methodology

3.1 Materials

An intensive survey of literature from published articles, books, thesis and dissertation was carried out based on the project.

3.2 Methodology

3.2.1 Analytical

In this thesis one of the method or approach used to solve the problem is analytical method. We have determined the energy eigen value of ground and excited state energy of triangular quantum well by exactly solving Schrodinger equation analytically.

3.2.2 Computational

The ground and excited state energy of triangular quantum well for applied electric field was calculated numerically. Both numerical and graphical methods have been used to solve the intended research problem. For numerical calculation and graphical method software's MATHEMATICA and MATLAB were used respectively.

Chapter 4

Energy eigen value of Triangular Quantum Well using Variational Techniques

4.1 Introduction

Semiconductor quantum well have been the object of detailed experimental and theoretical investigations. The studies on quantum heterostructure have opened a new field in fundamental physics, and also provide a wide range of potential application for optoelectronic devices[24]. Quantum well, heterostructures which are classified as low-dimensional semiconductor quantum systems have become an important part with in semiconductor studies[2-20]. The theoretical and experimental investigation gives some possibilities to produce high quality quantum heterostructures. Some visible lasers based on the electronic transition between levels of the conduction band. Among the other quantum heterostructures, the triangular quantum well(s) is also important systems since the absorption coefficient value is reduced in the experimental measurement of the electro absorption when a triangular quantum well is

used. Among the approaches and methods used to study the quantum heterostructures, our formalism is based on solving the schroendinger equation coming from the Hamiltonian written for the case of position of dependent mass. Here, we study, numerically the optical properties of the inter subband transition in ZnMgO/ZnO triangular quantum well nanostructure. Numerically the energy of eigen value of ground and excited states of triangular quantum well are calculated. Depending on this energy eigen value the refractive index and absorpction coefficient are calculated for triangular quantum well by using density matrix formalism.

4.2 Mathematical Formulation of the Problem

The lowest energy eigen values, the ground and first excited states are determined with respect to two trial chosen wave functions. Let us consider the following trial ground and excited state wave functions.

$$\begin{aligned}\psi_0(x, y, z) &= AZe^{\left(\frac{-\alpha z}{2}\right)}\phi_0(x, y) \\ \psi_1(x, y, z) &= BZ\left(1 - \frac{\alpha + \beta}{6}z\right) e^{\left(\frac{-\beta z}{2}\right)}\phi_1(x, y)\end{aligned}\quad (4.2.1)$$

Normalization is given by,

$$\int_{-\infty}^{\infty} \langle \psi^*(z)|\psi(z) \rangle dz = 1 \quad (4.2.2)$$

where A and B are the normalization constants, with

$A = \left(\frac{\alpha^3}{2}\right)^{\frac{1}{2}}$ and $B = \left(\frac{3\beta^5}{2(\alpha^2 + \beta^2 - \alpha\beta)}\right)^{\frac{1}{2}}$ It is observable that both $\psi_0(z)$ and $\psi_1(z)$ are zero at $z=0$, as they should be neither wave functions can penetrate the barrier at the hetro interface if it is very high. Moreover both the ground and excited state wave

functions are orthogonal.

$\phi_0(x, y)$ and $\phi_1(x, y)$ are two dimensional plane-wave functions. On the basic effective mass approximation (m^*), the Hamiltonian of the electron, for the triangular quantum well is given by,

$$\hat{H} = \frac{-\hbar^2}{2m^*} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + V(z) \quad (4.2.3)$$

where

$$V(z) = \begin{cases} eFz, & z > 0 \\ \infty, & z \leq 0 \end{cases}$$

Here z - represents the triangular quantum well's growth direction, F is the magnitude of the applied electric field parallel to z -direction.

A simple variational calculation is to minimize the total energy of the electrons was performed to determine the value of the parameter. The solution of the schrodinger equation for the Hamiltonian (4.2.3) is given by

$$E_{n,k} = E_n + \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) \quad (4.2.4)$$

where k_x and k_y are the wave vectors correspond to the plane waves. E_n is the solution of one dimensional schrodinger equation.

$$H_z \psi_0(z) = E_n \psi_0(z) \quad (4.2.5)$$

where H_z is the z part of the Hamiltonian \hat{H} , and it is given

$$\hat{H}_z = \frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} + eFz \quad (4.2.6)$$

