Stockholm University

Licentiat Thesis

Many-Body effects in Semiconductor Nanostructures

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Akademisk avhandling för avläggande av licentiatexamen i fysik vid Stockholms Universitet

April 2014
“För när som faran är som störst,
så räddas man av kaffetörst.”

Ronny Åström
Low dimensional semiconductor structures are modeled using techniques from the field of many-body atomic physics. B-splines are used to create a one-particle basis, used to solve the more complex many-body problems. Details on methods such as the Configuration Interaction (CI), Many-Body Perturbation Theory (MBPT) and Coupled Cluster (CC) are discussed. Results from the CC singles and doubles method are compared to other high-precision methods for the circular harmonic oscillator quantum dot. The results show a good agreement for the energy of many-body states of up to 12 electrons.

Properties of elliptical quantum dots, circular quantum dots, quantum rings and concentric quantum rings are all reviewed. The effects of tilted external magnetic fields applied to the elliptical dot are discussed, and the energy splitting between the lowest singlet and triplet states is explored for varying geometrical properties. Results are compared to experimental energy splittings for the same system containing 2 electrons.
Contents

Abstract ii

Contents iii

List of Papers iv

1 Introduction 1
  1.1 Low Dimensional Semiconductor Structures ..................... 1

2 Computational Methods 4
  2.1 One-Particle Treatment ........................................ 4
     2.1.1 Polar coordinates ........................................ 5
     2.1.2 Cartesian coordinates .................................... 7
     2.1.3 B-spline Basis .......................................... 8
     2.1.4 Magnetic Field .......................................... 10
  2.2 Many-Body Treatment ........................................... 12
     2.2.1 Configuration Interaction ................................. 13
     2.2.2 Perturbation Theory ...................................... 15
     2.2.3 Coupled Cluster .......................................... 22

3 Effective Potentials 25
  3.1 Quantum Dot .................................................. 25
     3.1.1 Harmonic Oscillator ...................................... 26
     3.1.2 Elliptic Harmonic Oscillator ............................... 28
     3.1.3 Hard Wall ................................................ 31
  3.2 Quantum Ring .................................................. 32
     3.2.1 Concentric Rings ......................................... 33

4 Outlook 35
  4.1 Outlook ....................................................... 35

Acknowledgements 36

Bibliography 37

Paper I 40

Paper II 52
List of Papers

Paper I  Performance of the coupled-cluster singles and doubles method applied to two-dimensional quantum dots
E. Waltersson, C. J. Wesslén, and E. Lindroth

Paper II  Two-electron quantum dot in tilted magnetic fields: Sensitivity to the confinement model
T. Frostad, J. P. Hansen, C. J. Wesslén, E. Lindroth and E. Räsänen
DOI: 10.1140/epjb/e2013-40677-x
Chapter 1

Introduction

1.1 Low Dimensional Semiconductor Structures

Low dimensional semiconductor structures are key building blocks in modern electronic technology, being the basis of several applications such as solar cells, light-emitting diodes and transistors. Quantum mechanical effects are of special importance in semiconductor structures and a proper understanding of these become important when creating more complex devices.

The important properties of semiconductor materials lie in the so called band structure. By adjusting the availability of electrons in the conduction band and holes in the valance band, control of the materials conductivity may be achieved. This is often done by doping the semiconductor, placing impurities into the bulk and thereby injecting conductive electrons or holes into the band structure.

The conducting particles in a semiconductor material, such as electrons in the conduction band or holes in the valence band, can usually be modeled as a free electron gas. If one constrains the motion of the particles, only allowing them to move in two of the material’s three dimensions, a partial quantization of energy is achieved. The resulting potential is called a quantum-well, the density of state of which can be seen in Fig. 1.1. By constraining the particle motion to one and then zero dimensions further quantization occurs until one has fully discretized energy levels in the zero-dimensional quantum dot. Details regarding this can be found in most textbooks on semiconductor physics, such as [1]. The term Quantum Dot (QD) was introduced in [2], and has become an established term when describing highly constrained, artificial, atom like systems. QD:s are not only formed by low dimensional semiconductor structures, however these are the ones handled in this thesis.
Discretized energy levels are normally something you find in atoms, but in the quantum dot they come with the advantage of being adjustable. The effective potential constructed due to the 0D confinement of the dot will largely determine the energy level structure in the dot, but also material properties such as the effective electron mass and the material’s dielectric constant come into effect. A more detailed discussion regarding the shape of the effective potential, and the effects of these on the conducting electrons, can be found in Chapter ??.

Another property that the quantum dot shares with the atom is the existence of a shell structure. Much as the noble gases of the periodic table, quantum dots with certain numbers of confined electrons also display spikes in addition energy, i.e. the energy required to add another electron to the system. This was experimentally demonstrated by Tarucha in 1996 [3], and has been subject to many theoretical studies as reviewed in [4]. When calculating the addition energy spectra for the electrons in the quantum dot, precise calculations of the Coulomb interaction is required. Methods of handling these are discussed in Chapter 3 of the thesis and the results from one such method, the Coupled Cluster Singles and Doubles method, are presented in paper I.
Chapter 1. Introduction

The effects of an applied magnetic field to a QD are of great importance when manufacturing spintronic devices, and are also discussed in the thesis. In paper II, experimental results by Meunier on an elliptical QD with a tilted magnetic field, [5], are compared to theoretical results.

These atom-like properties give the QDs the name artificial atoms, and many theoretical methods used in atomic physics are also very suitable when handling them. But semiconductors can also be used to form more exotic potential structures, displaying qualities usually not found in nature. An example of such a system is the Quantum Ring (QR). The QR is a toroid (donut-shaped) potential, where the electrons are confined in a ring of arbitrary size. The two extreme limits of the ring are: a dot in the case of a ring with zero radius, and a quantum wire for a ring of infinite radius. By adjusting the QRs features, it can have different interesting properties. Experimentally rings of different shapes and sizes have been manufactured in a number of ways, [6, 7], one of the more exotic being the concentric rings manufactured by Mano in 2002, [8]. Both normal quantum rings and concentric quantum rings are discussed more in Chapter ??.

The science of low dimensional semiconductor structures is still quite young and the full potential has not yet fully been explored. Except applications such as those already mentioned, a novel area of use is in quantum computing. Quantum computing is a hot topic that can be read about in most popular science literature and can be reviewed in [9]. A key component behind a quantum computer is the so called quantum bit, or qbit. Quantum dots are one of several qbit candidates, exhibiting desired qualities such as coherence and high controllability. Success in implementing them will however require a great deal of experimental technique and theoretical understanding of their properties.
Chapter 2

Computational Methods

2.1 One-Particle Treatment

Here the one-electron quantum dot is introduced and the corresponding single-particle Hamiltonian is defined to calculate the systems eigenstates and energies. The one-electron eigenstates will form a basis later to be used when treating the many electron dot and will include all effects except the electron-electron interaction, which will be added in in section 2.2.

