LOW LYING ENERGY STATES OF TWO ELECTRON QUANTUM DOTS WITH RIGID CONFINEMENT

By

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Abstract

The energy spectra of two electron system confined in a semiconductor quantum dot is studied using variational method under the assumption of spherically symmetric rigid confinement potential. It is shown that the ground state energy level for rigid confinement is calculated with the help of perturbation method. The quantum states of the dots are treated as the singlet and triplet states like in the theory of helium atom. The phase transitions from the triplet state to singlet states are possible only with the account of spin-orbit interaction. The corresponding eigen value problem with rigid boundary condition is solved by numerical integrations. It is observed that the results obtained for variational ground state energy is in agreement with exact energy values, suggesting that variational approach works well for rigid confinement of two electrons quantum dot.

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Above all, I would like to thank the almighty; God, for letting me accomplish this stage.

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Chapter 1

Introduction

1.1 Physics in Quantum System of Low Dimensions

The Physics of low dimensional systems is often different from $3D$. The term low-dimensional system refers to those materials that exhibit unusual structure because of the confinement of electrons to less than three directions from their ordinary bulk materials[1,2]. Depending on how many dimensions lay within the range of nanoscale (i.e. nanometer, nm), one generally speaks of quantum wells (2D), quantum wires (1D), and quantum dots (0D).In line with this, low dimensional systems can be thought as those materials whose electronic states are somewhat confined in one or more directions [1-3]. As a result, low dimensional system is referred as systems having at least one dimension that is intermediate between those characteristics of atoms or molecules and those of bulk materials. At such intermediate state, some of the properties of low dimensional systems become very different from those of their original molecular and bulk counterparts. As such nanometer scales, one important effect is the so called quantization effect will be observed as a result of the confined electrons movements along the unconfined directions [3,4]. In the range of nanometer scales, properties like mechanical, electrical, magnetic, optical, and melting as well as boiling points and etc becomes size dependent. This phenomenon would be crucial for both practical and theoretical applications in varieties field of study. For instance, theoretical understandings of optical and electronic properties of nanostructures are basic in optoelectronic materials. Thus, it is clear to say that such distinctive (peculiar) property leads to a host of useful phenomena in the area of optoelectronic engineering material devices [1-4]. At this point, it is important to note that, the dimension of confinement in the nanometer range must be comparable with de-Broglie wave length so as to exhibit the above mentioned properties. For low dimensional systems in the range of 1 and 100nm-scale, the effect of quantum confinement gives rise to many distinctive and interesting physical properties namely energy level quantization and the existence of discrete energy states around a given semiconductor nanostructures. This leads to the ideas that emission and absorption could be size dependent phenomena [1-4]. The study of semiconductor quantum dot (QDs) and nanocrystals have been of a great interest from the experimental and theoretical point of view. The interest arises from the size quantization of solids. As a result,the electronic spectrum of quantum dot consists a set of discrete energy levels[1,3]. This makes semiconductors quantum dot very important in the application of optical and transport properties of semiconductors [1].

The carrier motion is restricted to a narrow region of few nanometers in dimension and the correlation among electrons shown to be interesting in quasi zero dimensional system [23].In recent years, the study of two electrons quantum dot have been the subject of intensive research activity in modern science and technology .The electron electron interaction plays essential role in quantum dot with two electrons ;and hence it is interesting to study this phenomena.

So far the physics behind two electrons quantum dot semiconductors has been widely investigated by different scholars. A large portion of the studies conducted earlier were based on the models of infinite barriers potential with square well confinement and parabolic confinement potential[12].With this regard Bryant[22] studied the energy levels of two electrons in square well quantum box. In addition ,the effect of dielectric mismatch between the dot material and the surrounding has been studied by Brus[23]and Cantele et al.[24] for Cds and CdSe dots,respectively. The significance of the size as well as shape effects of electron electron interactions over the dot in parabolic confinement have pointed out by Zhu et al,[26]. Theoretical studies on singlet-triplet splitting,degree of entanglement and correlation in GaAs/ InAs quantum dot molecules are discussed in detail in Ref[20].Many experimental works revealed that there were field tunable phases in few electron quantum dot systems.

The speculation in nanoscience and technology shows that the behavior of nanomaterials/ nanoparticles and bulk matters are different. Because the ratio of surface atom to the interior atoms causes the surface energy to be increased with overall surface area which gives raise to nanomaterials dimension dependent character, but this may not the case for bulk materials [1,3-4]. Consequently, it is known that particles in the range of below 100nm are controllable size and are said to be nanoparticles. Accordingly, total surface area is negligible for bulk materials from technological point of view. However, the total surface area of nanoparticles is significant due to their size dependency. This situation makes nanostructures ease of control [1,2]. Evidently nanostructure consists large surface area and posses large surface energy due to this, they become thermodynamically unstable or metastable. Therefore the increase in surface area to volume ratio plays a great role in modern science and nanotechnology. To illustrate the situation let us consider a rectangular cube of a solid divided into two equal parts each having new structures with sides of 1cm and hence its volume be $1cm^3$ as shown below [1-3].

The number of atoms in such a volume will be $\frac{10^{23} atoms*(1cm^3)}{cm^3}/10^{-7}cm^3 \sim 10^{23}/10^{-7}cm^3$ atoms.Also, the surface atoms in a unit area is $6*10^{15}atoms/\frac{10^{15}atoms*6(10^{-7cm})^2}{cm^3} \sim 6*10^{15}atoms \sim \frac{10^{15}atoms}{60atoms}$ Therefore, $\frac{(S/V)_{nano}}{(S/V)_{bulk}} \sim \frac{6*10^{15}}{6*10^{8}} \sim 10^7 \Rightarrow \left(\frac{S}{V}\right)_{nano} \sim (10^7)\left(\frac{S}{V}\right)_{bulk}$ Thus, we see that the surface to volume ratio of the number of atoms in the nanomaterials is greater than by the order of that of the bulk counterpart. Generally speaking as the size of the system decreases, the fraction of atoms on the surface will increase [1].

1.2 The Physics of Quantum Dot

The simpler way to study the properties of quantum dot is modeling a confining potential that traps an electron in to the dot as well as an interaction potential that characterizes the repulsion between those electrons. The confinement of particles in $1D$, $2D$ and $3D$ provides size quantization effect,which in turns gives discrete energy levels [2,3].The limiting size of confinement so that such quantum confinement effects are observable at the energy spacing $\varDelta E$ is much greater than the thermal energy which is in the order of magnitude K_BT[1,4].

$$\varDelta E \gg K_BT \tag{1.2.1}$$

Therefore,at a very low temperature it is possible to create a quantum dot small enough to observe size quantization effect. In semiconductors,the dielectric constant is generally large, and as a result,screening tends to reduce the coulomb interaction between electrons and holes.The result is a Mott-Wannier exciton. As a consequence,the effect of lattice potential can be incorporated into the effective mass of electron and/or hole,because the lower mass and the screened coulomb interaction,the binding energy is much less than hydrogen atom,typically the order of $0.1eV$[11,13]. From the theory of quantum mechanics,the positions of electron and hole is described by their wave functions. Quantum size effect occurs when the size exceeds the particle diameter.So,the size limit for quantum confinement can be approximated by using de Broglie wavelength equation given below[12-18].

$$\lambda_B = \frac{h}{p} = \frac{\hbar}{m^*\omega} \tag{1.2.2}$$

where λ_B is the de Broglie wavelength(the wavelength associated to a particle with momentum p), $\hbar$ is the reduced Planck constant,and ω is the angular frequency of the particle. In this paper, the writers considered the low lying energies/states of two electron quantum dots with spherically symmetric rigid confinement potential and the wave function is assumed to be zero on the surface of quantum dots. Noting that in reduced dimensions the coulomb interaction of semiconductors quantum dot with a typical length $10nm$ cannot be treated as small.The variational method approach is used to solve the problem stated above.

1.3 Organization of the Thesis

This thesis is concerned with objects small enough that quantum mechanics is essential to understand their behavior, but large enough to contain many particles. Complete understanding of the physical situation is essential. Thus, the idea behind this thesis is organized as follows:

Chapter One:briefly reviews the concept of low dimensional systems in general and introduces the ideas of length scales in particular. The section ends with illustrations of the effect of surface area to volume ratio.

Chapter Two:discuss the calculations of density of states in bulk materials, quantum wells, wires and quantum dots. In addition this chapter deals about the properties of nanostructures such as quantum wells, wires and dots. Moreover the applications of quantum dots are discussed in detail under this section of the thesis. Finally the history of quantum dots is briefly reviewed.

Chapter Three:is concerned with single-particle electron states including calculations of wave functions and ground state energy by solving a Hamiltonian constructed by neglecting coulomb type potential for a single particle confined in spherical quantum dot. In addition models are reviewed based on the theoretical and physical concepts/facts that help to study single electron quantum dot.

Chapter Four :introduces a many body Hamiltonian to correct the electronic state of two electron quantum dots with rigid confinement. In addition variational method is employed to approximate the ground state energy levels of two electron systems by adopting variational parameters.

Chapter Five:displays the results on the energy levels of two electron quantum dots with rigid confinement and energy correction. The section ends with drawing conclusions that stress on the main findings of this Thesis.

Chapter 2

Density of States

2.1 Introduction

The peculiar characters between systems with different dimensions is their density of states $\rho(\varepsilon)$,which is the number of states per unit volume L^D in the energy $\varepsilon + \varepsilon + d\varepsilon$ divided by d where L is the linear size of the system,and D can be either $1, 2, 3$ dimension [1-4].

The basic idea here is that while restricting the motion of electron in one, two and three dimensions gives rise to discrete energy levels, in situations such as quantum well and quantum wire, there are additional degrees of freedom along unconfined directions. As a result one can get the concepts of density of states. So the calculation of density of states provide a more detail description of what the electrons structures as well as the energies of $3D$,$2D$,$1D$ and $0D$ and materials looks like [1-4].

