THE LOW LYING STATES OF TWO-ELECTRON QUANTUM DOT WITH PARABOLIC CONFINEMENT

By

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Abstract

In this thesis we study the first two low lying states of the two-electron quantum dot with parabolic confinement. We use Harmonic oscillation model in spherical coordinates due to its symmetry. With the help variational method, we find the ground state and first excited state energy correction since the interaction between the two electrons is not small in nano lengths. We determine the energy as a function of Coulomb interaction scale. We calculate numerical values and propose interpolation formula for energies. It is found that the electron-electron interaction affects not only the energy and the radius of the quantum dots but also the dielectric constant of the nanostructures.

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Chapter 1

Introduction

1.1 Low Dimensional Crystals

Low dimensional crystals such as Quantum wells (Q-wells),Quantum wires (Q-wires), and Quantum dots (Q-dots) are semiconductor crystals whose size confined and limited to atomic sizes (a few nanometers) in one, two, and three dimensions respectively [1-3]. Quantum-dot, a three dimensional midget, is a sphere with a radius of few nanometer(typical sizes of 2 $\sim$ 100nm, containing 100 to 10,000 atoms). It can be said that electrons in quantum dots are confined to zero-dimension. Quantum dots have quantized energy levels and discrete density states due to the three dimension confinements unlike one- and two-dimensions where density states and energy levels are continuous [1, 2].

The physical properties of nano structures is effectively controlled by their nano-dimensional size which is impossible for bulk semiconductors [2]. In the case of quantum dots the electric and optoelectronic properties are effectively controlled by their dimensions. The main features that makes quantum dots, in both applications and science, interesting is that [1, 2]:

• The physical properties of quantum dots are size, dimension and electrons density dependant .

• The size, dimension and electrons density of quantum dots can be controlled effectively.

It was in early 1980s that the first quantum dots were successfully made in a research laboratory . The main thing was to grow a semiconductor crystal of atomic dimensions. The construction of Quantum-dots took two separate paths. In the first method ,the dot is constructed using lithography techniques of microchip manufacturing; creating one Quantum-dot at a time. In the second method,chemical processes are used to grow Quantum-dots in bulk semiconductors [2- 4].

The main applications of quantum dots are for optoelectronic, medical imaging, information storage and quantum computing [2]. Even if bulk semiconductors have optoelectronic application the controllable properties of the quantum dots makes them preferable, since quantum dots of the same material but different size have completely different properties [1-4].

1.2 Electronic Properties of Quantum Dots

Quantum mechanics is a tool that helps us to understand how quantum dots are different from bulk semiconductors [1,2]. Quantum mechanics describes electron in the semiconductor crystal has a wavelike representation [1,2]. The wave length , λ, of this wave is inversely proportional to electron's momentum, P [6- 7].

$$\lambda = \frac{h}{p} \tag{1.2.1}$$

Also, according to Heisenberg's Uncertainty Principle, position x and momentum p of the electron are correlated in that confinement to electron in a space x_{min} results in a maximum possible energy for the electron [1].

$$\Delta E \Delta t = \Delta x \Delta p \tag{1.2.2}$$

Based on this uncertainty principle, We can write

$$\Delta E = \frac{hp}{m^* \Delta x}. \tag{1.2.3}$$

In the above h is Planck's constant and m^* is the electron effective mass. Fortunately, in semiconductor the electron's mass is reduced to an effective value, called the effective mass, to around 10 % of its value in free space. Because of this, room-temperature confinement of electron can take place in nanometer size crystals with single particle energy level spacing, $\Delta\epsilon$,[2]

$$\Delta\epsilon >> k_B T \tag{1.2.4}$$

where k_B is the Boltzmann factor and T is the temperature.

To examine the effects of this confinement we need to restore to a model description of a trapped particle in the quantum world [1, 2]. One model describing confinement of electron to a quantum dot is that of a particle trapped inside a box. In this model quantum mechanics predicts quantized energy levels similar to the simpler one-dimensional case. Another model describing this confinement is based on the electron-hole attraction, or the energy quantization of exciton.

In the study of quantum wires and quantum wells the one-dimensional and two-dimensional potential well models could be applied to predict energy levels due to the confinement. In the case of quantum dots the exciton model is a more realistic one. When an electron is promoted to the conduction band in bulk semiconductor material a hole is created in the valence band. The absence of negative charge in the valence band makes the hole's effective charge to be positive, thus attracting the electron. This pair form a hydrogenic atom that is relatively loosely bound. In the quantum dot where the size of the nanocrystal is comparable to the effective Bohr radius a_0 of the exciton, the binding is stronger

[10]; where the Bohr radius a_0 in semiconductors given as

$$a_0 = \frac{\varepsilon \hbar^2}{m^* e^2}. \tag{1.2.5}$$

where ε is the dielectric constant. Below is a list of effective Bohr radii for different nano crystals. [1-2]

Materials	Bohr radius (nm)
$CdSe$	6
PbS	20
$InAs$	34
$PbSe$	46

Table 1.1: Bohr Radius of some materials (Extracted from [1, 2] and organized in table form).

In contrast, the Bohr radius for hydrogen atom is about **0.05 nm**. The difference in the Bohr radii in different materials is solely due to the effective mass of the electron in that material [10]. This difference is also exhibited in the hydrogenic energy levels [1, 2]. These values are given by [1,2]:

$$E_n = -13.6 \frac{m^*}{\varepsilon^2 n^2} eV. \tag{1.2.6}$$

n=1,2,3.....

where m^* is the effective mass of the electron in the bulk material and ε is the dielectric constant.

Semiconductor quantum dots, as compared to semiconductor lattice(unit cell), have characteristic size at least one-two order of magnitude bigger than the characteristic length of the semiconductor lattice (unit cell). Hence the quantum dots has a macroscopic size in

comparison to the unit cell, but it is small on all macroscopic scales. One can often calls quantum dots mesoscopic structures, since quantum dots contains up to 10,000 atoms, which is neither microscopic nor macroscopic size.

It is reasonable to start the study of electronic states of quantum dots(mesoscopic structures) with the help of the usual bulk-semiconductor equation for the spatial single-particle wave function $\Psi(r)$ [1, 2];

$$\Psi_K(r) = \psi(r)U_k(r). \tag{1.2.7}$$

where r is the position of the electron, $U_k(r) = u_k e^{ik.r}$ is the rapidly oscillating periodic part of the Bloch function and $\psi(r)$ is the envelope function, which varies on the scale of several unit cells implies that we have a non degenerate conduction band with edge at $K = 0$ in the reciprocal space, as it is the case in usual GaAs/GaAlAs heterostructures, and that the Bloch function $U_k(r)$ refers to the state $K = 0$ [2].

In the spirit of the equation (1.2.7), it seems sensible to assume that the energy eigenvalues of the electron in the periodic lattice, i.e. the energy bands, are not appreciably modified by the quantum confinement [2].

The envelope eigenfunction $\psi(r)$ in Eq.(1.2.7) inside the quantum dots do satisfies the following equation (Schrodinger equation) for N number of electrons in a quantum dots or in a system of coupled quantum dots [1, 2];

$$H\psi = E\psi. \tag{1.2.8}$$

with $\psi = \psi(r_1 s_1, r_2 s_2, r_3 s_3 ... r_N s_N)$ total envelope wave function of electrons at position r_i and spin projection along z-axis $s_i = \pm\frac{1}{2}$ (i=1,2,3.....) and E total eigenvalue.

Then the total Hamiltonian H in Eq.(1.2.8) is the sum of the spatial Hamiltonian (which acts on the spatial coordinates) and spin Hamiltonian (which acts on spin coordinates).

$$H = H_{space} + H_{spin}. \tag{1.2.9}$$

The spin-orbit coupling is ignored since smaller for single conduction band and small number of electrons [1]. The spatial part of the Hamiltonian $\mathbf{H_{space}}$ is simply the sum of the single particle Hamiltonian, $\sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{H}(\mathbf{r_i})$, and the two-body Coulomb interaction potential [8-11];

$$H_{space} = \sum_{i=1}^{N} H(r_i) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\varepsilon |r_i - r_j|} \tag{1.2.10}$$

The Schrodinger equation corresponding to this Hamiltonian can be solved exactly for one particle. In the case of many electrons there is no exact solutions, can be solved approximately with the help of the numerical methods [8-11].

1.3 Outlines of The Thesis

The behavior of Quantum dot is understandable by the use of its wave function and energy levels of the electrons and protons which gives us information about its optoelectronic properties. In the case of single particle Quantum-dots, the confinement of electron to zero-dimension is that of a particle trapped inside a box. In this model quantum mechanics predicts quantized energy levels similar to the simpler one-dimensional case. Another model describing this confinement is based on the electron-hole attraction, or the energy quantization of exciton. In this paper we use the Harmonic oscillator model for the parabolic confinement of electrons to zero-dimension.

A Quantum-dot with two or more electrons, in addition to kinetic energy and confining potential, possesses an electron-electron interaction which has also contribution to the

wave functions and energy levels.

In this thesis we study the first two low lying states of the two- electron quantum dot with parabolic confinement. This work highlights single particle (electron) quantum dot which is a base for further investigation. The Coulomb interaction in the typical **10nm** semiconductor quantum dot can not be treated as small. We employ the variational method to approximate the modifications, in the ground and first excited states, resulted from the electron-electron interaction potential. We also investigate the effect of the electron-electron interaction on the dielectric constant ε of the material; since as in [10], for single electron quantum dot confinements, as size of nanostructure decrease the dielectric constant of the nanostructure also decreases.

In the introduction part, we have discussed the definitions of low dimensional system, better alternative applications of quantum dots and the electronic properties of quantum dots.

Chapter 2 , the main purpose of this chapter is to evaluate and study a single -electron quantum dot with parabolic confinement. We discuss the energy levels and wave functions of the single-electron quantum dots. The wave function of the system appears as power series and have the energy range with $\hbar\omega$.