Using the variational technique the ground state energy for triangular quantum well is:

$$\langle \hat{H}_z \rangle = \langle \psi_0 | H_z | \psi_0 \rangle = \langle \psi_0 | \frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} | \psi_0 \rangle + \langle \psi_0 | eFz | \psi_0 \rangle \quad (4.2.7)$$

$$\langle \hat{H}_z \rangle = \langle \hat{K} \rangle + \langle \hat{V} \rangle \quad (4.2.8)$$

In this case

$$K = \langle \psi_0 | \frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} | \psi_0 \rangle \text{ and } V = \langle \psi_0 | eFz | \psi_0 \rangle$$

$$K = \int (\frac{\alpha^3}{2})^{\frac{1}{2}} z e^{-\frac{\alpha z}{2}} (\frac{-\hbar^2}{2m^*}) (\frac{\alpha^3}{2})^{\frac{1}{2}} \frac{d^2}{dz^2} (z e^{-\frac{\alpha z}{2}}) dz$$

$$K = \frac{-\hbar^2}{2m^*} (\frac{\alpha^3}{2}) \int z e^{-\frac{\alpha z}{2}} \frac{d^2}{dz^2} (z e^{-\frac{\alpha z}{2}}) dz$$

$$K = \frac{-\hbar^2}{2m^*} (\frac{\alpha^3}{2}) \int z e^{-\frac{\alpha z}{2}} (\frac{z}{4} \alpha^2 e^{-\frac{\alpha z}{2}} - \alpha e^{-\frac{\alpha z}{2}}) dz$$

$$K = \frac{-\hbar^2}{2m^*} (\frac{\alpha^3}{2}) \int_0^\infty [\frac{1}{4}(z^2 \alpha^2 e^{-\alpha z}) - \alpha z e^{-\alpha z}] dz$$

$$K = \frac{-\hbar^2}{2m^*} (\frac{\alpha^3}{2}) (\frac{-1}{2\alpha}) = \frac{\hbar^2}{2m^*} (\frac{\alpha^2}{4})$$

$$K = \frac{\hbar^2 \alpha^2}{8m^*} \quad (4.2.9)$$

Similarly

$$V = \int_0^\infty (\frac{\alpha^3}{2})^{\frac{1}{2}} z e^{-\frac{\alpha z}{2}} eFz (\frac{\alpha^3}{2})^{\frac{1}{2}} z e^{-\frac{\alpha z}{2}} dz$$

$$V = \frac{\alpha^3}{2} eF \int_0^\infty z^3 e^{-\alpha z} dz$$

$$V = \frac{\alpha^3}{2} eF \frac{6}{\alpha^4} \text{ since } \int_0^\infty z^3 e^{-\alpha z} dz = \frac{6}{\alpha^4}$$

$$V = \frac{3eF}{2\alpha} \quad (4.2.10)$$

substituting equation (4.2.9) and (4.2.10) into equation (4.2.8) then $\langle \hat{H}_z \rangle$ becomes

$$\langle \hat{H}_z \rangle = \frac{\hbar^2 \alpha^2}{8m^*} + \frac{3eF}{2\alpha} \quad (4.2.11)$$

To find α derivate equation (4.2.11) and equate with zero (i.e $\frac{d}{d\alpha}(\langle \hat{H}_z \rangle) = 0$)

$$\begin{aligned}\frac{\hbar^2\alpha}{4m^*} - \frac{3eF}{2\alpha^2} &= 0 \\ \frac{\hbar^2\alpha}{4m^*} &= \frac{3eF}{2\alpha^2} \\ \alpha &= \left(\frac{6eFm^*}{\hbar^2} \right)^{\frac{1}{3}}\end{aligned}\quad (4.2.12)$$

$$E_0 = \langle \hat{H}_z \rangle = \frac{\hbar^2\alpha^2}{8m^*} + \frac{3eF}{2\alpha} \quad (4.2.13)$$

using equation (4.2.12)into (4.2.13)

$$\begin{aligned}E_0 &= \frac{\hbar^2}{8m^*} \left(\frac{6eFm^*}{\hbar^2} \right)^{\frac{2}{3}} + \frac{3eF}{2} \left(\frac{6eFm^*}{\hbar^2} \right)^{\frac{1}{3}} \\ E_0 &= \frac{3(3)^{\frac{2}{3}}}{4(2)^{\frac{1}{3}}} \frac{(eF\hbar)^{\frac{2}{3}}}{m^{*\frac{1}{3}}} = 1.23822 \left(\frac{e^2 F^2 \hbar^2}{m^*} \right)^{\frac{1}{3}}\end{aligned}\quad (4.2.14)$$

