NONLINEAR OPTICAL PROPERTIES OF ZNO CYLINDRICAL QUANTUM WIRE USING PARABOLIC CONFINING POTENTIAL

By

Maru Zewude

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This is to certify that the thesis prepared by **Maru Zewude** Graduate Studies entitled "**Nonlinear Optical properties of ZnO cylindrical quantum wire using parabolic confining potential**" in fulfillment of the requirements for the degree of **Master of Science in physics(Condensed Matter)** complies with the regulations of the University and meets the accepted standards with respect to originality and quality. .

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Supervisor: _____
Dr. Menberu Mengesha

cosupervisor: _____
Dr. Nebiyu Gemechu

External Examiner _____

To my wife and childern

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Abstract

One of the most intensively explored classes of semiconductor structures is the class of quantum wires. With the advances in semiconductor growth techniques it is possible to fabricate quantum wires of different sizes and geometries from different materials. Cylindrical quantum wire made of ZnO is one of such geometries. This cylindrical structure can be described using a parabolic potential model. In this study the energy eigenvalue of restricted electrons was calculated for ZnO cylindrical quantum wire. Using this energy eigenvalue the nonlinear optical properties such as susceptibility, index of refraction and absorption coefficient were investigated with the help of density matrix formalism. From the result of this study the change in index of refraction $\Delta n(\omega)$ and absorption coefficient $\Delta\beta(\omega)$ were calculated numerically and represented graphiclly. The changes in both cases are the difference of nonlinear and linear. The changes are very large and nonlinear, in general, this tells us our case material(ZnO cylindrical quantum wire) exhibits nonlinear optical properties.

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Chapter 1

Introduction

1.1 General Background

The ancient Greek philosopher Democritus can be considered as a father of modern nanotechnology, since he was the first to use the name "atom" to characterize the smallest particle of matter [1]. In modern history the first practical breakthrough in nanotechnology was made by the American inventor George Eastman, who in 1884 fabricated the first roll film for a camera. This film contained a photosensitive layer of silver bromide nanoparticles. The notion of "nanotechnology" was introduced for the first time by Richard Feynman in 1959 in his famous Caltech lecture "There's plenty of room at the bottom", showing his vision towards small sized. Richard Feynman imagined the world of the nanoscale where the fundamental laws of quantum physics define the behavior of a single atom and control the formation of different structures from individual atoms. Nanotechnology is the art and science of manipulating matter at the nanoscale. Nanotechnology also defined as use of technology to create materials on an atomic scale. It is based on the ability to manipulate individual atoms and molecules in order to assemble them into bigger structures. Such artificial nanoscale structures, usually fabricated using self-assembly phenomena. Therefore, from the

formal point of view nanostructures can be any objects with size (at least in one of the directions) of the order of 100nm or less. Thus, nanostructures are objects whose sizes range from individual atoms (the size of an atom is about 0.1nm) to large clusters consisting of up to 10^8 atoms or molecules. The transition of material structures from macroscale to nanoscale results in sharp changes of their properties. These changes are due to two reasons. The first reason is the increase of the proportion of surface atoms in the structure. The surface of the material can be considered as a special state of matter. The higher the proportion of atoms on the surface, the stronger are effects connected with the surface of a specimen. The ratio of the number of atoms located within a thin near-surface layer($\sim 1nm$)to the total number of atoms in a specimen increases with decreasing volume of the specimen. Also the surface atoms are under conditions, which are very different from the conditions for the bulk atoms, because they are bound to the neighboring atoms in a different way. Atoms in the surface layer have some of their chemical bonds broken and therefore they are free to make new bonds. Recent advances in semiconductor technology have made possible the fabrication of low-dimensional semiconductor heterostructures [2, 3], because the main objects of research in nanoelectronics are quantum-dimensional structures [1]. A low dimensional system is one in which microscopic degrees of freedom of carriers is restricted from moving in the full 3D space due to quantum confinement [4, 5]. The dimensionality refers to the number of degrees of freedom in the electron momentum. Artificial structures where the electrons motion is made to be restricted to move in less than three spatial dimensions, Such structures are called nanostructures [1, 6]. Low dimensional structures can be classified based on the number of dimensions, which are not confined to the nanoscale range dimensions. Such as 2D, 1D, and 0D

are quantum wells, quantum wires, and quantum dots, respectively. In the case when electrons motion along only one direction is limited to nanoscale(for example, along the z-direction) i.e., when the condition, $L_z \leq \lambda$ is satisfied, where λ is the electron de Broglie wavelength, the electron energy states corresponding to this direction are quantized. At the same time, the electrons motion in the other two directions(x- and y-directions) stays free, with the continuous energy spectrum. Such a structure is called a quantum well(QW).

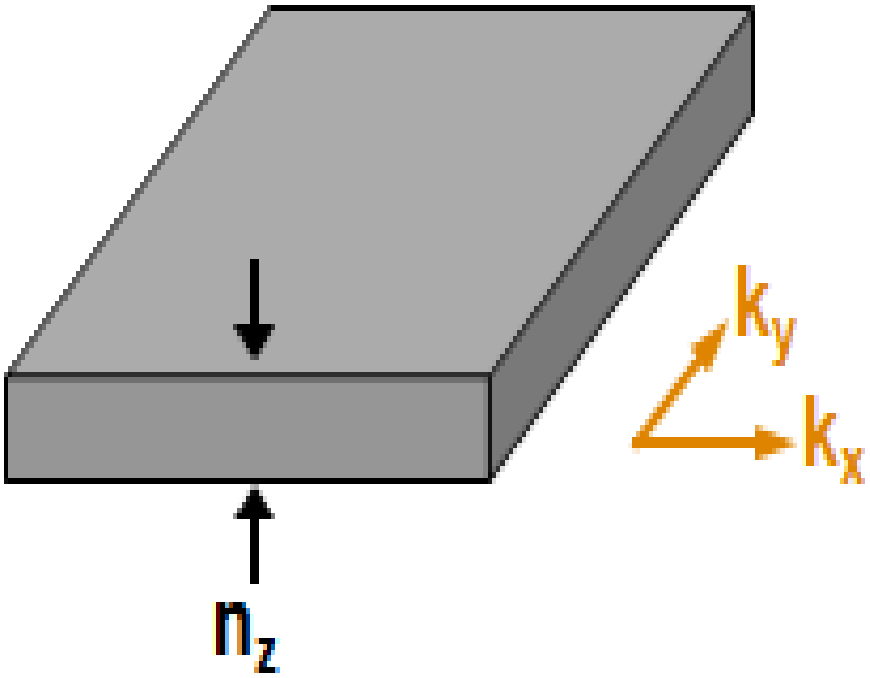

Figure 1.1: Quantum well(thin film)

In the case when the electrons motion is restricted along two directions (for example, along the y- and z-directions), i.e., when the conditions $L_y \leq \lambda$ and $L_z \leq \lambda$ are

satisfied, the energy which corresponds to these two directions of motion is quantized. At the same time, the electrons motion in the other one direction(x-direction) stays free, with the continuous energy spectrum. Such a structure is called a quantum wire (QWR).