2.2 Density of States in Three Dimensions (Bulk Materials)

In three dimensions, there is no confinement in the direction of motion of electrons. The only constrains is the periodic boundary conditions. Consider the volume in **k**-space

$\mathbf{V}_k = \frac{4}{3}\pi k^3$ and then each allowed value of $\mathbf{k}$-space occupies a volume of

$$\left(\frac{2\pi}{L_x}\right)\left(\frac{2\pi}{L_y}\right)\left(\frac{2\pi}{L_z}\right) = \frac{8\pi^3}{V} = \mathbf{k_x k_y k_z} \tag{2.2.1}$$

The number of modes (N) in the sphere is then;

$$N = \frac{V_k}{\mathbf{k_x k_y k_z}} = \frac{\frac{4}{3}\pi k^3}{8\pi^3}\mathbf{L_x L_y L_z} \tag{2.2.2}$$

Assuming that the particle is an electron and we consider the spin of degeneracy (up and down), then we multiply N by 2.

$$N' = 2\left(\frac{\frac{4}{3}\pi k^3}{8\pi^3}\mathbf{L_x L_y L_z}\right) = \frac{\pi k^3}{3\pi^3}\mathbf{L_x L_y L_z} \tag{2.2.3}$$

this is the total number of states in sphere.

From the definition of the density, which is the number of states per unit volume, we get

$$\rho = \frac{N'}{\mathbf{L_x L_y L_z}} = \frac{k^3}{3\pi^2} \tag{2.2.4}$$

Since the density of states, $\rho'(\varepsilon)$ is defined as the number of allowed states with in energy range $d\varepsilon$. Thus,

$$\rho'(\varepsilon) = \frac{d\rho}{d\varepsilon} = \frac{d\left(\frac{k^3}{3\pi^2}\right)}{d\varepsilon} = \frac{1}{3\pi^2}\frac{dk^3}{d\varepsilon} \tag{2.2.5}$$

where $k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$ alternatively, $k^3 = \left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2}$.

The expression becomes,

$$\rho'(\varepsilon) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{d\varepsilon^{3/2}}{d\varepsilon} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}\varepsilon^{1/2} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}\sqrt{\varepsilon} \tag{2.2.6}$$

The above equation tells that the density of states in $3D$ is square root dependent on energy. It is known that the unconfined wave functions within $3D$ box are plane waves in all three dimensions. Therefore, the wave functions could be described as

$$\Phi(x, y, z) = \psi e^{i\mathbf{k}_x\mathbf{x}}e^{i\mathbf{k}_y\mathbf{y}}e^{i\mathbf{k}_z\mathbf{z}} \tag{2.2.7}$$

Substituting in the Schrdingers equations gives;

$$\frac{-\hbar}{2m}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right)\Psi = \varepsilon\Psi \tag{2.2.8}$$

which gives

$$\frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)=\varepsilon \tag{2.2.9}$$

After rearranging, energies of the system are

$$\varepsilon=\frac{\hbar^2 k^2}{2m} \tag{2.2.10}$$

where $\mathbf{k}=\sqrt{k_x^2+k_y^2+k_z^2}$ and $\mathbf{k}_{x,y,z}=\frac{2m}{L_{x,y,z}}$

$$\rho'_{3D}=\frac{1}{2\pi^2}\left(\frac{2m}{\hbar}\right)\sqrt{\varepsilon-\varepsilon_g} \tag{2.2.11}$$

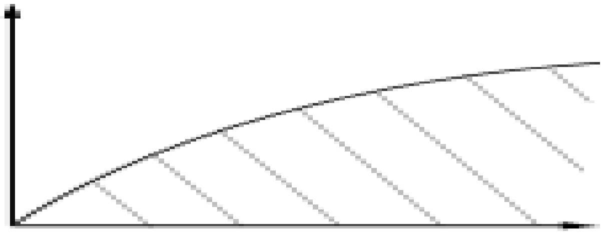

Figure 2.1: The Density of state of Bulk materials (3D)

2.3 The 2D DOS: Quantum Wells Confined in 1D

In quantum wells, the electrons motion is confined into two dimensions and unconfined in the other dimensions; lets assume its motion in the z-direction. Thus, the total energy of the system is the sum of the energy along the quantized direction and the energy along the other two directions. Therefore, the total energy is expressed as[1,2];

$$\varepsilon_{tot}=\frac{\hbar^2 k_z^2}{2m^*}+\frac{\hbar^2 k^2}{2m^*}=\varepsilon_n+\varepsilon_{x,y}=\frac{\hbar^2 k_z^2}{2m^*}+\frac{\hbar^2}{2m^*}\left(k_x^2+k_y^2\right) \tag{2.3.1}$$

where $k^2=k_x^2+k_y^2, k_z=\frac{n\pi}{L_z}, k_x=\frac{2\pi}{L_x}$,and $k_y=\frac{2\pi}{L_y}$

Suppose now two areas in the $\mathbf{k}$-space is given as $\mathbf{A}_k=\pi k^2$, The area of a given mode is then $\mathbf{k}_x k_y$ with the total number of modes (N)

$$N = \frac{\pi \mathbf{k}^2}{4\pi^2}\mathbf{L}_x\mathbf{L}_y = \frac{\mathbf{k}^2\mathbf{L}_x\mathbf{L}_y}{4\pi} \tag{2.3.2}$$

And again multiplying N by 2 accounts for the electrons spin to get the total number of states

$$N' = 2\left(\frac{\pi \mathbf{k}^2}{4\pi^2}\mathbf{L}_x\mathbf{L}_y\right) = \frac{\mathbf{k}^2\mathbf{L}_x\mathbf{L}_y}{2\pi} \tag{2.3.3}$$

We know that the total number of states per unit area gives, the density, ρ. i.e. $\rho = \frac{N'}{\mathbf{L}_x\mathbf{L}_y}$ recalling that $k = \sqrt{\frac{2m\varepsilon}{\hbar}}$ Substituting the equation gives $\rho = \frac{m\varepsilon}{\hbar^2\pi}$, which is number of states per unit area

From the definition of the energy density, the density of the state per unit area per unit energy becomes;

$$\rho' = \frac{d\rho}{d\varepsilon} = \frac{m}{\hbar^2\pi}. \tag{2.3.4}$$

One can observe that the energy density of the sub-band given by the above equation (2.3.4). For each successive $\mathbf{k}_z$, there will be an additional $\frac{m}{\hbar\pi}$ term and hence another sub-band. Therefore, the density of states can be written as

$$\rho'_{2D} = \frac{m}{\hbar\pi}\sum_n \Theta(\varepsilon - \varepsilon_n). \tag{2.3.5}$$

where Θ is the heavy-side function

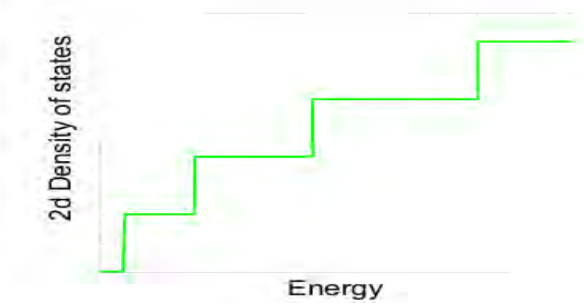

Figure 2.2: The density of state of quantum wells (2D).

2.4 Two Dimensional Quantum system, Quantum Wells (QWs)

If a given semiconductor material with small energy gap is sandwiched between energy barriers from a semiconductor material with a larger energy gap and layers thickness (are just a few atomic layers), the carriers are confined to the layered with lower energy. This situation gives the so called quantum wells [1-3].

Based on the above facts, QWs can be formed by preparing materials such as GaAs (gallium arsenide) sandwiched between two layers of materials with a wider band gap, like AlAs (aluminum arsenide) and etc [3,4]. From the knowledge of quantum mechanics, it can be clear that the spectral properties of quantum wells is derived from the confinement of charge carriers(electrons and holes).This shows that quantum confinement effect plays essential role to determine the spectral properties of quantum wells [2-4].

Another consequence of the quantum confinement is the modification of the density of states (DOS).In quantum wells the general shape of density of states modified as a step functions because of quantum confinement [3].

In addition, the possibility of manipulating the sizes associated with the quantum well, changing the semiconductor material composition can also be a tool to fine tune the property of these quantum structures [4].

One of the peculiar features of quantum wells is the restriction on the movement of the electron into two directions and the other direction being confined. This in turns will result in allowed energy bands, whose energy positions are dependent on the height and width of the barrier. Therefore, restriction on the movement of electron affects electrons energy [2].

The most useful techniques for studies of the properties of nanostructures are based on the optical transitions between the discrete electronic levels/band gaps and thereby also an increase in gap energy due to confinement effects [1-4].

Optical properties of quantum wells shows absorption effect and used to further investigation of unusual phenomena in this materia

2.5 The 1D DOS: Quantum Wires Confined in 2D

In the situation where, the electrons motion is confined in two dimensions and only have one degree of freedom (say the x-direction), one can get quantum wire. The total energy of the system can be written as

$$\mathbf{E}_{tot} = \frac{\hbar^2 k_z^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{\hbar^2 k^2}{2m} \tag{2.5.1}$$

where $\mathbf{k} = \mathbf{k}_x = \frac{2\pi}{L_x}$

Furthermore along the confined directions $\mathbf{k}_z = \frac{2\pi}{L_z}$, and $\mathbf{k}_y = \frac{2\pi}{L_y}$. From the concept of quantum mechanics, the length in the **k**-space is given as $\mathbf{L} = 2\mathbf{k}$

The number of modes along this length is $N = \frac{2\mathbf{k}}{\frac{2\pi}{\mathbf{L}_x}} = \frac{\mathbf{k}\mathbf{L}_x}{\pi}$ which is the number of states along a line.

Now if we consider an electron, ensure to take into account the spin degeneracy.

$$N' = 2N = \frac{2\mathbf{k}\mathbf{L}_x}{\pi} \tag{2.5.2}$$

The number of states per unit length call it density is given by

$$\rho = \frac{N'}{\mathbf{L}_x} = \frac{2\mathbf{k}}{\pi} = \frac{2}{\pi}\sqrt{\frac{2m\varepsilon}{\hbar^2}} \tag{2.5.3}$$

Therefore, based on similar definition given above, the energy density becomes

$$\rho' = \frac{d\rho}{d\varepsilon} = \frac{2}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{d\sqrt{\varepsilon}}{d\varepsilon} \tag{2.5.4}$$

Thus, the complete expression taking into account all **m**, and **n** and combinations for the energy density for quantum wire is written as :

$$\rho'_{1D} = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{\sqrt{\varepsilon - \varepsilon_{n,m}}}\Theta(\varepsilon - \varepsilon_{n,m}) \tag{2.5.5}$$

Where again Θ is the heavy-side function. It is clear to observe that the density of state is inversely proportional to the square root of energy.