The one particle Hamiltonian in a magnetic field reads:

\[ \hat{h}_{\text{op}} = \frac{1}{2m^*} (\hat{p} - ieA)^2 + V(x), \]  

(2.1)

where \( \hat{A} \) is the field vector potential and \( V(x) \) is the effective potential of the dot. Both \( \hat{A} \) and \( V \) will be discussed in further detail later on. The focus for now will be on the case of no magnetic field and \( V \) being a two dimensional harmonic oscillator potential. The Hamiltonian now reads:

\[ \hat{h}_{\text{op}}(\mathbf{r}) = \frac{\hat{p}^2}{2m^*} + \frac{1}{2} m^* \omega^2 r^2, \]  

(2.2)
in polar coordinates and:

\[
\hat{h}_{op}(x) = \frac{\hat{p}^2}{2m^*} + \frac{1}{2}m^*\omega^2(x^2 + y^2),
\]

(2.3)
in Cartesian coordinates.

Inserting the Hamiltonian into the Schrödinger equation,

\[
\hat{h}_{op}\Psi = \epsilon \Psi,
\]

(2.4)
one hopes to find the wave functions \( \Psi \) and their corresponding energies \( \epsilon \).

### 2.1.1 Polar coordinates

As the 2D harmonic oscillator potential has a cylindrical symmetry, it is natural to solve the problem using polar coordinates. Since the Hamiltonian is separable in a radial part and an angular part one expects to find solutions of the form:

\[
\Psi_{nm\ell m_s}(r,\phi) = u_{nm\ell m_s}(r)e^{im\phi}|m_s\rangle,
\]

(2.5)
divided into a radial part \( u_{nm\ell m_s} \), an angular part, \( e^{im\phi} \) and a spin part \( |m_s\rangle \).

The non trivial part to solve now is the radial eigenvalue problem:

\[
\left[ \frac{\hbar^2}{2m^*}(-\vec{\partial}_r\partial_r + \frac{m_l^2}{2r^2}) + \frac{1}{2}m^*\omega^2r^2 \right] u_{nm\ell}(r) = \epsilon_{nm\ell}u_{nm\ell}(r),
\]

(2.6)
Where \( \vec{\partial}_r \) and \( \partial_r \) represent differential operators working to the left or right respectively.

Solving this, one finds the wave functions to eq. 2.4:

\[
\Psi_{nm\ell}(r,\phi) = \frac{1}{\sqrt{\pi}}\sqrt{\frac{2n!}{n + |m_l|!}} \frac{(r)}{\sqrt{l}}^{|m_l|} L_n^{|m_l|}(r/l)^2e^{-(r^2/2l^2)}e^{im\phi} \sqrt{2\pi}
\]

(2.7)
Chapter 2. Computational Methods

\[ n,m_l=0,1 \]

\[ n,m_l=1,1 \]

\[ n,m_l=0,1 \]

\[ n,m_l=1,0 \]

Figure 2.1: Plots of the real part of four of the wave functions acquired using eq. 2.7, labeled using the \( n \) and \( m_l \) quantum numbers.

and the corresponding eigenvalues:

\[ \epsilon_{nm_l} = \hbar \omega (2n + |m_l| + 1) . \]  

(2.8)

Where \( L_n^{|m_l|} \) are the associated Laguerre polynomials, and \( l \) is the typical harmonic oscillator length: \( l = \sqrt{\frac{\hbar}{m \omega}} \).

Details on how eq. 2.6 is solved can be found in quantum mechanical textbooks such as [10]. The real part of some of these wave functions can be seen in figure 2.1.

The polar solution is powerful since it has a trivial solution in the angular regime, reducing our problem from two dimensions into one radial dimension. This solution is also useful when introducing a magnetic field, since these states are also eigenstates to the \( L_z \) operator. However any change to the potential that breaks the cylindrical symmetry, such as the elliptical dot or the tilted magnetic field introduced later on,
disables us from using the cylindrical symmetry property required for this separation
into an angular and a radial part.

2.1.2 Cartesian coordinates

By solving the Schrödinger equation in Cartesian coordinates the problem separates
into two one dimensional harmonic oscillator potentials:

\[
\frac{1}{2m^*} \frac{\partial^2}{\partial x^2} \psi_{n_x}(x) + \frac{1}{2} m^* \omega^2 x^2 \psi_{n_x}(x) = \epsilon_{n_x} \psi_{n_x}(x),
\]

(2.9)

for the \(x\) and \(y\) coordinate separately. The solution, once again in atomic units, has the
eigenstates:

\[
\psi_{n_x}(x) = \frac{1}{\sqrt{2^{n_x} n_x!}} \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} H_{n_x}(m \omega x / \hbar) e^{-m \omega x^2 / 2 \hbar},
\]

(2.10)

where \(H_{n_x}(x)\) are Hermite polynomials. And the eigenvalues are:

\[
\epsilon_{n_x} = \hbar \omega (n_x + \frac{1}{2})
\]

(2.11)

The solution to the Schrödinger equation in both dimensions will then have the wave
functions:

\[
\Psi_{n_x,n_y}(x,y) = \psi_{n_x}(x) \cdot \psi_{n_y}(y),
\]

(2.12)

with the energies:

\[
\epsilon_{n_x,n_y} = \hbar \omega (n_x + n_y + 1)
\]

(2.13)

Once again, details can be found in text books such as [10], and the wave functions can
be found in figure 2.2.
This solution is equivalent to the polar one, but requires the solutions to two sets of eigenvalue problems. If we were to change the parameters of the harmonic oscillator, separating the harmonic oscillator strength, $\omega$, into two parameters in the different dimensions, $\omega_x$ and $\omega_y$, we can write the harmonic potential: 

$$V_{HO}(x,y) = \frac{1}{2} m^* \left( \omega_x^2 x^2 + \omega_y^2 y^2 \right).$$

We now have the option to use different oscillator strengths in the two different dimensions, creating an elliptic dot. More details regarding this can be found later on in Chapter ??.

### 2.1.3 B-spline Basis

As we have seen, the 2D harmonic oscillator is exactly solvable, but for practical reasons we would rather have a numerical basis. Partly to be able to chose more exotic potentials that are not exactly solvable, and partly to be able to exploit the completeness property of the numerical basis.

So as a numerical basis we chose the so called B-spline basis. B-splines are piecewise polynomials of some order defined on grid, called a knot sequence. Details on the
properties of the basis and how it is applied in atomic physics can be reviewed in [11], what follows will be a very short summation of the application to our situation.

Any function $f(x)$ can be approximated using $N$ splines of order $k$ as:

$$f(x) = \sum_{i=1}^{N} c_i B_{i,k}(x), \quad (2.14)$$

The splines, $B_{i,k}$, are polynomials of order $k$, defined between the knot points $i$ and $i+k$. With more splines, another knot sequence or higher order polynomials, more complex functions can be approximated to a better accuracy. So we may now project our basis functions in the previous sections to our B-spline basis, as an example we chose the one dimensional wave functions from our solution using Cartesian coordinates:

$$|\psi_{n_x}\rangle = \sum_{i=1}^{N} c_{i,n_x} |B_{i,k}\rangle, \quad (2.15)$$

This new representation of the wave functions reduces the problem of the Schrödinger equation into finding the set coefficients belonging to each eigenstate. This is done by applying either of the one-particle Hamiltonians 2.2 or 2.3 to our new basis, 2.15, and taking the dot product with the basis set bras from the left to form the matrix equation as follows:

$$hc = \epsilon B c, \quad (2.16)$$

where the elements of $h$ are $h_{j,i} = \langle B_{j,k} | h_{op}(x) | B_{i,k} \rangle$, $B$ are $B_{j,i} = \langle B_{j,k} | B_{i,k} \rangle$ and $c$ contains the coefficients we are trying to find.

