國　立　交　通　大　學

電子工程學系　電子研究所碩士班

碩 士 論 文

外加磁場下多電子量子點之能量和束縛電子數目的關係

The addition energy of a few electrons' quantum dot in an external magnetic field

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摘要

在這個報告中，我們提出了在外加磁場下三維 InAs/GaAs 量子點的 addition energy，在此我們利用 exact diagonalization 方法來求得多電子量子點的束縛能階隨外加磁場的變化，這方法首先是找出單電子量子點的能階和對應的波函數，在列式的過程中我們將以下三點考慮進去：(1)電子的有效質量和 Lande' factor 是隨著總能和位置改變的(2)有限的 hard wall 限制位能(4)外加磁場跟磁動量的交互作用產生的 Zeeman effect。我們利用非線性遞迴方法來解決這個問題。由於電子間的交互作用對多電子量子點磁變能階，在我們求出單電子量子點的能階和對應的波函數後，我們利用這些結果去計算電子間的庫倫作用力，並利用以上所有相關數據來建構多電子量子點的 Hamiltonian，然後就可以算出 Addition energy 了。所有的結果在這個報告中都會呈現出來，我們發現 Addition energy 跟束縛電子的數量之關係符合 Shell 結構。然而，有一點值得注意的是，當外加磁場為零時某些 addition energy 的值會微微小於零，這是由於我們在計算過程中假設不同的單電子量子點的波函數之間是彼此正交的，但這只是個估計，與實際情形有微小差距，這導致我們用來創造多電子量子點 Hamiltonian 的基底並非如我們假設般彼此正交，然而，當我們將這些基底正交化後，預料便能將 addition energy 往上提升。

The addition energy of a few electrons' quantum dot in an external magnetic field

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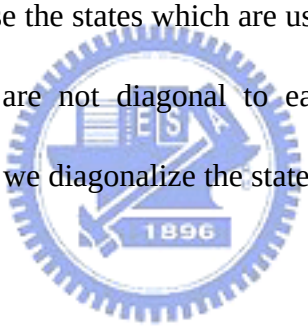
ABSTRACT

In this report, we present a study on the addition energy of interacting electrons for a realistic three-dimensional (3D) model of semiconductor nano-scale InAs/GaAs quantum dots under an external magnetic field. We supposed the interaction between electrons are totally caused by Coulomb effect. Here we use the exact diagonalization method to obtain the confined energy states of few electrons that exists in a quantum dot as a function of external magnetic fields. The first step is to find the eigenstates of a single electron. The model formulation includes (i) the energy and position dependent effective mass and Lande' factor for electrons (ii) finite hard wall confinement potential (iii) the Zeeman effect caused by interaction between the mesoscopic angular momentum and the magnetic field. We apply the non-linear iterative method to obtain self-consistent solutions of this 3D problem. The interaction

between electrons has important effects on the magnetic field dependence of the energy spectrum. After finding out the energy states of single electron confined in the dot and corresponding wave function dependence on an external magnetic field, we make use of these results to evaluate the Coulomb potential between electrons and construct the Hamiltonian of multi-electrons quantum dot. Then we obtain the energy states of few electrons confined in a dot and take all these data to get the addition energy for different applied magnetic field. All the results will be presented. We found that there are some values of addition energy are slightly negative when the external magnetic field is zero. However, the addition energy in a quantum dot should be always positive. This is because the states which are used to create the Hamiltonian of multi-electrons quantum dot are not diagonal to each other. We expect that the addition energy will shift up if we diagonalize the states.



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Chapter 1

Introduction

During the past years, the application of new and extraordinary experimental tools to nano-science has generated great interest in some special semiconductor electronic systems, called quantum dots. Because of the impressive developments in nano fabrication technology, quantum dots and coupled quantum dots can be designed at the nano scale and much of their behavior can be precisely tuned by using standard fabrication methods. Quantum dots can contain electrons from only one to more than thousands. The number of electrons in a quantum dot,denoted N, can be controlled precisely via external potential experimentally, affect many physical properties of the quantum dot. [1, 2] There is a strong interest in the study of quantum dots both from the technological and theoretical point of view. From the technological point of view, quantum dots are related to the field of quantum computing, especially after being shown that two-electron quantum dots have the potential to form the basis of scalable quantum bits in a future quantum computing. They also offer the potential to build faster electronic devices, such as single-electron transistors [3]. Moreover, quantum dots become more and more interesting topics in physics, especially in the field of lasers and photonics. From the

theoretical point of view, they represent a unique opportunity to study fundamental quantum phenomena in a tunable atomic-like energy level and this is the reason why, sometimes, they are referred to as artificial atoms [4].