In chapter 3 and chapter 4, Extending the concept of chapter one, we apply to a two-electron quantum dots parabolic confinement. The dimensionless Hamiltonian of the two-electron quantum dots with the electron-electron interaction potential, $V(|r_1 - r_2|) = \frac{e^2}{\varepsilon|r_1 - r_2|}$ becomes;

$$H = -\frac{1}{2}\left(\bigtriangledown_1^2 + \bigtriangledown_2^2\right) + \frac{1}{2}\left(\rho_1^2 + \rho_2^2\right) + \frac{\lambda}{|\rho_1 - \rho_2|}. \tag{1.3.1}$$

where we use λ, the dimensionless Coulomb interaction scale which gauges the strength

of the coulomb interaction;

$$\lambda = \sqrt{\frac{1}{\varepsilon^2}\frac{m^* e^4}{\hbar^2}\frac{1}{\hbar\omega}} \tag{1.3.2}$$

Here the dimensionless coordinates of the first and second electrons ρ_1 and ρ_2 are measured in units $\sqrt{\frac{\hbar}{m^*\omega}}$, ε is the dielectric constant of quantum dots and m^* is the effective mass of the electron. Taking the Rydberg constant $R_y = \frac{me^4}{\hbar^2} = 27.2eV$ and setting $\omega = 10THz$, we obtain $\lambda \simeq \frac{20}{\varepsilon}$. For the typical case if we assume $\varepsilon = 14$ then $\lambda = 1.43$, which is not small, this means that the Schrodinger equation corresponding to Hamiltonian (1.3.1) for the semiconductor quantum dot would be solved using Variational or numerical methods which we use in this paper.

The quantum state of the two-electron quantum dots can be constructed from a single-electron state in the case of non-interacting electrons. We use the Variational method approach to approximate the modification to the wave function and energy levels of the system due to electron-electron interaction.

Chapter 5 presents the conclusion of the final result.

Chapter 2

Single-Electron Quantum Dot With Parabolic Confinement

In this section we carefully inspect the solution of Eq.(1.2.8) for the spatial single-electron quantum dots in parabolic confinement potential $V(r)$. We investigate the wave functions and energy levels for the single electron in detail since a complete understanding of single-particle energy spectrum and related degeneracies is the basis for further study.

Starting from the spatial single-electron Hamiltonian of a quantum dots in spherically symmetric harmonic potential (parabolic confinement potential) V(r) [1, 2],

$$H = -\frac{\hbar^2}{2m^*} \bigtriangledown^2 + \frac{1}{2} m^* \omega^2 r^2. \tag{2.0.1}$$

where the first term, $-\frac{\hbar^2}{2m^*}\bigtriangledown^2$, is the kinetic energy of the electron , the second term , $\frac{1}{2}m^*\omega^2 r^2$, is the harmonic confinement potential of a quantum dot and m^* is the effective mass of the electron in the conduction band(for typical semiconductors $m^* = 0.13m_e$).

Defining the coordinate system in spherical coordinate for the advantage of its symmetry, $r = (r, \theta, \varphi)$ where $\mathbf{r}$ is the radial coordinate and (θ, φ) are polar coordinates of the electron.

$$\bigtriangledown^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial \theta}\left(sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial \varphi^2}. \tag{2.0.2}$$

Then using Eq.(2.0.2) at Eq. (2.0.1) the Hamiltonian of the system in spherical coordinates becomes,

$$H = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial \theta}\left(sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{1}{2}m^*\omega^2 r^2. \tag{2.0.3}$$

Introducing the dimensionless quantities,

$$\rho = \sqrt{\frac{m^*\omega}{\hbar}}r. \tag{2.0.4}$$

Where ρ is the dimensionless coordinate.

With the help of dimensionless coordinate (2.0.4), We obtain the dimensionless Hamiltonian

$$\begin{aligned}\hat{H} &= -\frac{1}{2}\bigtriangledown_\rho^2 + \frac{1}{2}\rho^2, \\ \hat{H} &= -\frac{1}{2}\left(\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2 sin\theta}\frac{\partial}{\partial \theta}\left(sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\rho^2 sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{1}{2}\rho^2. \end{aligned} \tag{2.0.5}$$

The Schrodinger equation of the single-electron quantum dots corresponding to the Hamiltonian (2.0.5) has the form

$$\{-\frac{1}{2}\left(\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2 sin\theta}\frac{\partial}{\partial \theta}\left(sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\rho^2 sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{1}{2}\rho^2\}\psi(r) = E\psi(r). \tag{2.0.6}$$

where E is the dimensionless energy quantity (eigenvalues), measured in units of $\hbar\omega$.

2.1 Solutions of Schrodinger Equations of single-electron Quantum Dot in Parabolic Confinement

The Schrodinger equation for the the single-electron quantum dot in the parabolic confinement can be solved expressing $\psi(r)$ as a product of the radial coordinate wave function and the angular coordinate wave function with the help of separation of variables[1 -7],

$$\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi). \tag{2.1.1}$$

where $\mathbf{R(r)}$ is the radial wave function and $Y(\theta,\varphi)$ is the spherical harmonics part which is a product of the azimuthal components and angular component, $Y(\theta,\varphi) = P(\theta)\phi(\varphi)$.

Substituting Eq.(2.1.1) at the Eq.(2.0.6) and dividing again by Eq.(2.1.1) we obtain

$$-\frac{1}{2}[\{\frac{1}{R}\frac{\partial^2}{\partial\rho^2}+\frac{2}{R\rho}\frac{\partial}{\partial\rho}\}R+\{\frac{1}{P\rho^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)\}P+\{\frac{1}{\phi\rho^2 sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\}\phi]+\{\frac{1}{2}\rho^2-E\}=0. \tag{2.1.2}$$

2.1.1 Solutions of the Spherical Harmonics

The Schrodinger equation (2.1.2) above contains the functions, $\mathbf{R}$ which is the function of r only,$\mathbf{P}$ which is the function of θ only and ϕ is the function of φ only. So, we can solve this equation by re-arranging the equation as [5-7],

$$-\rho^2 sin^2\theta\{\frac{1}{R}\frac{\partial^2}{\partial\rho^2}+\frac{2}{R\rho}\frac{\partial}{\partial\rho}\}R+\{\frac{sin\theta}{P}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)\}P+\rho^2 sin^2\theta\{2E-\rho^2\}=-\frac{1}{\phi}\frac{\partial^2\phi}{\partial\varphi^2}. \tag{2.1.3}$$

Since both sides contain independent functions, lets take both sides equals to a constant m [5-7], so we can have the equation

$$\frac{1}{\phi}\frac{\partial^2\phi}{\partial\varphi^2} = -m. \tag{2.1.4}$$

The solution for this equation has the form

$$\phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}. \tag{2.1.5}$$

where m is azimuthal quantum number $(= 0, \pm 1, \pm 2.....)$ [5-7].

Similarly separating Eq.(2.1.2) to the radial and spherical harmonics; we can obtain,

$$\{\frac{1}{sin\theta}(sin\theta\frac{\partial}{\partial\theta}) - \frac{m^2}{sin^2\theta}\}P(\theta) = \iota(\iota+1)P(\theta). \tag{2.1.6}$$

where we obtain Eq.(2.1.6) which is the equation of the Associated Legendre differential equation and has the solution Legendre polynomials $P_\iota^{|m|}(cos\theta)$ [6,7].

Then the spherical harmonics wave function $Y_{\iota m}$ becomes [1-7];

$$Y_\iota^m(\theta,\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} P_\iota^{|m|}(cos\theta). \tag{2.1.7}$$

where ι is the angular quantum number (=0,1,2,3.....).

2.1.2 Solutions for Radial Component Equation

Using Eq.(2.1.6) at the Eq.(2.1.3), the Schrodinger equation of the radial component becomes

$$\frac{\partial^2 R}{\partial\rho^2} + \frac{2}{\rho}\frac{\partial R}{\partial\rho} - \frac{\iota(\iota+1)}{\rho^2}R + \{2E - \rho^2\}R = 0. \tag{2.1.8}$$

Expressing the above equation again we can have

$$R''(\rho) + \frac{2}{\rho}R'(\rho) + \{\nu - \frac{\iota(\iota+1)}{\rho^2} - \rho^2\}R = 0. \tag{2.1.9}$$

Where we use dimensionless quantity $\nu = 2E$.

This differential equation can be solved with the use the power series expansion , with the help of the boundary conditions to obtain a meaningful physical wave function. The wave functions should be finite near the two extremes [6 ,7].

Boundary conditions

• If one looks at the differential Eq.(2.1.9)in the neighborhood of infinity ($|\rho| \to \infty$) , the differential equation (2.1.9) reduced to

$$R''(\rho)_\infty - \rho^2 R_\infty = 0. \tag{2.1.10}$$

This is the second order two term differential equation whose solution can be expressed in the form

$$R_\infty \to e^{-\frac{\rho^2}{2}}. \tag{2.1.11}$$

which has the behavior of rapid convergence as the dimensionless variable ρ increases to large value since the wave function at infinity should be finite [5-7].

