

ENERGY EIGENVALUE AND TUNNELING EFFECT OF RECTANGULAR DOUBLE QUANTUM WELL

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Abstract

In this research paper ,we study the energy eigenvalue and tunneling effect of rectangular double quantum well (RDQW) heterostructures composed of two different semiconductors. The heterostructure is denoted as B/W/B/W/B, where the heterostructure W and B acts as crystal wells and barriers, respectively. This confined heterostructure wells have quantized states. For this research we used analytical method and determined two transdental equations, and numerically we determined the energy eigenvalues of RDQW. We obtained wave states and energy eigenvalues with their transmission and reflection coefficients in the RDQW hetrostructure. However, we have also observed how the width of the wells can affect the transmission by increasing the thickness of the barriers. This study is important in developing photocells, photoswitching devices, optical filters, and other optoelectronic devices.

Chapter 1 Introduction

1.1 Background of the study

In 1924 De Broglie suggested that a particle of momentum p has an associated wave of wavelength λ given by the following $\lambda = \frac{\hbar}{P}$. In considering such one dimensional motion of particle that is restricted by the reflecting well that terminates a region of constant potential energy, such a system is called quantum well. And quantum well might have two type of potential that means finite and infinite at its potential energy. The quantum well can have different geometrical shape. If its geometrical shape of a layer is triangular we call it triangular quantum well, is square we call it square quantum well and is rectangular we call it rectangular quantum well. Its simplest form is single quantum well [1]

Hetrostructure formed from multiple heterojunction, like GaAs/AlGaAs (from III-V) can give us quantum well. If a thin layer of narrower-band gap material, say a sandwich between two layers of wider band gap material and form a double heterojunction. Still more complete structure can be formed such as double quantum well or multiple quantum wells or supper lattice, the difference between the lattices is the extent of the interaction between the quantum well, in particular, a multiple quantum well exhibits the properties of the properties of a collection of isolated single quantum well do interact [1]. In 1928 and 1929 there were published papers pointing out the quantum tunneling [2]. At the same time Gurney was developing idea about resonant tunneling. In 1930's and 1940's there were many attempt to relate the dynamics of the electron current in a system of metal-semiconductor which was used in rectifying the current, to the tunneling of electrons in solid. With the discovery of transistors in 1947, the tunneling of electrons received renewed attention [2]. In 1950 the construction of semiconductor like Ge and Si had advanced to a point that it was possible to manufacture semiconductors of given characteristics [2].

In 1957 L. Esaki discovered tunnel diode and this discovery proved the electron tunneling in solid determinedly. Then in 1960 I. Giaever observed that if one or both of metals are super conduction then voltage-current curve provides fascinating information on the subject of the state of super conductor(s). This experiment of Giaever was sufficiently precise that it enables one to measure the energy gap in superconductor [2]. The other major result was the theoretical work of B.D. Josephson in 1962 connection with the tunneling between two superconductors separated by thin layer of insulating oxide which serves as the barrier and he was able to forecast the existence of second current [2].

A new technique, molecular beam epitaxy (MBE) opened the way to the growth of semiconductors atomic layer up on atomic layer. In 1974 two basic experiments were accepted out: Esaki and Chang reported the oscillatory behavior of the perpendicular differential conductance due to resonant electron tunneling across potential barriers, and theoretical measurement of Dingle showed directly the quantization of energy levels in quantum wells [3] . The negative differential resistance of resonant-tunneling diode (a double barrier diode) was recommended by Tsu and Esaki in 1973, following their pioneering work on super lattices in the late 1960s and early 1970s. Mereover the structure and characteristics of this diode were first established by numerous authors in the early 1980, research interest escalated, partially due to the maturing MBE and metal organic chemical vapor deposition (MOCVD) technologies. In 1985 room temperature of negative differential resistance in this structure was reported [4].

After the first experimental realization of $GaAs/Ga_{1-x}Al_xAs$ made as quantum wells (QWs), and double quantum wells (DQWs) have been a subject of vast theoretical and experimental studies. As QWs show effect of tunneling coupling fairly interestingly, the wave function of the different wells overlap in the barrier region and show splitting of sub-band energy levels. This splitting depends on number of factors such as ratio of well widths, doping concentration, and barrier width etc. The understanding of such quantum wells led to the progress of many new optoelectrical devices such as photodetectors, semiconductor diodes etc [5].

In addition; this development of tunneling effect became means to various devices to be fabricated and by means of the potential profile of a DQW system and multiple quantum wells. Then electric field effects on the refractive index and optical absorption coefficient has been investigated by Kanel in 1987. Chuang and Ahn reported the difference of linear refractive index and absorption coefficients in parabolic quantum well. Linear and nonlinear optical absorption in semiconductor super lattice systems were also lately investigated [5].

In 2010 one study showed that the optical properties namely linear and nonlinear absorption coefficients and changes in the refractive index of DQW system having different well shapes have been studied theoretically in detail for varies quantum well and laser parameters in the existence of external electromagnetic field applied along the growth direction. And it recommended that the external electromagnetic field has influences on absorption coefficients and refractive index and modify quite strongly as compared to the cases in its absences [5].

Recently, there has been a new surge in the field effect of shape of the DQW on optical properties. And also had been reported the effect of asymmetry on its optical properties of a rectangular DQW system in the presence of external electromagnetic field. In addition to asymmetry, the applied static field greatly modifies the energy levels and the transition matrix element between levels [6].

One of the key approaches to understand optical materials with satisfactory value and usefully figure is that of quantum engineering of semiconductor nanostructure. Quantum wells are one instance of hetero-structures complete by joining different materials, usually in large, and with the materials connected directly at the atomic level. This can be achieved by placing a thin layer of semiconductor between two layers of a semiconductor material sandwiched between two layers of another semiconductor. When two semiconductors are connected, it is not clear in advance how the different bands in the two materials will line up in energy with one another, and there is no accurate projecting theory in practice [7].

The rectangular double quantum well is shaped by the alternating GaAs and GaAlAs layers with their different energy gaps. There is much larger barrier with in supper lattice, and a voltage can be functional between two adjacent potential wells to form RDQW. In this study we use Schrödinger equation and its solution to analyze the energy eigenvalue of RDQW. Next we establish the effect of tunneling in the DQW with calculation of transmission coefficient. Finally we illustrate the optical properties of DQW; it is important to find out the absorption coefficient and refractive index; and to analyses symmetry and asymmetry effects and linear and nonlinear photon nature.