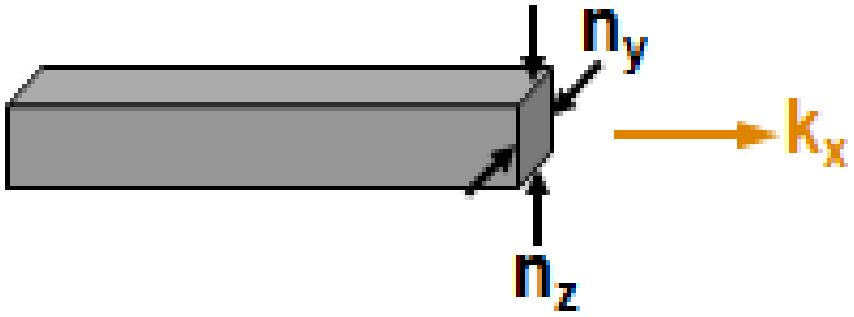

Figure 1.2: Quantum wire

In the case when the electrons motion is restricted along all three directions, i.e., when the conditions $L_x \leq \lambda$, $L_y \leq \lambda$ and $L_z \leq \lambda$ are satisfied, the energy spectrum of such a structure, which is called a quantum dot(QD), is totally quantized. This means reducing the degrees of freedom to zero.

Quantum dots can be regarded as artificial atoms to which the electrons are bound by a "manufactured" confining potential. They are a new class of artificially structured materials with atomic-like discrete states which is ideal for use in laser structures [4, 7]. Usually arrays of such dots are prepared on semiconductor heterostructures, such that all of them contain the same number of electrons. The spatial confinement of carriers enhances the coulomb interaction between the electron and hole, which

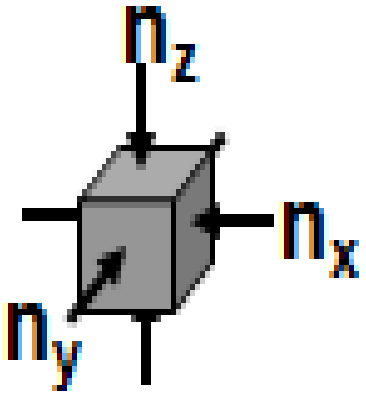

Figure 1.3: Quantum dot

leads to an increase in the exciton binding energy and oscillator strength [8, 9]. As more number of the dimension is confined, more discrete energy levels can be found, that is carrier movement is strongly confined in a given dimesion. The energy band structure of bulk semiconductor materials is almost continuous. In nano-size particles, the bands are split into sublevels because of the quantum confinement. The oscillator strengths increase as the confinement increases from bulk→quantum well→ quantum wire→quantum dot. The oscillator strength can be regarded as a measure of strength of a transition from an initial state with energy E_i to a final state with energy E_f [10]. The smaller the dimensions of the nanostructure (smaller L), the wider is the separation between the energy levels, leading to a spectrum of discreet energies. The band gap of semiconductor materials increase with decreasing size, and discrete energy levels arise at the band age [11]. In general, confinement produces a blue shift of the band-gap. One reason is that quantum confinement of carriers in

the low-dimensional system leads to the formation of discrete energy levels and the drastic changes of physical and chemical properties such as the novel nonlinear optical effects [12]. On the other hand the nonlinear optical properties in the low-dimensional materials have the potential for device applications in laser amplifiers, infrared photo detectors, high-speed electro-optical modulators, light emitting diode, single electron transistors and so on. As we make a semiconductor "crystal" smaller and smaller, the physical properties change in many ways. In a large crystal, the overall shape and size of the crystal make little or no difference to its internal properties. As the crystal becomes smaller, however, the effects of the surface become increasingly important. The most extreme consequence is that as the fraction of atoms at the surface becomes larger, the arrangement of the nuclei changes in order to relax the energy of the system as a whole, i.e., a transition from crystalline to molecular (cluster) behavior takes place [13].

1.2 Statement of the problem

The nonlinear optical properties in the low-dimensional materials have the potential for device applications in laser amplifiers, photodetectors, high-speed electro-optical modulators, and so on [12]. Recent advances in nanotechnology have made it possible to fabricate nanowires of different sizes and geometries [13, 14]. In nanostructures cylindrical surfaces show physical interesting properties. These structures can be described using a parabolic potential model and it is one of the types confining potentials [9, 15]. The parabolic confining potential is also introduced for technological reasons. With recent advances in material growth techniques, such as atomic layer epitaxy, etc., the growth of single atomic layers of good quality has become possible,

which has allowed potential profiles with reasonable shapes such as parabolic shapes and stepped shapes, etc[11]. Most of the studies that are mentioned in [2, 7, 9, 11, 16, 17] have been done on the optical properties of cylindrical quantum wires, with different kinds of confining potential, made of different kinds of materials and using different methods. However in this study we have determined the optical properties of ZnO cylindrical quantum wire in parabolic confining potential using density matrix formalism. The main purpose of this study is calculating the energy eigenvalue of ZnO cylindrical quantum wire, and determining its nonlinear optical properties. Research questions:

- What was the confining potential which we used to describe cylindrical quantum wire?
- How could we calculate energy eigenvalue of confined electrons?
- What are the linear and nonlinear optical properties of ZnO cylindrical quantum wire?
- Which method is important and effective for the determination of optical properties of ZnO cylindrical quantum wire?
- What are the applications of nonlinear optical properties of ZnO cylindrical quantum wire?

1.3 Objectives

1.3.1 General Objective

The general objective of this study is

- To study the nonlinear optical properties of ZnO cylindrical quantum Wire

1.3.2 Specific Objectives

The specific objectives of this study are:

- To calculate energy eigenvalue of ZnO cylindrical quantum wire
- To determine linear and nonlinear susceptibilities of ZnO cylindrical quantum wire
- To determine linear and nonlinear refractive indices of ZnO cylindrical quantum wire
- To determine linear and nonlinear absorption coefficients of ZnO cylindrical quantum wire

1.4 Significance of the study

Optical properties of low-dimensional semiconductor structures are important part of the modern physics of semiconductors. A large number of theoretical and experimental works have been devoted to the study of optical properties in low dimensional semiconductor nanostructures. It is to be noted that the study of optical properties of low dimensional semiconductor structures is important, not only to know, but also in the fabrication and subsequent working of electronic and optical devices based on such systems. Also this study helps us to know the energy eigenvalue and nonlinear optical properties of ZnO cylindrical quantum wire.

1.5 Limitation of the study

Due to time constraint, the scope of this study was limited only to determining nonlinear optical Properties of ZnO cylindrical quantum wire for confide electrons in parabolic confining potential using density matrix formalism.

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Chapter 2

Literature Review

2.1 Introduction

Due to the rapid advances of nanotechnology, it is possible to fabricate low-dimensional quantum system structures, such as quantum wells(QW), quantum wires(QWW), and quantum dots(QD) [12]. Because of their many properties different from bulk system structures, the investigation on low-dimensional semiconductor has attracted much interest in recent years. There are two approaches to fabricate these low dimensional systems. One is the top-down approach where small structures are obtained from a large structure by using lithographic patterning, which is based on the sequential decrease of the object's size for the fabrication of objects of nanoscale size and the other is the bottom-up approach where small structures are made by letting atoms or molecules self-assemble into the desired form [1, 18]. That means the bottom-up technology is based on the self-assembly phenomenon. The main idea of technology is in the development of the controlled self-assembly of the atoms, molecules, and molecular chains into nanoscale objects. The bottom-up technology allows the fabrication of nanoobjects, such as quantum dots, quantum wires, and super lattices [1].