• Near the origin,$\rho \to 0$ (small values of ρ), the differential equation (2.1.9) becomes

$$R''_{\to 0} + \frac{2}{\rho} R'_{\to 0} - \frac{\iota(\iota+1)}{\rho^2} R_{\to 0} = 0. \tag{2.1.12}$$

The behavior of the solution for this differential equation has the form;

$$R_{\to 0} \to \rho^\iota. \tag{2.1.13}$$

Now we can combine the two results and postulate the true wave function as [6, 7]:

$$R(\rho) = \rho^\iota e^{-\frac{\rho^2}{2}} f(\rho). \tag{2.1.14}$$

Where a function $f(\rho)$ can be expanded in power series in any powers of ρ , should be non-zero constant near the origin and cannot diverge faster than $e^{-\frac{\rho^2}{2}} f(\rho)$ [6, 7] .

$$f(\rho) = \sum_{k=0}^{\infty} a_k \rho^k. \tag{2.1.15}$$

Substituting Eq.(2.1.15) into Eq.(2.1.9), we obtain the differential equation

$$f''(\rho) + 2\{\frac{\iota - 1}{\rho} - \rho\}f'(\rho) + \{\nu - 2\iota - 3\}f(\rho) = 0. \tag{2.1.16}$$

letting $\rho^2 = \xi$ and also $f(\rho) = f(\sqrt{\xi}) = g(\xi)$, Eq.(2.1.16) can be expressed as:

$$\xi g''(\xi) + \{\iota - \frac{1}{2} - \xi\}g'(\xi) + \{\frac{\nu}{4} - \frac{\iota}{2} - \frac{3}{4}\}g(\xi) = 0. \tag{2.1.17}$$

letting

$$\begin{aligned} k &= \iota - \frac{3}{2}. \\ n_\rho &= \frac{\nu}{4} - \frac{\iota}{2} - \frac{3}{4} \end{aligned} \tag{2.1.18}$$

Substituting Eq.(2.1.18) at Eq.(2..1.17), we obtain the differential equation

$$\xi g''(\xi) + \{k + 1 - \xi\}g'(\xi) + n_r g(\xi) = 0. \tag{2.1.19}$$

This is the equation of the Associated Laguerre differential equation whose solution is the Laguerre polynomials L_n^k satisfying the physically accepted wave function and discreteness of the energy, with $n = n_r + \iota$ and $k = 2\iota + 1$ for the termination of the series [5- 7].

$$L_n^k = L_{n_\rho+\iota}^{2\iota+1}(\rho^2). \tag{2.1.20}$$

Then the radial wave function using Eq.(2.1.14) and (2.1.20) has the form of

$$R_{n_\rho,\iota} \to \rho^\iota e^{-\frac{\rho^2}{2}} L_{n_\rho+\iota}^{2\iota+1}(\rho^2). \tag{2.1.21}$$

where n_ρ is the radial quantum number(=0,1,2,3.....)

The normalization constant can be found from the orthogonality property of the Laguerre polynomials:

$$R_{n_\rho,\iota}(\rho) = \{\frac{2(\alpha)^{\iota+\frac{3}{2}} n_\rho!}{\Gamma(n_\rho - \iota + \frac{3}{2})}\}^{\frac{1}{2}} \rho^{|\iota|} e^{-\frac{1}{2}\rho^2} L_{n_\rho+\iota}^{2\iota+1}(\rho^2) \tag{2.1.22}$$

2.1.3 The Wave Functions and Energy Levels

The energy levels spectrum, for the single-electron quantum dot with parabolic confinement, using Eq. (2.1.18) can be expressed as

$$\begin{aligned} \nu &= 2E. \\ E &= \{2n_\rho + \iota + \frac{3}{2}\}. \\ E &= N + \frac{3}{2}. \end{aligned} \tag{2.1.23}$$

where $N = 2n_\rho + \iota$ is the quantum numbers(=0,1,2,3,....).

And the wave function for the single-electron quantum dots, using Eq.(2.1.7) and (2.1.22) at the Eq. (2.1.1), becomes

$$\psi_{N,\iota,m}(\rho,\theta,\varphi) = \{\frac{2(\alpha)^{\iota+\frac{3}{2}} n_\rho!}{\Gamma(n_\rho - \iota + \frac{3}{2})}\}^{\frac{1}{2}} \rho^{|\iota|} e^{-\frac{1}{2}\rho^2} L_{n_\rho+\iota}^{2\iota+1}(\rho^2) Y_{\iota m}(\theta,\varphi). \tag{2.1.24}$$

The eigenvalues of Eq. (2.1.23) depends only on N, and so are degenerate with respect to both ι and m. For each values of N, the general degeneracy g is [6, 7],

$$g = \frac{(N+1)(N+2)}{2}. \tag{2.1.25}$$

Table of the three low lying states of the single-electron quantum dots, with parabolic confinement, wave functions and energy levels using Eq. (2.1.23), (2.1.24) and (2.1.25).

N	n_ρ	ι	m	E	g	$\psi_{N,\iota,m}(\rho,\theta,\varphi)$.
0	0	0	0	$\frac{3}{2}$	1	$\psi_{000}(\rho,\theta,\varphi) = \{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi}\}^{\frac{3}{4}} e^{-\frac{1}{2}\rho^2}$.
1	0	1	0	$\frac{5}{2}$	3	$\psi_{110}(\rho,\theta,\varphi) = \sqrt{2}\{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi}\}^{\frac{3}{4}} \rho e^{-\frac{1}{2}\rho^2} cos\theta$.
			± 1			$\psi_{11\pm1}(\rho,\theta,\varphi) = \mp\{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi}\}^{\frac{3}{4}} \rho e^{-\frac{1}{2}\rho^2} sin\theta e^{\pm i\varphi}$.
2	1	0	0	$\frac{7}{2}$	6	$\psi_{200}(\rho,\theta,\varphi) = \sqrt{2}\{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi^2}\}^{\frac{3}{4}} \{\frac{3}{2} - \sqrt{\frac{m^*\omega}{\hbar}}\rho^2\} e^{-\frac{1}{2}\rho^2}$.
	0	2	0			$\psi_{220}(\rho,\theta,\varphi) = \frac{1}{2}\sqrt{5}\{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi^2}\}^{\frac{7}{4}} \rho^2\{3cos^2\theta - 1\} e^{-\frac{1}{2}\rho^2}$.
			± 1			$\psi_{22\pm1}(\rho,\theta,\varphi) = \mp\sqrt{15}\{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi^2}\}^{\frac{7}{4}} e^{-\frac{1}{2}\rho^2} \rho^2 sin\theta cos\theta e^{\pm i\varphi}$.
			± 2			$\psi_{22\pm2}(\rho,\theta,\varphi) = \frac{1}{2}\sqrt{15}\{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi^2}\}^{\frac{7}{4}} \rho^2 e^{-\frac{1}{2}\rho^2} sin^2\theta e^{\pm i\varphi}$.

Table 2.1: The eigenfunctions and eigenvalues of the single electron quantum dots for $N = 0, 1$ and 2 levels. The spherical Harmonics wave functions are taken from [7], page 325 .

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The amplitude of the wave function decreases as the radius of the quantum dots increases as shown by Fig. (2.1) and (2.2); and the discrete energy level spacing, $\triangle E$, is 1 as displayed in table (2.1).

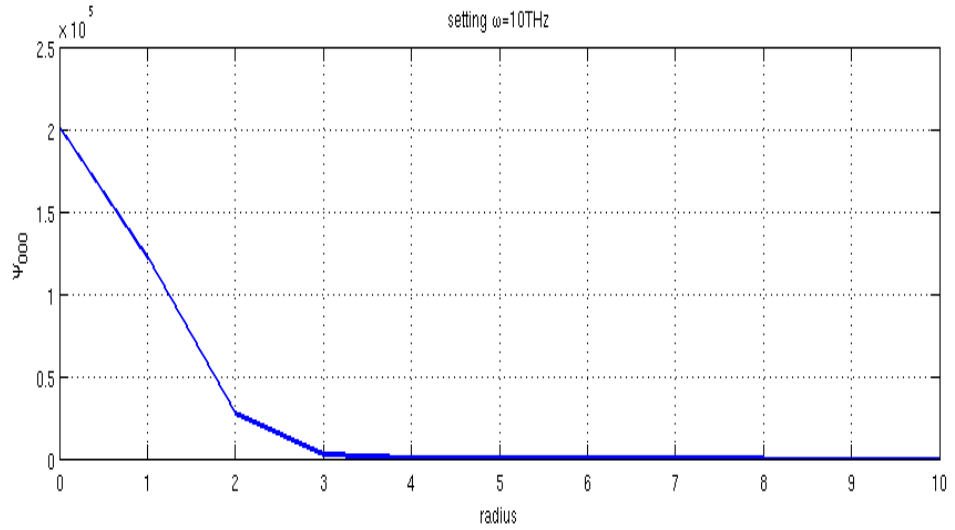

Figure 2.1: The plot of ground state eigenfunction versus ρ; setting $m^* = 0.13m_e$, $\omega = 10THz$.

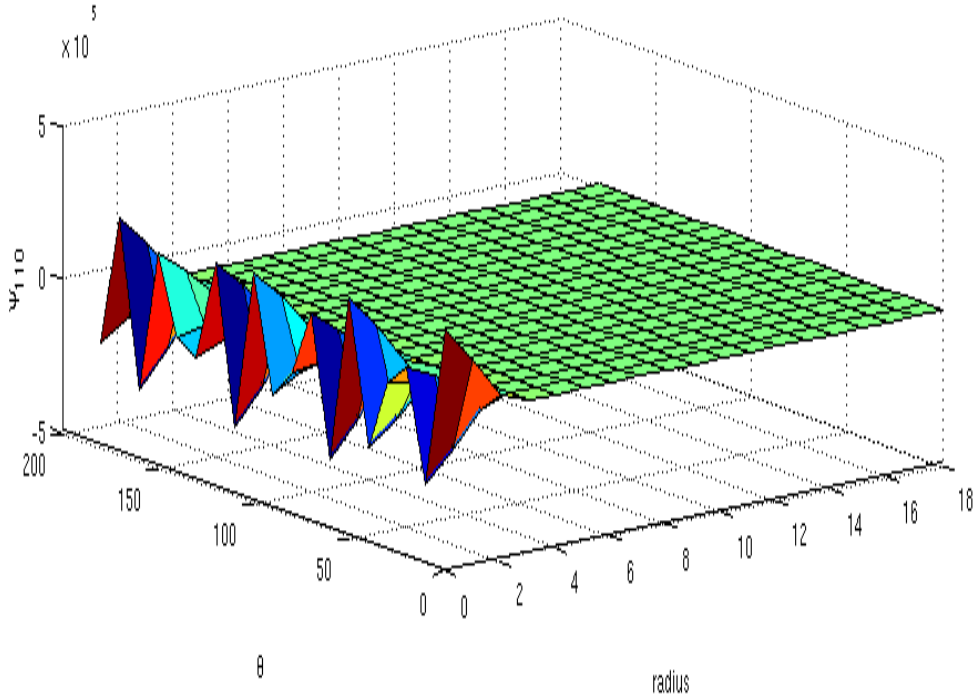

Figure 2.2: The 3D plot of the first excited state,($N = 1$, $\iota = 1$ and $m = 0$), eigenfunction versus ρ and θ ; setting $m^* = 0.13m_e$, $\omega = 10THz$.