1.2 Statement of the problem

For our rectangular double quantum well, we consider a double finite depth potential as an approximation of the GaAs/AlGaAs potential. Next it will be considered that discontinuous potential and its general analytical solution, as well as the continuity and smoothness condition imposed on the solution of the Schrödinger equation by the quantum mechanical postulate. Then, we believe the boundary condition that yield the allowed quantum energy, and we calculate the steps by steps the resultant transcendental equation for the case of infinite depth and energy greater than the barrier height and it is straight forward in addition to accessible to physics students. Then we calculate numerically the allowed energies and construct the first few normalized wave functions and their energy eigenvalue. Finally we describe the transmission and reflection rate and its numerical value in RDQW.

1.3 Objectives

1.3.1 General objectives

The main objective of this study is to determine energy eigenvalue and tunneling property of rectangular double quantum well.

1.3.2 Specific objectives

- Obtaining the energy eigenvalue of rectangular double quantum well.
- Analyzing numerically the energy eigenvalue of rectangular quantum well.
- Obtain the tunneling effects in terms of reflection and transmission coefficients of rectangular double quantum well.

1.4 Significant of the study

The rectangular double quantum well is one of the heterostructures of semiconductors. Heterostructures in general have many uses. They can be used for advanced electronic devices (e.g. Modulation-doper field-effect transistors, heterojunction bipolar transistors, resonant tunneling devices), optical components (e.g. Waveguides, mirrors, micro resonators), and optoelectronic devices and structures (e.g. laser diodes, photo detectors, quantum wells and super lattices optical and optoelectronic devices). Then in our study we make clear the rectangular double quantum wells and its associated application.

1.5 Limitation of the study

The limitation of the study is:

- Time constraint
- Lack of pre-knowledge to access some soft wares
- Lack of effective accessible internet connection

Chapter 2 LITRETURE REVIEW

2.1 Introduction

When one or more of the dimensions of a solid are classified to study, its physicochemical characteristics notably depart from those of the bulk solid. With reduction in size, novel electrical, chemical, mechanical, magnetic, and optical properties can be introduced. The resulting structure is then called a low-dimensional structure(or system). The confinement of particles, usually electrons or holes, to a low dimensional structure leads to a dramatic change in their behavior and to the manifestation of size effects that usually fall into the category of quantum-size effects [8].

The low dimensional mater exhibits new physicochemical properties not shown by the corresponding large-scale structures of the same compositions. Nanostructures constitute a bridge between molecules and bulk materials. Suitable control of the properties and responses of nanostructures can lead to new devices and technologies [8]

2.1.1 Classification of low-dimensional materials

Low-dimensional structures are usually classified according to the number o reduced dimensions they have more precisely, the dimensionality refers to the number of degrees of freedom in the particle momentum. According, depending on the dimensionality, the following classification is made:

- Three-dimensional (3D) structure or bulk structure: No quantization of the particle motion occurs, i.e, the particle is free
- Two-dimensional (2D) structure or quantum well: Quantization of the particles motion occurs in one direction, while the particle is free to move in the other two directions.
- One dimensional (1D) structure or quantum wire: Quantization of occurs in two directions, leading to free movement along one direction.

2.1.2 Why we need quantum mechanics?

As a spatial dimension approaches the atomic scales a transition occurs from the classical law to the quantum mechanical laws of physics [8]. Phenomena that occur on the atomic or subatomic scale cannot be explained outside the framework of quantum mechanical laws. For example: physical behavior at the nanoscale is accurately predicted by quantum mechanical as represented by the Schrödinger equation, which therefore provides a quantitative understanding of the properties of low-dimensional structures. In quantum mechanics, the trajectory of a moving particle loses its meaning when the distance over which potential energy varies is on the order of De Broglie wavelength:

$$\lambda = \frac{2\pi}{\sqrt{2mE}}\hat{h} \tag{2.1.1}$$

The quantum effects of confinement become significant when at least one of the dimensions of a structure is comparable in length to the de Broglie wavelength. If at least one dimension of the solid is comparable to the de Broglie wavelength of the particle motion becomes necessary [8].

2.1.3 Quantum wells

The most significant nanostructure required to design nanoelectronic device are quantum wells, quantum wires and quantum dots. They are the basic building blocks of nanoelectric devices. Nanoelectronic also we are going to control the transfer of electron. But how can to confine them? How to activate them?, how to fix the threshold level for conductance? This entire quantum will be answered when we understand the physics of this quantum structure.

What is quantum well?

The term " well" refers to a semiconductor region that is grown to possess a lower energy, so that it acts as a trap for electrons and holes (electrons and holes gravitate towards their lowest possible energy positions). They are referred to as "quantum well" because these semiconductor region are only a few atomic layers thick; in turn, this means that their properties are governed by quantum mechanics, allowing only specific energies and band gaps. Because quantum well structures are very thin, they can be modified very easily [8].

Quantum wells are real-world implementation of the "particles in the box" problems;

they act as potential wells for charge carriers and are typically experimentally realized by epitaxial growth of a sequence of ultrathin layers consisting of semiconducting materials of varying two dissimilar semiconductors with different band gaps can be joined to form a heterojunction.



Figure 2.1: Quantum well

The discontinuity in either the conduction or the valence band can be used to form a potential well. If a thin layer of a narrower-band gap material "A" say, is sandwiched "B", then they form a double heterojunction. If layer "A" is sufficiently thin for quantum properties to be exhibit, then such a band alignment is called a single quantum well [8].

Additional semiconductor layer can be included in the heterostructures, for example a stepped or asymmetric quantum well can be formed by the inclusion of an alloy between materials A and B. Still more complex structure can be formed, such as symmetric or asymmetric double quantum well and multiple quantum wells or super lattices. The difference between the latter is the extent of the interaction between the quantum wells; in particular, a multiple quantum well exhibits the properties of a collection of isolated single quantum well do interact. The motivation behind introducing increasingly complicated structure in an attempt of tailor the electronic and optical properties of these material for exploitation in devices [8].