2.2 Quantum wire

One of the most intensively explored classes of semiconductor structures is the class of quantum wires [12]. In a quantum wire the electrons motion is free along the length of the wire while its motion in the plane normal to the length is confined [16, 19]. Quantum confinement of charge carriers in these structures leads to formation of discrete energy levels, the enhancement of the density of states at specific energies and the drastic change of optical absorption spectra [20]. In quantum wires, due to dimension decreasing in contrast to quantum well, the electron hole interaction is enhanced by two-dimensional confinement. As a result, the wave function overlap of the electron and the hole is enhanced, namely, the exciton effect becomes especially prominent. Many authors found that the binding energy and polaronic effect of an exciton are greatly larger in quantum wire than in quantum well and predicted application to electronic and optoelectronic devices. Among the low-dimensional structures, there has been a great deal of interest in the investigation of quantum wires [21]. So far, many investigators studied the properties of quantum wires using several theoretical and experimental methods. The study of quantum wires has been revolutionary in the fundamental sciences due to the potential applications of these structures in the technology of electronic and optoelectronics devices and fundamental physics investigations [17, 21]. We know that Sakaki proposed the concept of quantum wires for the first time in 1975. After this, with the advances in semiconductor growth techniques like chemical lithography, molecular-beam epitaxy, and etching, researchers could fabricate quantum wires of nanometre size with various cross-sections such as circular, V-shape, triangular, parallelogram, T-shape, and hexagonal shape [21, 22]. Recent advances in nanotechnology have made it possible to fabricate nanowires of

different sizes and geometries [1, 14, 23]. Nanowires have a variety of novel properties, rendering them invaluable in diverse disciplines like medicine, optoelectronics and energy physics, among others. However, due to the small dimensions concerned, it is very difficult to fabricate nanostructures with controllable and uniform cross-sectional area, to which some effort has been directed. Apart from the difficulty in fabricating nanowires of uniform cross-sectional area, it may be beneficial to produce nanowires with non-uniform cross-sectional area.

2.2.1 Cylindrical quantum wire

In nanostructures, cylindrical surfaces show physical interesting properties [13]. These structures can be described using a parabolic potential model and it is one of the types confining potentials [9, 15, 16]. The parabolic confinement potential is also introduced for technological reasons. Electron confinement is selected in the form of transverse parabolic potential, since there are no rigid interface boundaries. At the same time according to Kohn theorem, optical properties of the systems are independent of both electron-electron interaction and the number of electrons in the layer; i.e., it can be neglected. The parabolic potential is equivalent to the potential produced by a positive charge uniformly distributed over an infinite layer. However, we note that the Kohn theorem is not true for two basic cases: for multicomponent systems (such as double quantum wells and for a nonparabolic well). In such systems, electronelectron interaction can have a strong effect on the optical properties of electrons. At small values of the radius of the quantum wire the parabolic confining potential can be regarded as a model for the real potential.

2.3 Optical Properties

2.3.1 General optical Properties of semiconductor

A full understanding of the optical properties of semiconductors is thus deeply rooted in the foundations of modern solid-state physics [24]. The optical properties of a semiconductor can be defined as any property that involves the interaction between electromagnetic radiation or light and the semiconductor, including absorption, diffraction, polarization, reflection, refraction, and scattering effects. From the macroscopic viewpoint, the interaction of matter with electromagnetic radiation is described by Maxwell's equations. The optical properties of matter are introduced into these equations as the constants characterizing the medium such as the dielectric constant, magnetic permeability, and electrical conductivity. From our optical viewpoint, we choose to describe the solid by the complex dielectric constant or complex dielectric function $\varepsilon(\omega)$. The complex refractive index is the complex square root of the dielectric function. Its real and imaginary parts are the refractive index n and the extinction coefficient k. These optical constants describe an electromagnetic wave in the medium of propagation; the refractive index n gives the phase shift of the wave, and the extinction coefficient k gives the attenuation of the wave. The field of optical spectroscopy is a very important area of science and technology since most of our knowledge about the structure of atoms, molecules, and solids is based upon spectroscopic investigations. Since the early 1950s, detailed knowledge about the various eigenstates present in semiconductors has emerged including energy bands, excitonic levels, impurity and defect levels, densities of states, energy-level widths (lifetimes), symmetries, and changes in these conditions with temperature, pressure,

magnetic field, electric field, etc. Most optical properties of semiconductors are integrally related to the particular nature of their electronic and vibrational structures. These electronic and vibrational dispersion relations are in turn related to the type of crystallographic structure, the particular atoms, and their bonding. The optical properties of semiconductors are often subdivided into those that are electronic and those that are vibrational (lattice related) in nature. The electronic properties concern processes involving the electronic states of the semiconductor, while the lattice properties involve vibrations of the lattice (absorption and creation of phonons). Lattice properties are of considerable interest for heat dissipation, electronic transport, and lifetimes (broadenings) of electronic states, but it is the electronic properties which receive the most attention in semiconductors because of the technological importance of their practical applications. Modern-day semiconductor optoelectronic technologies include lasers, light-emitting diodes, photodetectors, optical amplifiers, modulators, switches, etc., all of which exploit specific aspects of the electronic optical properties. The phenomena usually studied to obtain information on the optical properties of semiconductors are absorption, reflection or ellipsometry, photoconductivity, emission, light scattering, and modulation techniques.

2.3.2 Optical Properties of quantum wire

Optical and electronic properties of low-dimensional semiconductor structures are important part of the modern physics of semiconductors [24]. The effect of confinement on the electronic and optical properties increases as one goes from quantum wells to quantum dots [23]. A large number of theoretical and experimental works has been devoted to the study of optical properties in low dimensional semiconductor nanostructures [11]. The linear and nonlinear optical properties of low dimensional

semiconductor structures have been widely studied in the last few years, due to their potential applications in optoelectronic and photonic devices [11]. It is to be noted that the study of optical properties of low dimensional semiconductor structures is important, not only to know, but also in the fabrication and subsequent working of electronic and optical devices based on such systems. The decrease in dimensionality of system for semiconductors can lead to a dramatically enhancement of nonlinearities. So the nonlinear optical properties of semiconductor quantum wells, quantum wires, and quantum dots have attracted much attention in the past few years in theoretical and applied physics sides [12]. One reason is that quantum confinement of carriers in the low-dimensional system leads to the formation of discrete energy levels and the drastic changes of physical and chemical properties such as the novel nonlinear optical effects. Another reason is that the nonlinear optical properties in the low-dimensional materials have the potential for device applications in laser amplifiers, photo detectors, high-speed electro-optical modulators, and so on. The confinement of electrons in these systems changes the electron mobility remarkably. This results in a number of new phenomena, which concern a reduction of the sample dimensions. These effects, for example, electron-phonon interaction and scattering rates, the linear and nonlinear optical properties, differ from those in bulk semiconductors.

2.3.3 Optical processes

When light beam incident on optical medium, it may be: reflected, propagated and transmitted [25]. Absorption occurs during the propagation if the frequency of the light is resonant with the transition frequencies of the atoms in the medium. When light of sufficient energy shines on to a material, it induces transitions of electrons from occupied(lower level) states below the Fermi energy to unoccupied(higher level)

states above the Fermi energy. Photon is absorbed by exciting an electron from a lower level to higher level. Therefore optical absorption can lift electrons from completely full valence band to empty conduction band. Exciting electrons in a solid in addition to by photon absorption is exciting electron by other electron. This done by shining a beam of mono energetic electron at a sample. The conduction band and valence band are separated by an energy called band gap $E_g = E_c - E_v$, where E_c and E_v are energy of conduction band and valence band respectively. Absorption can occur $\hbar\omega > E_g$. Absorption can not occur at $\hbar\omega = E_g$, where $\hbar\omega$ is the energy of the photon. 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, $\hbar\omega_n = Een - Ehn$. The energy of the photons matches the difference in electric energy level. It is given by $\hbar\omega_n = E_{e2} - E_{e1}$. Atoms jump to an excited stated state by absorption of photon, then relax to an intermediate state, before re-emitting a photon by spontaneous emission as it falls back to the ground state. In solids this the re-emission process is called luminescence. In other words luminescence is the general name given to the process of spontaneous emission of light by excited atoms in a solid state materials. The photon emitted has a smaller energy than the absorbed photon. This reduction in the photon energy is called Stoke's shift. Note Materials with direct band gaps are better than those with indirect band gaps because their absorption is higher [25]. In a direct band gap semiconductor, large number of electrons are excited from the valence band to conduction band. In semiconductor physics a direct band gap means that