Chapter 3

Noninteracting Two-Electron Quantum Dots With Parabolic Confinements

3.1 Introduction

We shall primarily develop an understanding of identical quantum particles by considering a system of two particles (electrons) 1 and 2. All the properties of such system may be extracted from a two-electron wave function $\psi(r_1, s_1; r_2, s_2)$, where r_1 is the position of particle 1, r_2 is the position of particle 2 and s_1, s_2 are the spin vectors.

Since Fermions (electrons) are identical quantum particles ,their wave function must give rise to identical properties for each particle. Thus the two electrons always have an anti-symmetric function [6, 7].

$$\psi(r_1, r_2) = -\psi(r_2, r_1). \tag{3.1.1}$$

under the exchange of the two electrons.

3.1.1 Wave Function of The Two-Electron System

The quantum state of a single-particle state when the spatial and spin properties of a particle are independent of each other may be represented by a product [6, 7];

$$\psi(r,s) = \psi(r)\chi(s). \tag{3.1.2}$$

where the first term , $\psi(r)$, describes the spatial properties with quantum numbers n, ι, m and the second term ,$\chi(s)$, could be a spin state with quantum numbers s and $m = \pm\frac{1}{2}$.

Now, we can write down expressions for quantum states $\psi(r_1, s_1; r_2, s_2)$ which describe the spatial and spin properties of two-identical electrons in terms of the single-electron quantum state. The quantum state of two-electron system is always anti-symmetric $\psi_a(r_1, s_1; r_2, s_2)$ [6, 7]. This would occurs only if either spatial state is symmetric ,$\psi_s(r_1, r_2)$, and spin state is anti-symmetric, $\chi_a(s_1, s_2)$, or spatial state is ant-symmetric, $\psi_s(r_1, r_2)$, and spin state is symmetric, $\chi_s(s_1, s_2)$. The spin symmetric state(also called triplet state), is when the two electrons occupies different energy levels, has total spin one(**S=1**); and the ant-symmetric spin state, called singlet state, is when two electrons occupies the same energy levels, has total spin zero (S=0) [6, 7].

Then quantum state of the two-electrons system can be expressed as [6, 7]

$$\psi_a(r_1, s_1; r_2, s_2) = \begin{cases} \psi_a(r_1, r_2)\chi_s(s_1, s_2). \\ \psi_s(r_1, r_2)\chi_a(s_1, s_2). \end{cases} \tag{3.1.3}$$

Eq. (3.1.3) can be expressed with the single particle eigenstates, where we use ψ_{N_1} and ψ_{N_2} are the eigenstates of electron 1 and electron 2 respectively [6- 7].

$$\psi_a(r_1, s_1; r_2, s_2) = \frac{1}{\sqrt{2}} \begin{cases} \{\psi_{N_1}(r_1)\psi_{N_2}(r_2) - \psi_{N_1}(r_2)\psi_{N_2}(r_1)\}\chi_s(s_1, s_2). \\ \{\psi_{N_1}(r_1)\psi_{N_2}(r_2) + \psi_{N_1}(r_2)\psi_{N_2}(r_1)\}\chi_a(s_1, s_2) \end{cases} \tag{3.1.4}$$

where N_1 and N_2 are the energy levels of the first and the second particles respectively.

The spin states ,the three states (triplet states) that are symmetric, χ_s[6,7];

$$\chi(s_1, s_2)_{triplet} = \begin{cases} \chi_\uparrow(1)\chi_\uparrow(2). \\ \frac{1}{\sqrt{2}}\{\chi_\uparrow(1)\chi_\downarrow(2) + \chi_\downarrow(1)\chi_\uparrow(2)\}. \\ \chi_\downarrow(1)\chi_\downarrow(2). \end{cases} \tag{3.1.5}$$

And the singlet state ,that is anti-symmetric,χ_a ,is also [6,7]

$$\chi(s_1, s_2)_{singlet} = \frac{1}{\sqrt{2}}\{\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\downarrow(1)\chi_\uparrow(2)\}. \tag{3.1.6}$$

3.2 Schrodinger Equation for Two-electron Quantum Dot With Parabolic Confinements

In this section we consider a two-electrons quantum dots confinement in parabolic potential, $V(r_1, r_2)$,

$$V(r_1, r_2) = \frac{1}{2}m^*\omega^2(r_1^2 + r_2^2). \tag{3.2.1}$$

Where we consider both electrons have equal effective mass m^* and oscillates with equal angular frequency ω, with the first electron at position r_1 and the second electron at position r_2.

The Hamiltonian of the two-electron quantum dots can be expressed as the sum of the single electron Hamiltonian including the interaction potential between the two electron [2].

$$H = \frac{\hbar^2}{2m^*}\{\bigtriangledown^1 + \bigtriangledown^2\} + \frac{1}{2}m^*\omega^2\{r^1 + r^2\} + V_{12}(|r_1 - r_2|). \tag{3.2.2}$$

where the last term represents the electron-electron interaction and given as

$$V_{12}(|r_1 - r_2|) = \frac{e^2}{\varepsilon|r_1 - r_2|}, r_1 \neq r_2. \tag{3.2.3}$$

where ε is the dielectric constant in quantum dots.

Introducing the dimensionless coordinate Eq.(2.0.4) at Eq.(3.2.2), we obtain the dimensionless Hamiltonian

$$\hat{H} = -\frac{1}{2}\{\bigtriangledown^2_{\rho_1} + \bigtriangledown^2_{\rho_2}\} + \frac{1}{2}\{\rho_1^2 + \rho_2^2\} + \frac{\lambda}{|\rho_1 - \rho_2|}. \tag{3.2.4}$$

where we use the interaction scale $\lambda = \sqrt{\frac{m^* e^4}{\varepsilon^2 \hbar^2}\frac{1}{\hbar\omega}}$

The Schrodinger equation corresponding to the Hamiltonian (3.2.4) cannot be solved exactly. In this section we discuss the noninteracting two-electron quantum dots with the help of Schrodinger equation.

3.2.1 Solutions of Schrodinger Equation for Noninteracting Two-electron Quantum Dots

We can solve the Schrodinger equation for the noninteracting two-electrons quantum dots can be solved with the help of the solutions of Schrodinger equation of a single particle,since the kinetic energy and potential energy term of the two non-interacting electron's Hamiltonian is independent. The total energy of the noninteracting two-electrons quantum dot becomes the sum of the individual electron's energy. The wave function of the noninteracting two-electrons quantum dot could be constructed with the help of Eq.(3.1.4).

Starting from the single particle Schrodinger equation,

$$\begin{aligned} \hat{H_{01}}\psi^0_{N_1}(r_1) &= E^0_{N_1}\psi^0_{N_1}(r_1). \\ \hat{H_{02}}\psi^0_{N_2}(r_2) &= E^0_{N_2}\psi^0_{N_2}(r_2). \end{aligned} \tag{3.2.5}$$

where $\hat{H_{01}}$, $\hat{H_{02}}$ are the Hamiltonian of the first and the second particle, and $E^0_{N_1}$, $E^0_{N_2}$ are the corresponding energy eigenvalues. The superscript ($\mathbf{0}$) is to indicate the absence

of interaction. Using the advantage of Eq.(2.0.5), the dimensionless Hamiltonian of the electrons becomes

$$\hat{H_{01}} = -\frac{1}{2}\{\frac{\partial^2}{\partial\rho_1^2} + \frac{2}{\rho_1}\frac{\partial}{\partial\rho_1} - \frac{\iota_1(\iota_1+1)}{\rho_1^2}\} + \frac{1}{2}\rho_1^2.$$
$$\hat{H_{02}} = -\frac{1}{2}\{\frac{\partial^2}{\partial\rho_2^2} + \frac{2}{\rho_2}\frac{\partial}{\partial\rho_2} - \frac{\iota_2(\iota_2+1)}{\rho_2^2}\} + \frac{1}{2}\rho_2^2. \tag{3.2.6}$$

where ι_1,ι_2 are the angular quantum number (=0,1,2,3.....).

The Schrodinger equation corresponding the Hamiltonian (3.2.6) is similar to the equation we have discussed in Chapter 2. Using the the advantage of Eq.(2.1.23), we obtain the energy level spectrum of the electrons,

$$E_{N_1}^0 = N_1 + \frac{3}{2}.$$
$$E_{N_2}^0 = N_2 + \frac{3}{2} \tag{3.2.7}$$

where $N_1 = 2n_{\rho_1} + \iota_1$ and $N_2 = 2n_{\rho_2} + \iota_2$ are the quantum numbers (=0,1,2,3.....).

The total energy of the noninteracting two-electron quantum dots is the sum of the energies of the two electrons.

$$E_N^0 = N + 3. \tag{3.2.8}$$

where $N = N_1 + N_2$ is the two-electron quantum dots quantum numbers (=0,1,2,3.....).