The excited state energy, E_1 is determined using the excited state wave function.

$$E_1 = \langle \hat{H}'_z \rangle = \langle \psi_1 | \frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} | \psi_1 \rangle + \langle \psi_1 | eFz | \psi_1 \rangle \quad (4.2.15)$$

Again in equation (4.2.15) $K = \langle \psi_1 | \frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} | \psi_1 \rangle$ and $V = \langle \psi_1 | eFz | \psi_1 \rangle$

$$\begin{aligned}K_1 &= \frac{-\hbar^2}{2m^*} \left(\frac{3\beta^5}{2(\alpha^2 + \beta^2 - \alpha\beta)} \right) \int_0^\infty z \left(1 - \frac{\alpha + \beta z}{6} \right) e^{-\frac{\beta z}{2}} \frac{d^2}{dz^2} \left(z \left(1 - \frac{\alpha + \beta z}{6} \right) \right) e^{-\frac{\beta z}{2}} dz \\ K_1 &= \frac{-\hbar^2}{2m^*} \left(\frac{3\beta^5}{2(\alpha^2 + \beta^2 - \alpha\beta)} \right) \left[\frac{1}{144} \left(\frac{-8(\alpha^2 + \beta^2 - \alpha\beta)}{\beta^3} \right) \right] \\ K_1 &= \frac{-\hbar^2 \beta^2 (\alpha^2 + 7\beta^2 - \alpha\beta)}{24m^* (\alpha^2 + \beta^2 - 2\alpha\beta)}\end{aligned}\quad (4.2.16)$$

$$V_1 = \frac{3\beta^5 eF}{2(\alpha^2 + \beta^2 - \alpha\beta)} \int_0^\infty z^3 \left(1 - \frac{\alpha + \beta z}{6} \right)^2 e^{-\beta z} dz$$

$$V_1 = \frac{eF(5\alpha^2 - 2\alpha\beta + 2\beta^2)}{\beta(\alpha^2 - 2\alpha\beta + \beta^2)} \quad (4.2.17)$$

$$\langle \hat{H}'_z \rangle = \langle \hat{K}_1 \rangle + \langle \hat{V}_1 \rangle \quad (4.2.18)$$

Using equation (4.2.16) and (4.2.17) into (4.2.18) then $\langle \hat{H}'_z \rangle$ becomes,

$$\langle \hat{H}'_z \rangle = \frac{-\hbar^2 \beta^2 (\alpha^2 + 7\beta^2 - \alpha\beta)}{24m^* (\alpha^2 + \beta^2 - 2\alpha\beta)} + \frac{eF(5\alpha^2 - 2\alpha\beta + 2\beta^2)}{\beta(\alpha^2 - 2\alpha\beta + \beta^2)} \quad (4.2.19)$$

Table 4.1: Ground and excited state energies of triangular quantum well for applied electric field.

| $Fx10^7 \frac{v}{m}$ | α | β | $E_0(J)$ | $E_1(J)$ | $\Delta E(E_1 - E_0)(J)$ |
|----------------------|-------------------------|------------------------|---------------------------|--------------------------|---------------------------|
| 1 | 5.48208x10 ⁸ | 1.8696x10 ⁸ | 6.56685x10 ⁻²¹ | 8.997x10 ⁻²⁰ | 0.834x10 ⁻¹⁹ |
| 5 | 9.37423x10 ⁸ | 3.197x10 ⁸ | 1.9202x10 ⁻²⁰ | 2.631x10 ⁻¹⁹ | 2.438x10 ⁻¹⁹ |
| 10 | 1.1811x10 ⁹ | 4.028x10 ⁸ | 3.0481x10 ⁻²⁰ | 4.1761x10 ⁻¹⁹ | 3.871x10 ⁻¹⁹ |
| 15 | 1.352x10 ⁹ | 4.611x10 ⁸ | 3.994x10 ⁻²⁰ | 5.472x10 ⁻¹⁹ | 5.073x10 ⁻¹⁹ |
| 20 | 1.488x10 ⁹ | 5.075x10 ⁸ | 4.8385x10 ⁻²⁰ | 6.629x10 ⁻¹⁹ | 6.145x10 ⁻¹⁹ |
| 25 | 1.603x10 ⁹ | 5.467x10 ⁸ | 5.6146x10 ⁻²⁰ | 7.6925x10 ⁻¹⁹ | 7.13104x10 ⁻¹⁹ |
| 30 | 1.703x10 ⁹ | 5.809x10 ⁸ | 6.340x10 ⁻²⁰ | 8.687x10 ⁻¹⁹ | 8.053x10 ⁻¹⁹ |
| 35 | 1.793x10 ⁹ | 6.116x10 ⁸ | 7.026x10 ⁻²⁰ | 9.627x10 ⁻¹⁹ | 8.924x10 ⁻¹⁹ |
| 40 | 1.875x10 ⁹ | 6.394x10 ⁸ | 7.681x10 ⁻²⁰ | 1.052x10 ⁻¹⁸ | 9.755x10 ⁻¹⁹ |
| 45 | 1.950x10 ⁹ | 6.650x10 ⁸ | 8.308x10 ⁻²⁰ | 1.138x10 ⁻¹⁸ | 10.55x10 ⁻¹⁹ |