the minimum of the conduction band lies directly above the maximum of the valence band in the k space. In contrast, an indirect semiconductor refers to a semiconductor with a band gap in which the minimum energy in the conduction band is shifted by a k vector relative to the top of the valence band. Indirect transitions(nonvertical transition) Semiconductors such as GaP, Ge, and Si have indirect gaps where the maximum valence band energy and minimum conduction band energy do not occur at the same k value. In this case, the electron cannot make a direct transition from the top of the valence band to the bottom of the conduction band because this would violate conservation of momentum. Such a transition can still take place but as a two-step process requiring the cooperation of another particle and which can then be described by second-order perturbation theory. Semiconductor nanowires (NWs) are usually characterized by anisotropic optical properties like optical absorption, photoluminescence, photoconductivity, as well as generation of higher harmonics, and strongly depend on the polarization of exciting light [26].

2.4 Zinc Oxide (ZnO) and its application in technology

Zinc oxide is a transparent piezoelectric semiconductor which occurs naturally in the mineral called zincite [27]. Zinc oxide(ZnO) is one of II-IV semiconductor material and it is an important semiconductor material with a wide and direct band gap of 3.44 eV at low temperatures and 3.37 eV at room temperature, and it has relatively high Curie temperature, which has a large exciton binding energy of 60 meV at room temperature, even larger than the ionization energy at the same temperature [27-30]. This makes it especially suitable for room temperature optoelectronics in

the near UV spectral region. Having large exaction binding energy of ZnO, implies that it emits more excitons at room temperature when compared to others [31]. Note Materials with direct band gaps are better than those with indirect band gaps because their absorption is higher [25]. In a direct band gap semiconductor, large number of electrons are excited from the valence band to conduction band. ZnO is a key technological material[27, 32], because ZnO has attracted more and more attention due to its interesting properties. The growth of nano sized ZnO, including the ZnO quantum well, ZnO nano wire, and ZnO quantum dots have been investigated widely and used as transparent conductors in solar cell, as a component in UV light emitters and high-power electronics. Recently, ZnO nano structures attracted attention for possible applications in optoelectronic and spintronic devices, such as light emitting and laser diodes, spin-based memory, and logic [33]. When the size of ZnO nano particles is smaller than the Bohr radius, the quantum confinement has a notable influence on the band gap and further causes a series of novel characteristics such as the blue-shift of luminescence in the cathode luminescence(CL) spectrum which implies that ZnO QDs would be applicable to optoelectronic and spintronic devices [34]. In general a partial lists of the properties of ZnO that distinguish it from other semiconductors or oxides: direct and wide band gap, large exciton binding energy, large piezoelectric constant, strong luminescence, the high electron mobility, high thermal conductivity, large non-linear optical coefficients, has high conductance, chemical and thermal stability, a good radiation resistance and is harmless to the environment, it has been also observed that ZnO exhibits exceptionally high radiation hardness, which is important for application at high altitude or in space and so on [27, 30].

2.5 Nonlinear optics

The optical properties of semiconductors at low light levels are often referred to as linear properties in contrast to the nonlinear optical properties described later[24]. There are many physical processes that control the amount of absorption or other optical properties of a semiconductor. In turn, these processes depend upon the wavelength of radiation, the specific properties of the individual semiconductor being studied, and other external parameters such as pressure, temperature, etc. Just as the electrical properties of a semiconductor can be controlled by purposely introducing impurity dopants (both p and n type) or affected by unwanted impurities or defects, so too are the optical properties affected by them. Thus, one can talk about intrinsic optical properties of semiconductors that depend upon their perfect crystalline nature and extrinsic properties that are introduced by impurities or defects.

Properties such as the refractive index, absorption coefficient and reflectivity are independent of optical power [25]. Linear optics [35]:

- Optical properties, such as the refractive index and the absorption coefficient are independent of light intensity.
- The principle of superposition, a fundamental tenet of classical, holds.
- If input A produces response X and input B produces response Y then input (A + B) produces response (X + Y)→ image.
- The frequency of light cannot be altered by its passage through the medium.
- Light cannot interact with light; two beams of light in the same region of a linear optical medium can have no effect on each other.

- Thus light cannot control light.

This approximation is only valid at low power levels [25]. With a high power laser, it is possible to enter a different realm of behavior called nonlinear optics. 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 [33]. In other words nonlinear optics is the study of the interaction of intense laser light with matter [24]. Typically, only laser light is sufficiently intense to modify the optical properties of a material system [33]. The beginning of the field of nonlinear optics is often taken to be the discovery of second-harmonic generation. We are concerned with the effects that light itself induces as it propagates through the medium. Nonlinear optical phenomena are "nonlinear" in the sense that they occur when the response of a material system to an applied optical field depends in a nonlinear manner on the strength of the optical field. For example, second-harmonic generation occurs as a result of the part of the atomic response that scales quadratically with the strength of the applied optical field. Consequently, the intensity of the light generated at the second-harmonic frequency tends to increase as the square of the intensity of the applied laser light. Nonlinear optics (When E is very high) [35]:

- The refractive index, and consequently the speed of light in an optical medium, does change with the light intensity.
- The principle of superposition is violated.
- Light can alter its frequency as it passes through a nonlinear optical material (e.g., from red to blue!).
- Light can control light; photons do interact

The optical properties of materials are described through the real and imaginary parts of the dielectric constant ϵ_r. The dielectric constant is derived from the polarization p of the medium. In linear optics, we assume that P depends linearly on the electric field of the light wave, so that we can write:

$$\overrightarrow{P}(t) = \epsilon_0 \chi \overrightarrow{E}(t) \tag{2.5.1}$$

Where χ is the electric susceptibility. We derive the usual relationship between ϵ_r and 2 χ namely:

$$\epsilon_r = 1 + \chi \tag{2.5.2}$$

In nonlinear optics we consider the possibility that relationship between $\overrightarrow{P}(t)$ and $\overrightarrow{E}(t)$ is more general than that given by equation 2.6.2.

$$\overrightarrow{P}^{nonlinear}(t) = \overrightarrow{P}^{1}(t) + \overrightarrow{P}^{2}(t) + \overrightarrow{P}^{3}(t) + ... \tag{2.5.3}$$

We now introduce nonlinear susceptibility $\chi^{nonlinear}$: $\overrightarrow{P}^{nonlinear}(t) = \epsilon_0 \chi^{nonlinear} \overrightarrow{E}(t)$

$$= \epsilon_0(\chi^{(1)} \overrightarrow{E}(t) + \chi^{(2)} \overrightarrow{E}^2(t) + \chi^{(3)} \overrightarrow{E}^3(t) + ...) \tag{2.5.4}$$

where E is the magnitude of the applied electric field. The various terms in equations 2.6.3 and 2.6.4 correspond directly with each other so that

$$\overrightarrow{P}^{1}(t) = \epsilon_0 \chi^{(1)} \overrightarrow{E}(t) \tag{2.5.5}$$

$$\overrightarrow{P}^{2}(t) = \epsilon_0 \chi^{(2)} \overrightarrow{E}^2(t) \tag{2.5.6}$$

$$\overrightarrow{P}^{3}(t) = \epsilon_0 \chi^{(3)} \overrightarrow{E}^3(t) \tag{2.5.7}$$