The wave functions of the electrons with the advantage of Eq. (2.1.24) can be expressed as:

$$\psi^0_{N_1,\iota_1,m_1}(\rho_1,\theta_1,\varphi_1) = \{\frac{2(\sqrt{\frac{m^*\omega}{\hbar}})^{\iota_1+\frac{3}{2}}n_{\rho_1}!}{\Gamma(n_{\rho_1}-\iota_1+\frac{3}{2})}\}^{\frac{1}{2}}\rho_1^{|\iota_1|}e^{-\frac{1}{2}\rho_1^2}L^{2\iota_1+1}_{n_{\rho_1}+\iota_1}(\rho_1^2)Y_{\iota_1 m_1}(\theta_1,\varphi_1).$$
$$\psi^0_{N_2,\iota_2,m_2}(r_2,\theta_2,\varphi_2) = \{\frac{2(\sqrt{\frac{m^*\omega}{\hbar}})^{\iota_2+\frac{3}{2}}n_{\rho_2}!}{\Gamma(n_{\rho_2}-\iota_2+\frac{3}{2})}\}^{\frac{1}{2}}\rho_2^{|\iota_2|}e^{-\frac{1}{2}\rho_2^2}L^{2\iota_2+2}_{n_{\rho_2}+\iota_2}(\rho_2^2)Y_{\iota_2 m_2}(\theta_2,\varphi_2) \tag{3.2.9}$$

3.2.2 Ground State

For the ground state of the two-electron quantum dots, $N = 0$, both electrons occupies the lowest energy level $N_1 = N_2 = 0$. The spin state is singlet state(anti-symmetric)[5-7]. Such type the states are also called para-state like in the theory of helium atom.
From Eq. (3.2.8) ground state energy becomes

$$E_0^0 = 3. \tag{3.2.10}$$

And the wave function, with the help of Eq.(3.1.4) becomes

$$\psi_{000}(\rho_1, \rho_2) = \{\frac{\sqrt{\frac{m^*\omega}{\hbar}}}{\pi}\}^{\frac{3}{2}} e^{-\frac{1}{2}\{\rho_1^2+\rho_2^2\}} \chi_{singlet}. \tag{3.2.11}$$

Where the singlet spin state expressed as

$$\chi(s_1, s_2)_{singlet} = \frac{1}{\sqrt{2}}\{\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\downarrow(1)\chi_\uparrow(2)\}. \tag{3.2.12}$$

3.2.3 First excited states

The first excited state corresponds to when one electron occupies the next level leaving the second electron on the ground state; i.e either $N_1 = 0$ and $N_2 = 1$ or $N_1 = 1$ and $N_2 = 0$. In this case the spin state is triplet (symmetric state), which can be called ortho-state and the spatial state is ant-symmetric. The quantum numbers associated to this state are $N_1 = 1, \iota_1 = 1, m_1 = 0, \pm 1$; $N_2 = 0, \iota_2 = 0, m_2 = 0$ and $N_1 = 0, \iota_1 = 0, m_1 = 0$; $N_2 = 1, \iota_2 = 1, m_2 = 0, \pm 1$.

The first excited state energy for the noninteracting two-electron quantum dots, from Eq. (3.2.8), becomes

$$E_1^0 = 4. \tag{3.2.13}$$

The wave function inferring to Eq.(3.1.4) and (3.2.9) can be expressed as:

$$\Psi_1(\rho_1, s_1; \rho_2, s_2) = \frac{1}{\sqrt{2}}\{\psi_0(\rho_1)\psi_1(\rho_2) \pm \psi_1(\rho_1)\psi_0(\rho_2)\}^{\chi_{singlet}}_{\chi_{triplet}}.$$

$$\Psi_1(\rho_1, s_1; \rho_2, s_2) = \frac{1}{\sqrt{2}}\{\psi_{000}(\rho_1)\psi_{11m}(\rho_2) \pm \psi_{11m}(\rho_1)\psi_{000}(\rho_2)\}^{\chi_{singlet}}_{\chi_{triplet}}. \quad (3.2.14)$$

Chapter 4

Interacting Two-electron Quantum Dots With Parabolic Confinement

We now consider the Hamiltonian (3.2.4) which includes the electron-electron interaction which complicates the Schrodinger equation we have discussed. In this section, with the help of variational method, we solve the ground state and the first excited state mean energy and wave function for the interacting two-electron quantum dots with parabolic confinement .

4.1 Ground State Energy Correction Using Variational Method

Lets take the trial ground state wave function for the two-electron quantum dots

$$\psi_{000}(\rho_1, \rho_2) = Ce^{-\frac{\beta}{2}(\rho_1^2+\rho_2^2)}\chi_{singlet}. \tag{4.1.1}$$

where we use, C normalization constant and β is the variational parameter to be optimized.Here we consider the spatial states.

The trial ground state wave equation has the form of Eq.(3.2.24) which is the combination of the two single spatial particle state. Using this we can write Eq.(4.1.1) separately as

$$\psi_{000}(\rho_1) = C_1e^{-\frac{\beta}{2}\rho_1^2}.$$
$$\psi_{000}(\rho_2) = C_2e^{-\frac{\beta}{2}\rho_2^2}. \tag{4.1.2}$$

where we take C_1 and C_2 are the normalization constants of the first and the second particles respectively. with $C = C_1C_2$.

The normalized wave function should satisfies:

$$\langle\psi_{000}(\rho_1)|\psi_{000}(\rho_1)\rangle = 1.$$
$$\langle\psi_{000}(\rho_2)|\psi_{000}(\rho_2)\rangle = 1 \tag{4.1.3}$$

Then the above Eq.(4.1.3) can be expressed in position space integral

$$\int \psi^*_{000}(\rho_1)\psi_{000}(\rho_1)d\tau_1 = 1.$$
$$\int \psi^*_{000}(\rho_2)\psi_{000}(\rho_2)d\tau_2 = 1. \tag{4.1.4}$$

Using Eq.(4.1.2) at Eq.(4.1.4) and changing $d\tau = d\varphi sin\theta d\theta\rho^2 d\rho = d\Omega\rho^2 d\rho$ where $d\Omega$ is the solid angle and $\int d\Omega = 4\pi$..

$$4\pi C_1^2 \int_0^\infty e^{-\beta\rho_1^2}\ \rho_1^2 d\rho_1 = 1.$$
$$4\pi C_2^2 \int_0^\infty e^{-\beta\rho_2^2}\ \rho_2^2 d\rho_2 = 1. \tag{4.1.5}$$

Evaluating the integral and solving for the normalization constant we obtain

$$C_1 = \{\frac{\beta}{\pi}\}^{\frac{3}{4}}.$$
$$C_2 = \{\frac{\beta}{\pi}\}^{\frac{3}{4}}. \tag{4.1.6}$$
$$C = \{\frac{\beta}{\pi}\}^{\frac{3}{2}}. \tag{4.1.7}$$

Then the normalized wave function of the trial ground state wave function Eq.(4.1.2) and (4.1.1) becomes

$$\psi_{000}(\rho_1) = \{\frac{\beta}{\pi}\}^{\frac{3}{4}} e^{-\frac{\beta}{2}\rho_1^2}.$$
$$\psi_{000}(\rho_2) = \{\frac{\beta}{\pi}\}^{\frac{3}{4}} e^{-\frac{\beta}{2}\rho_2^2}. \tag{4.1.8}$$

Now,the normalized two-electron quantum dots ground state wave function attains the form

$$\psi_{000}(\rho_1, \rho_2) = \{\frac{\beta}{\pi}\}^{\frac{3}{2}} e^{-\frac{\beta}{2}(\rho_1^2+\rho_2^2)}\chi_{singlet}. \tag{4.1.9}$$

4.1.1 Mean Ground State Energy

The average Value of the Hamiltonian (3.2.5) of the two-electrons quantum dots can be expressed as

$$E_0 = \langle\psi|\hat{H}|\psi\rangle. \tag{4.1.10}$$

The Hamiltonian $\hat{H}$ can expanded as for simplicity

$$\hat{H} = \hat{T_1} + \hat{T_2} + \hat{V}_{01} + \hat{V}_{02} + \hat{V}_{12}. \tag{4.1.11}$$

where T_1 and T_2 are the kinetic energy and $\hat{V}_{01}$ and $\hat{V}_{02}$ are the potential energies of the first and second particles respectively;the last term $\hat{V}_{12}$ is the interaction potential.
For the ground state since $\iota = 0$ we have the kinetic energy term ,with the help of Eq.(3.2.6)

$$\begin{aligned}\hat{T_1} &= -\frac{1}{2}\{\frac{d^2}{d\rho_1^2} + \frac{2}{\rho_1}\frac{d}{d\rho_1}\}.\\ \hat{T_2} &= -\frac{1}{2}\{\frac{d^2}{d\rho_2^2} + \frac{2}{\rho_2}\frac{d}{d\rho_2}\}\end{aligned} \tag{4.1.12}$$

And the potential energy terms are

$$\begin{aligned}\hat{V_{01}} &= \frac{1}{2}\rho_1^2.\\ \hat{V_{02}} &= \frac{1}{2}\rho_2^2.\end{aligned} \tag{4.1.13}$$

The electron-electron potential V_{12}

$$V_{12} = \frac{\lambda}{|\rho_1 - \rho_2|}. \tag{4.1.14}$$

Then Eq.(4.1.10), with the help of Eq.(4.1.11), can be expressed as

$$E_0 = \langle\psi_{000}(\rho_1, \rho_2)|\hat{H}_0 + V_{12}|\psi_{000}(\rho_1, \rho_2)\rangle. \tag{4.1.15}$$

For the case of independent Hamiltonian ,since T_1 and V_{01} are independent of $\psi_0(\rho_2)$ and T_2 and V_{02} are independent of $\psi_0(\rho_1)$, we can rewrite the $\langle H_0\rangle = \langle H_{01}\rangle + \langle H_{02}\rangle$.Then,we have

$$\langle E_0 1\rangle = \int \psi^*_{000}(\rho_1)\hat{T}_1\psi_{000}(\rho_1)d\tau_1 + \int \psi^*_{000}(\rho_1)\hat{V_{01}}\psi_{000}(\rho_1)d\tau_1.$$
$$\langle E_0 2\rangle = \int \psi^*_{000}(\rho_2)\hat{T}_2\psi_{000}(\rho_2)d\tau_2 + \int \psi^*_{000}(\rho_2)\hat{V_{02}}\psi_{000}(\rho_2)d\tau_2. \quad (4.1.16)$$

First lets evaluate E_{01} letting $E_{01} = T_1 + U_1$.