The integrals needed to be solved to create the matrix equation can be calculated exactly using Gaussian quadrature since the B-splines are polynomials. This means that the source of approximation in the method is the representation of the wave functions in the new basis. By modifying the knot point sequence and the polynomial order we have a way of optimizing the wave function representation to suite the accuracy required. We will to a good approximation reproduce a certain number of lower lying states, but due to the knot sequence the states will become less and less accurate as they increase in energy. Eventually the states are becoming fully unphysical and are mainly determined by the
boundaries of the knot-sequence, the so called numerical box. However these states are still required and useful to construct the complete and finite basis, a property we eventually want to be able solve the many-body Hamiltonian in Section 2.2 accurately.

2.1.4 Magnetic Field

We now want to add a general time-independent magnetic field potential to the dot. The most trivial magnetic field is one lying in the z-direction, however we chose a more general field:

\[
B = B_0 \left( \cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta \right),
\]

(2.17)

giving us the vector potential:

\[
A = \frac{B_0}{2} \left( z \cos \phi \sin \theta - y \cos \theta, x \cos \theta - z \sin \phi \sin \theta, y \sin \phi \sin \theta - x \cos \phi \sin \theta \right),
\]

(2.18)

In our convention \( \theta \) is the inclination angle and \( \phi \) is the azimuthal angle from the x-axis, as seen in figure 2.3. The Hamiltonian in equation 2.1 can be rewritten:

\[
\hat{h}_{op} = \frac{\hat{p}^2}{2m^*} + V(x) + \frac{e^2}{2m^*} A^2 + \frac{e}{2m^*} B \cdot L + g^* \mu_B B \cdot S.
\]

(2.19)
Now if we assume an almost two-dimensional dot, the contributions in the z-direction vanish, leaving us with the quadratic coupling:

\[ A^2 = \frac{B_0^2}{4} \left( (x^2 + y^2) \cos^2 \theta + \sin^2 \theta (y \sin \phi - x \cos \phi)^2 \right), \tag{2.20} \]

the linear coupling:

\[ \mathbf{B} \cdot \mathbf{L} = B_0 \cos \theta L_z \tag{2.21} \]

and the spin coupling:

\[ g^* \mu_b \mathbf{B} \cdot \mathbf{S} = g^* \mu_b B_0 \cos \theta \hat{s}_z. \tag{2.22} \]

The quadratic term will act as an anisotropic two-dimensional harmonic potential, where the angles \( \theta \) and \( \phi \) will control the direction of the anisotropy. This is easily seen by fixing \( \phi \) to zero and ending up with the potential:

\[ A^2 = \frac{B_0^2}{4} \left( x^2 + y^2 \cos^2 \theta \right), \tag{2.23} \]

where the harmonic potential in the y-direction is dampened by a factor \( \cos \theta \). With a general azimuthal angle \( \phi \) an equivalent elliptical potential is created but with its axis in the direction of \( \phi \). So for a tilted magnetic field the dominating effect will be that of an anisotropic harmonic oscillator potential with its axis in the \( \phi \)-direction.

A Cartesian basis will be more natural to use when a tilted magnetic filed is involved, since the quadratic magnetic effect only has a cylindrical symmetry in the case when \( \theta \) is zero. The first part of eq. 2.20 is separable and can be added to the two one-dimensional Schrödinger equations (2.9). The second part of eq. 2.20 and the linear magnetic term both mix in the x-y-dimensions and need to be added separately, mixing the states produced in subsection 2.1.2.
2.2 Many-Body Treatment

In the previous section a single-particle basis has been created, which we may now use in an attempt to solve the many-body Hamiltonian:

\[ H_{MB} = \sum_i^N h_i + \sum_{i<j}^N \frac{e^2}{4\pi\epsilon\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} \tag{2.24} \]

Here we have separated the Hamiltonian into two parts, the non-interacting, one-body part, \( h_i \) that we have already solved, and the many-body, electron-electron interaction. Some of the simpler methods used to do solve this problem are so called mean-field methods, where the electron-electron interaction is simplified to a one-body interaction with a total potential created by all the other electrons collectively. Hartree-Fock (HF) and Density Function Theory (DFT) are two such methods, but both lack accuracy to one degree or the other. HF does not include any correlation effects and will be a fairly bad method when we increase our number of particles. DFT can produce very high quality results, but they are dependent on the functionals used and the accuracy of the method is hard to determine beforehand.

In this work, focus is on more exact numerical many-body methods; Configuration Interaction (CI), Many-Body Perturbation Theory (MBPT) and Coupled Cluster (CC).

To start out we should define some things. First off a many-body wave function for a system consisting of \( N \) electrons can be written as a product of single-body functions as a slater determinant:

\[ \Psi_0 = |\psi_a \cdot \psi_b \cdot ... \cdot \psi_N| \tag{2.25} \]

So the wave function in eq. 2.25 is a \( N \)-electron wave function where the orbitals \( a, b, ...N \) are occupied. We also divide the space constructed by the one-electron states into two parts, the model space and the function space. The model space is spanned by model functions, which are states used as starting-points in our numerical routines when searching for exact many-body wave functions. These are approximations of the exact wave functions, and the choice of these will be discussed in further detail below. The function space is the complementary space to the model space, spanned by all the other wave functions created using our one-body states.
We use the convention of denoting electron orbitals occupied in the model space with the letters \(a, b, c,\ldots\) and orbitals unoccupied in the model space using the letters \(r, s, t,\ldots\). When describing a general case where an orbital may be either occupied or unoccupied the letters \(m, n, o,\ldots\) will be used. A many-body state in the function space, where the electron occupying the orbital \(a\) in the model space, is instead occupying the excited orbital \(r\), is written as the Slater determinant:

\[
\Psi_a^r = |\psi_r \cdot \psi_b \cdot \ldots \cdot \psi_N|.
\]

Due to the completeness of the basis, any state, such as the solution the many-body Hamiltonian in eq. 2.24, can be written as:

\[
\Psi = c_0 \Psi_0 + \sum_{ar} c_a^r \Psi_a^r + \sum_{abrs} c_{ab}^{rs} \Psi_{ab}^{rs} + \sum_{abcrst} c_{abc}^{rst} \Psi_{abc}^{rst} + \ldots = \sum_i \Psi_i
\]

So the exact many-body state can be written as a superposition of states in our model and function space. We can see the different parts as the original non-interacting state and excitations from this configuration, these excitations may be one-electron, two-electron or more electron excitations. The division based on the degree of excitation will be useful later on, but for simplicity it is enough to describe them as some excitation \(\Psi_i\) from \(\Psi_0\).

### 2.2.1 Configuration Interaction

In a similar fashion as previously done when switching basis to the B-spline basis in subsection 2.1.3, we can now construct an eigenvalue problem on matrix form where we now search for the coefficients of eq. 2.27.

\[
HC = EC
\]

(2.28)
Thanks to the orthogonality of the many-body states in the model and function space, \( C \) will only be a vector containing the coefficients, \( E \) will contain the many-body energies and \( H \) is:

\[
H = \begin{pmatrix}
\langle \Psi_0 | H_{MB} | \Psi_0 \rangle & \langle \Psi_0 | H_{MB} | \Psi_1 \rangle & \cdots \\
\langle \Psi_1 | H_{MB} | \Psi_0 \rangle & \langle \Psi_1 | H_{MB} | \Psi_1 \rangle & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix}
\]

(2.29)

Using the Configuration Interaction method, one constructs this matrix and diagonalizes it to form the exact many-body solution to eq. 2.24.