In this report, we will consider a quantum dot with more than one electron confined in an external magnetic field. The electron-electron interaction is highly important and leads to unusual magnetic-field dependence of the ground state and it's excitations. Since the interaction between electrons is mostly caused by Coulomb effect, here we ignore the other kinds of interaction such as weak interaction, gravitation and strong nuclear interaction. Studies of quantum dots with even few confined electrons meet many challenges, for the simple reason that, sometimes, standard techniques of condensed matter physics, such as Hartree-Fock methods [5], are not sufficiently accurate. Therefore, a more accurate quantum mechanical treatment is needed, and inevitably this requires the use of numerical methods. The first pioneering work on such systems is done by Bryant [6] in which the electronic structure of up to $N \leqq 6$ electrons confined in a 2D infinite rectangular potential well was calculated. A Coulomb potential screened by the background dielectric constant was chosen as the form of the electron-electron interaction. In particular, the problem of two interacting electrons in a 2D parabolic well confinement potential both in the absence and in the presence of a perpendicular magnetic field has previously been studied by using several methods. Then the exact closed-form solution for the problem of two interacting electrons in both uniform magnetic field and external 2D parabolic potential has been reported. Recently, the problem of electrons in a three dimensional(3D) parabolic confinement potential has also been studied.[7]

There are two 'exact' (in the numerical sense) methods have been successfully applied to multi-electrons quantum dots: one is the exact numerical di-

agonalization technique[8, 9], and the other one is the quantum Monte Carlo (QMC)[10, 11] method. Here, we choose the exact numerical diagonalization method to solve our problem. Though there are some researches investigating interacting electrons in a quantum dot by the same method. Most of them consider the dot with parabolic confinement potential. However, the quantum dot more likely form the finite hard-wall confinement potential. Especially when we make the size of the dot quite small. Therefore, in our case, we assume that electrons in the quantum dot are confined with finite hard-wall potential. It is worth noting that, not only does the results get from each kind of confinement potential diverse, but also the approximation we make in our computation is different. According to exact diagonalization method, the Hamiltonian of multi-electrons system is represented in the basis which is constructed by eigenfunctions of the single electron Hamiltonian. But there is some limitation of this method which may result in somewhat inaccuracy. That is, the eigenfunctions we get from single electron problem do not span all the space of the multi-electrons' problem. In the case of parabolic confinement potential, infinite energy states will be found confined in the dot when there is one electron inside. Therefore, the basis set we build for multi-electron problem is infinite. However, we can select the lowest few eigenfunctions and build a finite basis set to achieve the desired accuracy. It is different in the case of hard wall confinement potential where there would be finite energy states confined in the dot. Moreover, the number of the states would be less if we make the size of the dot smaller. Therefore, we can only build finite basis set for multi-electron Hamiltonian in this case. The accuracy and the complexity of our computation depends on the size of the dot(the interaction between electrons) we decide, so we will compare the interaction energy to the energy of single electron in this report.

In the creation of quantum dots with a molecular beam epitaxy chamber, by spraying a surface with layers of atoms under high temperature, a residue is produced on the surface called wetting layer, which can interfere with the stimulation of the dots in order to control their state for quantum computation. In our model, the size of the dot is so small that we can not neglect the wetting layer. However, we supposed that the length of wetting layer is long enough and we made an approximation that the the length extends to infinity.

In this report, we propose a model of InAs/GaAs quantum dot with wetting layer. Fig1.1 is the 3D configuration of the dot. We supposed the quantum dot is of cylindrical symmetry about z axis. The cross-section of z-axis is an ellipse.

This report is organized as follows: in chapter 2, we present the essential formalism for our study and the numerical approach we use to calculate the tunnelling transmission probability. The calculation results and discussions are shown in chapter 3. Finally, we summarize our work in chapter 4.

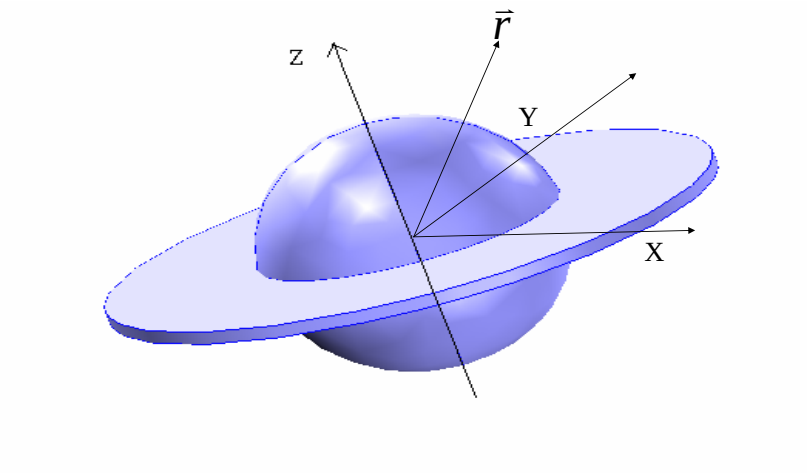

Figure 1.1: the figure of the 3D quantum dot with wetting layer

Chapter 2

Theory

The objective of our work is to study few interacting electrons in a quantum dot by using the exact numerical diagonalization technique. We are interested in confined energy states which are exact solutions (or good approximations) to them of the many-body problem defined by the Hamiltonian