Now lets solve for T_1, kinetic energy term,

$$T_1 = \int \psi^*_{000}(\rho_1)\hat{T}_1\psi_{000}(\rho_1)d\tau_1. \quad (4.1.17)$$

Using Eq.(4.1.8) and (4.1.12) at Eq.(4.1.17) and using $d\tau_1 = d\Omega\rho_1^2 d\rho_1$, we obtain

$$T_1 = \frac{1}{2}\{\frac{\beta}{\pi}\}^{\frac{3}{2}}\beta 4\pi\int_0^\infty \rho_1^2 e^{-\beta\rho_1^2}d\rho_1 -$$
$$\frac{1}{2}\{\frac{\beta}{\pi}\}^{\frac{3}{2}}\beta^2 4\pi\int_0^\infty \rho_1^4 e^{-\beta\rho_1^2}d\rho_1 + \{\frac{\beta}{\pi}\}^{\frac{3}{2}}\beta 4\pi\int_0^\infty \rho_1^2 e^{-\beta\rho_1^2}d\rho_1 \quad (4.1.18)$$

Evaluating integral (4.1.18), we obtain

$$T_1 = \frac{3}{4}\beta. \quad (4.1.19)$$

The same procedure for the second particle also gives us the same average kinetic energy.The total average kinetic energy becomes twice .

$$T = T_1 + T_2 = \frac{3}{2}\beta. \quad (4.1.20)$$

The average value of potential energy U_1 ,the second term of Eq.(4.1.16) , using Eq.(4.1.8) and (4.1.13):

$$U_1 = \langle\frac{1}{2}\rho_1^2\rangle = \frac{1}{2}\{\frac{\beta}{\pi}\}^{\frac{3}{2}}\beta\int_0^\infty \rho_1^4 e^{-\beta\rho_1^2}d\rho_1 \quad (4.1.21)$$

Evaluating the integral we obtain

$$U_1 = \frac{3}{4\beta}. \quad (4.1.22)$$

The average potential energy of the second particle results the same value. Then the total average potential energy becomes

$$U = U_1 + U_2 = \frac{3}{2\beta}. \quad (4.1.23)$$

Then the average Hamiltonian of the two-electron quantum dots ,using Eq.(4.1.20)and(4.1.23) at Eq.(4.1.15), becomes

$$E = \frac{3}{2}\{\beta + \frac{1}{\beta}\} + \langle V_{12}\rangle. \tag{4.1.24}$$

The average value for the interaction potential, $\langle V_{12}\rangle$,due to electron-electron interaction,w ith the help of Eq.(4.1.15), expressed as

$$\langle V_{12}\rangle = \int\int \psi_0^0(\rho_1)^*\psi_0^0(\rho_2)^* V_{12}\psi_0^0(\rho_1)\psi_0^0(\rho_2) \tag{4.1.25}$$

where $V_{12} = \frac{\lambda}{|\rho_1-\rho_2|}$ is the interaction potential.

We carry out the integral with the help of the identity

$$V(k) = \int \frac{1}{|\rho_1 - \rho_2|} e^{-ik.|\rho_1-\rho_2|} d\rho_1 d\rho_2 = \frac{4\pi}{k^2} \tag{4.1.26}$$

Which is a Fourier transform and rearranging for our aim ;

$$V(|\rho_1 - \rho_2|) = \frac{\lambda}{\{2\pi\}^3}\int V(k) e^{ik.(\rho_1-\rho_2)} d^3k. \tag{4.1.27}$$

Using Eq.(4.1.8) and (4.1.27) at Eq.(4.1.25), we obtain

$$\langle V_{12}\rangle = \frac{\beta^3\lambda}{2\pi^5}\int \frac{d^3K}{k^2}\int\int e^{ik.\{\rho_1-\rho_2\}} e^{-\beta\{\rho_1^2+\rho_2^2\}} d^3\rho_1 d^3\rho_2. \tag{4.1.28}$$

then with the help of the relations $d^3\rho = d\varphi sin\theta d\theta \rho^2 d\rho$ Eq.(4.1.28) becomes

$$\begin{aligned}\langle V_{12}\rangle = \frac{\beta^3\lambda}{2\pi^5}\int_0^{2\pi} d\varphi_1 \int_0^{\pi} sin\theta_1 d\theta_1 \int_0^{\infty} \rho_1^2 d\rho_1 e^{-\beta\rho_1^2 + ik.\rho_1} \\ * \int_0^{2\pi} d\varphi_2 \int_0^{\pi} sin\theta_2 d\theta_2 \int_0^{\infty} \rho_2^2 d\rho_2 e^{-\beta\rho_2^2 - ik.\rho_2}.\end{aligned} \tag{4.1.29}$$

Since $\int_0^{2\pi} d\varphi = 2\pi$ and the exponential terms have the same expression except the $+/-$ terms then we can rewrite the integral as

$$\langle V_{12}\rangle = \frac{2\beta^3\lambda}{\pi^3}\int \frac{d^3k}{k^2} I. \tag{4.1.30}$$

where we use I

$$\begin{aligned} I &= \int_0^{\pi} sin\theta_1 d\theta_1 \int_0^{\infty} \rho_1^2 d\rho_1 e^{-\beta\rho_1^2 + ik.\rho_1} \int_0^{\pi} sin\theta_2 d\theta_2 \int_0^{\infty} \rho_2^2 d\rho_2 e^{-\beta\rho_2^2 - ik.\rho_2} \\ &= |\int_0^{\pi} sin\theta_1 d\theta_1 \int_0^{\infty} \rho_1^2 d\rho_1 e^{\beta\rho_1^2 + ik.\rho_1}|^2. \end{aligned} \tag{4.1.31}$$

Lets take that $I = |J|^2$ then using this

$$J = \int_0^{\pi} sin\theta_1 d\theta_1 \int_0^{\infty} \rho_1^2 d\rho_1 e^{-\beta\rho_1^2 + ik.\rho_1}. \tag{4.1.32}$$

Using the relations $d(cos\theta_1) = -sin\theta_1 d\theta_1$ and $ik.\rho_1 = ik\rho_1 cos\theta_1$ at Eq.(4.1.32)we obtain

$$J = -\int_0^{\pi} d(cos\theta_1) \int_0^{\infty} \rho_1^2 d\rho_1 e^{-\beta\rho_1^2 + ik\rho_1 cos\theta_1} \tag{4.1.33}$$

letting $cos\theta = w$ and evaluating first the trigonometric term of integral (4.1.33);

$$\int_{-1}^{1} e^{ik\rho_1 w} dw = \frac{1}{ik\rho_1}(e^{ik\rho_1 - e^{-ik\rho_1}}) \tag{4.1.34}$$

Then using Eq.(4.1.34) at (4.1.33) we obtain

$$J = \frac{1}{ik}\int_0^{\infty} \rho_1 d\rho_1 e^{-\beta\rho_1^2}(e^{ik\rho_1} - e^{-ik\rho_1}) = \frac{1}{ik}\int_0^{\infty} \rho_1 d\rho_1 e^{-\beta\rho_1^2 + ik\rho_1} - \frac{1}{ik}\int_0^{\infty} \rho_1 d\rho_1 e^{-\beta\rho_1^2 - ik\rho_1}. \tag{4.1.35}$$

Lets substitute ρ_1 by $-\rho_1$ at the last term of Eq.(4.1.35),then we obtain

$$\int_0^{\infty} \rho_1 d\rho_1 e^{-\beta\rho_1^2 - ik\rho_1} = -\int_{-\infty}^{0} \rho_1 d\rho_1 e^{-\beta\rho_1^2 + ik\rho_1} \tag{4.1.36}$$

Then using this at Eq.(4.1.35) we obtain

$$J = \frac{1}{ik}\int_{-\infty}^{\infty} \rho_1 d\rho_1 e^{-\beta\rho_1^2 + ik\rho_1} \tag{4.1.37}$$

Using the Gaussian square completing method we can write Eq.(4.1.37) as

$$J = \frac{1}{ik} e^{\frac{-k^2}{4\beta}} \int_{-\infty}^{\infty} e^{-\beta(\rho_1 - \frac{ik}{2\beta})^2}(\rho_1 - \frac{ik}{2\beta} + \frac{ik}{2\beta}) d(\rho_1 - \frac{ik}{2\beta}) \tag{4.1.38}$$

letting $b = \rho_1 - \frac{ik}{2\beta}$ Eq.(4.1.38) becomes

$$J = \frac{1}{ik} e^{\frac{-k^2}{4\beta}} \{\int_{-\infty}^{\infty} e^{-\beta b^2} b db + \int_{-\infty}^{\infty} e^{-\beta b^2} \frac{ik}{2\beta} db\}. \tag{4.1.39}$$

The first term of the integral(4.1.39) vanishes since it contains both even and odd functions. Evaluating the second term of the integral (4.1.39), gives

$$J = \frac{1}{2\beta} e^{\frac{-k^2}{4\beta}} \sqrt{\frac{\pi}{\beta}}. \tag{4.1.40}$$

Thus the value the integral (4.1.31) using Eq.(4.1.40) becomes

$$I = |J|^2 = \frac{\pi}{4\beta^2} e^{-\frac{k^2}{2\beta}}. \tag{4.1.41}$$

Now substituting Eq.(4.1.41) at Eq.(4.1.40) we obtain

$$\langle V_{12} \rangle = \frac{\lambda}{2\pi^2} \int_0^\infty \frac{d^3k}{k^2} e^{\frac{-k^2}{2\beta}}. \tag{4.1.42}$$

Using $d^3k = d\varphi \; sin\theta \; d\theta k^2 dk$ at Eq.(4.1.42)

$$\langle V_{12} \rangle = \frac{2\lambda}{\pi} \int_0^\infty dk e^{\frac{-k^2}{2\beta}}. \tag{4.1.43}$$

Now evaluating the integral(4.1.43) we obtain

$$\langle V_{12} \rangle = \lambda \sqrt{\frac{2}{\pi}} \beta^{\frac{1}{2}}. \tag{4.1.44}$$

Then the ground state energy of two-electron quantum dots, using Eq.(4.1.44) at (4.1.24), becomes

$$E_0 = \frac{3}{2}\{\beta + \frac{1}{\beta}\} + \lambda \sqrt{\frac{2}{\pi}} \beta^{\frac{1}{2}}. \tag{4.1.45}$$

The variational parameter β,that minimizes the ground state energy (4.1.45), is obtained by setting $\frac{dE_0}{d\beta} = 0$, which gives us the equation [18]

$$\beta^2 + \frac{\lambda}{3} \sqrt{\frac{2}{\pi}} \beta^{\frac{3}{2}} - 1 = 0. \tag{4.1.46}$$