Table 4.1 shows the energy eigen value, Transition energy and parameters α and β

4.3 Optical Properties of Triangular Quantum Wells

Triangular quantum wells are formed by continuously changing the allow composition from the center to edge of the wells. The effective masses of electrons and the dielectric constant of materials vary with the allow composition as well as the positions of the electrons. The interest in the quantum wells composed of the II-VI materials has increased, because of their wide band gap and the applications on potential devices such as high brightness blue light emitting diodes and laser diodes. Here, we study numerically the optical properties of the intersubband transitions in ZnMgO/ZnO triangular quantum well nanostructure. The refractive index and absorption coefficient are calculated for triangular quantum well using density matrix formalism. In order to calculate these optical constants we used the ground and excited state energies calculated previous section, which one related to the transition dipole frequencies

$\omega_{ji} = \frac{(E_j - E_i)}{\hbar}$. Moreover, the transition dipole moment $\mu_{ij} = \langle \phi_j(z) | ez | \phi_i(z) \rangle$ is determined. We assume that the system is excited by applying an oscillatory field $\vec{E}(t) = \varepsilon e^{i\omega t}$, Decomposing the Hamiltonian in to the unperturbed Hamiltonian \hat{H}_0 and the time dependent interaction potential $\hat{H}_1(t)$ representing the perturbation.

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t) \quad (4.3.1)$$

where $\hat{H}_1(t) = -\mu \cdot \vec{E}(t)$ The density of matrix operator $\hat{\rho}$ is defined as:

$$\hat{\rho} = |\psi \rangle \langle \psi| \quad (4.3.2)$$

The time evolution of the density matrix operator, including phenomenological damping constant is [7].

$$\left(\frac{d\rho}{dt}\right)_{nm} = \frac{-i}{\hbar} [\hat{H}, \hat{\rho}]_{nm} - \gamma_{nm}(\hat{\rho}_{nm} - \rho_{nm}^{eq}) \quad (4.3.3)$$

where $\left(\frac{d\rho}{dt}\right)_{nm}$ is the nm element the evolution of the density matrix operator, ρ_{nm}^{eq} is the equilibrium value of ρ_{nm} and γ_{nm} is the decay rate of ρ_{nm} .

The electric polarization to the quantum system due to $\vec{E}(t)$ can be expressed as

$$\vec{P}(t) = \epsilon_0 \chi^{(1)}(\omega) \varepsilon(i\omega t) + \epsilon_0 \chi^{(2)}(\omega) \varepsilon(i\omega t) + \epsilon_0 \chi^{(3)}(\omega) \varepsilon(i\omega t) + \dots \quad (4.3.4)$$

The linear response of the triangular quantum well system to the applied fields is determined by the linear susceptibility $\chi^{(1)}$ and given by,

$$\chi^{(1)} = \frac{N |\mu_{ij}|^2}{\epsilon_0} \left[\frac{1}{\Delta E_{ij} - \hbar\omega - i\hbar\gamma_{ij}} \right] \quad (4.3.5)$$

where N is the number of carriers per unit surface.