$$H = \sum_{i=1}^{N} H_0(\vec{r_i}) + \frac{1}{2}\sum_{i\neq j} V(\vec{r_i}, \vec{r_j}), \tag{2.1}$$

Where H_0 is the Hamiltonian of single electron. $V(\vec{r_i}, \vec{r_j})$ is the energy due to the interaction between electrons. $\vec{r_i}$ is the position vector of the i'th electron in the quantum dot. We supposed $V(\vec{r_i}, \vec{r_j})$ is totally decided by Coulomb potential. The first step is to find the energy states and the corresponding wave function of single electron problem. In the presence of an external magnetic field B, by including the Zeeman term, an approximate effective Hamiltonian can be obtained in the form

$$\hat{H} = -\frac{\hbar^2}{2}\frac{1}{m_i(E)}\left(\frac{\partial^2}{\partial^2\rho} + \frac{\partial^2}{\rho^2\partial^2\phi} + \frac{\partial^2}{\partial^2 z}\right) + B^2\frac{e^2\rho^2}{8m_i(E)} - i\frac{e\hbar}{2m_i(E))}B\frac{\partial}{\partial\phi}$$
$$+\frac{sg_i(E)\mu B}{2} + V_c(\rho, z), i = 1, 2, \tag{2.2}$$

Where i=1 represent the Hamiltonian inside the dot and i=2 represent the Hamiltonian outside the dot. The coordinate system of the above eqation is cylindrical coordinate. The quantum dot we consider is ploted in Fig1.1. Where ρ is the length of the projection of $\vec{r_j}$ on the x-y plane, ϕ is the angle between the axis x and the projection of $\vec{r_j}$ on the x-y plane. $V_c(\rho, z)$ is the finite confinement potential, and is set for 0 inside the dot. So the $V_c(\rho, z)$ outside the dot is the potential difference between the conduction band of GaAs and InAs. The first two terms of the Hamiltonian are due to the interaction of the orbital motion and the magnetic field. The last terms represent the energy caused by Zeeman effect. Where $\mu = \frac{e\hbar}{2m_0}$ is the Bohr magneton, and m_0 is the free-electron mass. $g(E, \rho, z)$ and $m(E, \rho, z)$ stand for the energy and position dependent mass and Lande factor, respectively. It is given by

$$\frac{1}{m(E)} = \frac{1}{m(0)} \frac{E_g(E_g + \Delta)}{3E_g + 2\Delta} \left(\frac{2}{E + E_g} + \frac{1}{E + E_g + \Delta}\right), \tag{2.3}$$

$$g(E) = 2\left(1 - \frac{1}{m(E)} \frac{\Delta}{3(E_g + E) + 2\Delta}\right), \tag{2.4}$$

$m(0)$ is free electron mass of designated material which is made by InAs inside the dot and GaAs outside in this report. Δ is spin-orbit splitting in the valence band , E_g is energy band.

The Ben Daniel-Duke boundary conditions for the electron and hole wave functions $\Psi(\mathbf{r})$ are given by

$$\Psi_1(\vec{r_s}) = \Psi_2(\vec{r_s}) \qquad and$$

$$\frac{1}{m(E)} \left(\frac{\partial \Phi(\rho, z)}{\partial \rho} + \frac{df(\rho)}{d\rho} \frac{\partial \Phi(\rho, z)}{\partial z}\right)_{z=f(\rho)} = const, \tag{2.5}$$

$\vec{r_s}$ is an arbitrary position of the surface of the dot. $f(\rho)$ is a function that shows how z is dependent upon rho on the surface. Solutions of these eigen-systems provide the single-electron energies and the spinor wave functions. By the cylindrical symmetry of the system, the energy eigenfunction takes the well-known form

$$\Psi_{n,l,s}(\mathbf{r}) = exp(il\phi)\Phi_{n,l,s}(\rho, z), \tag{2.6}$$

where $l = 0, 1, 2, ...$is the quantum number of the projection of the angular momentum on to the magnetic field B axis, n is the main quantum number, with $\Phi_{n,l,s}(\rho, z)$ that satisfies