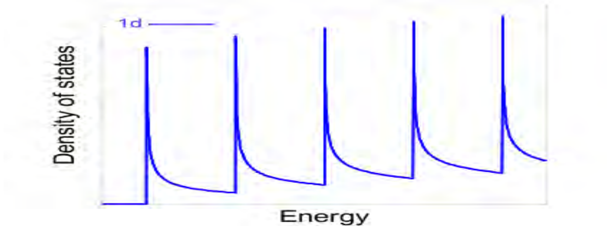

Figure 2.3: The Density of state of quantum wire (1D).

2.6 One Dimensional Quantum System, Quantum Wires (QWR's)

In quantum wires it is clear to observe that the motion of electrons is restricted only in one direction while leaving the other two directions confined. Thus, quantum wires can be defined as extremely narrow wires in which the free motion of carriers is only possible in one direction, along the wire, but confined in the other two directions. It can also be defined as structures that have a thickness or diameter constrained to tens of nanometers or less and an unconstrained length [5,6]. Many different structures of nanowires exist, including metallic (e.g., Ni, Pt, Au), semiconducting (e.g. Si, InP, GaN, etc.), and insulating (e.g. SiO2, TiO2) and etc [9]. These structures are usually referred to us one-dimensional (1D) materials and have many interesting properties that make them different from their corresponding bulk materials in the sense that QWRs are confined laterally and thus occupies discrete energy levels/bands which are by far different from their original bulk materials [7,8].

One of the peculiar features of this quantum confinement exhibited by certain nanowires manifest themselves in discrete values of the electrical conductance. In this regard (Dereselhaustal, 2002) found that when electron free path is much longer than the wire length,the conduction is a pure quantum phenomenon [8,9].

As nano-wire shrinks in size, the surface of atoms become more numerous compared to the atoms with in the nano-wire, and edge effect becomes more important.Additional properties observed in QWRs are transport properties, electrical properties and many others [5-9]. The transport properties in nano-wires are affected by wire diameter, material compositions, surface conditions, quality of the crystal and etc [7]. Optical properties raises in QWR's often show intense features at specific energies near singularities in the joint density of states formed under strong quantum confinements. Optical methods provide an easy and sensitive tool for measuring the electronic structure of nanowires, since optical measurements are sensitive to quantum effects [5-9].

2.7 The 0D- DOS: Particles Confined in 3D

The $0D$- DOS is special case because the motion of the particle confined in all directions. The density of states is basically a series of Delta-functions[10]. The total energy of the system becomes

$$\mathbf{E}_{tot} = \frac{\hbar^2 \mathbf{k}_x^2}{2m} + \frac{\hbar^2 \mathbf{k}_y^2}{2m} + \frac{\hbar^2 \mathbf{k}_z^2}{2m} = \mathbf{E}_l + \mathbf{E}_m + \mathbf{E}_n \tag{2.7.1}$$

where l, m, and n are integers, and

$$k_x = \frac{2\pi}{\mathbf{L_x}}, k_x = \frac{2\pi}{\mathbf{L_y}}, k_z = \frac{2\pi}{\mathbf{L_z}} \tag{2.7.2}$$

The density of states in $0D$(quantum dot) is written as

$$\rho'_{0D} = \delta\Theta\left(\varepsilon - \varepsilon_{l,m,n}\right) \tag{2.7.3}$$

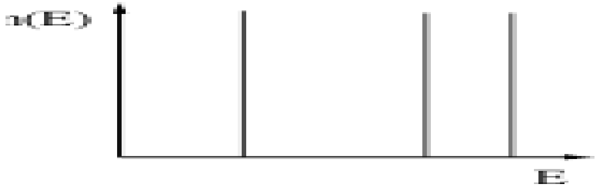

Figure 2.4: The Density of state of quantum dot (0D).

2.8 Zero Dimensional Quantum System,Quantum Dots

Quantum dots are man-made droplets of charge that contains anything from a single electron to collections of several thousands [10]. In quantum dots electrons are confined in all three directions and hence they are known as zero (0D) dimensional systems. Different people give different names for quantum dots such as nanoparticles, clusters, colloids and etc. Depending up on their applications, the total diameter of quantum dots varies from 2-10nm corresponding to 10-50 atoms and several thousand nanometers for 100-100,000 atoms, etc [12-15].

Since quantum dots are extremely confined in all the three directions, they exhibit excellent quantization behavior. However, the only thing that behaves like this is a real atom; and hence quantum dots are known as artificial atoms [16-19]. As explained above quantum dots have an interesting confinement behavior which in turn has many applications in nanoworld. Some of these applications are: in modern laser science, imaging optics, medicine and etc [20,21]. By zero dimensionality, means that, the carrier confinement of the dot give rise for a dozens of new optical, electronic, and transport properties that differ from its original bulk property of semiconductor material [18]. These new properties of quantum dots lead us to exploit them in different fields of studies as well as device applications in various areas of interest. For instance quantum dot lasers for telecom and data-com applications. Another quantum dot applications resulted from its optical behavior is infrared photo detectors. In addition to these, its imaging behavior also used in optical amplifications in quantum computing. Furthermore, its electronic behavior is used in quantum dot nano-structure [20-21].

2.9 History of Quantum dot

The first theoretical studies of artificial system began in late 50's.In the 60's, the techniques of epitaxial decompositions were developed and with it, the first optical properties were discovered and the two dimensional character of the sample was realized [16,19-21]. At the beginning of 80's, there was rapid progress in technology. As a result the first quasi one dimensional quantum wire was developed [18].

During 1918s colloidal quantum dot were developed. The particles obtained from quantum dot displayed unique properties called fluorescence emissions. This provided a method to choose excitation and emissions wavelength and particle band gaps [10,11].

The first quantum dot was fabricated using etching techniques in the middle of 80's(Zhu et al ;1986).As a result a complete quantization of free electron motion becomes possible. At the end of 80's and at the beginning of 90's light lithography was evolved and resulted in an increased precision than the previously developed ion lithography[15]. Quantum dots are fabricated in varieties of ways. To mention some of them such as using lithography techniques, getting one QD at particular instance and etc [50-55].

In 1998 quantum dots were used in biomedicine as fluorescent indicators. Early 2009 the smallest quantum dots with diameter less than previously created QDs. Until now, quantum dots have been used only at empirically low temperatures, but the newly developed atomic size quantum dots work at room temperature evidently Silicon crystal used in today's computers [12,14].

2.10 Some Applications of Quantum dots

Recently in nano-technologies especially quantum dots are the most applicable, functional and reproducible nano-materials in many areas of science and technology. Evidently, quantum dots become usable in experiment and theory. To mention some of the applications where quantum dots intensively used in electronic devices, medicine, optics, optical imaging, communications, quantum computations, information and etc [20,21].

Several experiments reveal that quantum dots can be used in the area of biomedicine. In the sense that the particles could be targeted to particular parts of the cell so that quantum dots can be helpful in many antibodies and proteins to produce fluorescence indicators. In electronic devices, exceptional electrical and optical properties of the dots make them to be attractive in various area of interest [18,21].

In addition, quantum dots are important for wavelength selection so that people can interconnect light and electricity in tunable manner. As a result, quantum dots are highly applicable in the area of laser, LEDs, photovoltaics, transistors and so on. Moreover, one of the interesting applications of quantum dots in the area of biology is to investigate various cellular labeling mechanism (for example in cancer treatment) and developing drugs [15-21]. Generally speaking the applications of quantum dots are diverse and all could not be listed here in detail.

Chapter 3

A Single Electron Quantum Dot with Spherically Symmetric Rigid Confinement

This section gives brief review of the theoretical back ground as well as the basic concepts behind the physics of a single electron quantum dot. Because it helps us to grasp the main ideas, as a result we can extend the existing facts and/or knowledge of single electron quantum dot to few electron quantum dots. In addition determining the energy levels together with wave functions of a single quantum particle in a dot serves as standing point to study two electron quantum dot. Therefore giving highlights regarding to one electron QDs models have great importance to investigate the properties of many electron quantum dots[1,3].

3.1 The Particle in a Box

Modeling our electronic material as a box allows us to ignore atoms and assume that the material is perfectly homogeneous[4]. We will consider boxes in different dimensions: three dimensions (typical bulk materials), 2-d (quantum wells), 1-d (quantum wires), or 0-dimensions (quantum dot). The label quantum here refers to the confinement of electrons.

When we say that an electron is confined in a low dimensional material we mean that critical dimensions of the material are on the order of the wavelength of an electron[1,2]. We know that when particles are confined, their energy levels become discrete. In quantum dots, electrons are confined in all three dimensions, in quantum wires, electrons are confined in only two dimensions and so on. So when we say that a given structure is 2-d, we mean that the electron is unconfined in 2 dimensions. In the unconfined directions, we will assume that the electron described by a plane wave [1,2].

3.2 The Schrodinger Equation

Analyzing quantum particle in a box and bulk materials requires that solving the Schrodinger equation in 1-D 2-D and 3-D. The Schrodinger equation in $1-D$ is given by;

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\Psi(x)=E\Psi(x) \tag{3.2.1}$$

The above equation can be extended to higher dimensions $(3D)$ as

The kinetic energy operator in $3D$ is given as

$$\hat{T}=\frac{\hat{p_x^2}}{2m}+\frac{\hat{p_y^2}}{2m}+\frac{\hat{p_z^2}}{2m}=-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right) \tag{3.2.2}$$

Where p_x ,p_y and p_z are the components of momentum on the x, y and z axes, respectively. Suppose the potential is given by

$$\hat{V}(x,y,z)=\begin{cases} 0, 0<x<L, 0<y<L, 0<z<L. \\ \infty, otherwise. \end{cases} \tag{3.2.3}$$

The above potential can be separated into x, y, and z dependent terms

$$V(x,y,z)=V(x)+V(y)+V(z) \tag{3.2.4}$$

For a potential of this form the Schrodinger equation can takes the following forms:

$$-\left[\frac{\hbar^2}{2m}\right]\left[\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right]\left[V(x)+V(y)+V(z)\right]\Psi(x,y,z)=E\Psi(x,y,z) \tag{3.2.5}$$

where $E = -\left[\frac{\hbar^2}{2m}\right]\left[\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right][V(x) + V(y) + V(z)] = E_z + E_y + E_z$