2.1.4 potential step

For better understanding of the role that the potential acting, let us consider a simple step potential, in which the potential is define as V(x) as shown in Fig.2.2



Figure 2.2: Schematic view of the potential of which is non-zero card constant only in the positive half space

Thus the potential has a height of V(x) for positive x, and is zero for the negative x-region. This potential creates a barrier to the wave function, and a wave incident from the left (the negative region) will have part (or all) of its amplitude reflected from the barrier. The result that obtained depended up on the relative energy of

the wave. If the energy is less than V(x), the wave cannot propagate in the region of positive x axis. This is clearly seen from the Fig. 2.2; where the wave vector is imaginary for V. Only one exponent can be retained, as we required that the wave can be retained, as we require that the wave function remain finite (but zero) as $x \to \infty$. From Fig.2.2 the various wave vectors are related to the energy of the wave [9]. Let us consider the low-energy case, whose wave is a non propagating wave for x > o. In the negative half -space, we consider the wave function to be the form of,

$$\Psi(x) = A \exp(ikx) + B \exp(-ikx) \tag{2.1.2}$$

Composed of an incident wave (the position exponent term) and a reflected wave (the negative-exponent term). That are, we write the wave function for x < 0 where the energy E and the wave vector K are related by

$$E = \frac{\hbar^2 K^2}{2m} \tag{2.1.3}$$

Then it gives us $K = \sqrt{\frac{2mE}{\hbar^2}}$. This behavior is shown in Fig 2.2. In the positive half-space, the solution of the Schrdinger equation is given by

$$\Psi(x) = C \exp(-\gamma(x)) \tag{2.1.4}$$

where $\gamma = \sqrt{\frac{2m(E-V)}{\hbar^2}}$

Here, we have defined a wave function in two separate regions, in which the potential is constant in each region. These two wave functions must be smoothly joined where at two region meet. While three constant are defined (A, B, C), one of these is defined by the resultant normalized of the wave function (For example let A=1 without loss of generally). Two boundary conditions are required to evaluate the other two coefficient in terms of A. The boundary conditions can vary with the problem, but



Figure 2.3: The various wave vectors are related to the energy of the wave

one must describe the continuity of the probability of occurring at interfere between the two regions. Thus, one boundary condition, as there may not be a sufficient number of constant to evaluate this will be one case in the next section [9]. Equating the derivatives of the wave function at the interface leads to

$$\frac{d\Psi_I}{dx}|_{x=0} = \frac{d\Psi_{II}}{dx}|_{x=0}$$
(2.1.5)

This last equation can be rearranged by placing the momentum term in the determined on the right hand side. Then adding these equations leads to

$$\frac{C}{A} = \frac{2ik}{ik - \gamma} \tag{2.1.6}$$

This result can now be used in, A + B = C. To find

$$\frac{B}{A} = \frac{ik + \gamma}{ik - \gamma} \tag{2.1.7}$$

The amplitude of the reflected wave is unity, so there is no probability amplitude transmitted across the interface. In fact, the only effect of the interface is the plan shift the reflected wave; that the wave function is (x < 0)

$$\Psi_I = A(\exp(ik + ik\theta) \tag{2.1.8}$$

Where $\theta = 2 \arctan(\frac{\gamma}{\kappa})$

The probability amplitude is given by

$$|\Psi|^2 = 2A^2 [1 + 2\cos(2kx + \theta)], X < 0$$
(2.1.9)

2.1.5 Finite quantum well

Now let us turn to the situation in which the potential is finite in amplitude and hence the wave function penetrates to the regions under the barrier. We continue to treat the potential as a symmetric potential centered about the point x = 0. However, it is clear that we want to divide out treatment in to two cases one for energies that lie above the top of the barriers and a second for energies that confine the particle into the potentials which in this regard, the system is precisely like a single finite barrier. When the energy is below the height of the barrier, the wave must decay into the region where the barrier exist [9].// On the other hand, when the energy is greater than the barrier height, the propagating waves exist in all regareds but there is a mismatch in the wave vectores, which leads to the quasi- bount stats and reflection from the interface which begin with the case for the energy below the barrier height, which is the case shown in Fig.2.4. For energies below the potential, (0 < E < V), the particle has free propagating charactertices only for the range |x| < a, for which the schrodinger equation becomes

$$\frac{d^2\Psi}{dx^2} + K^2\Psi = 0 (2.1.10)$$



Figure 2.4: The various wave vectors are related to the wave for the case of $E < V_o$ a quantum well

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. In equation 2.1.10 it must be remembered that V_o is the magnitude of the potential barrier, and is a positively similarly, in the range |x| < a, the Schrodinger equation comes [9]

$$\frac{d^2\Psi}{dx^2} - \gamma^2\Psi = 0 \tag{2.1.11}$$

where $\gamma = \sqrt{\frac{2m(E-V)}{\hbar^2}}$. We saw at the end of the last section that with the potential begin a symmetry quantity, the solution for the schrodinger equation would have either even or odd symmetry. The last the basic properties of section will carry over to the present case and we expect the solutions in the well region to be either sines or cosines. Of course these solutions have the form $\Psi = C \exp(-\gamma |x|)$, |x| < a, we can match this to the proper sine or cosine function. However, in the normal case, both the wave function and its derivative are matched at each boundary. If we attempt to do the same here, this will provide four equations. However, these are only two unknowns the amplitude of C relative to that of either the sine or cosine wave and

the allowed value of the wave vector k and hence since it is not two unknowns-the amplitude of C relative to that of either the sine or the cosine wave and the allowed value of the wave K(and hence since it is not independent of k) for the bound- state energy level. We can get around this problem in one fashion, and that is to make the ratio of the continuous. That is, we make the boundary condition is logarithmic derivative $\frac{\Psi}{\varphi}$ continuous. (This is obviously called the logarithm of Ψ .) Of course, if we choose the solutions to have even or odd symmetry, the redundant, as if is the same as that at these symmetry relations. Let us consider the even-symmetry wave functions for which the logarithmic derivative is

$$\frac{-k\sin(kx)}{\cos(kx)} = -k\tan(kx) \tag{2.1.12}$$

the logarithmic derivative of the damped function is merely $(-\gamma)sgn(x)$ where sgn(x) is the sign of x and a rises because of the magnitude in the argument of the exponent [9]. We note that we can match the boundary condition is just, $k \tan(kx) = \gamma$. This transidental equation now determines the allowed value of the energy for the boundary states. If we define the new, reduced variable then this equation becomes

$$\tan(\xi) = \frac{\gamma}{k} = \sqrt{\frac{\beta^2}{\xi^2} - 1}$$
(2.1.13)

where $\beta^2 = \frac{2mV_0a^2}{\hbar^2}$. The right-hand side of the transcendental equation is a decreasing function, and it is only those values for which the energy lies in the range [9]. In recent years, there is express progress in nanoelectronic which is already on the way to continue the outstanding successes of microelectrics. This became possible among others, due to the development of technologies and techniques. The approach to the semiconductors design comes into being, which perhaps could be termed as smart design and whose aim is to tail the heterostructures shape in order to gain the

predetermined characteristics [1].