From the above equation we get,

$$\chi^{(1)} = \frac{N|\mu_{ij}|^2}{\epsilon_0} \left[\frac{\Delta E_{ij} - \hbar\omega + i\hbar\gamma_{ij}}{(\Delta E_{ij} - \hbar\omega)^2 + (\hbar\gamma_{ij})^2} \right] \quad (4.3.6)$$

from equation (4.3.6) the Real and Imaginary are as follows:

$$Re\chi^{(1)}(\omega) = \frac{N|\mu_{ij}|^2}{\epsilon_0} \left[\frac{\Delta E_{ij} - \hbar\omega}{(\Delta E_{ij} - \hbar\omega)^2 + (\hbar\gamma_{ij})^2} \right] \quad (4.3.7)$$

$$Im\chi^{(1)}(\omega) = \frac{N|\mu_{ij}|^2}{\epsilon_0} \left[\frac{\hbar\gamma_{ij}}{(\Delta E_{ij} - \hbar\omega)^2 + (\hbar\gamma_{ij})^2} \right] \quad (4.3.8)$$

The change in the refractive index is related to the susceptibility

$$\Delta n(\omega) = Re \frac{\chi(\omega)}{2n_r} \quad (4.3.9)$$

where n_r is the medium index of refraction.

Using equations (4.3.7) and (4.3.9)

$$\Delta n^{(1)}(\omega) = \frac{N|\mu_{ij}|^2}{2n_r\epsilon_0} \left[\frac{\Delta E_{ij} - \hbar\omega}{(\Delta E_{ij} - \hbar\omega)^2 + (\hbar\gamma_{ij})^2} \right] \quad (4.3.10)$$

where $\Delta E_{ij} = E_j - E_i$ is the energy interval of two different electronic states, μ_{ij} is the dipole matrix element and γ_{ij} is the damping rate.

Absorption coefficient is given by,

$$\beta^{(1)}(\omega) = \frac{\omega Im\chi^{(1)}(\omega)}{n_r c} \quad (4.3.11)$$

The absorption coefficient $\beta^{(1)}(\omega)$ is related to the susceptibility by, using equation (4.3.8) in to (4.3.11) and C is speed of light given by $C = \frac{1}{\sqrt{\mu\epsilon_0}}$ where μ is permeability and ϵ_0 is permittivity of free space, finally absorption coefficient becomes,

$$\beta^{(1)}(\omega) = \frac{\omega}{n_r} \sqrt{\frac{\mu}{\epsilon_0}} \left[\frac{N|\mu_{ij}|^2 \hbar\gamma_{ij}}{(\Delta E_{ij} - \hbar\omega)^2 + (\hbar\gamma_{ij})^2} \right] \quad (4.3.12)$$

where μ is the permeability of the system.

Now will investigate the linear response of the triangular quantum well which is coupled by laser field. We solved the effective mass schroendinger equation already obtained the energy eigen value. Moreover we calculated the transition dipole moment using wave functions. As we know the real and imaginary part of $\chi^{(1)}$ accounts for the linear dispersion and absorption, respectively.

The numerical solution of linear change in refractive index absorption coefficient is carried out for different values transition energies $\Delta E_{ij} = 8.34 \times 10^{-20} J$, $10.17 \times 10^{-20} J$ and $12.15 \times 10^{-20} J$, the transition dipole moment $\mu_{ij} = 2.436 \times 10^{-28} \text{c.m}$, $2.677 \times 10^{-28} \text{c.m}$ and $2.88 \times 10^{-28} \text{c.m}$, $N = \frac{5.0 \times 10^{12}}{\text{cm}^2}$