The wave function can also be written as

$$\Psi(x, y, z) = \Psi(x)\Psi(y)\Psi(z) \tag{3.2.6}$$

The wave function $\Psi(x, y, z)$ must vanish at the wall of the cubic box. The solution for one dimensional potential is given by

$$X(x) = \sqrt{\frac{2}{a}} sin\left(\frac{n_x \pi}{L} x\right), n_x = 1, 2, 3, ... \tag{3.2.7}$$

and the corresponding energy eigen-values becomes

$$E_{n_x} = \frac{\hbar^2 n_x^2}{2m^* L^2} \tag{3.2.8}$$

From the expression above we can write the normalized three dimensional eigen functions and their corresponding energies as

$$\Psi_{n_x n_y n_z}(x, y, z) = \sqrt{\frac{8}{L^3}} sin\left(\frac{n_x \pi}{L} x\right) sin\left(\frac{n_y \pi}{L} y\right) sin\left(\frac{n_z \pi}{L} z\right) \tag{3.2.9}$$

$$E_{n_x n_y n_z} = E_{n_x} + E_{n_y} + E_{n_z} = \frac{\hbar^2 \pi^2}{2m^* L^2}\left(n_x^2 + n_y^2 + n_z^2\right) \tag{3.2.10}$$

where $n_x, n_y, n_z = 1, 2, 3, ...$

The ground state energy becomes

$$E_{111} = \frac{3\pi^2 \hbar^2}{2m^* L^2} = 3E_1 \tag{3.2.11}$$

Where,$E_1 = \frac{\pi^2 \hbar^2}{2m^* L^2}$, is the zero point energy of a particle in one dimensional box. The first excited state has three possible sets of quantum numbers $n_x, n_y, n_z = (2, 1, 1), (1, 2, 1)(1, 1, 2)$,Correspon to three different states $\Psi_{211}(x, y, z)$,$\Psi_{121}(x, y, z)$,and $\Psi_{112}(x, y, z)$.

The first quantum state is given by

$$\Psi_{211}(x, y, z) = \sqrt{\frac{8}{L^3}} sin\left(\frac{2\pi}{L} x\right) sin(\left(\frac{\pi}{L} y\right) sin\left(\frac{\pi}{L} z\right) \tag{3.2.12}$$

3.3 Particles Confined in Spherical Quantum Dots

The Schrodinger equation [1,2] for $3D$ spherically symmetric motion is given by

$$\frac{-\hbar^2}{2m}\nabla^2\psi(r,\theta,\varphi)+V(r)\psi(r,\theta,\varphi)=E\psi(r,\theta,\varphi) \tag{3.3.1}$$

The Laplacian ∇^2 in spherical coordinate is given by:

$$\nabla^2=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\left[\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{3.3.2}$$

After substitution the above equations , the Hamiltonian of the system becomes

$$\hat{H}=-\frac{\hbar^2}{2m*}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{3.3.3}$$

using a spherical coordinate,the free particle wave equation can be written as

$$-\frac{\hbar^2}{2m*}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Psi(r,\theta,\phi)=E\Psi(r,\theta,\phi) \tag{3.3.4}$$

Applying separation of variables, the above equation separated into the angular and radial parts.

$$\begin{cases}\frac{1}{sin\theta}\frac{d}{d\theta}\left(sin\theta\frac{\partial}{\partial\theta}Y_{lm}\right)+\frac{1}{sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+l(l+1)Y_{lm}=0.\\ \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{nl}}{dr}\right)\left(\frac{2mE_{nl}}{\hbar^2}-\frac{l(l+1)}{r^2}\right)R_{nl}=0.\end{cases} \tag{3.3.5}$$

The Hamiltonian separates into angular and radial parts, giving the eigen states;

$$\Psi(r,\theta,\phi)=R_{nl}(r)Y_{lm}(\theta,\phi) \tag{3.3.6}$$

Where,$Y_{lm}(\theta,\phi)$ is spherical harmonics, and $R_{nl}(r)$ is radial wave function. The solution to the angular part of the Schrodinger equation is

$$Y_{lm}(\theta,\varphi)=p_l^m cos\theta e^{im\varphi}. \tag{3.3.7}$$

The radial part of the Schrodinger equation is given by

$$\left\{-\frac{\hbar^2}{2m^*}\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-l(l+1)\right]\right\}R(r)=ER(r) \tag{3.3.8}$$

Multiplying the above equation by $\frac{2m^*}{\hbar^2}$ and introducing the dimensionless variable $\rho = kr$.

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2}\right] R_{nl}(\rho) = 0 \tag{3.3.9}$$

The above equation looks like the Bessel function except that $l(l+1)$ is not the square of an integer. The solutions are the spherical Bessel functions.

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{sin\rho}{\rho}, \tag{3.3.10}$$

which is regular at the origin and

$$n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{cos\rho}{\rho}, \tag{3.3.11}$$

which is irregular solution , Neumann Function. The first few functions are:

$$j_0(\rho) = \frac{sin\rho}{\rho},\ j_1(\rho) = \frac{sin\rho}{\rho} - \frac{cos\rho}{\rho},\ j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right) sin\rho - \frac{3cos\rho}{\rho} \tag{3.3.12}$$

$$n_0(\rho) = \frac{cos\rho}{\rho}, n_1(\rho) = \frac{-cos\rho}{\rho^2} - \frac{sin\rho}{\rho}, n_2(\rho) = -\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right) cos\rho - \frac{3sin\rho}{\rho} \tag{3.3.13}$$

The general solution with function number l in region $r \leqslant R$ is:

$$R_{nl}(\rho) = Aj_l(\rho) + Bn_l(\rho) \tag{3.3.14}$$

As

$$\rho \to 0, j_l(\rho) = \frac{(\rho)^l}{(2l+1)!!} \tag{3.3.15}$$

$$\rho \to \infty, j_l(\rho) = \frac{sin\rho}{\rho} \tag{3.3.16}$$

$$\rho \to \infty, n_l \to \infty \tag{3.3.17}$$

So that we must choose solution that satisfy the boundary condition $rR(r) = U(r)$ vanish at $r = 0$ therefore, we must discard the spherical Neumann functions.Thus, the radial function will be given by:

$$R_{nl}(\rho) = Aj_l(\rho), r \leqslant R \tag{3.3.18}$$

The energy eigen values are then determined by requiring that$j_l(kr) = 0$. The allowed values of k are determined from the boundary conditions which now reduced to

$$\frac{d}{dr} j_l(kr)|_{kr=R} = 0 \tag{3.3.19}$$

$$j_0(kR) = \frac{sin(kR)}{kR} = 0 \Rightarrow kR = sin(kR) = 0 \tag{3.3.20}$$

$$sin(kR) = 0 \Rightarrow \beta_{nl} \Rightarrow k = \frac{\beta_{nl}}{R} \tag{3.3.21}$$

Thus, the eigen state and energy levels are given by:

$$R_{nl}(r) = j_l \left(\frac{\beta_{nl} r}{R} \right), r \leqslant R \tag{3.3.22}$$

$$E_{nl} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*} \left(\frac{\beta_{nl}}{R} \right)^2 = \frac{\hbar^2 \beta_{nl}^2}{(2m^* R^2)} \tag{3.3.23}$$

Where, the function $j_l(\rho)$ is the l^{th} spherical Bessel function and the coefficient β_{nl} is the n^{th} zero of $j_l(\rho)$.Some of the coefficients are; $\beta_{0,1} = 4.5$ and $\beta_{0,2} = 5.8$, $\beta_{0,1} = 2\pi$, $\beta_{1,1} = 7.7$ and etc.

Chapter 4

Three Dimensional Quantum dot With Two Interacting Electrons with Rigid Confinement

4.1 Conceptual Literature of Two Electron Quantum dots

Introduction

The models of quantum wells and quantum dots with one electron are widely used in nano physics[1,2]. The modern technology provides possibility to fabricate quantum dots with two and more electrons where the coulomb interaction between them must be taken into account[4].

It is clear that quantum dots can be studied through a number of methods such as electron tunneling and others. If we have relatively high potential barrier to tunnel the dot from a source, the tunneling effect will be dependent on the numbers of electrons and hence the number of electrons N which is well defined in the situation[20]. Here, the number of electrons to tunnel will be dependent on many parameters. For example in two electron quantum dot, the properties that influence the electron-electron interactions are spatial confinement, geometrical shape, the presence of impurities, the existence of external electric/magnetic fields, and many more [18,19]. Different theoretical methods and models have been used to study the problem of two electrons confined in a quantum dot, both with a soft wall (parabolic confinement) as well as a hard wall (rigid circular wall with radius a) in plane of confinement[26]. Therefore the types of confinement potential used affect the types of quantum dots intended to be fabricated. Several investigations on the properties of circular and spherical quantum dots have been made in the last decades. For example, Adamowski et al[25] have studied two electrons confined in quantum dots under an assumption of a Gaussian confining potential and its parabolic approximation. They have calculated the energy levels of singlet and triplet states as functions of the range and depth of the confining potential in the two-dimensional (circular) and three-dimensional (spherical) quantum dots. One important effect in the properties of electron-electron interaction in the dot is Coulombic interactions and spin effect inside the dot. In line with this, Szafran et al [25] have proposed perturbation method to calculating the energy of a quantum dot using electron-electron interaction. They have used this method to calculate the ground and several excited states of a quantum dot consisting of two electrons. Excess electrons introduced into a semiconductor quantum dot (QD) are subjected to three dimensional spherical confinement potential can be studied by considering many body identical particle systems. Since the wave functions of systems of identical particles are either totally symmetric or anti symmetric[24]. However in the case where two interacting electrons (A and B) confined in quantum dot their total wave is anti symmetric under interchange of the two electrons. Due to the fact that electrons are indistinguishable fermions,requires that the two electron wave function must be anti symmetric with respect to exchange of electron A and B i.e $\Psi(\rho_1, \rho_2) = -\Psi(\rho_2, \rho_1)$[23].

4.2 Wave functions of two electron Quantum dots

The quantum state of a single electron ,if both the spatial and spin parts are independent of each other, the total wave function is given as the product spatial and spin part [1-3].

$$\Psi = \Psi_{spatial}(\rho_1, \rho_2) * \chi_{spin}(s_1, s_2) \tag{4.2.1}$$

where $\psi(\rho)$is the spatial part of the wave function and described by quantum number n ,l_m and $\chi(s)$ is the spin part and described by quantum number S and $m = \pm\frac{1}{2}$.

The quantum state two identical electrons expressed in terms of single electron states, which is always anti symmetric. These happens only if and only if either the spin part anti symmetric or spatial part symmetric or vis-versa.

The triplet state (spin symmetric state) occurs when the two electrons are found to be in different quantum state with different energy levels in which the total spin $S = 1$ and while the anti symmetric counter part occurs if the two electrons are found in the same quantum state having the same energy levels and the total spin $S = 0$.