Figure 2.5: The graphical solution of single quantum well is indicated by the circle crossings. Here , we have used the value of a = 5nm, $v_o = 0.3ev$, and $m^* = 0.067m_0$, appropriate to a GaAs quantum well between two two layers of GaAlAs. The two circled crossing indicate that there are two even -symmetry solution [9].

Many of the quantum wells and super lattices that are commonly studied today do not occur in nature, but are deliberately structured materials. In the case of super lattices formed by molecular beam epitaxy, the quantum well results from different band gaps of the two constituents materials [11]. The double quantum well (DQW) represents a typical example of a bi-layer system. These structures are characterized by two dimensional translation symmetry amended by an additional binary degree of freedom due to the possible tunneling between layers. The presence of a quantized motion in the growth direction of these structures has a huge impact on their physical properties, which strongly differ from properties of narrow single quantum wells [10]. The quantum well structures are usually realized as sandwich-like semiconductor devices, where the width of individual wells is controlled with the precision of single atomic layers. Among materials used for their preparation appear usually in group of III-V semiconductors type. The most frequent methods of growth are without any double the molecular beam epitaxy (MBE). Other methods such as the metal organic chemical vapor deposition (MOCVD) or the liquid phase epitaxy are now a day very rarely used for the preparation of high quality sample and are especially important in the industrial use. In this thesis we discuss results achieved on rectangular double quantum wells structure by MBE using GaAs/AlGaAs ternary system, which is the most common combination of technology and materials at all. Its materials parameters such as electron and hole effective masses or band offsets are relatively well known [10].

A schematic representation of a semiconductor hetero-structure super lattice is shown as Fig.2.6. Because of the different band gap in the two semiconductors potential well and barriers are formed.

The barrier height in the conduction and valance bands are E_c and E_v respectively. We see that the difference in band gaps between the two semiconductors gives rise to bands. In principle, these band offsets are determined Fermi level are and highly sensitive to impurities, defects change transfer at the heterojunction interface. Because of the different band gap in the two semiconductors potential well and barriers are formed. The barrier height in the conduction and valance bands are E_c and E_v respectively. We see that the difference in band gaps between the two semiconductors gives rise to bands. In principle, these band offsets are determined Fermi level are



Figure 2.6: Heterojunction super lattice of periodicity

and highly sensitive to impurities, defects change transfer at the heterojunction interface [10].

The two semiconductors of a heterojunction super lattice could be different semiconductors such as binding semiconductors with ternary alloy semiconductors such as binary semiconductors with a ternary alloy semiconductor, as GaAs/AlGaAs. The period thicknesses typically vary between a few and many layers $(10\text{\AA} \text{ to } 500\text{\AA})$ The electron states corresponding to the of hetero junction super lattice are two fundamental types bound stats in quantum wells and nearly free electrons states in zone-folded energy bands. Multiple quantum wells will be made subsequently. The eigenfunction and bound state energies of an infinitely deep potential well used as an approximation to the states in two finite wells. The upper well applies to electrons and the lower one to holes. This Fig.2.6 is a schematic representation of quantum well in the GaAs region formed by a adjacent wide gap semiconductor AlGaAs [11].



Figure 2.7: Each super lattice unit cell consists of a thickness L of material AlGaAs, because of the diffracted band gaps a periodic array of potential well and potential barrier is formed.

GaAs/AlGaAs is the most popular material combination used as rectangular double quantum well structure semiconductor type. It is geometrically at the middle this quantum well thickness is typically around 5nm, and the barrier layer ranges from 1.5nm-5nm [3]. The rectangular double quantum well semiconductor can serve as a filter, which only transmits electrons of energy close to the determinable resonance value [2].

The application of double quantum well is also exist in emitting laser light in wide range of wavelength including $1.3\mu m - 1.5\mu m$ which is very useful in optical communication. It also use to terahertz detectors fabrication [5]



Figure 2.8: The eigenfunction and bound states energies of a infinitely deep potential well used as approximation to the states in two finite quantum wells

2.2 Energy eigenstate and energy eigenvalue of the Schrödinger equation for RDQW

The main equation of non-relativistic quantum mechanics is known as the Schrödinger equation. It allows us to find the wave state of a particle or system of particles in a stationary state as well as its evolution in time. This equation has an operator form since in quantum mechanics each physical quantity corresponds to own operator. The description of an electron's behavior is very simple if the corresponding probability current density, J, is constant.

In this case we studies and determines the electron wave function $\Psi(x)$ that is the solution of Schrödinger equation. Depending on the configuration of the potential with in which the electron motion take place, the solution of the time-independent Schrödinger equation defines the allowed energy state and corresponding wave functions. In the complete energy eigenvalue study of the rectangular double quantum well determine of its eigenstates important. The Schrödinger equation in one dimension for the particles of interest in quantum well is

$$\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$
(2.2.1)

Here is the structure potential or quantum well. The technology of fabrication of planer layer structures with given physical properties allows the experimental realization of the confinement of electrons inside potential well of various profile for practical realization are two-dimensional potential profile of rectangular double quantum well can be studied by dividing it into five region the quantum well, and setting general differential equation from Schrödinger equations can be constructed a general solution. The boundary condition of the potential is taken

$$V(x) = \begin{cases} 0, \ 0 < x < L, \ 0 < x < L \\ V_o, \ \text{otherwise} \end{cases}$$
(2.2.2)

Where V_o is the depth or dissociation energy and it is also the height of the central separating two equivalent spatial regions. Also notice that the potential is an even function of position. Due to this symmetry, the solution of Schrödinger equation is either odd or even function of position. Then considering the five potential regions we determine the energy eigenfunction using SE. These functions are well known sine and cosine, or the hyperbolic sine and cosine functions. And they are general solution of the SE in each potential region. In these linear combination functions we have six unknown coefficients that must be determined. These coefficients must be determined and should satisfy the required conditions at the region of boundaries. And about eight conditions help us to determine the ten coefficients of the general solution of the SE for DQW potential. The boundary conditions can complete the general solution of SE [12].