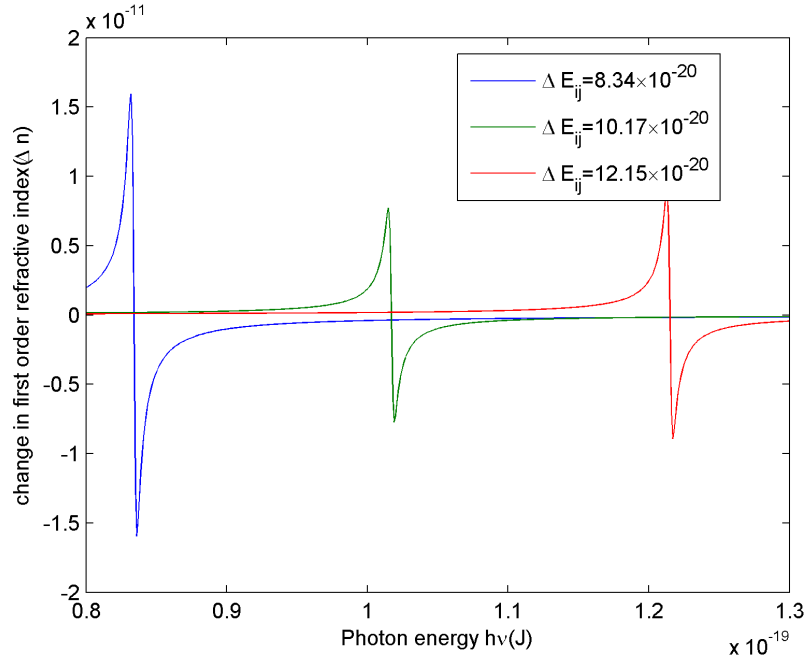


Figure 4.1: The change in first order refractive index ($\Delta n^{(1)}$) versus photon energy ($\hbar\omega$) in (J)

The change in linear refractive index is plotted as a function of photon energy ($\hbar\omega$) for transition energies ($\Delta E_{ij} = 8.34 \times 10^{-20} \text{ J}$, $10.17 \times 10^{-20} \text{ J}$ and $12.15 \times 10^{-20} \text{ J}$ respectively as shown in Figure 4.1. Figure 4.1 describes that the change in linear refractive index depends on the transition energy of triangular quantum well. As the transition energy or frequency increases, the peak of the spectra of the change in refractive index move toward the high energy regions.

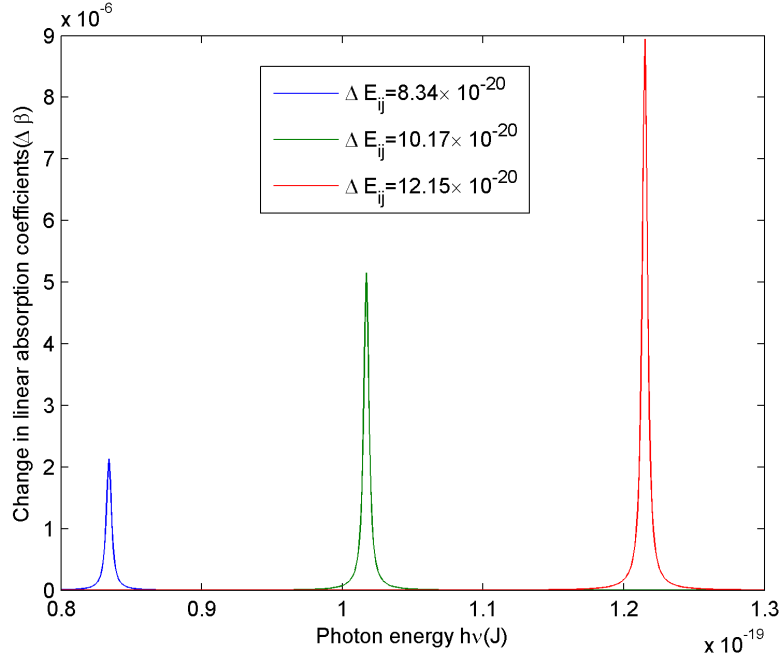


Figure 4.2: The change in linear absorption coefficient ($\Delta\beta^{(1)}$) versus photon energy ($\hbar\omega$) in (J)

In Figure 4.2 the linear absorption coefficient of a triangular quantum well is plotted as a function of photon energy for transition energies of ($\Delta E_{ij} = 8.34 \times 10^{-20} \text{ J}$, $10.17 \times 10^{-20} \text{ J}$, $12.15 \times 10^{-20} \text{ J}$ respectively. As the transition energy increases the peak of the spectra of the change in linear absorption coefficient shows blue shift. Moreover, the magnitude of the absorption coefficient increases with an increment of photon energy.

Chapter 5

Conclusion

In this thesis energy eigen value of triangular quantum well with an applied electric field has been calculated analytically and numerically. We have worked out the ground and excited state energy of triangular quantum well. Depending on this ground and excited state energy and by using a compact density matrix formalism, the change in linear refractive index and absorption coefficient is studied. The energy eigen value increase with an increment of the applied electric field. As the transition energy or frequency increases, the peak of the spectra of the change in refractive index move toward the high energy regions. Moreover, the magnitude of the absorption coefficient increases with an increment of transition energy.

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I hereby declare that this Msc dissertation is my original work and has not been presented for a degree in any other University and that all source of materials used for the dissertation have been duly acknowledged.

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