The eigen state of two electrons system is given by [1,2]

$$\psi_a^s(r_1, s_1; r_2, s_2) = \frac{1}{\sqrt{2}} \{\psi_1(r_1)\psi(r_2) \pm \psi_1(r_1)\psi(r_2)\chi_s^a(s_1, s_2)\} \tag{4.2.2}$$

The spin symmetric state (triplet state) χ_s [6,7].

$$\chi_{triplet}(s_1, s_2) = \begin{cases} \chi(1) \uparrow \chi(2) \uparrow . \\ \frac{1}{\sqrt{2}} \{\chi \uparrow (1)\chi \downarrow (2) + \chi \downarrow (1)\chi \uparrow (2)\} . \\ \chi \downarrow (1)\chi \downarrow (2) \end{cases} \tag{4.2.3}$$

The singlet state (anti-symmetric state)

$$\chi_{singlet}(s_1, s_2) = \frac{1}{\sqrt{2}} \{\chi \uparrow (1)\chi \downarrow (2) - \chi \downarrow (1)\chi \uparrow (2)\} \tag{4.2.4}$$

4.3 Systems of Two Interacting Electrons in 3D Spherical Quantum dot

A system of two interacting identical spin-1/2 particles in three dimensional spherical quantum dot with rigid confinement potential of radius a can be described by a Hamiltonian as follows

$$\hat{H} = \frac{p_1^2}{2m^*} + \frac{p_2^2}{2m^*} + \frac{e^2}{\varepsilon\left|\rho_1 - \rho_2\right|} \tag{4.3.1}$$

where, the third term is known as coulomb repulsion energy between the two electrons (electron-electron interaction), and $|\varepsilon|$is dielectric constant of quantum dot. The dimensionless Hamiltonian can be written as

$$\hat{H} = -\frac{\hbar^2}{2m^*}(\nabla_1^2 + \nabla_2^2) + \frac{e^2}{\varepsilon\left|\rho_1 - \rho_2\right|} \tag{4.3.2}$$

The Laplacian is given as

$$\nabla_i^2 = \frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\rho_i^2\frac{\partial}{\partial\rho_i}\right) + \frac{1}{\rho_i^2}\left[\frac{1}{sin\theta_i}\frac{\partial}{\partial\theta_i} + \frac{1}{sin^2\phi_i}\frac{\partial^2}{\partial\phi_i^2}\right] \tag{4.3.3}$$

,where $i = 1, 2$ and multiplying the above equation by $\frac{m^*}{\hbar^2}$ we get a dimensionless expression for H

$$\hat{H} = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{e^2 m^* a^2}{\varepsilon\hbar^2\left|\rho_1 - \rho_2\right|} \tag{4.3.4}$$

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{2}\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\rho_i^2\frac{\partial}{\partial\rho_i}\right) + \frac{1}{\rho_i^2}\left[\frac{1}{sin\theta_i}\frac{\partial}{\partial\theta_i} + \frac{1}{sin^2\phi_i}\frac{\partial^2}{\partial\phi_i}\right] + \frac{\lambda}{\left|\rho_1 - \rho_2\right|} \tag{4.3.5}$$

where $\lambda = \frac{e^2 ma}{\varepsilon\hbar^2}$, and the energy is measured in $\frac{\hbar^2}{2m^*}$ Here m^* is an effective mass of electron,e is the charge of electron. In this model the wave function must vanish on the surface of the sphere. This type of confinement is known as ridged confinement. Therefore, the Schrdinger equation of the total Hamiltonian takes this form.

$$\hat{H} = H_0 + H', \tag{4.3.6}$$

where $H_0 = H_0^2 + H_0^2$ is the unperturbed Hamiltonian.

$$\hat{H} = H_0^1 + H_0^2 + H', \tag{4.3.7}$$

where $H' = \frac{\lambda}{\varepsilon|\rho_1-\rho_2|}$, is the perturbation.

4.4 Solving the Schrodinger Equations for Non Interacting Electrons Confined in Spherical Quantum dot

It is clear that the total Hamiltonian for non interacting electrons in the dot treated as the sum of the Hamiltonian of single electron to get solutions to the Schrodinger equation. According to the previous knowledge of quantum mechanics the total wave functions of two electron system must be symmetric or anti-symmetric. Thus the wave function of the system should be expressed as a one electron quantum state. The Schrodinger equation for the unperturbed system has the form

$$\hat{H}^0\Psi^0(\rho_1,\rho_2) = E^0\Psi^0(\rho_1,\rho_2) \tag{4.4.1}$$

where E^0 is the dimensionless energy corresponding to dimensionless Hamiltonian. Solving the Schrodinger equations for one electron confined in spherical quantum dot

$$H_{01}\Psi^0_{n_l}(r_1) = E^0_{n_l}\Psi^0_{n_l}(r_1) \tag{4.4.2}$$

The above equation can be written as

$$\left[-\frac{1}{2}\left(\frac{1}{\rho_1}\frac{\partial}{\partial\rho_1}\left(\rho_1^2\frac{\partial}{\partial\rho_1}\right)+\frac{1}{\rho_1^2}\left[\frac{1}{sin\theta_1}\frac{\partial}{\partial\theta_1}+\frac{1}{sin^2\psi_1}\frac{\partial^2}{\partial\psi_1^2}\right]\right)\right]\Psi(\rho_1) = E^0_{n_1}\Psi^0_{n_1}(\rho_1) \tag{4.4.3}$$

From which follows that the Hamiltonian takes this form

$$H^0_1 = -\frac{1}{2}\left[\frac{\partial^2}{\partial\rho_i^2}+\frac{2}{\rho_i}\frac{\partial}{\partial\rho_i}-\frac{l(l+1)}{\rho_i^2}\right] \tag{4.4.4}$$

This can be extended for two electrons confined in spherical quantum dot. As a matter of fact previous studies exactly solved the Schrdinger equation for a single electron confined in spherical quantum dot. However, the Schrdinger equation for two electron quantum dot has been not yet solved exactly.

$$H^2_{i=1,2} = \sum_{i=1}^{2} -\frac{1}{2}\left[\frac{\partial^2}{\partial\rho_i^2} + \frac{2}{\rho_i}\frac{\partial}{\partial\rho_i} - \frac{l(l+1)}{\rho_i^2}\right] \tag{4.4.5}$$

The overall solution of the problem in spherical coordinates is given by the standard form as

$$\Psi(\rho,\theta,\varphi) = R(\rho)Y(\theta,\varphi) \tag{4.4.6}$$

Using separation of variable, the radial part of the wave function for a single particle becomes

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2}\right]R_{nl}(\rho) = 0 \tag{4.4.7}$$

We look solutions of the form

$$R_l(\rho) = A_l j_l(\rho) + B_l n_l(\rho) \tag{4.4.8}$$

Since the function $n_l(\rho)$ is not finite at $\rho = 0$ so that it is must be discarded by setting $B_l = 0$ So, the ground state wave function of the radial part becomes

$$R_{n0}(\rho) = A_l j_l(\rho) = A\frac{sin\pi\rho}{\rho}, n = 1,2,3,.... \tag{4.4.9}$$

The normalization of $R(\rho)$ $\int_0^1 |R_{n0}(\rho)|^2 \rho^2 d\rho = 1$ leads to

$$1 = |A|^2 \int_0^1 \frac{1}{\rho^2} sin^2(\rho)\rho^2 d\rho = |A|^2 \int_0^1 sin^2\rho d\rho = |A|^2 \left[\frac{\rho}{2} - sin2\rho\right]_0^{\rho=1} = \frac{1}{2}|A|^2 \Rightarrow A = \sqrt{2} \tag{4.4.10}$$

Therefore the normalized form of the radial wave function becomes

$$R_{00}(\rho) = \sqrt{2}\frac{sin\pi\rho}{\rho} \tag{4.4.11}$$

Thus,$\frac{sin\kappa.1}{1} = 0 \Rightarrow \kappa = \pi$ and the ground state energy becomes

$$E^0_{n_1} = \frac{\hbar^2\kappa^2}{2m^*a^2} = \frac{\hbar^2\pi^2}{2m^*a^2} \tag{4.4.12}$$

$E^0_{n_1} = \frac{\pi^2}{2}$, (is dimensionless energy)

4.5 The Wave Functions of Non-interacting System of Two Electrons

The essential point must be considered in the study of two electrons is that the singlet and triplet states have different spatial wave functions. This has a strong effect on the energy of the system. Basically the spatial and spin coordinates are independent of each other. The wave functions for the two electrons if the electron occupies the same energy state meaning that the spatial part is symmetric while the spin part is anti symmetric, the wave function will be given by:

$$\Psi^0(r_1, r_2) = (\Psi^0_{n_1,l_1,m_1}(\rho_1) * \Psi^0_{n_2,l_2,m_2}(\rho_2))\chi_a(s_1, s_2) \tag{4.5.1}$$

On the other hand if the electrons occupy different energy states meaning that spatial part is anti symmetric and spin part are symmetric the wave function becomes

$$\Psi^0(r_1, r_2) = \frac{1}{\sqrt{2}}\left(\Psi_0^{n_1,l_1,m_1}(\rho_1) * \Psi_0^{n_2,l_2,m_2}(\rho_2) - \Psi_0^{n_2,l_2,m_2}(\rho_2) * \Psi_0^{n_1,l_1,m_1}(\rho_1)\right)\chi_s(s_1, s_2) \tag{4.5.2}$$

4.6 The Ground State Wave Functions and Energy for Non Interacting Two Electron System

Suppose the two electrons occupies the lowest energy states $n_1 = n_2 = 0$,$l_1 = l_2 = 0$,$m_1 = m_2 = 0$ the normalized ground state exact wave function of two electron quantum dot is given by

$$\Psi^0_0(\rho_1, \rho_2) = R_{00}(\rho)Y_{00}(\theta, \phi) = (2)\left(\frac{sin\pi\rho_1}{\rho_1}\right)\left(\frac{sin\pi\rho_2}{\rho_2}\right) \tag{4.6.1}$$

and the energy becomes

$$E_0 = E^0_{n_1} + E^0_{n_2} = \frac{\pi^2}{2} + \frac{\pi^2}{2} = \pi^2 \tag{4.6.2}$$

As stated above,the dimensionless Hamiltonian of two electrons in spherically symmetric quantum dot with rigid confinement potential of radius are expressed as

$$H = -\frac{1}{2}\bigtriangledown_1^2 - \bigtriangledown_2^2 + \frac{\lambda}{|\vec{\rho_1} - \vec{\rho_2}|} \tag{4.6.3}$$

where $\vec{\rho_1}$ and $\vec{\rho_2}$ are the dimensionless coordinates of electron 1 and electron 2 measured in units of the radius of quantum dot a ,and $\lambda = \frac{1}{\varepsilon}\frac{e^2 m^* a}{\hbar^2}$,and the dimensionless energy is measured in $\frac{\hbar^2}{m^* a^2}$;where m^* is an effective mass of electron, e is the charge of electron and ε is the dielectric constant.