However, this is a very expensive method. Even though we have a finite one-body basis, the number of many-body functions we can create using these grows very large when more than a few active electrons are allowed. This usually requires a truncation of some aspect of the problem, usually by only allowing a certain degree of excitations in the function space. This is done by removing some of the terms in eq. 2.27, and reducing the dimensionality of the \( H \)-matrix.

But by doing this, certain problems will arise in regards to the solution. The most obvious is that the complete basis is required to form the exact wave function, however we must always trade accuracy for speed when using numerical methods, so some loss in accuracy can be acceptable. A less obvious drawback is lack of size consistency, [12], that is, truncated CI does not conserve energy when dividing something into several separate subsystems, [13]. Since we will study potentials with some degree of separation later on, this may be important. So the only CI used will be non-truncated, Full CI (FCI).

The matrix-elements of \( H \) will consist of the one-electron Hamiltonians from the previous section and the electron-electron interaction. Since the many-body wave functions are eigenstates to the sum of one-electron Hamiltonians, this part falls out into a diagonal matrix.

The non trivial part that is left is the ee-interaction:

\[
\langle \Psi_k | \sum_{i<j}^{N} \frac{e^2}{4\pi\epsilon\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} | \Psi_l \rangle
\]

(2.30)
The electron-electron interaction is actually a two particle operator, so the matrix element will be a sum of all possible two-particle combinations belonging to the states $\Psi_k$ and $\Psi_l$ such as:

$$\langle op|\frac{1}{r_{12}}|mn\rangle_l,$$  \hspace{1cm} (2.31)

where particles $op$ belong to state $k$ and particles $mn$ belong to state $l$. Depending on the configuration of the one-particle states, these $1/r_{12}$ matrix elements will be added with different signs, or may be zero.

When using the polar solutions to the one-body Hamiltonians we can use the expansion suggested by Cohl et al. in [14] and write the $1/r_{12}$ matrix elements as:

$$\langle op|\frac{1}{r_{12}}|mn\rangle = \frac{e^2}{4\pi \epsilon \epsilon_0} \sum_{m_l=-\infty}^{m_l=\infty} \langle u_o(r_1), u_p(r_2)|Q_{m_l-1/2}(\xi)\frac{\pi}{\sqrt{r_1 r_2}}|u_m(r_1), u_n(r_2)\rangle$$

$$\cdot \langle e^{im_1 \phi_1} e^{im_2 \phi_2}|e^{im_l \phi_1 - \phi_2}|e^{im_m \phi_1} e^{im_n \phi_2}\rangle \langle m_o|m_m\rangle \langle m_p|m_n\rangle.$$  \hspace{1cm} (2.32)

Here the numbers 1 and 2 denote the first and second particle, $u_o(r)$, $m$ and the $m_s$ quantum numbers are defined as in eq. 2.5. The $Q_{m_l-1/2}(\xi)$ functions are Legendre functions of the the second kind and half integer degree solved using software from [15]. Thanks to the use of B-splines, the radial integrals that need to be evaluated are polynomial, allowing the use of exact Gaussian integration. The angular integrals will only be non-zero given certain quantum numbers, leading us to some selection-rules, namely: $m_l - m_{m_l} = m_l = m_{m_l} - m_{m_l}$, $m_s = m_{m_l}$ and $m_s = m_{m_l}$.

In the case of Cartesian coordinates the process is more straight forward however special care must be taken when operating close to the poles in the $1/r_{12}$ operator, to circumvent division by zero.

### 2.2.2 Perturbation Theory

Moving on to the many-body perturbation theory, the idea is to perturbatively add the ee-interaction to an already known solution. This presents a number of options on what to do and the work done here is based on Lindgren and Morrisons textbook on many-body atomic physics, [16]. The goal is to achieve a perturbation expansion to all order, that is including all possible linked Coulomb interactions. If electron pair $a$ and $b$ couple...
to pair $r$ and $s$, we should also include the effect from the subsequent coupling $r$ and $s$ to all other pairs. In CI this is included in the diagonalization of the Hamiltonian matrix, and therefore all interactions are included. With perturbation theory we hope to achieve the same thing without the computational expenses of FCI or the drawbacks of truncated CI.

To start of we want to divide the complete Hamiltonian into two parts, $H = H_0 + V$, with the exact unknown eigenstate $\Psi$. Here $H_0$ has a known solution $\Psi_0$ that is an approximation of $\Psi$, and $V$ is treated as a perturbation to $H_0$. We have the option to either place the entire electron-electron interaction in $V$ or place some of it in $H_0$ by first using something simpler, such as the Hartree-Fock method that includes some, but not all ee-effects. Hence, $V$ becomes:

\[
V = \sum_{i<j \leq N} \frac{1}{r_{ij}} - \sum_{i \leq N} u_i,
\]

where $u_i$ is some one-particle potential already included in the solution of $H_0$. The reason to do this is to possibly include some of the ee-interaction in the model function, by using solutions from some mean-field method, such as Hartree-Fock. This will not effect the solution since all interactions are included in the MBPT method but may speed up the process.

In the previous subsection, the concept of model-space and function-space have already been defined. The model space may span any number of many-body functions, but for simplicity we start of by investigating the case where it only contains one model function $|\Psi_0\rangle$. It becomes useful to create some projection-operators associated to these spaces, $P = |\Psi_0\rangle\langle\Psi_0|$ which projects onto the model function, and $Q = \sum_{\beta \neq \Psi_0} |\beta\rangle\langle\beta|$ which projects onto the complimentary functions. The two projection operators form a complete space, i.e. $P + Q = 1$. We also chose to normalize our functions in such a way that $\langle\Psi_0|\Psi\rangle = 1$. This allows us to write the exact solution as the model function plus a correction in function space:

\[
|\Psi\rangle = (P + Q)|\Psi\rangle = |\Psi_0\rangle + Q|\Psi\rangle
\]

Finally we define the wave operator $\Omega$ and the correlation operator $\chi$. The wave operator has the property that it creates the exact state when operating on the model function, i.e. $\Omega|\Psi_0\rangle = |\Psi\rangle$. The correlation operator is defined by $\Omega = 1 + \chi$, and will when
operating on the model function, create the correction in function space to the model function:

\[
\chi|\Psi_0\rangle = (\Omega - 1)|\Psi_0\rangle = |\Psi\rangle - P|\Psi\rangle = |\Psi_0\rangle + Q|\Psi\rangle - |\Psi_0\rangle = Q\Omega|\Psi_0\rangle \quad (2.35)
\]

We can now rewrite the Schrödinger equation onto a, for the purpose, more useful form called the Bloch equation, formulated in [17]. The SE in our operator form reads:

\[
H|\Psi\rangle = H_0|\Psi\rangle + V|\Psi\rangle = E|\Psi\rangle, \quad (2.36)
\]

or

\[
(E - H_0)|\Psi\rangle = V|\Psi\rangle, \quad (2.37)
\]

we now project onto our model space using the \( P \) operator, which commutes with \( H_0 \) since \( \Psi_0 \) is an eigenfunction.