Comparing equations 2.6.3 and equation 2.6.5, we see that:

$$\epsilon_r^{nonlinear} = 1 + \chi^{nonlinear} \tag{2.5.8}$$

2.6 Density matrix formalism of the third order susceptibility

We calculate the nonlinear optical susceptibility through use of the density matrix formulation of quantum mechanics [36]. We use this formalism because it is capable of treating effects, such as collisional broadening of the atomic resonances, that cannot be treated by the simple theoretical formalism based on the atomic wave function. Let us begin by reviewing how the density matrix formalism follows from the basic laws of quantum mechanics. If a quantum-mechanical system (such as an atom)is known to be in a particular quantum-mechanical state that we designate S, we can describe all of the physical properties of the system interms of the wave function $\psi_S(r,t)$ appropriate to this state. This wavefunction obeys the Schrdinger equation

$$i\hbar\frac{\partial\psi_s(r,t)}{\partial t} = \hat{H}\psi_s(r,t) \tag{2.6.1}$$

where $\hat{H}$ denotes the Hamiltonian operator of the system. We assume that $\hat{H}$ can be represented as

$$\hat{H} = \hat{H}_0 + \hat{V}(t) \tag{2.6.2}$$

where $\hat{H}_0$ is the Hamiltonian for a free atom and $\hat{V}(t)$ represents the interaction energy. Third-order nonlinear optical interactions (i.e., those described by a $X^{(3)}$ susceptibility) can occur for both centrosymmetric and noncentrosymmetric media. In order to describe more precisely what we mean by an optical nonlinearity, let us consider how the dipole moment per unit volume, or polarization $\overrightarrow{p}(t)$, of a material

system depends on the strength $\overrightarrow{E}(t)$ of an applied optical field. In the case of conventional(i.e, linear) optics, the induced polarization depends linearly on the electric field strength in manner that often be described by the relationship

$$\overrightarrow{p}(t) = \varepsilon_0 \chi^{(1)} \overrightarrow{E}(t) \tag{2.6.3}$$

where the constant of proportionality $\chi^{(1)}$ is known as the linear susceptibility and ε_0 is the permittivity of free space. In nonlinear optics, the optical response can often be described by the polarization $\overrightarrow{p}(t)$ as a power series in the field strength $\overrightarrow{E}(t)$ as

$$\overrightarrow{p}(t) = \varepsilon_0[\chi^{(1)} \overrightarrow{E}(t) + \chi^{(2)} \overrightarrow{E}^2(t) + \chi^{(3)} \overrightarrow{E}^3(t) + ...] \tag{2.6.4}$$

$$\overrightarrow{P}^3(t) = \varepsilon_0 \chi^{(3)} \overrightarrow{E}^3(t) \tag{2.6.5}$$

as the third-order nonlinear polarization. The third-order correction to the density matrix is given by

$$\rho^{(3)}_{nm} = \exp[-(\omega_{nm} + \gamma_n m)t] \int_{-\infty}^{t} \frac{-i}{\hbar} [\hat{V}, \hat{\rho}^2]_{nm} \exp(i\omega_{nm} + \gamma_{nm})t' dt' \tag{2.6.6}$$

where the commutator can be represented explicitly as

$$[\hat{V}, \hat{\rho}^2]_{nm} = -\sum_{\nu} (\mu_{n\nu} \rho^{(2)}_{\nu m} - \rho^{(2)}_{n\nu)} \mu_{\nu m}).\tilde{E}(t) \tag{2.6.7}$$

Expressions for $\rho^{(2)}_{\nu m}$ and $\rho^{(2)}_{n\nu}$ are very complicated, we use the abbreviated notation introduced there:

$$\rho^{(2)}_{\nu m} = \sum_{l} \sum_{pq} K_{\nu l m} \exp -i(\omega_p + \omega_q)t \tag{2.6.8}$$

where $K_{\nu m l}$ has been displayed explicitly. We also represent the electric field as

$$\tilde{E}(t) = \sum_{r} E(\omega_r) e^{-i\omega_r t} \tag{2.6.9}$$

The commutator thus becomes

$$[\hat{V},\hat{\rho}^2]_{nm} = -\sum_{\nu l}\sum_{pqr}[\mu_{n\nu}.E(\omega_r)]K_{\nu ml}e^{-i(\omega_p+\omega_q+\omega_r)t}+\sum_{\nu l}\sum_{pqr}[\mu_{\nu m}.E(\omega_r)]K_{n\nu l}e^{-i(\omega_p+\omega_q+\omega_r)t} \tag{2.6.10}$$

The nonlinear polarization oscillating at frequency $\omega_p+\omega_q+\omega_r$ is given by

$$P(\omega_p+\omega_q+\omega_r) = N\langle\mu(\omega_p+\omega_q+\omega_r)\rangle \tag{2.6.11}$$

We express the nonlinear polarization in terms of the third-order susceptibility defined by

$$P_k(\omega_p+\omega_q+\omega_r) = \epsilon_0\sum_{hij}\sum_{pqr}\chi^{(3)}_{kjih}(\omega_p+\omega_q+\omega_r,\omega_r,\omega_q,\omega_p)\times E_j(\omega_r)E_i(\omega_q)E_h(\omega_p) \tag{2.6.12}$$

where ω_p, ω_q and ω_r are permutation frequencies.

Chapter 3

Materials and Methodology

3.1 Materials

The study is purely theoretical.

- An intensive survey of literature from published articles, books, thesis and dissertation have been carried out.
- MATLAB and MATHEMATICA softwares and computers are the other very important and necessary instruments those have been used for numerical calculations and generation of graphs

3.2 Methodology

3.2.1 Analytical

In this thesis one of the methods or approaches that we have used to solve the problem was analytical method. We have calculated the energy eigenvalues of ZnO cylindrical quantum wire by exactly solving *Schrödinger* equation analytically. And its optical properties have been calculated analytical using density matrix formalism.

3.2.2 Computational(Graphical)

Both numerical and graphical methods have been used to solve the intended research problem. For numerical calculation and generation of graphs softwares MATHEMATICA and MATLAB have been used. Change in index of refraction, absorption coefficient and photon energy are calculated numerically and these numerically calculated values were represented graphically.

Chapter 4

Energy eigenvalue and optical properties of ZnO cylindrical quantum wire

4.1 Introduction

One of the most intensively explored classes of low dimensional semiconductor structures is the quantum wire [23]. In recent years, quantum wires have attracted great attention due to their potential applications in optoelectronic devices and fundamental physics investigations [17]. With the advances in semiconductor growth techniques it has been made possible to fabricate a wide variety of heterostructures with well-controlled dimension and composition. Among heterostructures, quantum wires with rectangular, T-shaped, V-groove, and other cross sections have received lots of attention by researchers during the last decade [20]. Optical and electronic properties of low-dimensional semiconductor structures are important part of the modern physics of semiconductors. The linear and nonlinear optical properties of low dimensional semiconductor structures have been widely studied in the last few years, due to their potential applications in optoelectronic and photonic devices [2]. It is to be noted

that the study of optical properties of low dimensional semiconductor structures is important, not only to know, but also in the fabrication and subsequent working of electronic and optical devices based on such systems [14]. In this study, the selected heterostructure of quantum wire is cylindrical with parabolic confining potential. The energy eigenvalues of ground and excited states of cylindrical quantum wire were calculated. Depending on these energy eigenvalues the refractive index and absorption coefficient are calculated for cylindrical quantum wire by using density matrix formalism.