The type of confinement in which the wave function should be zero on the surface of the sphere is referred as rigid confinement.

The trial wave function when the electrons are in the ground state may be given as;

$$\Psi_0(\rho_1, \rho_2) = A_n(1 - \rho_1^\alpha)(1 - \rho_2^\alpha) \tag{4.6.4}$$

where A_n is the normalization constant and determined by the following relation.

$$A_n^2 \int_0^1 (1 - \rho_1^\alpha)(1 - \rho_2^\alpha) \left(\int_0^1 (1 - \rho_1^\alpha)(1 - \rho_2^\alpha)\rho_2^2 d\rho_2 \right) \rho_1^2 d\rho_1 = 1 \tag{4.6.5}$$

$$A_n^2 \left(\frac{2\alpha^2}{6\alpha^2 + 27\alpha + 27} \right)^{1/2} \left(\frac{2\alpha^2}{6\alpha^2 + 27\alpha + 27} \right)^{1/2} = 1 \tag{4.6.6}$$

$$A_n = \frac{6\alpha^2 + 27\alpha + 7}{2\alpha^2} \tag{4.6.7}$$

Here α is the variational parameter.The above wave function (4.6.4) vanishes on the surface of the sphere (Q.D) where $\vec{\rho_1}$ and $\vec{\rho_2} = 1$.

The exact ground state wave function for this kind of one-electron Q.D [11] is given by

$$\Psi_0(\rho_1) \approx \frac{sin(\pi\rho_1)}{\rho_1} \tag{4.6.8}$$

The above function is non-zero as $\vec{\rho} \to 0$ and zero at $\vec{\rho} = 1$, which means the wave function becomes zero on all the surface of the QD. According to the above fact, the exact wave function for two non- interacting electrons is given by;

$$\Psi_0(\vec{\rho_1}, \vec{\rho_2}) = 2\frac{sin(\pi\rho_1)}{\rho_1}\frac{sin(\pi\rho_2)}{\rho_2} \tag{4.6.9}$$

Evaluating the average of the Hamiltonian using the trial wave function (4.6.4), one can obtain the variation energy of the ground state E_0^v. Since the Hamiltonian for two-electron is given by;

$$H = -\frac{1}{2} \bigtriangledown_1^2 - \bigtriangledown_2^2 + \frac{\lambda}{|\vec{\rho_1} - \vec{\rho_2}|} \tag{4.6.10}$$

The first two terms are the average kinetic energy of a single electron, and the last term is the interaction energy. So, therefore, the average ground state energy becomes

$$E_0^v = T + J \tag{4.6.11}$$

But, for a single electron the average kinetic energy is given by;

$$T = \langle \Psi_0(\rho_1) | T | \Psi_0(\rho_1) \rangle \tag{4.6.12}$$

$$T = \int_0^1 A_1(1-\rho^\alpha) \left(\frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho} \right) A_1(1-\rho^\alpha)\rho^2 d\rho \tag{4.6.13}$$

$$T = \int_0^1 A_1(1-\rho^\alpha) \left\{ (\rho^{\alpha-1})(\alpha^2 - \alpha) + \frac{2\alpha}{\rho} \rho^{\alpha-1} \right\} \rho^2 d\rho \tag{4.6.14}$$

After evaluating the above integral the average kinetic energy for a single electron is given by

$$T_1 = \frac{1}{2} \frac{A_n \alpha^2}{2\alpha + 1}, and\ T_2 = \frac{1}{2} \frac{A_n \alpha^2}{2\alpha + 1} \tag{4.6.15}$$

$$T_{tot} = \frac{1}{2} \frac{A_n \alpha^2}{2\alpha + 1} + \frac{1}{2} \frac{A_n \alpha^2}{2\alpha + 1} = \frac{A_n \alpha^2}{2\alpha + 1} \tag{4.6.16}$$

Following similar procedure the average energy of coulomb interaction is evaluated as follows.

$$J = \int_0^1 \Psi_0(\rho_1, \rho_2) \frac{\lambda}{\rho_{12}} \Psi_0(\rho_1, \rho_2) d\tau_1 d\tau_2 \tag{4.6.17}$$

where $\vec{\rho}_{12} = |\vec{\rho_1} - \vec{\rho_2}|$

$d\tau_1 = sin\theta_1 d\theta_1 d\varphi_1 \rho^2 d\rho_1 = 4\pi^2 d\rho_1$,simillarly $d\tau_2 = 4\pi^2 d\rho_1$.

Using the Legendary polynomial expansion

$$\vec{\rho}_{12} = \frac{1}{\rho_1} \sum_{i=1}^{\infty} \left(\frac{\rho_2}{\rho_1} \right)^l p_l(cos\theta), \rho_1 > \rho_2 \tag{4.6.18}$$

$$\vec{\rho}_{12} = \frac{1}{\rho_1}\sum_{i=1}^{\infty}\left(\frac{\rho_1}{\rho_2}\right)^{l} p_l(cos\theta), \rho_1 < \rho_2 \tag{4.6.19}$$

where θ is the angle between $\vec{\rho_1}$,and $\vec{\rho_2}$. Based on the addition theorem for spherical harmonic [2,3] and

$$p_l(cos\theta) = p_l(cos\theta_1)p_l(cos\theta_2) + 2\sum_{m=1}^{l}\frac{(l-m)!}{(l+m)!} * p_l^m cos\theta_1)p_l^m(cos\theta_2)cos(\Phi_1 - \Phi_2) \tag{4.6.20}$$

where θ_1,ϕ_1 and θ_2 ,ϕ_2 are polar angles of the vectors $\vec{\rho_1}$ and $\vec{\rho_2}$,respectively. Substituting the above relation in equations (4.6.17) and integrating with respect to ϕ_1 ,ϕ_2 and θ_1, θ_2 one can obtain the second term of equation (4.6.20)vanishes and only the contribution of $p_l(cos\theta_2) = 1$ lefts.

Therefore, the general expression for the interaction energy is given by

$$J_0 = \int_0^1 \left[\int_0^{\rho_1} \frac{1}{\rho_1}\psi_0^2(\vec{\rho_1},\vec{\rho_2})\rho_2^2 d\rho_2 + \int_{\rho_1}^1 \psi_0^2(\vec{\rho_1},\vec{\rho_2})\rho_2 d\rho_2\right]\rho_1^2 d\rho_1 \tag{4.6.21}$$

The trial wave function for the ground state is:

$$\Psi_0(\rho_1,\rho_2) = A_n(1-\rho_1^\alpha)(1-\rho_2^\alpha) \tag{4.6.22}$$

using the above equation in equation(4.6.17)

$$\frac{\lambda}{|\vec{\rho_1}-\vec{\rho_2}|} = \int_0^1 \Psi_0(\vec{\rho_1},\vec{\rho_2})\frac{\lambda}{\rho_{12}}\Psi_0(\vec{\rho_1},\vec{\rho_2})d\tau_1 d\tau_2 \tag{4.6.23}$$

$$J = \int_0^1 (1-\rho_1^\alpha)^2\left\{\frac{1}{\rho_1}\left(\int_0^{\rho_1}(1-\rho_2^\alpha)^2\rho_2^2 d\rho_2\right) + \left(\int_{\rho_1}^1 (1-\rho_2^\alpha)^2\rho_2^2\right)\right\}\rho_1^2 d\rho_1 \tag{4.6.24}$$

Evaluating the above integral using Mathematica yields

$$J = \int_0^1 (1-\rho_1^\alpha)^2\left(\frac{1}{3}\frac{1}{\rho_1}\rho_1^3\left(\frac{1-6\rho_1^\alpha}{3+\alpha}\right) + \frac{3\rho_2^{2\alpha}}{3+2\alpha}\right)\rho_1^2 d\rho_1 \tag{4.6.25}$$

The expression above after evaluating using Mathematica also yields

$$J = \frac{4}{3}\frac{A_n^2\alpha^4(124+\alpha(89+12\alpha))}{(5)(3+\alpha)(5+\alpha)(3+2\alpha)(5+2\alpha)(5+3\alpha)(5+4\alpha)} \tag{4.6.26}$$

The interaction energy can be rewritten as

$$J = \frac{4\lambda A_n^2\alpha^4\left(124\alpha+\alpha(89+12\alpha)\right)}{\prod_{i=0}^{3}(3+i\alpha)\prod_{j=0}^{4}(5+j\alpha)} \tag{4.6.27}$$

where $\prod_i$ and $\prod_j$ are the product of the function with respect to i and j, respectively. What comes next is minimizing the energy value of equation (4.6.11) using the condition:

$$\frac{dE_0^v(\alpha)}{d\alpha} = 0 \tag{4.6.28}$$

using the above condition, one can determine, first the variational parameter α for different values of λ.And then ,substituting the values of α and λ in equation(4.6.11) one can get the variational ground state energy,E_0^v for different values of α.

The variational ground state energy using equation (4.6.11) is presented below for different values of α and λ.

Table 4.1: The ground state energy E_0^v and variational parameyter α for different λ.

λ	0	0.5	1	1.5	2	2.5	3	3.5	4
α	1.08114	1.13453	1.18887	1.24404	1.29993	1.35643	1.41342	1.47081	1.5285
E_0^v	9.9934	10.7641	11.6408	12.5123	13.3800	14.2407	15.1080	16.0505	16.8087

From the above table, it is clear to see that the variational ground state energy of the trial wave function is found to be $E_0^v = 9.993$.While the ground state energy of the exact wave function gives $E_0 = \pi^2$. Therefore, the numerical data in the above table shows that the ground state energy obtained from equation(4.6.8) is lower than the variational ground state energy. The reliability of the result obtained through variational method shows only small deviation from the exact value.

Figure 4.1 is the graphic representation of the numerical data for the ground state energy and exact value. As indicated,the result obtained through variational method is more or less in agreement with the interplotation of the exact wave function with a slight difference.