\[
P(E - H_0)|\Psi\rangle = (E - H_0)|\Psi_0\rangle = PV|\Psi\rangle. \quad (2.38)
\]

Next step is to use the definition of the wave operator:

\[
P(E - H_0)|\Psi\rangle = E|\Psi_0\rangle - H_0|\Psi_0\rangle = PV\Omega|\Psi_0\rangle, \quad (2.39)
\]

and then operate with \( \Omega \):

\[
E\Omega|\Psi_0\rangle - \Omega H_0|\Psi_0\rangle = E|\Psi\rangle - \Omega H_0|\Psi_0\rangle = \Omega PV\Omega|\Psi_0\rangle. \quad (2.40)
\]
We now replace $E|\Psi\rangle$ with the SE in eq. 2.36 and once again use the definition of the wave operator:

$$E|\Psi\rangle - \Omega H_0|\Psi_0\rangle = (H_0 + V)|\Psi\rangle - \Omega H_0|\Psi_0\rangle = (H_0 + V)\Omega|\Psi_0\rangle - \Omega H_0|\Psi_0\rangle = \Omega PV\Omega|\Psi_0\rangle,$$

(2.41)

and by shuffling the terms we get:

$$H_0\Omega|\Psi_0\rangle - \Omega H_0|\Psi_0\rangle = \Omega PV\Omega|\Psi_0\rangle - V\Omega|\Psi_0\rangle.$$

(2.42)

We bring in a $\langle \Psi_0|$ from the right and switch signs to write this with a commutator on the form:

$$[\Omega, H_0]P = V\Omega P - \Omega PV\Omega P.$$

(2.43)

Finally we want to use a formalism where we create excitations from the model space $P$ onto the function space $Q$, therefor we use our definition of $\chi$ to rewrite this onto its final form, the Bloch equation:

$$[\Omega, H_0]P = QV\Omega P - \chi PV\Omega P.$$

(2.44)

We can now divide the wave operator order by order, $\Omega = 1 + \Omega_1 + \Omega_2 + ..., and likewise for the correlation operator, $\chi = \Omega_1 + \Omega_2 + ...$. Here the order of the operator denotes the number of ee-interactions involved in the operator. The point of this is to create an order-by-order scheme to construct our wave operator, so by inserting the expanded operator into the Bloch equation we may identify connections between different parts of the two sides of the equation:

$$[(1 + \Omega_1 + ...), H_0]P = QV(1 + \Omega_1 + ...)P - (\Omega_1 + ...)PV(1 + \Omega_1 + ...)P$$

(2.45)
\[ [1, H_0] P = 0 \]
\[ [\Omega_1, H_0] = Q V P \]
\[ [\Omega_2, H_0] = Q V \Omega_1 P - \Omega_1 P V P \]
\[ [\Omega_3, H_0] = Q V \Omega_2 P - \Omega_2 P V P - \Omega_1 P V \Omega_1 P \]

\[ : \]

By calculating all the matrix elements \( Q V P \) we can now create the first order wave operator, and by using \( \Omega_1 \) we can continue constructing \( \Omega_2 \) and so on. When evaluating the operators, certain parts of the right hand side of the expressions may be found to have so called unlinked or disconnected parts. These are called the unlinked diagrams when applying a diagrammatic approach to the problem.

The clearest case are of the variety \( \Omega_2 P V P \), here the \( V \) operator operates between the model functions only creating an energy contribution of the form of a constant number. Also the \( \Omega_1 P V \Omega_1 P \) term has a similar closed off part, here created by the \( \Omega_1 \) and subsequent \( V \) operator, creating another energy contribution. If the \( Q V \Omega_2 P \) term is expanded, the same parts with the same closed of energy contribution will be found, but only if we allow for the Pauli exclusion principle to be violated. That is, we allow for unphysical states where several particles are allowed to occupy the same orbitals at once. If this is done in all terms of eq. 2.44, we will get a cancellation between the disconnected parts of first term and the entire second term of the right hand side. This is called the linked-diagram theorem and details may be found in [16]. This allows us to formulate the Bloch equation in a new way:

\[ [\Omega_i, H_0] P = (Q V \Omega_{i-1} P)_{\text{linked}}, \quad (2.47) \]

where only the linked diagrams, but all Pauli principle violating diagrams are included in the right hand side. Note that the resulting wave operator is not Pauli violating, these terms are only there to ensure the cancellation of the second term in eq. 2.44.

We now wish to utilize the wave operator expansion to find the exact wave function \( |\Psi\rangle \) and the states energy \( E \). The wave operator has been divided order-by-order, and so
can the wave function:

\[ |\Psi\rangle = \Omega |\Psi_0\rangle = |\Psi_0\rangle + \Omega_1 |\Psi_0\rangle + \Omega_2 |\Psi_0\rangle + \ldots = |\Psi_0\rangle + \chi |\Psi_0\rangle \]  \hspace{1cm} (2.48)

Now, \(\chi |\Psi_0\rangle\) operates from \(P\) space to \(Q\) space as in eq. 2.35 so we are only interested in the parts of the wave operator doing the same. If we operate with the \(Q\)-operator from the left-hand side of eq. 2.46, we can investigate the effects on the first order operator:

\[ Q[\Omega_1, H_0] = Q\Omega_1 H_0 P - Q H_0 \Omega_1 P \]  \hspace{1cm} (2.49)

By letting the \(H_0\) operator operate to the right on \(P\) in the first term and to the left on \(Q\) in the second term, we can replace the \(H_0\) operator with its eigenvalues:

\[
Q\Omega_1 H_0 P - Q H_0 \Omega_1 P = Q\Omega_1 E_P P - QE_Q \Omega_1 P = \\
= \sum_{\beta \neq \Psi_0} (|\beta\rangle \langle \beta| \Omega_1 \epsilon_0 |\Psi_0\rangle \langle \Psi_0| - |\beta\rangle \langle \beta| \epsilon_\beta \Omega_1 |\Psi_0\rangle \langle \Psi_0|) = \\
= (\epsilon_0 - \epsilon_\beta) \sum_{\beta \neq \Psi_0} |\beta\rangle \langle \beta| \Omega_1 |\Psi_0\rangle \langle \Psi_0| \hspace{1cm} (2.50)
\]

If we also rewrite the right hand side of the corresponding row of eq. 2.46, we can express the first order wave function as:

\[
|\Psi_1\rangle = Q\Omega_1 |\Psi_0\rangle = \sum_{\beta \neq \Psi_0} |\beta\rangle \langle \beta| \Omega_1 |\Psi_0\rangle = \sum_{\beta \neq \Psi_0} \frac{|\beta\rangle \langle \beta| V |\Psi_0\rangle}{(\epsilon_0 - \epsilon_\beta)} \hspace{1cm} (2.51)
\]

By doing the same thing for the other lines of eq. 2.46 we now have a way of constructing the complete wave function, order by order.