This is the transcendental equation,we see that if $\lambda = 0$ we have $\beta = 1$ but if $\lambda << 1$ the above equation can be solved with the help of expansion of β by small parameter [18]

$$\beta = 1 + \beta_1 \lambda + \beta_2 \lambda^2 + ... \tag{4.1.47}$$

Using this expansion we find the expansions for β^2 ignoring higher order terms since $\lambda << 1$;

$$\beta^2 = 1 + 2\beta_1 \lambda + 2\beta_2 \lambda^2 + \beta_1^2 \lambda^2 + ... \tag{4.1.48}$$

and also we find the values $\beta^{\frac{3}{2}}$ using Binomial expansions ignoring higher order terms as

$$\begin{aligned}\beta^{\frac{3}{2}} &= \{1+\beta_1\lambda+\beta_2\lambda^2+..\}^{\frac{3}{2}}.\\ &= 1+\frac{3}{2}\beta_1\lambda+\frac{3}{2}\beta_2\lambda^2+..\end{aligned} \tag{4.1.49}$$

Substituting Eq.(4.1.49) and (4.1.48) at Eq.(4.1.46) and ignoring higher order terms

$$2\beta_1\lambda+2\beta_2\lambda^2+\beta_1^2\lambda^2+B\lambda+\frac{3}{2}B\beta_1\lambda^2=0. \tag{4.1.50}$$

where we use $B=\frac{1}{3}\sqrt{\frac{2}{\pi}}$,then rearranging Eq.(4.1.50) we obtain

$$\beta_1^2+\{\frac{2}{\lambda}+\frac{3}{2}B\}\beta_1+\{\frac{B}{\lambda}+2\beta_2\}=0. \tag{4.1.51}$$

Since $\lambda << 1$,we can estimate that $\frac{B}{\lambda}+2\beta_2 \simeq \frac{B}{\lambda}$ and $\frac{2}{\lambda}+\frac{3}{2}B \simeq \frac{2}{\lambda}$, then using this Eq.(4.1.50) reduced to

$$\beta_1^2+\frac{2}{\lambda}\beta_1+\frac{B}{\lambda}=0. \tag{4.1.52}$$

This is a quadratic equation and has two solutions β_1^+ and β_1^-;

$$\begin{aligned}\beta_1^+ &= -\frac{B}{2}.\\ \beta_1^- &= -\frac{2}{\lambda}-\frac{B}{2}.\end{aligned} \tag{4.1.53}$$

Here we see that the second solution β_1^- diverges for $\lambda << 1$,the physically accepted solution would be

$$\begin{aligned}\beta_1 &= -\frac{B}{2}.\\ &= -\frac{1}{6}\sqrt{\frac{2}{\pi}}.\end{aligned} \tag{4.1.54}$$

Now we use Eq.(4.1.54) at Eq.(4.1.51) and calculate for β_2. We find the physically accepted value

$$\begin{aligned}\beta_2 &= \frac{B^2}{4}.\\ &= \frac{1}{18\pi}.\end{aligned} \tag{4.1.55}$$

Then substituting Eq.(4.1.54) and (4.1.55) at the Eq.(4.1.47), we obtain the variational parameter β as a function of λ;

$$\beta(\lambda) = 1 - \frac{\lambda}{3\sqrt{2\pi}} + \frac{\lambda^2}{18\pi} + ... \tag{4.1.56}$$

Using Eq.(4.1.56), we can propose the interpolation formula for β;

$$\beta = \frac{1}{1 + \frac{\lambda}{3\sqrt{2\pi}}}. \tag{4.1.57}$$

Now we can find the ground state energy as a function of λ ,for $\lambda << 1$,using Binomial expansions for $\beta^{-1} = 1 + \frac{\lambda}{3\sqrt{2\pi}} - \frac{\lambda^2}{9\pi} + ...$ and $\beta^{\frac{3}{2}} = 1 - \frac{\lambda}{6\sqrt{2\pi}} + \frac{\lambda^2}{36\pi} + ...$ Then the ground state energy for the two-electron quantum dots as a function of λ , $E_0(\lambda)$, using Eq.(4.1.57) at Eq.(4.1.45),becomes

$$E_0(\lambda) = 3 + \lambda\sqrt{\frac{2}{\pi}} - \frac{\lambda^2}{12\pi}, \lambda << 1. \tag{4.1.58}$$

The above ground state energy is for $\lambda << 1$, but if λ is not small Eq.(4.1.45) can be solved numerically. Below we present the calculated values of ground state energy E_0 and variational parameter β for different values of λ.

λ	0	0.5	1	1.5	2	2.5	3	3.5	4
β	1.000	0.938	0.883	0.834	0.791	0.752	0.718	0.686	0.656
$E_0(\lambda)$	3.000	3.393	3.773	4.143	4.502	4.852	5.194	5.529	5.885

Table 4.1: The ground state energy E_0 and variational parameter β for different values of λ.

Comparing the data of table (4.1) with β given by Eq.(4.1.57) and the energy E_0 (4.1.45), with the help of graph (4.1), we obtain very good agreement for $0 \leq \lambda \leq 4$.

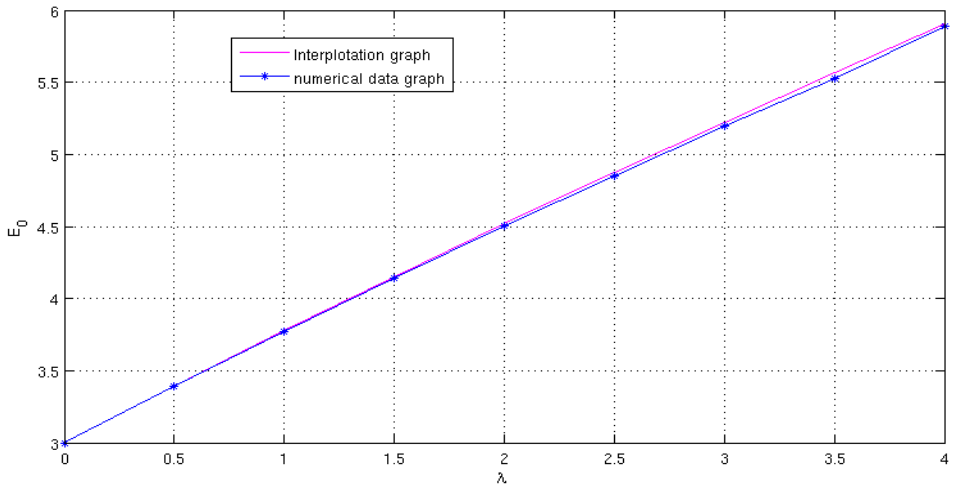

Figure 4.1: The plot of ground state energy versus λ using numerical data in table (4.1) and with β given by (4.1.57) .

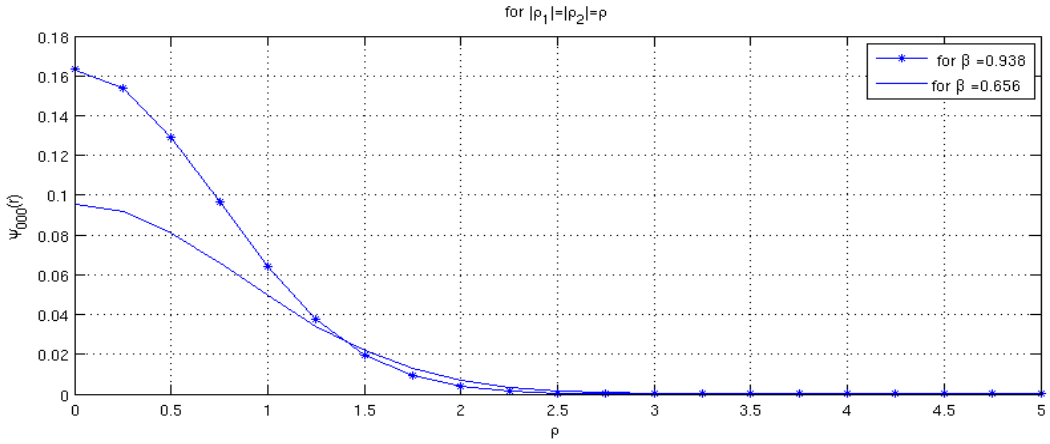

Figure 4.2: The plot of ground state wave function versus radius of the quantum dots for the high and low values of β.

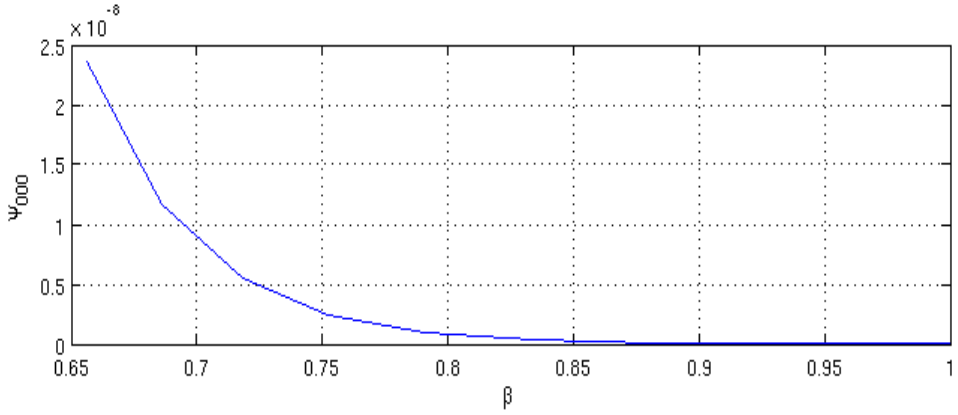

Figure 4.3: The plot of ground state wave function versus variational parameter β , setting $|\rho| = 5$.

4.2 Excited State(para-state) Energy Correction Using Variational Method

Lets take the trial first excited state wave function, with $m = 0, \iota = 1$ for simplicity, with the help of Eq.(3.2.9) and (3.2.14)

$$\Psi_1(\rho_1, \rho_2) = C\{e^{-\frac{\beta}{2}\rho_1^2} e^{-\frac{\gamma}{2}\rho_2^2} \rho_2 cos\theta_2 \pm e^{-\frac{\beta}{2}\rho_2^2} e^{-\frac{\gamma}{2}\rho_1^2} \rho_1 cos\theta_1\}^{\chi_{singlet}}_{\chi_{triplet}}. \tag{4.2.1}$$

Where C is the normalization constant, γ is the first excited state variational parameter relates to one electron wave function and β is the ground state variational parameter already calculated.