4.2 Mathematical formulation of energy eigen value

We consider a wire of ZnO with circular cross-section with radius "a" and a length "ℓ" embeded in ZnMgO. The carriers(electrons) are assumed to be confined by symmetric parabolic potential of the form:

$$\phi = \frac{1}{2} m^* \omega_0^2 r^2 \tag{4.2.1}$$

where m^* is the effective mass of electron , and ω_0 is parabolic confinement frequency of the potential well. Electrons in a ZnO cylindrical semiconductor quantum wire with two dimensional parabolic confinement potential along Z direction can be described by the effective mass Hamiltonian in a cylindrical co-ordinate system as:

$$\hat{H} = \frac{-\hbar^2}{2m^*}[\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}] + \frac{1}{2} m^* \omega_0^2 r^2 - \frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} \tag{4.2.2}$$

where m^* is the effective mass of electron in the conduction band of ZnO, ω_0 is parabolic confinement frequency, and the energy is continuous in Z-direction. However, our interest is to calculate energy eigenvalue of discrete energy levels, so that

Hamiltonian for these discrete energy level is:

$$\hat{H} = \frac{-\hbar^2}{2m^*}[\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}] + \frac{1}{2}m^*\omega_0^2 r^2 \tag{4.2.3}$$

Using the dimensionless variable $\rho = \sqrt{\frac{m^*\omega_0}{\hbar}}\ r$, then after some mathematical steps equation(4.2.3)can be rewritten as:

$$\hat{H} = \frac{-1}{2}[\frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho\frac{\partial}{\partial \rho}) + \frac{1}{\rho^2}\frac{\partial^2}{\partial \theta^2}] + \frac{1}{2}\rho^2 \tag{4.2.4}$$

The *Schrödinger* equation for this Hamiltonian is given as:

$$\hat{H}_{nm}\psi_{nm} = \frac{-1}{2}[\frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho\frac{\partial}{\partial \rho}) - \frac{1}{\rho^2}\frac{\partial^2}{\partial \theta^2} - \rho^2]\psi_{nm} = \epsilon\psi_{nm} \tag{4.2.5}$$

where, $\epsilon = \frac{E}{\hbar\omega_0}$. The envelop wave function that can satisfy the above *Schrödinger* equation in this case is given by

$$\psi_{nm}(\rho) = \sqrt{\frac{2n!}{(n+|m|)!}}e^{\frac{-\rho^2}{2}}\rho^{|m|}L_n^{|m|}(\rho^2)\frac{1}{\sqrt{2\pi}}e^{im\varphi} \tag{4.2.6}$$

where, $n = 0, 1, 2, ..., m = 0, \pm1, \pm2, ...$ and $L_n^{|m|}$ are generalized Lagure polynomials. The ground state wave function for parabolic confinement is given by

$$\psi_{00}(\rho) = \frac{1}{\sqrt{\pi}}e^{-\frac{\rho^2}{2}} \tag{4.2.7}$$

and also the ground state energy can be determined using

$$E_{nm} =< \psi_{nm}|\hat{H}|\psi_{nm} > \tag{4.2.8}$$

$E_{00} =< \psi_{00}|\hat{H}|\psi_{00} > =< \psi_{00}|\hat{K}|\psi_{00} > + < \psi_{00}|\hat{V}|\psi_{00} >$

$$E_{00} = \int_0^{2\pi}\int_0^{\infty}\frac{1}{\sqrt{\pi}}e^{-\frac{\rho^2}{2}}[\frac{-1}{2}(\frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho\frac{\partial}{\partial \rho}))]\frac{1}{\sqrt{\pi}}e^{-\frac{\rho^2}{2}}\rho d\rho d\theta + \int_0^{2\pi}\int_0^{\infty}\frac{1}{\sqrt{\pi}}e^{-\frac{\rho^2}{2}}(\frac{1}{2}\rho^2)\frac{1}{\sqrt{\pi}}e^{-\frac{\rho^2}{2}}\rho d\rho d\theta \tag{4.2.9}$$

$E_{00} = \frac{-1}{2}\int_0^{2\pi}\int_0^{\infty} e^{-\frac{\rho^2}{2}}(\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}))]e^{-\frac{\rho^2}{2}}\rho d\rho d\theta + \frac{1}{2}\int_0^{2\pi}\int_0^{\infty} e^{-\frac{\rho^2}{2}}(\rho^3)e^{-\frac{\rho^2}{2}}d\rho d\theta$

$= -\frac{1}{2\pi}(2\pi)(-\frac{1}{2}) + \frac{1}{2\pi}(2\pi)(\frac{1}{2})$

$= \frac{1}{2} + \frac{1}{2} = 1$ in the units of $\hbar\omega$. Therefore,

$$E_{00} = \hbar\omega_0 \tag{4.2.10}$$

The first excited state wave function of cylindrical quantum wire in the parabolic confinement is

$$\psi_{01} = \frac{1}{\sqrt{\pi}}\rho e^{-\frac{1}{2}\rho^2}e^{i\theta} \tag{4.2.11}$$

$$E_{nm} =< \psi_{nm}|\hat{H}|\psi_{nm} > \tag{4.2.12}$$

$E_{01} =< \psi_{01}|\hat{H}|\psi_{01} >$

$=< \psi_{01}|\hat{K}|\psi_{01} > + < \psi_{01}|\hat{V}|\psi_{01} >$, where $\hat{K}$ and $\hat{V}$ are the kinetic energy and potential energy operators of Hamiltonian respectively.

$$E_{01} = E_k + E_v \tag{4.2.13}$$

$$E_k =< \psi_{01}|\hat{K}|\psi_{01} > \tag{4.2.14}$$

$E_k = -\frac{1}{2}\int_0^{2\pi}\int_0^{\infty}\frac{1}{\sqrt{\pi}}\rho e^{-\frac{1}{2}\rho^2}e^{i\theta}(\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2})\frac{1}{\sqrt{\pi}}\rho e^{-\frac{1}{2}\rho^2}e^{i\theta}\rho d\rho d\theta.$

$= -\frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty}\rho e^{-\frac{\rho^2}{2}}e^{i\theta}(\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2})\rho e^{-\frac{\rho^2}{2}}e^{i\theta}\rho d\rho d\theta.$

$$E_k = -1(-1) = 1 \tag{4.2.15}$$

in the units of $\hbar\omega$.

$$E_v =< \psi_{01}|\hat{V}|\psi_{01} > \tag{4.2.16}$$

$= \frac{1}{2}\int_0^{2\pi}\int_0^{\infty}\frac{1}{\sqrt{\pi}}\rho e^{-\frac{1}{2}\rho^2}e^{i\theta}\rho^2\frac{1}{\sqrt{\pi}}\rho e^{-\frac{1}{2}\rho^2}e^{i\theta}\rho d\rho d\theta = \int_0^{\infty}\rho^5 e^{-\frac{\rho^2}{2}}d\rho d\theta$

$$E_v = 1 \tag{4.2.17}$$

in the units of $\hbar\omega$.