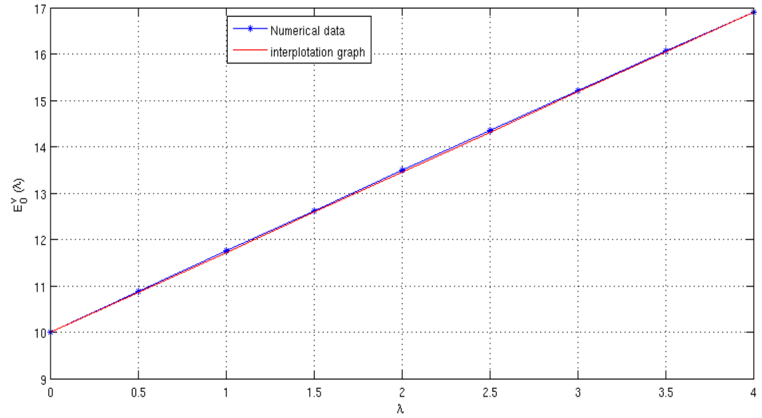

Figure 4.1: comparison of the numerical data with the interplotation result .

4.7 The First and Second excited state

When both non-interacting electrons are found in the first excited state,the trial wave function for the first exited state may be taken as [27]

$$\psi(\vec{\rho}_1, \vec{\rho}_2) = A_m \rho_1 \left(1 - \rho_1^{\beta}\right) \rho_2 \left(1 - \rho_2^{\beta}\right) cos\theta_1 cos\theta_2 \tag{4.7.1}$$

where A_m is the normalization constant and β is the variational parameter. Evaluating the normalization constant for equation (4.7.1) as follows.For a single particle, A_m is evaluated as

$$A_m^2 \int_0^1 \left(1 - \rho_1^{\beta}\right)^2 \rho_1^2 d\rho_1. \tag{4.7.2}$$

$$A_m^2 \left(\frac{2\beta^2}{5(5+\beta)(5+2\beta)}\right) = 1.$$

$$A_{m_1} = \sqrt{\frac{5(5+\beta)(5+2\beta)}{2\beta^2}} \tag{4.7.3}$$

Similarly, The normalized A_m is the product of A_{m_1} , A_{m_2} times the contribution of spherical harmonics for $l = 1$.

$$A_{m_2} = \sqrt{\frac{5(5+\beta)(5+2\beta)}{2\beta^2}}.$$

$$A_m = A_{m_1} A_{m_2} = \frac{5(5+\beta)(5+2\beta)}{2\beta^2} \tag{4.7.4}$$

$$A_m = \frac{3}{4\pi}\frac{5(5+\beta)(5+2\beta)}{2\beta^2} \tag{4.7.5}$$

Evaluating the average kinetic energy for the 1^{st} excited state using Hamiltonian (4.6.3) and the trial wave function (4.6.4)

$$T = \int_0^1 \langle\psi_1(\vec{\rho}_1)|\hat{T}|\psi_1(\vec{\rho}_1)\rangle \rho_1^2 d\rho_1 \tag{4.7.6}$$

$$T = (\frac{5(5+\beta)(5+2\beta)}{2\beta^2})\int_0^1 \left[\left(1-\rho_1^\beta\right)\rho_1\right]\left(\frac{d^2}{d\rho_1^2}+\frac{2}{\rho_1}\frac{d}{d\rho_1}\right)\left[\left(1-\rho_1^\beta\right)\rho_1\right]\rho_1^2 d\rho_1 \tag{4.7.7}$$

Evaluating the above equation using Mathematic gives

$$\begin{aligned} T = &\left(\frac{5(5+\beta)(5+2\beta)}{2\beta^2}\right)\int_0^1 \left(1-\rho^\beta\right)\rho_1 \\ &*\left[\left(-2\rho^{-1+\beta}\beta-\rho^{-1+\beta}(-1+\beta)\beta\right)+\left(\frac{2}{\rho}\left(1-\rho^\beta-\rho^\beta\beta\right)\right)\right]\rho_1^2 d\rho_1 \end{aligned} \tag{4.7.8}$$

$$T = \frac{5(5+\beta)(5+2\beta)}{2(3+2\beta)} \tag{4.7.9}$$

The average interacting energy is evaluated using Hamiltonian (4.6.3) and the trial wave function (4.7.1) becomes

$$J = \frac{\lambda 5(5+\beta)(5+2\beta)}{2\beta^2}\int_0^1 \left(1-\rho^\beta\right)^2\rho_1^2\left[\frac{1}{\rho_1}\int_0^{\rho_1}\left(1-\rho_2^\beta\right)^2\rho_2^3 d\rho_2+\int_{\rho_1}^1\left(1-\rho_2^\beta\right)\rho_2^4 d\rho_2\right]\rho_1^2 d\rho_1 \tag{4.7.10}$$

The result obtained after using Mathematica becomes

$$J = \left(\frac{\lambda 5(5+\beta)(5+2\beta)}{2\beta^2}\right)\left(\frac{2\beta^2\lambda(152020+129810\beta+39046\beta^2+4836\beta^3+208\beta^4)}{5(7)(7+\beta)(9+\beta)(9+2\beta)(9+4\beta)}\right) \tag{4.7.11}$$

After rearranging , the result will be rewritten as

$$J = (5+\beta)(5+2\beta)\left[\frac{\lambda\sum_{n=0}^4 C_n\beta^n}{\prod_{i=0}^2(7+i\beta)\prod_{j=0}^4(9+j\beta)}\right] \tag{4.7.12}$$

The total energy for the first excited state using the trial wave function (4.7.1) is the sum of the interaction energy plus the non-interaction energy, that is given by

$$E^v_{excited} = (5+\beta)(5+2\beta)\left(\frac{5}{2(3+2\beta)}+\frac{\lambda\sum_{n=0}^4 C_n\beta^n}{\prod_{i=0}^2(7+i\beta)\prod_{j=0}^4(9+j\beta)}\right) \tag{4.7.13}$$

where $C_0 = 152020$, $C_1 = 129810$, $C_2 = 39046$,$C_3 = 4836$, and $C_4 = 208$.

The minimum energy of equation is obtained from the condition ,

$$\frac{dE^v_{excited}(\beta)}{d\beta} = 0 \tag{4.7.14}$$

The numerical computation for the first excited state is carried out using the following procedure. Firstly, taking the first derivative of equation (4.7.14) with respect to β for different values of λ. Secondly, substitute the values of β and λ into equation (4.7.13) to get the value of the first excited state. In table-2 bellow, we present the calculated value the first excited state energy for different values of λ and β.

Table 4.2: The ground state energy of $E^v_{excited}$ and variational parameter β for different values of λ.

λ	0	0.5	1	1.5	2	2.5	3	3.5	4
β	0.3708	0.3919	0.4130	0.4343	0.4557	0.4774	0.499	0.5208	0.5427
$E^v_{excited}$	20.60	21.32	22.13	23.05	23.78	24.58	25.40	26.21	27.02

The result obtained above shows that the first excited state energy of two non-interacting electrons gives 20.60 while the exact wave function for non-interacting electrons gives 20.25 for the exact excited state.

The trial wave function of the first excited state for two non-interacting electrons when the first electron is in the ground state with $n = 0$,$l = 0$,$m = 0$ and the second electron is in the first excited state with $n = 0$,$l = 1$,$m = 0$. The wave function of two non-interacting electrons in the first excited state, the symmetric combination of the wave function is given by;

$$\psi_1(\vec{\rho_1}, \vec{\rho_2})^{(s,a)} = \frac{1}{\sqrt{2}} \left\{ \psi_0(\vec{\rho_1})\psi_1(\vec{\rho_2}) \pm \psi_0(\vec{\rho_2})\psi_1(\vec{\rho_1}) \right\}. \tag{4.7.15}$$

where s and a represents the symmetric and anti-symmetric wave functions.

The trial wave function may be taken as;

$$\psi_0(\vec{\rho_1})\psi_1(\vec{\rho_2}) = A_l \left(1 - \rho_1^{\alpha}\right) \rho_2 \left(1 - \rho_2^{\beta}\right) cos\theta_2 \tag{4.7.16}$$

where A_l is the normalization constant and determined from the relation

$$A_l^2 \int_0^1 \left(1-\rho_1^{\alpha}\right)^2 \rho_1^2 d\rho_1 = 1. \tag{4.7.17}$$

The normalization constant for particle-1 is

$$A_{l_1}^2 \left(\frac{2\alpha^2}{27+27\alpha+6\alpha^2}\right) = 1 \tag{4.7.18}$$

$$A_{l_1} = \left(\frac{27+27\alpha+6\alpha^2}{2\alpha^2}\right)^{1/2} \tag{4.7.19}$$

Using similar procedure the normalization constant for particle-2 is

$$A_{l_2}^2 \int_0^1 \rho_2^2 \left(1-\rho_2^{\beta}\right)^2 \rho_2^2 d\rho_2 = 1. \tag{4.7.20}$$

$$A_{l_2}^2 \left(\frac{2\beta^2}{5(5+\beta)(5+2\beta)}\right) = 1 \tag{4.7.21}$$

$$A_{l_2} = \left(\frac{5(5+\beta)(5+2\beta)}{2\beta^2}\right)^{1/2} \tag{4.7.22}$$

Thus, A_l is the product of A_{l_1} and A_{l_2} multiplied by the spherical harmonics for $l = 1$.

$$A_l = A_{l_1} A_{l_2} = \frac{\sqrt{3}}{4\pi} \left(\frac{27+27\alpha+6\alpha^2}{2\alpha^2}\right)^{1/2} \left(\frac{5(5+\beta)(5+2\beta)}{2\beta^2}\right)^{1/2} \tag{4.7.23}$$

where β is an additional parameter. It appears because the electrons are in different states.

The exact wave function of the first excited state for rigid confinement if one electron is in the excited state for small coupling constant λ the respective wave function is given by

$$\psi_1(\vec{\rho_1}, \vec{\rho_2}) = \frac{1}{\sqrt{2}} \left\{\psi_0(\vec{\rho_1})\psi_1(\vec{\rho_2}) \pm \psi_0(\vec{\rho_2})\psi_1(\vec{\rho_1})\right\} \tag{4.7.24}$$

where $\psi_0(\vec{\rho_1}) = \frac{A_0 sin\pi\rho_1}{\rho_1}$ and $\psi_1(\vec{\rho_2}) = A_1 \left[\frac{sink\rho_2}{(k\rho_2)^2} - \frac{cosk\rho_2}{k\rho_2}\right]$ are the ground and the first excited state wave functions, respectively. And $A_0 = \frac{1}{\sqrt{2\pi}}$, $A_1 = 6.51011\sqrt{\frac{3}{4\pi}}$ are the normalization constants and $k = 4.4934$ is the 2^{nd} root of the spherical Bessel's function. The wave functions vanishes at the surface of the quantum dot(i.e $\psi_0(1) = \psi_1(1) = 0$).