The quantum system allow only a discrete set of energies, $\{E_n\}$. And these E_n are consistent with the continuity and smoothness conditions at the potential boundaries. The most familiar boundary condition requires as in the case of the particle in a box, that the wave function become extinct at the edge of the box. Our derivation of boundaries equation gives us that

$$\eta = \frac{\xi^2 \cosh(\eta \frac{a}{L}) - \eta^2 \sinh(\eta \frac{a}{L})}{\xi \cot(\xi(1 - \frac{a}{l})) \exp(\eta \frac{a}{L})}$$
(2.2.3)

Where $\eta = k_1 L = \sqrt{\frac{2m^*(E-V_o)}{\hbar^2}}L$ and $\xi = k_2 L = \sqrt{\frac{2m^*E}{\hbar^2}}L$ for E < V then following the super lattice description curves the energy E of a particle as a function of its wave vector k, this can be solved numerically using a dimension [8]. And we fix the value of the mass, the length of the thickness and the height of the barrier, and the depth of the potential and E. And only a finite number of energies satisfy the relation expressed by Eq.2.2.3 [12].

2.3 Tunneling through a rectangular DQW

Quantum mechanics predict that even if the system has a finite probability to cross or tunnel the barrier to the other side of the potential barrier. For GaAs/AlGaAs there is minimum potential and quantum tunneling. Using the quantum tunneling effect and taking into account the tunneling of particle of mass, m, and energy, E, through an arbitrary potential barrier V_o , denoting the classical tunneling point and, the transmission coefficient is defined by relations [2],

$$T = \left|\frac{E}{A}\right|^2 = \left[1 + \left(\frac{1}{4}\left(\frac{k_1}{k_2} + \frac{k_2}{k_1}\right)^2\right)sinh^2 2k_1 a\right]^{-1}$$
(2.3.1)

Where E and A are coefficients of transmission and incident wave, respectively; and k_1 and k_2 are wave vectors at barrier and well, respectively. The double well is the simple system in which resonant tunneling involves coupling between two localized energy levels in addition to coupling between the continuums of energies in the potential well so it serves as a model for tunneling through super lattice. The results are important of the quantum wells and the electrons when optimize the performance of super lattice tunneling devices [13].

It can be seen that, away from a resonance an increasing barrier height read, as would be expected, to a decrease in the transmission coefficient T [14]. Tunneling through a barrier is described in terms of transmission coefficient which defined as the probability that any single electron impinging on barrier structure will tunnel and supply to the current flow through the barrier. Frey has produced a comprehensive analysis of transmission coefficient for rectangular double quantum well [2]. One important aspect of the resonance tunneling is structure is the traversal of the electron from one end of the device to the other tunneling process [15].

Quantum wells derive most of their special properties from the quantum confinement of charge carriers ("electrons" and "holes") in thin layers (e.g. 40 atomic layers thick) of one semiconductor "well" material sandwiched between other semiconductor "barrier" layers. They can be made to a high degree of precision by modern epitaxial crystal growth techniques. Many of the physical effects in quantum well structures can be seen at room temperature and can be exploited in real devices. For quantum well, the valance bands are known as the heavy and light hole bands. Notably for quantum wells, the electrons in the conduction band, and the positively charged in the valence band behave with valuable masses different from the free electron mass [16].

Chapter 3 Materials and Methodology

3.1 Materials

The study is purely theoretical. For understanding the energy eigenvalue and the tunneling effect of rectangular double quantum wells an intensive literature review is carried out. The main sources of 'literature review are the published articles, books, thesis and dissertations. MATLAB and MATHEMATICA software's and computers are additional instruments used to accomplish this 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. That is the Schrödinger equation of rectangular double quantum wells was solved using variational technique analytically.

3.2.2 Computational

The energy eigenvalue and tunelling effect of the rectangular double quantum wells for different values of variational Parameters was calculated numerically.

Chapter 4

Energy Eigen value of rectangular double quantum well

4.1 Introduction

Many of the quantum wells and superlattices that are commonly studied today do not occur in nature, but rather are deliberately structured materials. In the case of superlattices formed by molecular beam epitaxy, the quantum wells result from the different band gaps of the two constituent materials. The additional periodicity is in one dimension (1D) which we take along the x-direction, and the electronic behavior is usually localized on the base planes (x-y planes) normal to the x-dimensional behavior.

A schematic representation of a semiconductor hetrostructure superlattice is shown in Fig.4.1. where d is the superlattices periodicity composed of a distance 2a or, of semiconductor s_1 , and L of semiconductor s_2 . Because of the different band gaps in the two semiconductors, potential wells and barriers are formed. For example in the Fig.4.1., the barriers height in the conduction and valance bands are $\Delta(E_c)$ and $\Delta(E_v)$ respectively. We see that the difference in bandgaps between the two semiconductors gives rise to band offsets and for the conduction and valance bands. In principle, these band offsets ΔE_c and ΔE_v are determined by matching the Fermi levels for the two semiconductors. In actual materials, the Fermi levels are highly sensitive to impurities, defects and charge transfer at the heterojunction interface. The two semiconductors of a heterojunction super lattice could be different semiconductors such as InAs with GaP or a binary semiconductor with a ternary alloy

conductors such as InAs with GaP or a binary semiconductor with a ternary alloy semiconductor, such as GaAs with AlGaAs. In the typical semiconductor superlattices the periodicity d = 2a + L is the repeated many times. The period thicknesses typically vary between a few layers and many layers. Semiconductors superlattices are totally an extremely active research field internationally. The electronic states corresponding to the heterojunction superlattices are of two fundamental types-bound states in quantum wells and nearly free electron states in zone-folded energy bands. In this course, we limit our discussion to the band states a double finite quantum wells. Bound Electronic states From Fig.4.1 we see that the heterojunction superlattices consist of array of potential wells. The interesting limit to consider is the case where the width of the potential well contains only a small number of crystallographic unit cells, in which case the number of the bound states in the well is a small number.