$$-\frac{\hbar^2}{2}\frac{1}{m_i(E)}(\frac{\partial^2}{\partial^2\rho}+\frac{\partial^2}{\partial^2 z})\Phi_{n,l,s}(\rho,z)+\frac{\hbar^2 l^2}{2m_i(E)\rho^2}\Phi_{n,l,s}(\rho,z)+$$

$$B^2\frac{e^2\rho^2}{8m_i(E)}+\frac{e\hbar l}{2m_i(E)}B\Phi_{n,l,s}(\rho,z)+\frac{sg_i(E)\mu B}{2}$$

$$\Phi_{n,l,s}(\rho,z)+V_c(\rho,z)\Phi_{n,l,s}(\rho,z)=E\Phi_{n,l,s}(\rho,z), i=1,2 \tag{2.7}$$

The Ben Daniel-Dukeboundary conditions can be written as

$$\Phi_1(\rho,z)=\Phi_2(\rho,z), \qquad z=f(\rho)$$

$$\frac{1}{m_1(E)}(\frac{\partial\Phi_1(\rho,z)}{\partial\rho}+\frac{df(\rho)}{d\rho}\frac{\partial\Phi_1(\rho,z)}{\partial z})_{z=f(\rho)}=\frac{1}{m_2(E)}$$

$$(\frac{\partial\Phi_2(\rho,z)}{\partial\rho}+\frac{df(\rho)}{d\rho}\frac{\partial\Phi_2(\rho,z)}{\partial z})_{z=f(\rho)}, \tag{2.8}$$

To solve this 2D non-linear problem ,we apply the non-linear iterative method to obtain self-consistent solutions.

After we get the energy states and the corresponding wave function of single electron confined in a quantum dot, we use theses results to construct the Hamiltonian of multi-electrons system. The Hamiltonian is given by equation (2.1).

In order to obtain the mathematical form of H, we use exact diagonalization method and make an approximation that any wave function of H can be given as

$$\begin{aligned}\Psi(\mathbf{r_1},\mathbf{r_2},\ldots,\mathbf{r_k}) &= \sum_{p_1,p_2,\ldots,p_k} C_{p1,p2,\ldots,pk}\Psi_{p1}(\mathbf{r_1})\Psi_{p2}(\mathbf{r_2})\cdots\Psi_{pk}(\mathbf{r_k}) \\ &= \sum_{p1,p2,\ldots,pk} C_{p1,p2,\ldots,pk}\Psi_{p1,p2,\ldots,pk}(\mathbf{r_1},\mathbf{r_2},\ldots,\mathbf{r_k}), \qquad (2.9)\end{aligned}$$

Where $\Psi_p(\mathbf{r})$ is the normalized eigenfunction of single electron Q.D. in equation 2.6. Here, for simplicity, we use pi=n,l,s to collect all the three quantum number n,l,s of the ith electron confined in the dot. For example, p1=1 represent the quantum number (n,l,s)=(1,0,1) of the first electron, p1=2 represent the quantum number (n,l,s)=(1,0,-1) of the first electron, and so on. $C_{p1,p2,\ldots pk}$ is an arbitrary constant, k is the number of the electrons confined in the dot. Since we suppose the finite hard-wall confinement potential here, the maximum of k must be finite. There are finite numbers of m because we only consider the states confined in the Q.D.

If $\Psi_q(\mathbf{r})$ is orthogonal to $\Psi_p(\mathbf{r})$, $q \neq p$. $\Psi_{p1,p2\ldots pk}(\mathbf{r_1},\mathbf{r_2},\ldots,\mathbf{r_k})$ has the property

$$\langle\Psi_{p1,p2,\ldots,pk}(\mathbf{r_1},\mathbf{r_2},\ldots,\mathbf{r_k}) \mid \Psi_{q1,q2,\ldots,qk}(\mathbf{r_1},\mathbf{r_2},\ldots,\mathbf{r_k})\rangle = \delta_{p1,q1}\delta_{p2,q2}\cdots\delta_{pk,qk}, \qquad (2.10)$$

Where $\delta_{q,p} = 1$,$q = p$ and $\delta_{q,p} = 0, q \neq p$

We can express H approximately by matrix form with the orthonormal basis

$$\{\forall q1, q2, ..qk \mid \Psi_{q1,q2,...,qk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k})\}, \tag{2.11}$$

And the multi-electron Hamiltonian is

$$H = \sum_{q1,q2,\ldots,qk,p1,p2,\ldots pk} \mid \Psi_{p1,p2,...,pk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k})\rangle\langle\Psi_{q1,q2,\ldots,qk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k}) \mid$$

$$\langle\Psi_{p1,p2,\ldots,pk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k}) \mid H \mid \Psi_{q1,q2,\ldots,qk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k})\rangle, \tag{2.12}$$

However, since the Hamiltonian of single eletctron quantum dot in our problem depends on the electronic energy, the wavefunctions of the Hamiltonian with different energy level are not orthogonal to each other. Therefore, the eqation (2.10) can not be applied here. This results is overlap between the wavefunctions which we use to create the Hamiltonian of milti-electron quantum dot and may make the eqation (2.12) inccurate. However, this is our first step to analyze the addition energy of multi-electrons quantum dot. We just want to see a trend of the results here and supposed that all the wavefunctions we get from single electron problem are diagonal with each other. We will tell how to solve the problem of un-diagonalization of the wavefunctions in chapter 3 and will investigate more in the future.