With the same procedure in section (4.1), we obtain the one electron normalized trial wave functions:

$$\psi_0(\rho) = (\frac{\beta}{\pi})^{\frac{3}{4}} e^{-\frac{\beta}{2}\rho^2}.$$
$$\psi_1(\rho) = \sqrt{2}\{\frac{\gamma^{\frac{5}{4}}}{\pi^{\frac{3}{4}}}\} e^{-\frac{\gamma}{2}\rho^2} \rho cos\theta. \tag{4.2.2}$$

The normalized trial wave function corresponds to first excited state (4.2.1) attains the form

$$\Psi_1(\rho_1, \rho_2) = \frac{\beta^{\frac{3}{4}}\gamma^{\frac{5}{4}}}{\pi^{\frac{3}{2}}}\{e^{-\frac{\beta}{2}\rho_1^2} e^{-\frac{\gamma}{2}\rho_2^2} \rho_2 cos\theta_2 \pm e^{-\frac{\beta}{2}\rho_2^2} e^{-\frac{\gamma}{2}\rho_1^2} \rho_1 cos\theta_1\}^{\chi_{singlet}}_{\chi_{triplet}} \tag{4.2.3}$$

4.2.1 First Excited Para-State Mean Energy

The mean energy of the first excited para- state is given by

$$E_1^p = \langle \Psi_1(\rho_1, \rho_2) | H_0 + V_{12} | \Psi_1(\rho_1, \rho_2) \rangle. \tag{4.2.4}$$

The normalized trial wave function corresponds to the quantum numbers $N_1 = N_2 = 1, \iota_1 = \iota_2 = 1, m_1 = m_2 = 0, \pm 1$; for simplicity taking $m = 0$,

$$\psi_1(\rho_1, \rho_2) = \frac{2\gamma^{\frac{5}{2}}}{\pi^{\frac{3}{2}}} e^{-\frac{\gamma}{2}(\rho_1^2 + \rho_2^2)} \rho_1 cos\theta_1 \rho_2 cos\theta_2. \tag{4.2.5}$$

$$E_1^p = \langle \psi_1(\rho_1, \rho_2) | H_{01} | \psi_1(\rho_1, \rho_2) \rangle + \langle \psi_1(\rho_1, \rho_2) | H_{02} | \psi_1(r_1, r_2) \rangle + \langle \psi_1(\rho_1, \rho_2) | V_{12} | \psi_1(\rho_1, \rho_2) \rangle. \tag{4.2.6}$$

The first two terms can be expressed as twice of one of the expressions..

$$E_1^p = 2\langle \psi_1(\rho_1, \rho_2) | H_{02} | \psi_1(\rho_1, \rho_2) \rangle + \langle \psi_1(\rho_1, \rho_2) | V_{12} | \psi_1(\rho_1, \rho_2) \rangle. \tag{4.2.7}$$

With the help of Eq.(4.1.12),(4.1.13) and (4.2.5), Eq.(4.2.7) in the integral form becomes

$$E_1^p = 4\{\frac{\gamma^{\frac{5}{2}}}{\pi^{\frac{3}{2}}}\} \int d\tau_2 e^{-\frac{\gamma}{2}\rho_2^2} \rho_2 cos\theta_2 [-\frac{1}{2}\{\frac{d^2}{d\rho_2^2} + \frac{2}{\rho_2}\frac{d}{d\rho_2} - \frac{\iota_2(\iota_2+1)}{\rho_2^2}\} + \frac{1}{2}\rho_2^2] e^{-\frac{\gamma}{2}\rho_2^2} \rho_2 cos\theta_2 + \langle V_{12} \rangle. \tag{4.2.8}$$

With the help of Mathematica, for $\iota_{1,2} = 1$, the integral (4.2.8) gives

$$E_1^p = \frac{5}{2}(\gamma + \frac{1}{\gamma}) + \langle V_{12} \rangle. \tag{4.2.9}$$

Where the first term is the kinetic energy and the second term is the potential energy of the two noninteracting electrons in the first excited state.

The interaction potential term can be evaluated with the help of Eq.(4.1.27) and (4.2.5);

$$\langle V_{12} \rangle = 2(\frac{\gamma^5 \lambda}{\pi^5}) \int \frac{d^3k}{k^2} \int e^{ik.\rho_1 - \gamma\rho_1^2} \rho_1^2 cos^2\theta_1 d^3\rho_1 \int e^{-ik.\rho_2 - \gamma\rho_2^2} \rho_2^2 cos_2^2\theta d^3\rho_2 \tag{4.2.10}$$

Using the same procedure we have discussed in section (4.1) and with the help of Mathematica, We obtain

$$\langle V_{12} \rangle = 0.651\lambda\sqrt{\gamma} \tag{4.2.11}$$

The energy E_1^p, using Eq.(4.2.11)at Eq.(4.2.9), becomes

$$E_1^p(\lambda) = \frac{5}{2}(\gamma + \frac{1}{\gamma}) + 0.651\lambda\sqrt{\gamma} \tag{4.2.12}$$

The variational parameters γ is found from the condition $\frac{dE_1^p(\lambda)}{d\gamma} = 0$ with the help of Eq.(4.2.12). We obtain the equation

$$\frac{5}{2}(1 - \frac{1}{\gamma^2}) + \frac{0.3255\lambda}{\sqrt{\gamma}} = 0 \tag{4.2.13}$$

For $\lambda = 0, \gamma = 1$, for λ not small Eq. (4.2.13) can be solved numerically. Below we present the calculated values of the first excited state energy $E_1^{(1)}$ and variational parameter γ for different values of λ.

λ	0	0.5	1	1.5	2	2.5	3	3.5	4
γ	1.000	0.968	0.939	0.911	0.885	0.860	0.837	0.815	0.7943
$E_1^p(\lambda)$	5.000	5.323	5.641	5.954	6.263	6.566	6.866	7.163	7.454

Table 4.2: The first excited state energy E_1^p and variational parameter γ for different values of λ.

With the help of the numerical data displayed on table (4.2), We can propose the interpolation formula for variational parameter γ,

$$\gamma(\lambda) = \frac{1}{1 + 0.0650596\lambda} \tag{4.2.14}$$

Comparing data table (4.2) with the interpolation formula given by Eq. (4.2.14), we obtain an excellent agreement as shown in Fig (4.4).

These results coincides with the results of [18] obtained by another method.

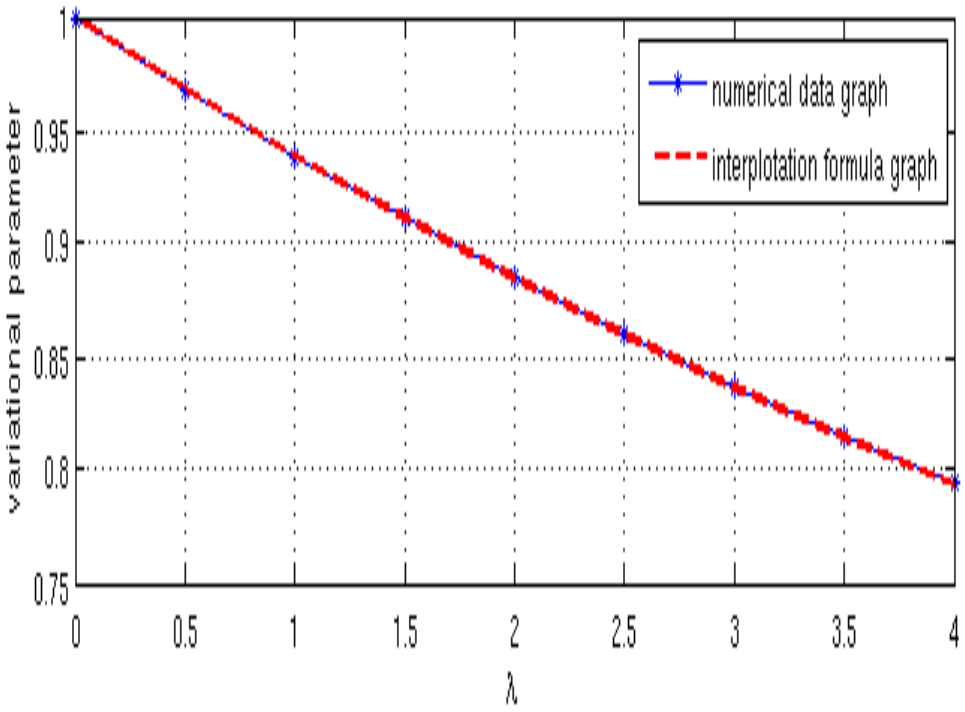

Figure 4.4: The first excited para-state variational parameter γ versus λ using the data table (4.2) and proposed interpolation formula (4.2.14)

Chapter 5

Conclusion

In this paper :

• We considered the general properties of low dimensional crystals.

• We discussed the electronic properties of quantum dots with one electron.

• we have studied the first two low lying para-states of the two-electron quantum dots with parabolic confinement. We employ the spherical coordinates for its symmetry.

We have obtained the first two low lying para-state wave function and energy using the Schrodinger equation for the noninteracting two-electron quantum dots. We have also derived the ground and first excited state energy for the interacting two-electron quantum dots with the help of Variational method approximation.

Employing the normalized trial wave function, we obtained the energy as a function of Gausian interaction energy scale λ. We also calculated the numerical values and propose interpolation formula .

Moreover, we have determined that for $\lambda = 1$ the energy calculated with the help of Schrodinger equation and variational method matches exactly. But for the interacting system, we have obtained the values in table (4.1) and (4.2); shows that as an interaction scale becomes stronger, the state energy increases.

In this work, we have found a good agreement with results of [18], where they consider different approach. Finally, we call attention about the gigantic dielectric constant quantum dots with parabolic confinement. In this case the Coulomb interaction becomes very small and it can be treated with the help of perturbation methods .

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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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