4.2 Mathematical formulation of the problem

From a mathematical stand point, the our case to consider is a finitely deep rectangular well. In this case, a particle of mass m* in a well of width L in the x direction satisfies the free particle Schrodinger equation as:-

Analytic solution: for rectangular double quantum well potential region, there are five special regions and we construct general analytical solutions from the Schrödinger



Figure 4.1: Rectangular double quantum well with barrier thickness 2a and width of wells L

equations. Even through the rectangular double quantum well potential is discontinuous function of position, it gives an appropriate description of the continuous double minima potential. It is a simplified model of potential found in molecular chemical systems where possible double rectangular well potential is described by the following piecewise constant potential in one dimension.

 V_o is the depth or dissociation energy and the height of the central barrier separating two equivalent spatial regions. In region(I) for $-\infty < x \leq -L$, the Schrdinger equation is

$$\frac{-\hbar^2}{2m^*}\frac{d^2\Psi_I}{dx^2} + V_o\Psi_I = E\Psi_I$$
(4.2.1)

For $E < V_o$ (that is classically forbidden region)

 $\frac{d^2\Psi_I}{dx^2} = k_1 \Psi_I$ with $k_1 = \sqrt{\frac{2m^*(v_o - E)}{\hbar^2}}$. The solution in this region is

$$\Psi_I = A e^{k_1 x} \tag{4.2.2}$$

In region (II) for -L < x < -a, the Schrödinger equation is

$$\frac{-\hbar^2}{2m^*} \frac{d^2 \Psi_{II}}{dx^2} = E \Psi_{II} \tag{4.2.3}$$

the general solution of this equation is,

$$\Psi_{II} = Be^{ik_2x} + ce^{-ik_2x} \tag{4.2.4}$$

with $k_2 = \sqrt{\frac{2m^*E}{\hbar^2}}$. In region(III), $(-a) \le (x) \le (a)$, the Schrödinger equation is ,

$$\frac{-\hbar^2}{2m^*} \frac{d^2 \Psi_{III}}{dx^2} + V_o \Psi_{III} = E \Psi_{III}$$
(4.2.5)

The general solution of this Schrodinger equation is ,

$$\Psi_{III} = De^{k_1 x} + Ee^{-k_1 x} \tag{4.2.6}$$

In region (IV) for a < x < L, the Schrödinger equation is,

$$\frac{-\hbar^2}{2m^*} \frac{d^2 \Psi_{IV}}{dx^2} = E \Psi_{IV} \tag{4.2.7}$$

And this solution is

$$\Psi_{IV} = F e^{ik_2 x} + G e^{-ik_2 x} \tag{4.2.8}$$

In region(V), $L \leq (x) < \infty$, the Schrödinger equation is,

$$\frac{-\hbar^2}{2m^*}\frac{d^2\Psi_V}{dx^2} + V_o\Psi_V = E\Psi_V \tag{4.2.9}$$

and its solution is

$$\Psi_V = H e^{-k_1 x} \tag{4.2.10}$$

Generally it is known that the wavefunction and the slope of the wavefunction must be continuous every where matching at the step x = -L, x = -a, x = a and x = Lgives

$$B = \frac{1}{2} \left(1 + \frac{k_1}{ik_2}\right) A e^{-k_1 L + ik_2 L}$$
(4.2.11)

$$C = \frac{1}{2} \left(1 - \frac{k_1}{ik_2}\right) A e^{-k_1 L - ik_2 L}$$
(4.2.12)

$$F = \frac{1}{2} \left(1 - \frac{k_1}{ik_2}\right) H e^{-k_1 - ikL_2L}$$
(4.2.13)

$$G = \frac{1}{2} \left(1 + \frac{k_1}{ik_2}\right) H e^{-k_1 - ikL_2L}$$
(4.2.14)

$$D = \frac{1}{2} \left(1 + \frac{ik_2}{k_1}\right) B e^{-ik_2 a + k_1 a} + \frac{1}{2} \left(1 - \frac{-ik_2}{k_1}\right) C e^{ik_2 a + k_1 a}$$
(4.2.15)

$$E = \frac{1}{2}\left(1 - \frac{ik_2}{k_1}\right)Be^{-ik_2a - k_1a} + \frac{1}{2}\left(1 + \frac{-ik_2}{k_1}\right)Ce^{ik_2a - k_1a}$$
(4.2.16)

$$D = \frac{1}{2} \left(1 + \frac{ik_2}{k_1}\right) F e^{ik_2 a - k_1 a} + \frac{1}{2} \left(1 - \frac{-ik_2}{k_1}\right) G e^{-ik_2 a - k_1 a}$$
(4.2.17)

$$E = \frac{1}{2} \left(1 - \frac{ik_2}{k_1}\right) F e^{ik + 2a + k_1 a} + \frac{1}{2} \left(1 + \frac{-ik_2}{k_1}\right) G e^{-ik_2 a + k_1 a}$$
(4.2.18)

Replacing equation (4.2.11) and (4.2.12) for B and C in equation(4.2.15) and we obtain

$$D = \frac{A}{2}e^{k_1(a-L)}\left[2\cos(k_2(a-L) + (\frac{k_2^2 - k_1^2}{k_1k_2})\sin(k_2(a-L))\right]$$
(4.2.19)

Similarly replacing equations (4.2.11) and (4.2.14) for B and C in equation (4.2.16)

$$E = \frac{-A}{2} e^{-k_1(a+L)} \left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right) \sin(k_2(a-L))$$
(4.2.20)

Inserting equations (4.2.13) and (4.2.14) in to equation(4.2.17) we obtain

$$D = \frac{-H}{2} \left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right) \left(e^{-k_1(a-L)}\right) \sin(k_2(a-L))$$
(4.2.21)

Using the same fashion inserting equations (4.2.13) and (4.2.14) in equation (4.2.18) we obtain

$$E = \frac{H}{2} e^{k_1(a-L)} [2\cos(k_2(a-L) + \frac{(k_2^2 - k_1^2)}{k_1 k_2)}\sin(k_2(a-L))]$$
(4.2.22)