$$E_{01} = E_{k_{01}} + E_{v_{01}} = 1 + 1 = 2 \tag{4.2.18}$$

in the units of $\hbar\omega$

$$E_{01} = 2\hbar\omega_0 \tag{4.2.19}$$

4.3 Optical properties of ZnO cylindrical quantum wire using density matrix formalism

In this part the linear and third order nonlinear susceptibility, refractive index and absorption coefficient are calculated using density matrix formalism. Density matrix formalism is capable of treating effects such as collision broadening of atomic resonances, that can not be analyzed by simple theoretical formalism with respect to atomic wave functions. Considering that the charge carriers in a cylindrical ZnO quantum wire are excited by laser field,

$$\overrightarrow{E}(t) = \check{E}e^{iwt} + \check{E}e^{-iwt} \tag{4.3.1}$$

where ω is the frequency of the external field with a polarization vector normal to the quantum wire. The time dependent equation of the density matrix operator is given by

$$\dot{\varrho}_{ij} = (i\hbar)^{-1}[\hat{H}_0 - er\overrightarrow{E}(t), \varrho]_i j - \gamma_{ij}(\varrho - \varrho^{(0)})_i j. \tag{4.3.2}$$

where $\hat{H}_0$ is unperturbed Hamiltonian, e is the electronic charge, $\varrho^{(0)}$ is the unperturbed density matrix and γ_{ij} is the relaxation rate representing the damping due

to the electro-phonon interaction or collision between electrons. The value of the relaxation rate is assumed $\gamma_{ij}= \gamma=\frac{1}{T}$, with T is the relaxation time. For analysis of equation(4.3.2) the usual iterative method is used [36]

$$\varrho(t) = \sum_n \varrho^{(n)}(t) \tag{4.3.3}$$

with

$$\dot{\varrho}_{ij}^{(n+1)} = (i\hbar)^{-1}\{[\hat{H}_0, \varrho^{(n+1)}]_{ij} - i\hbar\gamma_{ij}\varrho_{ij}^{(n+1)}\} - (i\hbar)^{-1}[er, \varrho^{(n)}]_{ij}\check{E}(t) \tag{4.3.4}$$

The electric polarization of the parabolic cylindrical quantum wire due to the time dependent electric field $\check{E}(t)$ can be expanded with respect to equation(4.3.3). We consider only the first three lowest orders, and the second order is usually zero due to the symmetry condition.

$$\overrightarrow{p}(t) = \epsilon_0\chi^{(1)}\check{E}e^{-iwt} + \epsilon_0\chi_{\omega}^{(3)}|\check{E}|^2\check{E}e^{-iwt} + \epsilon_0\chi_{3\omega}^{(3)}\check{E}^3e^{-3iwt} + cc \tag{4.3.5}$$

where $\chi^{(1)}$, $\chi_{\omega}^{(3)}$, and $\chi_{3\omega}^{(3)}$ are the linear and third order and third order harmonic order generation susceptibilities respectively, ϵ_0 is the permetivity of free space. The electronic polarization of the n^{th} order is given by

$$\overline{P}^{(n)}(t) = \frac{1}{V}Tr(\varrho^{(n)}\mu) \tag{4.3.6}$$

where μ is the transition dipole moment. The transition dipole moment is given by

$$\hat{\mu} =< \varphi_{nm}|er|\varphi_{nm} > \tag{4.3.7}$$

V is the volume of the interaction and Tr denotes the summation over the diagonal element of the matrix $\varrho^{(n)}\hat{\mu}$. The analytical expression for $\chi^{(1)}$ and $\chi^{(3)}$ are described by[36]

$$\chi^{(1)} = \frac{1}{\epsilon_0}\frac{N|\mu_{nm}|^2}{E_{nm} - \hbar\omega - i\hbar\Gamma_{nm}} \tag{4.3.8}$$

$$\chi^{(3)} = \frac{1}{\epsilon_0}\frac{N|\mu_{nm}|^2E^2}{E_{nm}-\hbar\omega-i\hbar\Gamma_{nm}}[\frac{4|\mu_{nm}|^2}{(E_{nm}-\hbar\omega)^2+(\hbar\omega)^2}]-\frac{(\mu_{nn}-\mu_{mm})^2}{(E_{nm}-i\hbar\Gamma_{nm})(E_{nm}-\hbar\omega-i\hbar\Gamma_{nm})} \tag{4.3.9}$$

The electric susceptibility $\chi(\omega)$ is connected with the change in refractive index as

$$\Delta n(\omega) = Re\frac{\chi(\omega)}{2n_r} \tag{4.3.10}$$

where n_r is the medium refractive index.

$$\Delta n^{(1)}(\omega) = \frac{1}{2n_r}|\mu_{nm}|^2N[\frac{E_{nm}-\hbar\omega}{(E_{nm}-\hbar\omega)^2+(\hbar\Gamma_{nm})^2}] \tag{4.3.11}$$

and

$$\Delta n^{(3)}(\omega) = \frac{-\mu c}{4n_r\epsilon_0}|\mu_{nm}|^2\frac{NI}{[(E_{nm}-\hbar\omega)^2+(\hbar\Gamma_{nm})^2]^2}\times[4(E_{nm}-\hbar\omega)|\mu_{nm}|^2 \tag{4.3.12}$$

$$-\frac{(\mu_{nn}-\mu_{mm})}{(E_{nm})^2+(\hbar\Gamma_{nm})^2}]\times\{(E_{nm}-\hbar\omega)E_{nm}[E_{nm}-\hbar\omega-(\hbar_\Gamma nm)^2]-\hbar_\Gamma nm)^2(2E_{nm}-\hbar\omega)^2\},$$

where $I = \frac{2n_r}{\mu c}|\check{E}(\omega|^2$, c is the speed of light in free space, N is the carrier density in the system , μ is the permeability of the system and E_{nm} is the energy difference of the two systems, and Γ_{nm} is the inverse of relaxation rate. Similarly the absorption coefficient can be given by

$$\beta^1(\omega) = \omega\sqrt{\frac{\mu}{\epsilon_r}}\frac{|\mu_{nm}|^2N\hbar\Gamma_{nm}}{(E_{nm}-\hbar\omega)^2+(\hbar\Gamma_{nm})^2} \tag{4.3.13}$$

$$\beta^3(\omega) = -\omega\sqrt{\frac{\mu}{\epsilon_r}}(\frac{I}{2\epsilon_0 n_r c})\frac{|\mu_{nm}|^2N\hbar\Gamma_{nm}}{[(E_{nm}-\hbar\omega)^2+(\hbar\Gamma_{nm})^2]^2}\times\{4|\mu_{nm}|^2 \tag{4.3.14}$$

$$-\frac{(\mu_{nn}-\mu_{mm})^2[3E_{nm}-4E_{nm}\hbar\omega+\hbar^2(\omega^2-\Gamma_{nm}^2)]}{E_{nm}^2+(\hbar\Gamma_{nm})^2}\}$$

4.3.1 Numerical results and discussions

In order to clarify the results that have been obtained in this section, we numerically calculated the linear and nonlinear optical absorption coefficients and index of refraction for a ZnO cylindrical quantum wire. The parameters used in our numerical work are : effective mass(m^*) of ZnO $= 0.21m_o \Rightarrow \frac{m^*}{m_0} = o.21$, $\epsilon(ZnO) = 8.5 \Rightarrow n_r = \sqrt{8.5} = 2.92$. The dipole moment(transition)$\approxeq 4.5 \times 10^{-28} cm$. The damping constant $\gamma_{nm} = 5 \times 10^{11}/s$, $\rho_v = 10^{22} m^3$. Since the radius of the cylindrical wire we are interested is 30nm, the relation between the parabolic confinement frequency ω_0 and the radius $a = 30nm$ should satisfy $\hbar\omega_0 = \frac{\hbar^2}{m^* a^2}$. This results in the confining frequency $\omega_0 = 6.16 \times 10^{11}/s$. The transition energy can be calculated: $E_{eg} = 2\hbar\omega_0 - \hbar\omega_0 = \hbar\omega_0 = 6.47429 \times 10^{-23}$.