Since

$$H_0(\mathbf{r_i}) \mid \Psi_{q1,q2,...,qk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k})\rangle = E_{qi} \mid \Psi_{q1,q2,...,qk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k})\rangle, \tag{2.13}$$

The problem reduces to the calculation of the matrix elements of each $V(\mathbf{r_i}, \mathbf{r_j})$, Where

$$V(\mathbf{r_i}, \mathbf{r_j}) = \frac{e^2}{4\pi\varepsilon|\mathbf{r_i} - \mathbf{r_j}|}, \tag{2.14}$$

The formulation of the energy of Coulomb interaction between electrons i and j written as

$$V_{qi,qj,pi,pj} = \langle \Psi_{p1,p2,\ldots,pk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k}) \mid V(\vec{r_i}, \vec{r_j}) \mid \Psi_{q1,q2,\ldots,qk}(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k}) \rangle$$

$$= \int d\mathbf{r_i} d\mathbf{r_j} \Phi^*_{pi}(\mathbf{r_i}) \Phi^*_{pj}(\mathbf{r_j}) V(\mathbf{r_i}, \mathbf{r_j}) \Phi_{qi}(\mathbf{r_i}) \Phi_{qj}(\mathbf{r_j})$$

$$= \int d\mathbf{r_i} d\mathbf{r_j} \Phi^*_{pi}(\mathbf{r_i}) \Phi^*_{pj}(\mathbf{r_j}) \frac{e^2}{4\pi\varepsilon|\mathbf{r_i} - \mathbf{r_j}|} \Phi_{qi}(\mathbf{r_i}) \Phi_{qj}(\mathbf{r_j}), \tag{2.15}$$

For convenient, we rewrite the above equation with simple symbol.

$$\langle pi, pj \mid V \mid qi, qj \rangle = \int \int \Psi^*_{pi}(\mathbf{r_i}) \Psi^*_{pj}(\mathbf{r_j}) \frac{1}{|\mathbf{r_i} - \mathbf{r_j}|} \Psi_{qi}(\mathbf{r_i}) \Psi_{qj}(\mathbf{r_j}) d\mathbf{r_i} d\mathbf{r_j}, \tag{2.16}$$

Consider equaton (2.6).

Here, we use the well-known presentation by Bessel functions of first kind $J_m(X)$

$$\frac{1}{|\mathbf{r_i} - \mathbf{r_j}|} = \sum_{m=-\infty}^{\infty} \int_0^{\infty} dk e^{im(\phi - \phi')} J_m(k\rho_i) J_m(k\rho_j) e^{-k|z_i - z_j|}, \tag{2.17}$$

We can transform (2.16) into

$$\langle pi, pj \mid V \mid qi, qj \rangle = (2\pi)^2 \delta_{L_{piqi}, L_{pjqj}} \int \rho_i \rho_j d\rho_i d\rho_j dz_i dz_j \Phi_{pi}(\rho_i, z_i) \Phi_{qi}(\rho_i, z_i) \Phi_{pj}(\rho_j, z_j) \Phi_{qj}(\rho_j, z_j)$$

$$\int_0^\infty dk J_{L_{piqi}}(k\rho_i) J_{L_{pjqj}}(k\rho_j) e^{-k|z_i - z_j|}, \tag{2.18}$$

Where L_{pq} is the angular momentum of the state p minus the angular momentum of the state q. By means of equations (2.1), (2.13), and (2.18). We construct the matrix form of the Hamiltonian with the basis given in equation (2.11). Then we solve the eigenvalue problem of the matrix, and get the energy states of multi-electrons confined in the dot. Finally we calculate the addition energy when we add another electron to a quantum dot.

The addition energy is defined by the difference of chemical potential when we add an electron into a quantum dot. The chemical potential for N electrons is given by

$$U(N) = E(N) - E(N-1), \tag{2.19}$$

where E(N) is the total energy of N electrons confined in a dot. Therefore, the formula of the addition energy is given as

$$A_E = U(N) - U(N-1)$$

$$= E(N+1) - 2E(N) + E(N-1) \tag{2.20}$$

Where A_E is the addition energy of the system and N the number of the electrons confined in a dot.