To find the corresponding energy we define a effective Hamiltonian, \(H_{eff}\), with the properties that its eigenvalue is the exact energy \(E\) corresponding to the exact wave
function $|\Psi\rangle$, and its eigenfunction is the model function $|\Psi_0\rangle$. To get these properties the effective Hamiltonian must be defined as follows:

$$H_{eff} = PH\Omega P = PH_0P + PV\Omega P$$  \hspace{1cm} (2.52)

In a similar way to how the wave function was treated, we now divide the energy into an order-by-order expansion:

$$\langle \Psi_0 | E | \Psi_0 \rangle = \langle \Psi_0 | H_{eff} | \Psi_0 \rangle =$$
$$= \langle \Psi_0 | H_0 | \Psi_0 \rangle + \langle \Psi_0 | V | \Psi_0 \rangle + \langle \Psi_0 | V \Omega_1 | \Psi_0 \rangle + \langle \Psi_0 | V \Omega_2 | \Psi_0 \rangle + ... =$$
$$= E_0 + E_1 + E_2 + E_3 + ... \hspace{1cm} (2.53)$$

Note that the first order wave operator, $\Omega_1$, produces the second order energy, $E_2$, since an additional electron-electron interaction is added to it.

Even though a scheme for finding the true many-body wave function and energy has been found, it is not a very practical one. Since the different order wave operators can be combined in more ways to form higher order operators, a computer algorithm will be tough to construct. A better form would be an iterative equation where one can insert one iteration of the solution once again into the same equation to form a higher order solution. Such a Bloch equation would instead be:

$$[\Omega^{(i)}, H_0]P = QV\Omega^{(i-1)}P - \chi^{(i-1)}PV\Omega^{(i-1)}P,$$ \hspace{1cm} (2.54)

where the starting point wave and correlation operators are $\Omega^{(0)} = 1$ and $\chi^{(0)} = 0$. By inserting the expressions for $\Omega$ iteration by iteration, one would find that the expressions do not match the order by order formalism in eq. 2.46. However, the sum of the all-order expansion of wave operators in both formalisms would be the same, i.e. given that a self consistent solution is reached through iteration, it will be equivalent to the one found order-by-order.

For an exact solution all orders of the wave operator need to be included, but the contribution to the energy and wave function will be smaller and smaller for each order as each higher order operator is built from lower order operators. However, size consistency once again may play an important roll. It has been shown, [13], that MBPT is only
size consistent if it includes simultaneous pair excitations in the separated subsystems. These are disconnected quadruple excitations i. e. two separate double excitation in the subsystems. So if we implement MBPT using the linked diagram theorem, and truncate it by the double excitations, we will not include these disconnected "double-double" excitations. To be sure to include this, we can not truncate the wave function before the fourth order. But by a slight modification to how we treat the wave operator, we may include all double excitations, even simultaneous ones we have thus far treated as quadruple excitations. This treatment is called the Coupled Cluster method.

2.2.3 Coupled Cluster

The Coupled Cluster method (CC), originates from the field of nuclear physics [18], and has since then been well used in atomic, molecular and chemical physics, see for instance [19] for a review of the use in these areas. Due to the atom-like properties of low dimensional semiconductor systems, and the theoretical modeling using an effective potential, the method has also seen some recent use in this area such as [20–22] and paper I in this thesis.

We define: \( S_N = \Omega_{N,\text{connected}} \), a cluster operator of order \( N \) is defined as the part of the wave operator that creates excitations of the \( N \):th order, that may not be subdivided into several disconnected lower order excitations. As an example, a double excitation from the model function, exciting electrons in orbitals \( a \) and \( b \) to \( r \) and \( s \), \( \langle \Psi_{ab}^r s | V | \Psi_0 \rangle \), is a pure double excitation included in the \( S_2 \) operator. However two single excitations, \( \langle \Psi_{b}^r | V | \Psi_0 \rangle \langle \Psi_{a}^s | V | \Psi_0 \rangle \), resulting in the same total excitation to the state \( \Psi_{ab}^r s \), will not be included, but will instead be a case of two single excitations \( \{ S_1 \}^2 \). Both of these are double excitations belonging to the \( \Omega_2 \) operator, but are built by two different classes of cluster operators.

We can write the entire wave operator as the exponential function of the sum of all cluster operators:

\[
\Omega = \{ e^S \} = \{ e^{S_1+S_2+S_3+...} \} = 1 + S_1 + S_2 + \frac{1}{2!}(S_1)^2 + S_3 + \{ S_1 S_2 \} + \frac{1}{3!}(S_1)^3 + ..., \quad (2.55)
\]

where the curly brackets denote anti-symmetrization of the operators. The right-hand side of eq. 2.55 can now be subdivided into the different orders of the the wave operator as follows:
\[ \Omega_1 = S_1 \]
\[ \Omega_2 = S_2 + \frac{1}{2!} \{ S_1 \}^2 \]
\[ \Omega_3 = S_3 + \{ S_2 S_1 \} + \frac{1}{3!} \{ S_1 \}^3 \]
\[ \Omega_4 = S_4 + \{ S_3 S_1 \} + \frac{1}{2!} \{ S_2 \}^2 + \frac{1}{2!} \{ S_2 S_1 \}^2 + \frac{1}{4!} \{ S_1 \}^4 \]  
(2.56)

If we truncate the cluster operator so as to only include single and double clusters (Coupled Cluster Singles and Doubles), we still include some higher order excitations. Better yet, we include the separated doubles required for our method to be size consistent as long as we include all combinations of singles and doubles up until \( \Omega_4 \). The cluster operator also satisfies the Bloch equation, [23]:

\[ [S_N, H_0] P = (QV \Omega P - \chi PV \Omega P)_{N,\text{connected}} \]  
(2.57)

Once again, connected denotes the excitations that can not be divided into several lower order disconnected parts. The linked diagram theorem, explained in the previous chapter can be applied to the equation too, canceling out the second right hand term.

Concentrating on the Coupled Cluster Singles and Doubles (CCSD), the most common CC method, truncating the cluster operator to include singles and doubles and only including intermediate excitations up to quadruples. We now want to write the iterative cluster equations for the \( S_1 \) and \( S_2 \) operators. Starting with the singles cluster, the goal is to achieve a similar expression as in eq. 2.51. However, it becomes more complicated since a single excitation can be created in various ways, with higher order intermediate excitations possible. For instance \( \langle \Psi_a | V | \Psi_{rs} \rangle \langle \Psi_{rs} | V | \Psi_0 \rangle \), has a net single excitation, but an intermediate double excitation. It becomes advantageous to divide the perturbation interaction \( V \) into components by the excitation created; \( V_0, V_1 \) and \( V_2 \), where the index represents the excitation order. \( V_0 \) will only interact between identical states such as the \( PVV \) terms canceled out with the linked diagram theorem, and will not appear in the expressions. Combining the perturbation operators and the wave operators we can write the iterative formula for the singles cluster operator as:
\[ \langle \Psi_r^i | S_1 | \Psi_0 \rangle_{i+1} = \frac{1}{\epsilon_a - \epsilon_r} \langle \Psi_r^i | V_1 + (V_1 + V_2) S_1 + (V_1 + V_2) S_2 + \]
\[ + \frac{1}{2!} (V_1 + V_2) \{S_1\}^2 + V_2 \{S_1 S_2\} + \frac{1}{3!} V_2 \{S_1\}^3 | \Psi_0 \rangle^i \]
\[ (2.58) \]

In the same way the doubles operator expression becomes:

\[ \langle \Psi_{ab}^s | S_2 | \Psi_0 \rangle^{i+1} = \frac{1}{\epsilon_a + \epsilon_b - \epsilon_r - \epsilon_s} \langle \Psi_{a}^r | V_2 + V_2 S_1 + (V_1 + V_2) S_2 + \]
\[ + \frac{1}{2!} V_2 \{S_1\}^2 + \frac{1}{3!} V_2 \{S_1 S_2\} + \frac{1}{2!} V_2 \{S_1\}^3 + \frac{1}{4!} V_2 \{S_1\}^4 | \Psi_0 \rangle^i \]
\[ (2.59) \]

Figuring out the ways to combine the operators to form the different orders of excitations is in no way a trivial matter, and is the greatest drawback of the CC method. But if this is done properly and the cluster expressions are implemented in a numerical routine very high accuracy results may be calculated fairly inexpensively. Such results may be viewed in comparison to other methods such as the FCI and Quantum Monte Carlo methods in paper I.
Chapter 3

Effective Potentials

The effective potential is the total interaction the electrons has with the surrounding material. Depending on the material properties, it may see some different potential structures. Here we investigate two of these, the quantum dot and the quantum ring, including some special cases of these to systems.