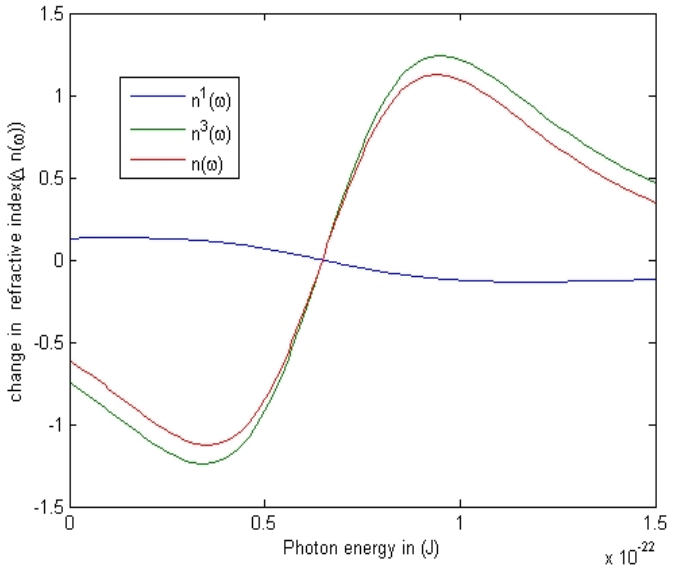

Figure 4.1: The change in refractive index $\Delta n(\omega)$ versus photon energy ($\hbar\omega$) in (J) for ZnO CQWR.

In Fig.4.1 the change in refractive index $\Delta n(\omega)$ versus photon energy $(\hbar\omega)$ in(J) is plotted and the change is nonlinear. The change $\Delta n(\omega)$ is the difference between the nonlinear $n^{(3)}(\omega)$ and linear $n^{(1)}(\omega)$ refractive indices. From the graph, as it has the larger nonlinear than linear, as a result of this the change becomes nonlinear.

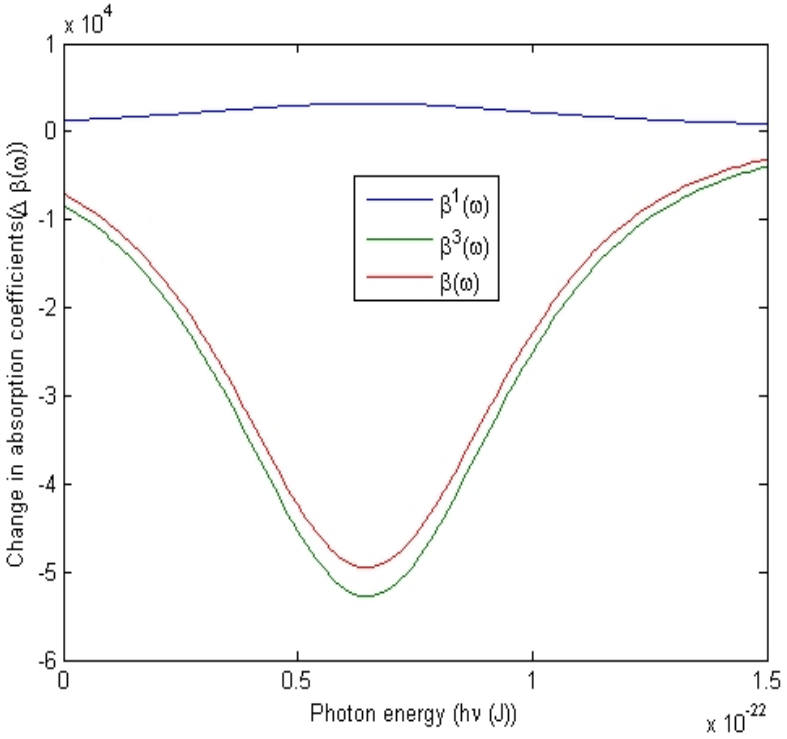

Figure 4.2: The change in optical absorption coefficient $\Delta\beta(\omega)$ versus photon energy $\hbar\omega$ in (J) for ZnO CQWR.

In Fig.4.2 the change in absorption coefficient $\Delta\beta(\omega)$ versus photon energy $\hbar\omega$ in(J) is plotted in parabolic potential well for ZnO cylindrical quantum wire and the change is very large and nonlinear. The change $\Delta\beta(\omega)$ is the difference between the nonlinear $\beta^3(\omega)$ and linear $\beta^1(\omega)$ absorption coefficients .

Chapter 5

conclusion

In this study, the nonlinear optical properties of ZnO cylindrical quantum wire in parabolic confining potential is calculated with help of density matrix formalism. Such nonlinear optical properties are susceptibility, index of refraction and absorption coefficient. These optical properties were calculated using its discrete energy eigenvalues. From the result of this study, the ZnO cylindrical quantum wire has a very large nonlinear $n^{(3)}(\omega)$ and a very small linear $n^{(1)}(\omega)$ indices of refraction. As a result of this change in index of refraction $\Delta n(\omega)$ is very large and nonlinear. And also it has a very large nonlinear $\beta^{(3)}(\omega)$ and a very small linear $\beta^{(1)}(\omega)$ absorption coefficients. As a result of this the change in absorption coefficient $\Delta\beta(\omega)$ is very large and nonlinear. From this point of view we can consider that the changes of both index of refraction and absorption coefficient are very large and nonlinear. These indicate that as a total the material (ZnO cylindrical quantum wire) exhibits nonlinear optical properties in our case. From this point of view we can conclude that due to these its nonlinear optical properties it is very important in modern theoretical and applied physics. So it has the potential for device applications in laser amplifiers, photodetectors, high-speed electro-optical modulators, and so on

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COLLEGE OF NATURAL SCIENCES
PERFORMANCE CERTIFICATE FOR MASTER'S DEGREE

Name of Student: **Maru Zewude** ID No. **RM 1197/09**

Graduate Program: **Regular, MSc.**

1. Course Work Performance

Course Code	Course Title	Cr. hr	Number Grade	Rank **	Remark
Phys799	**MSc. Thesis**	**6**	**78.5**	**Very good**	

Ecellent, Very Good, Good, Satisfactory, Fail.

Thesis Title

Nonlinear optical properties of ZnO cylindrical quantum wire using parabolic confining potential

2. Board of Examiners decision Mark in one of the boxes. Pass [x] Failed [ ]
   If failed, give reasons and indicate plans for re-examination.

   _____

   _____

3. Approved by: Name and Signature of members of the examining Board, and Deans, SGS

Committee member	Name	Signature	Date
Chairman	_____	_____	_____
External Examiner	Dr.Chernet Amente	_____	_____
Internal Examiner	Mr.Tolu Biressa	_____	_____
Major Advisor	Dr.Menberu Mengesha	_____	_____

_____ _____ _____

Department Head, Signature Date

School of Graduate Studies
Jimma University
College of Natural Sciences
MSc. Thesis Approval Sheet

We the undersigned, number of the Board of Examiners of the final open defense by **Maru Zewude** have read and evaluated his/her thesis entitled "**First Principle Calculations Of GaAs Using Density Functional Theory**" and examined the candidate. This is therefore to certify that the thesis has been accepted in partial fulfilment of the requirements for the degree Master of Science in **Physics (Condensed Matter Physics)**.

Name of the Chairperson	Signature	Date
Dr.Menberu Mengesha		
Name of the Major Advisor	Signature	Date
Mr.Tolu Biressa		
Name of Internal Examiner	Signature	Date
Dr.Chernet Amente		
Name of External Examiner	Signature	Date

SCHOOL OF GRADUATE STUDIES