Chapter 3

Results and discussions

We simulate the InAs/GaAs dot when the material parameters for InAs inside the dots are $g(E=0)=0.42$, $\Delta=0.38$, $V_c=0eV$, $m(E=0)=0.0665m_e$. m_e is free electron mass. The parameters for GaAs outside of the dots are $g(E=0)=1.52$, $\Delta=0.34$, $V_c=0.77eV$, $m(E=0)=0.0665m_e$. The geometry of the dot is like Figure 1.1. And the size for the dot is radius (x-y plane) : $7.5\cdot10^{-9}$ m ; radius (z-axis) : $1.5\cdot10^{-9}$ m ; thick : $5\cdot10^{-10}$ m.

First we solve the energy states and the corresponding wave functions of single electron confined in the dot with different magnetic field. The results with zero external magnetic field are plotted below. In our case, there are only 8 states confined. They are $(n,l,s)=(1,0,1),(1,0,-1),(1,1,1),(1,1,-1),(1,-1,1),(1,-1,-1),(2,0,1),(2,0,-1)$. For simplicity, we use the symbol p to substitute for each combination of (n,l,s) and q=1,2,3,...,8 represent $(n,l,s)=(1,0,1),(1,0,-1),(1,1,1),(1,1,-1),(1,-1,1),(1,-1,-1),(2,0,1),(2,0,-1)$ respectively. The case which magnetic field differ from 0 is similar. Fig 3.1 to Fig 3.3 shows the wave function of single electron quantum dot with external magnetic field B=0, and (n,l)=(1,0),(1,1),(2,0). The corresponding energy states are 0.5158 eV, 0.6350eV, and 0.71434 eV. Where n is main quantum

number and l is angular quantum number. Since the energy states are irrelevant to the spin and the sign of the angular quantum number when B=0. These three cases represent all the states confined in the dot.

After we get all the wavefunctions and the corresponding energy levels of an electron confined in the dot with specified magnetic field. We use these datas to calculate the coulomb energy with each specified normalized states. Table.3.1 shows the energy caused by the Coulomb effect of two electrons with specified normalized states confined in the quantum dot with magnetic field zero. We can see that the Coulomb energy between electrons is two order less than the energy states of single electron confined in a dot. Therefore, the approximation we make for the exact diagonalization method is negligible in our problem.

Finally, by means of exact diagonalization method and the above datas, we get the enegy states of this multi-electrons system and calculate the addition energy which is shown in Fig3.4 to Fig3.6. We can see from the figures that : when the external magnetic field equals to zero, the addition energy appears to be slightly negative at some value of N. This is because the Hamiltonian of single electron Q.D. in our problem depends on the elecronic energy, so the eigenstates of the Hamiltonian with different energy level are not orthogonal to each other. This result in overlap of the stateswhich we use to create the Hamiltonian of multi-electrons quantum dot and make our results inaccurate especially when external magnetic field B=0. However, if we diagonalize these states, we can shift the addition enrgy up and turn the negative part to positive.

Table 3.1: The energy (Unit :eV) caused by the Coulomb effect of pair electrons with specified normalized states confined in the quantum dot.

$(pi,pj)/(qj,qi)$	$(1,1)$	$(3,1)$	$(7,1)$	$(1,3)$	$(3,3)$	$(7,3)$	$(3,7)$	$(7,7)$
$(1,1)$	0.0273	0	0.0042	0	0.0231	0	0	0.0222
$(3,1)$	0	0.0060	0	0	0	0	-0.0023	0
$(7,1)$	0.0042	0	0.0038	0	0.0010	0	0	0.0021
$(1,3)$	0	0	0	0.0060	0	-0.0023	0	0
$(3,3)$	0.0231	0	0.0010	0	0.0216	0	0	0.0198
$(7,3)$	0	0	0	-0.0023	0	0.0024	0	0
$(3,7)$	0	-0.0023	0	0	0	0	0.0024	0
$(7,7)$	0.0222	0	0.0021	0	0.0198	0	0	0.0197

Table 3.2: Ground state energy of multi-electrons confined in a quantum dot with zero magnetic field. Num is the number of the electrons. E is the ground states energy.

Num	$E(ev)$
1	0.4094954
2	0.8453178
3	1.4003105
4	1.9552513
5	2.5522374
6	3.1490976
7	3.8976914

Table 3.3: Ground state energy of multi-electrons confined in a quantum dot with magnetic field B=1T.