3.1 Quantum Dot

In chapter 3 several methods capable of handling energy and wave function calculations on our desired two dimensional semiconductor systems have been presented. We now change our focus to some specific systems and start with the quantum dot. Two of the most common models for quantum dots are the harmonic oscillator potential and the hard wall potential.

The circular two dimensional harmonic oscillator has been shown to be in good agreement for few electron quantum dots in [24], and has already been briefly discussed previously in this work. It is also the model used in paper I for the high precision results discussed there. The hard wall and harmonic models are both used in paper II, and are compared to each other under the influence of a tilted magnetic field. Here, the harmonic oscillator will be the main focus, and the hard wall will mostly be compared to the harmonic model. Also the anisotropic, elliptic, harmonic oscillator will be discussed briefly.
3.1.1 Harmonic Oscillator

The two dimensional harmonic oscillator potential and the one particle solutions have already been discussed in subsections 2.1.1 and 2.1.2. Depending on the number of electrons in the quantum dot we want to use different methods to calculate the many-body energies.

For two electrons it is fully viable to use the complete one-electron basis constructed with B-splines to solve the problem with untruncated FCI. Modern computers and algorithms have very little trouble diagonalizing matrices with thousands of elements, so there is no real requirement to truncate the basis used in FCI. Due to the completeness of the basis, and the nature of the FCI method, near exact results should be obtained with this method. MBPT is also usable for two electrons, and given that it is allowed to iterate until a self consistent solution is obtained, it should yield the same results as FCI. CCSD will be identical to MBPT for two particles and is therefor mainly just a more complicated method that achieves the same results.

We may want to truncate the basis to increase the speed of the calculations and still achieve adequate results. Size consistency should not be an issue as no separated double excitations may occur, so both MBPT and FCI can be truncated without loosing any physical properties. A way to truncate the basis is by the energy of the states. In MBPT this becomes obvious in eq. 2.51, where the energy difference between the states in the model space and states in the function space are in the denominator. For FCI this can be shown by diagonalizing a matrix with only two states, where one will see that the coupling strength between the states decreases as the energy difference increases. However, since the two methods give the same results we also know this has to be true.

For more electrons it is possible to use untruncated FCI or MBPT, but due to the scaling relation of calculation time and the number of particles, this becomes more and more resource demanding, and will eventually be impossible due to the time and memory it would require from the computer to run it. Truncating the basis is still an option, but as can be seen in paper I, the size of the basis is often more important than using an exact method with respect to the accuracy of the orbital energy. So the better option for more than four electrons is to change to another method, such as the CCSD. In paper I, results for CCSD with as many as 12 electrons have been presented with good accuracy, compared to the FCI and Quantum Monte Carlo. In table 3.1 an outtake from the article can be seen, showing the comparison between the CCSD routine and previously published FCI results.

Some basis truncation will most often be needed or at least useful to speed up the calculations and it has already been declared that the energy of the one-particle states
### Table 3.1: Comparison between the Coupled Cluster Singles and Doubles method and Full Configuration Interaction according to Kvaal [25–27] and Rontani [28]. The basis is in all three cases defined by the one-electron harmonic oscillator Hamiltonian and is truncated after a specific number of major oscillator shells \( R = 2n + |m_l| \). Energies are given in units of \( \hbar \omega \) and the number of confined electrons is 2-6 and 8.

| \(|2S \ M_L\rangle\) | \(h\omega\) (meV) | Basis set | CCSD | FCI |
|-----------------|-----------------|----------|------|------|
|                 |                 | This work | Kvaal | Rontani et al. |
| N=2 | | | | |
| | (00) | 11.85720 | R=7 | 3.009234 | 3.009236 |
| | | 2.964301 | R=7 | 3.729323 | 3.729324 |
| | | 0.3293668 | R=5 | 5.784651 | 5.7850 |
| | | 0.1852688 | R=7 | 6.618089 | 6.6185 |
| N=3 | | | | |
| | (11) | 11.85720 | R=10 | 6.36773 | 6.365615 |
| | | 2.964301 | R=7 | 8.17635 | 8.166708 |
| N=4 | | | | |
| | (20) | 2.964301 | R=7 | 13.635 | 13.626 |
| N=5 | | | | |
| | (11) | 2.964301 | R=7 | 20.3467 | 20.33 |
| N=6 | | | | |
| | (00) | 2.964301 | R=5 | 28.0161 | 28.0330 |
| | | R=7 | | 27.9751 | 27.98 |
| | | R=15 | | 27.9390 | |
| N=8 | | | | |
| | (20) | 2.964301 | R=5 | 47.13801 | 47.14 |
| | | R=15 | | 46.67960 | |

is a natural method of doing this. The one electron energies for the Cartesian and polar solutions: \( \epsilon_{n_x,n_y} = (n_x + n_y + 1)\hbar \omega \) and \( \epsilon_{nm_l} = (2n + |m_l| + 1)\hbar \omega \), will yield identical results and degeneracies, so cutting at the same energy using the different methods will result in the same basis truncation. The polar one-electron energies can be seen plotted in figure 3.1. By observing the energy structure, we introduce a new compound quantum number \( R = 2n + |m_l| \). \( R \) scales with energy, so a truncation by \( R \) will ensure that all states of the energy \( E \leq (R+1)\hbar \omega \) will be included in the basis. The Cartesian energies may be mapped to the polar states and truncated in the same way with the same results.

More complex truncation methods can be devised and implemented to ensure that only states with important contributions are included, but will require some prior knowledge about the solution.

With \( R \) we have also found a possible shell-structure in the many-body energies. The idea behind a shell-structure, is inspired by the structure found in atoms. Assuming the non-interacting many-body energy is close to the final many-body energy with the ee-interactions included, one expects the addition energy to spike at 3, 7 and 13 electrons. The addition energy is the extra energy contribution a system requires to bind a new particle to it. These numbers come from figure 3.1 where each bar in the figure is capable of storing two electrons (one spin up and one spin down). So if the first two electrons are placed in the lowest energy states, the next electron to be added will need to be placed in a state of higher energy than the previous two. The same thing occurs again when the next two levels are filled, requiring the 7:th electron to have a higher energy.
Chapter 3. Effective Potentials

Figure 3.1: The one particle energies states of the quantum dot and their corresponding quantum numbers. In the x-axis the $m_l$ quantum number is increased and decreased, with the $n$ quantum number being constant in each marked "V", and the energy increases along the y-axis.