Equating (4.2.19) and (4.2.20)

$$A[2k_1k_2\cos(k_2(a-L)) + (k_2^2 + k_1^2\sin(k_2(a-L)))]e^{k_1a} = H(k_1^2 + k_2^2)\sin(k_2(a-L))e^{-k_1a}$$
(4.2.23)

Similarly relating (4.2.20) and (4.2.22)

$$A[(k_1^2 + k_2^2)\sin(k_2(L-a)]e^{-k_1a} = H[2k_1k_2\cos(k_2(L-a)) + (k_1^2 - k_1^2)\sin(k_2(L-a))]e^{k_1a}$$
(4.2.24)

After some mathematical manipulation (4.2.23) and (4.2.22) becomes

$$A[2k_1k_2\cot(k_2(L-a)) + (k_1^2 - k_2^2]e^{k_1a} - H(k_1^2 + k_2^2)e^{-k_1a} = 0$$
(4.2.25)

$$A[(k_1^2 + k_2^2)](e^{-k_1 a}) - H[2k_1k_2\cot(k_2(L-a)) + (k_1^2 - k_2^2)e^{k_1 a}] = 0$$
(4.2.26)

The solution of the determined of equation (4.2.25) and (4.2.26) is

$$[2k_1k_2\cot(k_2(L-a) + (k_1^2 - k_2^2)]e^{k_1a} = \pm (k_1^2 + k_2^2)e^{-k_1a}$$
(4.2.27)

From this we infer that we have two transdental equations,

$$k_1 k_2 \cot(k_2 (L-a)) e^{k_1 a} = k_2^2 \cosh(k_1 a) - k_1^2 \sinh(k_1 a)$$
(4.2.28)

and

$$k_1 k_2 \cot(k_2 (L-a)) e^{k_1 a} = k_2^2 \sinh(k_1 a) - k_1^2 \cosh(k_1 a)$$
(4.2.29)

Using dimensionless variables $\eta = k_1 L = \sqrt{\left(\frac{2m^*(v_o - E)}{\hbar^2}\right)}L$ and $\xi = k_2 L = \sqrt{\left(\frac{2m^*E}{\hbar^2}\right)}L$, we have

$$\eta^2 + \xi^2 = \frac{2m^* v_o L^2}{\hbar^2} = R^2 \tag{4.2.30}$$

Rewriting equations (4.2.28) and (4.2.29) with dimensionless variables ξ and η

$$\eta \xi \cot[\xi(1-\frac{a}{L})]e^{\eta \frac{a}{L}} = \xi^2 \cosh(\eta \frac{a}{L}) - \eta^2 \sinh(\eta \frac{a}{L})$$

$$(4.2.31)$$

$$\eta \xi(\xi(1-\frac{a}{L}))e^{\eta \frac{a}{L}} = \xi^2 \sinh(\eta \frac{a}{L}) - \eta^2 \cosh(\eta \frac{a}{L})$$

$$(4.2.32)$$

$$\eta = \frac{\xi^2 \cosh(\eta \frac{a}{L}) - \eta^2 \sinh(\eta \frac{a}{L})}{\xi \cot(\xi(1 - \frac{a}{L}))e^{\eta \frac{a}{L}}}$$
(4.2.33)

$$\eta = \frac{\xi^2 \sinh(\eta \frac{a}{l} - \eta^2 \cosh(\eta \frac{a}{L}))}{\xi \cot(\xi(1 - \frac{a}{L}))e^{\eta \frac{a}{L}}}$$
(4.2.34)

If we measure E in terms of V_o , then $\xi = R\sqrt{\frac{E}{v_o}}$ and $\eta = R\sqrt{1-\frac{E}{v_o}}$

4.3 Numerical Solution

The energy eigenvalues are found from a numerical or graphical solution of equations(4.2.33) and (4.2.34) with definitions k_1 and k_2 in the previous section. The graphical method for analytical equation that described in the previous section. The graphical method for describing the solution is given here as it reveals the way in which the number of is create energy levels depend on V_o an L. Further more tunneling effect over the barrier depends on the width of the barrier a and the potential V_o . In equation(4.2.30) ξ and η are restricted to position values, the energy levels may be found in this form the inter sections in the first quadrant of the curve of known radius $R = \sqrt{\frac{2m^*V_ol^2}{\hbar^2}}$. Similarly the odd part of the same circle with the curve of equation (4.2.34) in the first quadrant. For the values of $\frac{a}{l}=0.1$, 0.01, and 0.001 and $V_oL^2 = \frac{\hbar^2}{2m^*}$, $4\frac{\hbar^2}{2m^*}$ and $12\frac{\hbar^2}{2m^*}$, the graphical solutions are demonstrated in Fig.4.2, Fig.4.3, and Fig.4.4 respectively. In this computation the height of the barrier is given in units of $\frac{\hbar^2}{2m^*L^2}$.



Figure 4.2: Energy eigenvalues of even and odd and eigen states with $\frac{a}{L} = 0.1$



Figure 4.3: Energy eigenvalues of even and odd and eigen states with $\frac{a}{L} = 0.01$



Figure 4.4: Energy eigenvalues of even and odd and eigen states with $\frac{a}{L} = 0.001$

The intersection point(at which we determined our energy eigenvalue) of the graphes and the energy eigenvalues for different barrier width are explained in Table 1.