Num	$E(ev)$
1	0.4094308
2	0.8453020
3	1.3993759
4	1.9724783
5	2.5685960
6	3.1837163
7	3.9322930

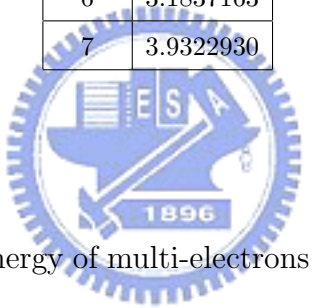

Table 3.4: Ground state energy of multi-electrons confined in a quantum dot with magnetic field B=5T.

Num	$E(ev)$
1	0.40927362
2	0.8455553
3	1.3959370
4	1.9679039
5	2.5655613
6	3.1847322
7	3.9334867

Table 3.5: Addition energy of multi-electrons confined in the quantum dot with Magnetic field B=0T. A_E means addition energy

Num	$A_E(ev)$
2	0.119170
3	−0.000052
4	0.042045
5	−0.00013
6	0.151734

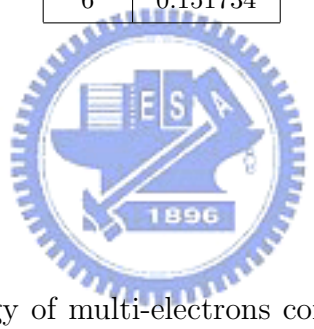

Table 3.6: Addition energy of multi-electrons confined in the quantum dot with Magnetic field B=1T.

Num	$A_E(ev)$
2	0.118203
3	0.019029
4	0.023015
5	0.019003
6	0.133456

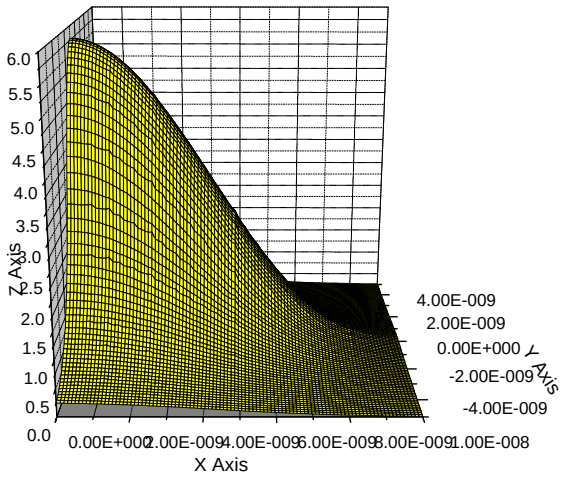

Figure 3.1: the wave function of single electron quantum dot with external magnetic field B=0T, and (n,l)=(1,0). n is angular quantum number and l is angular quantum number.

Table 3.7: Addition energy of multi-electrons confined in the quantum dot with Magnetic field B=5T.

Num	$A_E(ev)$
2	0.114100
3	0.021585
4	0.025691
5	0.021513
6	0.129584

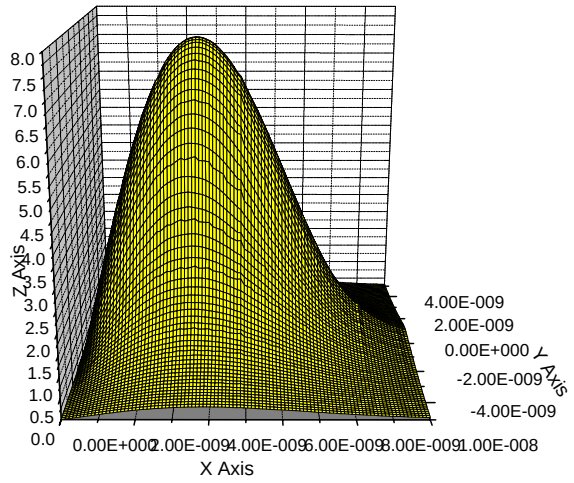

Figure 3.2: the wave function of single electron quantum dot with external magnetic field B=0T, and (n,l)=(1,1).

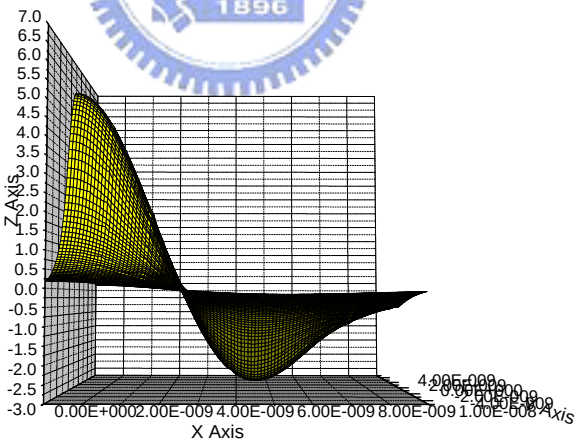

Figure 3.3: the wave function of single electron quantum dot with external magnetic field B=0T, and (n,l)=(2,0).