The calculation of the average Hamiltonian (4.6.3) with the help of symmetrized wave function (4.6.4) gives the following result[27].

$$E_1^v(\alpha,\beta) = \frac{(\alpha+1)(6\alpha^2+27\alpha+27)}{4(2\alpha^2+3\alpha+1)} + \frac{5(5+\beta)(5+2\beta)}{4(3+2\beta)} + J_1 \pm I_1 \tag{4.7.25}$$

where

$$J_1 = \int |\psi_1(\rho_1)|^2 \frac{\lambda}{\rho_{12}} |\psi_1(\rho_2)|^2 dv_1 dv_2 \tag{4.7.26}$$

$$I_1 = \int \psi_1(\rho_1)\psi_0(\rho_1) \frac{\lambda}{\rho_{12}} \psi_1(\rho_2)\psi_0(\rho_2) dv_1 dv_2 \tag{4.7.27}$$

After integrating using mathematic and rearranging the result yields

$$J_1 = \frac{3\lambda}{16\alpha^2\beta^2} A_k (C+D+E) \tag{4.7.28}$$

with

$$C = \frac{32}{21} + \frac{7+3\alpha}{\prod_{i=1}^2 (7+i\alpha)} - \frac{15(1+\alpha)}{\prod_{i=1}^2 (3+i\alpha)} \tag{4.7.29}$$

$$D = \frac{10(7+3\beta)}{3\prod_{i=1}^2 (7+i\beta)} - \frac{40}{6+5\alpha+\alpha^2}\left(\frac{7+\alpha+3\beta}{\prod_{i=1}^2 (7+\alpha+i\beta)}\right) \tag{4.7.30}$$

$$E = \frac{10}{3+5\alpha+2\alpha^2}\left(\frac{7+2\alpha+3\beta}{\prod_{i=1}^2 (7+2\alpha+i\beta)}\right) - \frac{10\alpha^2(5+3\beta)}{(2+3\alpha+\alpha^2)\prod_{i=1}^2 (5+i\beta)} \tag{4.7.31}$$

The energy exchange interaction A is given by

$$I = \frac{5\lambda}{4\alpha^2\beta^2} A_k (F+G+H), \tag{4.7.32}$$

with

$$F = \frac{2\alpha^2(17+2\alpha)}{35(5+\alpha)\prod_{i=1}^2 (7+i\alpha)} - \frac{5\alpha(\alpha-1)}{3(\alpha-3)(2+\alpha)(5+\beta)} \tag{4.7.33}$$

$$G = \frac{203+38\beta}{15\prod_{i=1}^2 (7+i\beta)} + \frac{4}{21+6\alpha+6\beta} + \frac{\alpha(5+\alpha)}{3(6+5\alpha+\alpha^2)(5+\alpha+\beta)}, \tag{4.7.34}$$

$$H = \frac{6(7+\alpha+\beta) - 3(20+\alpha(7+\alpha))(7+2\alpha+\beta))}{(2+\alpha)(5+\alpha)\prod_{i=1}^2 (7+\beta+i\alpha)} + \frac{24}{(-9+\alpha^2)(7+\beta^2)} \tag{4.7.35}$$

$$A_k = \prod_{i=1}^{2} (3+i\alpha) \prod_{j=1}^{2} (5+j\beta) \tag{4.7.36}$$

Table 4.3: The excited state energy of $E_1^{(s)}$,and $E_1^{(a)}$ variational parameter α and β,the normal Coulomb interaction energy J_1,and the exchange energy I_1 for different values of λ.

λ	J_1	I_1	$E_1^{(s)v}(\lambda)$	$E_1^{(a)v}(\lambda)$
0	0	0	15.298	15.298
0.5	0.798	0.1762	16.274	15.922
1	1.591	0.3529	17.249	16.542
1.5	2.379	0.529	18.222	17.542
2	3.164	0.707	19.194	17.780
2.5	3.943	0.884	20.165	18.395
3	4.719	1.062	21.1341	19.009
3.5	5.490	1.240	22.101	19.620
4	6.257	1.418	23.066	20.230

The result tabulated above(in table 4.3) shows that the first excited state of symmetric combination of the wave function is greater than the anti-symmetric counter parts. This indicates that the contribution of coulomb and exchange interactions are high for symmetric wave functions than the anti-symmetric combinations.

The energy of the exact wave function (4.6.9)of the first excited state studied under rigid confinement in which the 1^{st} electron is in the ground state and the 2^{nd} electron is found in the excited state. Solving equation (4.6.9) using the expression of Legendre polynomial in spherical harmonics [4.6.18], we get

$$J = 84.76\lambda \int_0^1 \left\{ \frac{sin^2\pi\rho_1}{\rho_1^3} \int_0^{\rho_1} \left(\frac{sink\rho_2}{(k\rho_2)^2} - \frac{cosk\rho_2}{k\rho_2} \right)^2 {\rho_2}^2 d\rho_2 + \frac{sin^2\pi\rho_1}{\rho_1^2} \int_{\rho_1}^1 \left(\frac{sink\rho_2}{(k\rho_2)^2} - \frac{cosk\rho_2}{k\rho_2} \right)^2 \rho_2 d\rho_2 \right\} \tag{4.7.37}$$

The above integral (4.7.37) is evaluated using Mathematica gives $J = 1.62159\frac{e^2}{\varepsilon a}$.And interchanging electrons state in equation (4.7.32) and (4.7.24), the gives a result to $I = 0.359656\frac{e^2}{\varepsilon a}$.

The calculation of the Hamiltonian (4.6.3) with the help of symmetrized wave function (4.7.24) yields,

$$E_1 = \left(\frac{\pi^2}{2} + \frac{4.5^2}{2} \right) \frac{\hbar^2}{m^*a} + 1.62159\frac{e^2}{\varepsilon a} \pm 0.359655\frac{e^2}{\varepsilon a}. \tag{4.7.38}$$

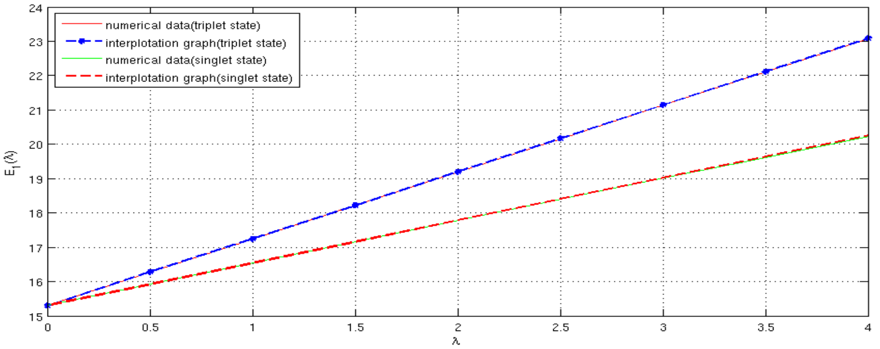

Figure 4.2: The figure shows the triple and singlet states of the excited state energy Vs λ.

Figure 4.2 is the graphical representation of the triplet and singlet states of the excited state energy. As shown,the excited state energy of the symmetric wave function is greater than its anti-symmetric counter part. This is due to the fact that the coulomb and exchange interactions for symmetric combinations is greater as compared to the corresponding anti-symmetric combination.

Chapter 5

Conclusion

In this paper we have studied theoretically a two electrons quantum dot using a three dimensional spherically symmetric rigid confinement potential.In particular,the researchers focused on the effect of electron-electron interaction on the ground and excited electronic state of the quantum system.

For this purpose, the writers have considered both the singlet and triplet state basis function

In this work the eigenvalue problem is solved for the Hamiltonian(4.6.3) using the variational method with trial wave function (4.6.4),[27], which is built from the wave function of one electron state for the rigid confinement potential. As a result, both the ground state wave function and energy levels are calculated for the non-interacting two electrons quantum dot.

In addition, both the variational ground state energy E_0^v and variational parameter α are calculated for different values of coupling constant λ for two non interacting electrons quantum dot with rigid confinement, table (4.1), with the help of equation given above. The results obtained in table (4.1) above shows that variation ground state energy increases with increasing coupling constant λ /interaction scale λ. To test the validity of the results,the results obtained using variational method is compared with the exact energies obtained using numerical integration of the Schrdinger equation. The variational method approach is in agreement with the results of exact energies. For instance, the ground state energy of the two non-interacting electrons is $E_0^v = 9.9993$ with trial wave function(4.6.4). However, the exact wave function(4.6.9) of non-interacting electrons gives the ground energy $E_0 = \pi^2$.

Based on this fact the writer can say that the accuracy of the variational method deviates from the exact value by 1.3 percent.

The change of dielectric constant leads to the induced electric polarization at the QD boundary[17]. The influence of the electric polarization on the electron states in spherical QD[19] under the assumption of rigid confinement potential is studied. Based on the these results [25],we can state that for QD embedded in a dielectric medium of smaller dielectric constant,the electric polarization contributes to an additional potential,which will repulse the electrons from the boundaries pushing them towards the dot center. As a result, the electron will be more localized inside QD.

The major conclusions of of this work are summarized as follows.

The dominant contribution to the total energy is coming from the electronic repulsion in QD.

The expectation values of electron-electron interaction for ground state increases almost linearly with the quantum dot radius a. The coulombic interaction energy more strongly depends on the quantum state for more separated electrons.

As shown in table(4.2) above, the result of the first excited state energy for two non interacting electrons with trial wave function(4.7.1) increases with increasing variational parameter β for different values of λ.

As we have stated above,the singlet and triplet states have different energies once the electron repulsion is taken in to account. So that the result obtained above confirms that the triplet(ortho) state energies lower than the energies of the singlet(para) state counter parts. It is interesting to note that both the coulomb integral and the exchange integral are non negative because they arise from electron-electron repulsion and the value of coulomb integral is greater than the exchange integral.Here the exchange integral arise when we have terms in the wave function where the two electrons have exchanged places.

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Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

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