$\frac{a}{L}$	ξ_n	η_n	E_n in $\frac{\hbar^2}{2m^*L^2}$
0.1	0.820	0.5903	0.6724
	1.120	1.704	1.2544
	1.320	3.273	1.7424
	1.56	1.297	2.4336
	1.62	3.062	2.6244
0.01	0.74	0.6728	0.54776
	1.04	1.759	1.0857
	1.22	3.320	1.4884
	1.50	1.381	2.250
	1.52	3.113	2.3104
0.001	0.74	0.6728	0.5476
	1.03	1.755	1.0609
	1.23	3.200	1.5129
	1.50	1.381	2.250
	1.53	3.121	2.3409

Table1: The energy eigen value of rectangular double quantum well for different values of $\frac{a}{L}$, $E_n = \frac{V_o \xi_n^2}{R_2^2}$

4.4 Tunneling effects in terms of transmission and reflection coefficient

Consider our rectangular double quantum well as Fig4.1 taking the regions II, III and IV, as a point of interest to derive our tunneling effect. Let's take for region -L < x < -a Schrödinger equation and derive wave states as

$$\Psi(II) = Ae^{ik_2x} + Be^{-k_2x} \tag{4.4.1}$$

then for region -a < x < a region using Schrödinger equation we have another equation as

$$\Psi_{III} = Ce^{k_1 x} + De^{-k_1 x} \tag{4.4.2}$$

at last for $a \leq (x) < L$ region we get

$$\Psi_{IV} = Ee^{ik_2x} \tag{4.4.3}$$

from the incident part at region II, and we have a transmission or at the region IV a wave state Ψ_{IV} , then to determine the transmission coefficient of this tunneling effect, we can use two boundary conditions at x = -a and x = -a. We can use $\Psi|_{x=(\pm)a}$ and $\frac{d\Psi}{dx}|_{x=\pm(a)}$ at two interfaces so that:

At x = -a using equations (4.4.1) and (4.4.2) we obtained that

$$A = \left(1 - \frac{k_1}{ik_2}\right) \frac{C}{2} e^{-k_1 a + ik_2 a} + \left(1 - \frac{k_1}{ik_2}\right) \frac{D}{2} e^{k_1 a + ik_2 a}$$
(4.4.4)

And at x = a using equation (4.4.2) and (4.4.3) we can get that

$$C = \left(1 + \frac{ik_2}{k_1}\right)\left(\frac{E}{2}\right)e^{ik_2a - k_1a} \tag{4.4.5}$$

and

$$D = \left(1 - \frac{ik_2a}{k_1}\right)\left(\frac{E}{2}\right)e^{ik_2a + k_1a} \tag{4.4.6}$$

Then substituting equations (4.4.5) and (4.4.6) in equation (4.4.4) and we obtained that

$$\left(\frac{A}{E}\right) = \frac{1}{4} \left[\left(\frac{k_1^2 - k_2^2}{ik_1k_2}\right) + 2\right] e^{2ik_2a - 2k_1a} - \left(\frac{1}{4}\right) \left[\left(\frac{k_1^2 - k_2^2}{ik_1k_2}\right) - 2\right] e^{2k_1a + 2ik_2a}$$
(4.4.7)

When the above equation squared and simplified gives us an equation of

$$\left(\frac{A}{E}\right)^2 = 1 + \left(1 + \frac{1}{4}\left(\frac{k_1^2 - k_2^2}{k_1 k_2}\right)^2 sinh^2(2k_1 a)\right)$$
(4.4.8)

And further can be simplified as

$$\left(\frac{A}{E}\right)^2 = \left[1 + \frac{1}{4}\left(\frac{k_1}{k_2} + \frac{k_2}{k_1}\right)^2 sinh^2(2k_1a)\right]$$
(4.4.9)

this means that our transmission coefficient(T) will be indicated in Equ.4.4.10

$$T = \left|\frac{E}{A}\right|^2 = \left[1 + \left(\frac{1}{4}\left(\frac{k_1}{k_2} + \frac{k_2}{k_1}\right)^2\right)sinh^2 2k_1 a\right]^{-1}$$
(4.4.10)

In addition; the probability of transmission and reflection is

$$T + R = 1 \tag{4.4.11}$$

where T and R are transmission and reflection coefficients, respectively across the barrier in the RDQW hetrostructure



Figure 4.5: Tunneling effects of rectangular double quantum well of central barrier thickness a = 3nm and a = 5nm

At this point, we denote our RDQW heterostructure as $B_1/W_2/B_3/W_4/B_5$ in order to clarify discussion. The width of the central barrier if it is taken to be 2a, while the width of the outer well (crystal W_2 and W_4) is given by $\pm L$. The transmission coefficient of the total RDQW heterostructure is analytically determined from the values ($\xi = 0.820$ and $\eta = 0.5903$) from the data given in Table 4.1 at the first row. Using the obtained equation analytically as transmission and plotting it over the range of the central barrier crystal then we can see the how thickness of the barrier affects the transmission rate in tunneling effects of particles in the system. As the thickness of the barrier increases the transmission decreases.

Chapter 5 Conclusion

In this thesis we have studied the rectangular double quantum well (RDQW) with the model of double finite potential of GaAs/AlGaAs. The simplicity of RDQW allow us to obtain relations from the required properties imposed to the solutions of the schrodinger equation by the quantum mechanical postulates analytically. The analytical manipulations are straight forward to obtain two transcedental equations. The numerical aspect of the analysis that include the solution of a transcedental equation and the solution of schrodinger equation with softwares results energies eigen value in RDQW. we have demonstrated how tunneling effect occurs in these heterostructure, where by wave states with their energies corresponding to bound states of the system undergo transmission through the structure. The degree of transmission can be controlled by varying the thickness of the central barrier and by modifying the width of the wells in the hetrostructure.

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JIMMA UNIVERSITY COLLEGE OF NATURAL SCIENCES PERFORMANCE CERTIFICATE FOR MASTER'S DEGREE

Name of Student: Tesfu Gudeta ID No. SMSC 00914/06

Graduate Program: Summer, MSc.

1. Course Work Performance

Course	Course Title	Cr. hr	Number	Rank **	Remark
Code			Grade		
Phys699	MSc. Thesis	6	82	V.good	

** Ecellent, Very Good, Good, Satisfactory, Fail.

Thesis Title

Energy eigenvalue and tunneling effect of rectangular double quantum well

- 2. Board of Examiners decision Mark \times in one of the boxes. Pass \times 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

<u>Committee member</u> Chairman	Name	Signature	Date
External Examiner			
Internal Examiner			
Major Advisor			
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 **Tesfu Gudeta** have read and evaluated his thesis entitled "**Energy eigenvalue and tunneling effect of rectangular double quantum well**" 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
Name of Major Advisor	Signature	Date
Name of Internal Examiner	Signature	Date
Name of External Examiner	Signature	Date

SCHOOL OF GRADUATE STUDIES

DECLARATION

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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This Msc dissertation has been submitted for examination with my approval as University advisor.

Name:Dr.Menberu Mengesha

Signature: _____

Place and date of submission:

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