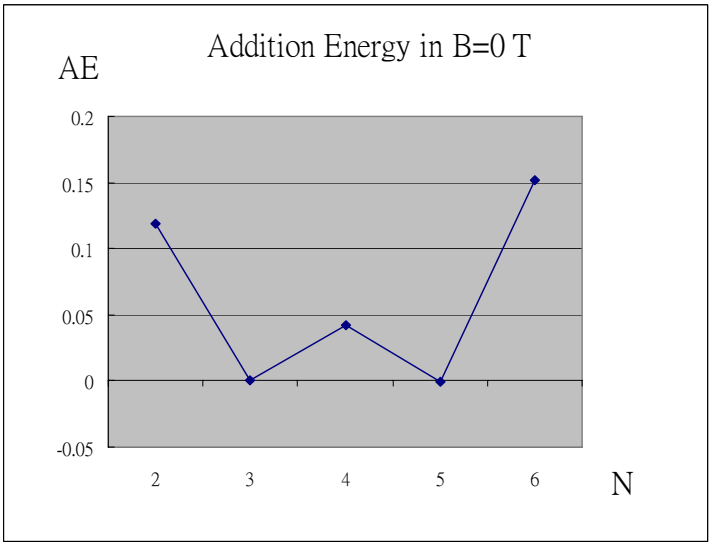

Figure 3.4: the addition energy of quantum dot with magnetic field B=0T

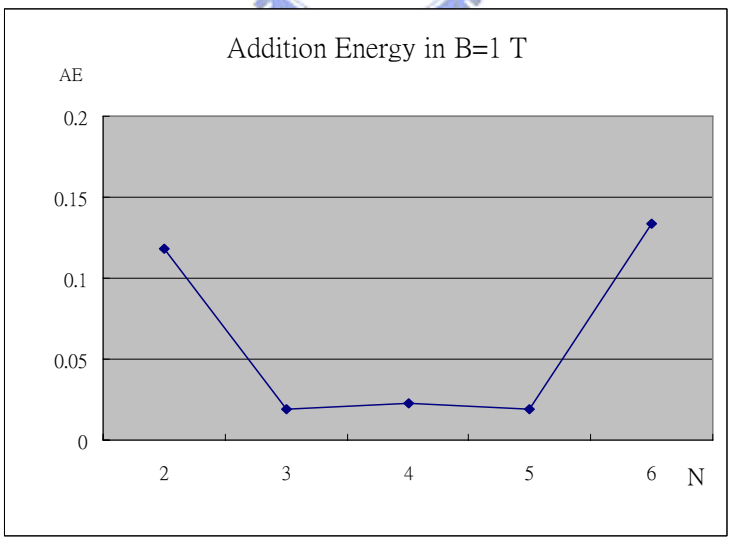

Figure 3.5: the addition energy of quantum dot with magnetic field B=1T

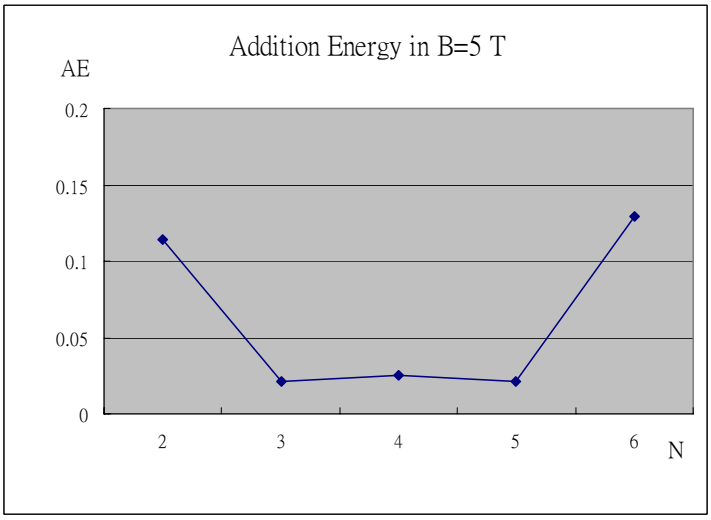

Figure 3.6: the addition energy of quantum dot with magnetic field B=5T

Chapter 4

Conclusions

We can find from the addition energy spectrum that structure in the addition energy for electrons in an external magnetic field as a function of electron number shows a clear progression from peaks consistent with shell structure to those consistent with the electrostatics of point particles. This should be observable in Coulomb blockade conductance measurements.

In this report, the basis we used to create the Hamiltonian of multi-electrons quatum dot are not diagonal. we will revise this in our next research. In addition, we will also find the addtion energy of the system with more than one quantum dots, even with the dots of different size.

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