If the electron-electron interaction eventually starts to dominate over the basis energy structure, some changes to the structure may occur. However studies show that the three lowest shells (2, 6 and 12 electrons) indeed seem to follow what is expected from the one-electron basis, [29].

3.1.2 Elliptic Harmonic Oscillator

The elliptic harmonic oscillator (EHO) has the potential shape: $V(x, y) = \frac{1}{2} m^* \omega^2 (\delta x^2 + (1/\delta)y^2)$. Since the EHO lacks cylindrical symmetry but is still parabolic in both the x and y-dimensions, the Cartesian coordinates solution may be used after scaling the potential strength in the x and y direction. The effects of the dots ellipticity has been studied somewhat before, [30–32], and even small elliptic effects have been shown to alter the shell structure noticeably.

In paper II this is of importance since a tilted magnetic field is applied to a two electron dot. The tilted field in itself will have a quadratic term that acts as an elliptic harmonic potential in the $\phi$ direction as seen in section 2.1.4. In paper II, experimental results are compared to results from a CI routine for both hard wall and harmonic potentials. The hard walls ellipticity is added as an extra harmonic perturbation in one dimension, $\epsilon x^2$, to the the potential described in section 3.1.3.

Further studies of the EHO dot with a tilted magnetic field has led to some further understanding of the different parameters. As in paper II, the energy splitting between the lowest lying singlet and triplet states are investigated. As the magnetic field is increased, these two states will eventually cross and the triplet state will become the
ground state. Figures 3.2, 3.3 and 3.4 show the experimental data from [5] and the results from CI calculations with different sets of parameters.

In figure 3.2 we see the effects of the dot parameters, i.e. the oscillator strength and ellipticity. In the left figure the oscillator strengths is varied with the result of translating the curve, increasing the splitting with higher oscillator strengths. This increase in splitting is however only valid for sufficiently large oscillator strengths, eventually non-linear energy contribution terms may start to dominate changing this behavior. The other figure shows the effect of the ellipticity, the energy splitting with no magnetic field is decreased with a higher degree of ellipticity, while the splitting at higher field strengths remains the same. The result of this is a small plateau at low magnetic fields, that is wider for more elliptic dots.

Figure 3.3 displays the effect the inclination angle has. In the left figure the azimuthal angle is perpendicular to the ellipticity, $\phi = 90^\circ$, and in the right figure this angle is $45^\circ$. The two angular parameters are naturally of no importance at zero magnetic field and will determine the slope of the curve for higher fields. A large inclination angle will reduce the magnetic fields z-component, thereby also reducing most of the fields effect on the energy, flattening the curve. This effect is seen in both figures, where the slope is flatter in the $65^\circ$ case than for $50^\circ$.

The last figure, 3.4, shows the effect of the azimuthal angle, i.e. the difference in orientation between the magnetic field and the ellipticity of the dot. The left graph shows an inclination angle of $50^\circ$ and the right graph $65^\circ$. Once again the effect of the angle grows in importance with the strength of the magnetic field, by changing the slope of the curve. This effect is more prominent for larger inclination angles, and once again the reason is the importance of the B-field z-component. The components of the field not in the z-direction make the magnetic field interaction elliptical, and this effect is competing against the elliptic form of the dot. Depending on the difference in orientation the magnetic field may either enhance the elliptical form, or weaken it. With a strong field, this effect is of less importance, making the curve in the graphs less sensitive to the angle.

The experimental data has an inclination angle of $\theta = 68^\circ \pm 5^\circ$ with an unknown azimuthal orientation and ellipticity. In paper II, good agreement was not found for the harmonic oscillator dot with no azimuthal angle. However with a new implementation we now have the possibility of investigating the different parameters, including the azimuthal angle in more detail.
Figure 3.2: The Singlet-Triplet energy splitting for an elliptic quantum dot with a tilted magnetic field. In the left, figure the strength of the confining potential has been varied between $\omega = 0.25 \text{ a.u.}$ and $0.26 \text{ a.u.}$. The figure to the right has its degree of ellipticity changed between $\delta = 1.2$ and $1.3$.

Figure 3.3: The Singlet-Triplet energy splitting for an elliptic quantum dot with a tilted magnetic field. In the left, figure the inclination angle of the magnetic field has been varied between $\theta = 50^\circ$, $60^\circ$ and $65^\circ$ for an azimuthal angle of $\phi = 90^\circ$. The figure to the right has its inclination angle changed between $\theta = 50^\circ$ and $65^\circ$ for an azimuthal angle of $\phi = 45^\circ$.

Figure 3.4: The Singlet-Triplet energy splitting for an elliptic quantum dot with a tilted magnetic field. In the left, figure the azimuthal angle of the magnetic field has been varied between $\phi = 0^\circ$, $45^\circ$ and $90^\circ$ for an inclination of $\theta = 50^\circ$. The figure to the right has its azimuthal angle changed between $\phi = 45^\circ$ and $90^\circ$ for an inclination of $\theta = 65^\circ$. 

Chapter 3. Effective Potentials
Chapter 3. Effective Potentials

3.1.3 Hard Wall

The results in paper II indicate that there may be a significant difference in using a hard wall (HW) or harmonic (HO) model to describe some QD systems. Due to this result the hard wall dot model will be discussed shortly.

The circular hard wall is written:

\[
V(r) = \begin{cases} 
0 & ; \quad r < r_0 \\
\infty & ; \quad r \geq r_0 
\end{cases}
\] (3.1)

An alternative to this is to use an anharmonic potential of the form:

\[
V(r) = \left(\frac{r}{r_0}\right)^{2n},
\] (3.2)

where \(n\) is a number larger than 1. In the limit of \(n \to \infty\), this will be identical to the potential described above, but will be sufficiently "hard" for lower \(n\)s. This is a more useful form when using a Cartesian basis where an ellipticity may be added as:

\[
V(x, y) = \frac{(\delta x^2 + 1/\delta y^2)^n}{r_0^{2n}},
\] (3.3)

The HW potential has analytical one-particle solutions, but it can also be solved using B-splines. The wave functions and energies are similar to the ones found solving the radial 2D harmonic oscillator potential. The main difference is the radial distribution. Due to the infinite walls in the circular HW potential the electrons wave functions will be strictly constrained within the limit of \(r_0\). In the HO case on the other hand, no such limitations exist, and high energy states may have their wave functions spread out over a much larger area. This stronger confinement on the hard wall wave functions will increase the effect of the electron-electron interaction strength. As this interaction is controlled by the factor \(\frac{1}{|r_1 - r_2|}\) in the denominator, the proximity of the states will be very important. As seen in paper II, there is some difference in the singlet-triplet energy splitting between the HW and HO models.
Chapter 3. Effective Potentials

3.2 Quantum Ring

The Quantum Ring (QR) can just as the quantum dot, be modeled in several ways. Using a harmonic oscillator form, one can write it in polar coordinates as: \( V(r) = \frac{1}{2} m^* \hbar \omega^2 (r - r_0)^2 \). It then simply takes the shape of a radially displaced harmonic oscillator rotated around the z-axis. The limit of the QR, when \( r_0 \to \infty \), will be the infinite one-dimensional quantum wire. The solutions to this is known, and the wave functions will be plane waves in the \( \phi \)-dimension and harmonic oscillator solutions in the \( r \)-dimension. Given this, we expect our one-particle ring solutions with the same radial, \( n \)-quantum number, to become more and more degenerate when \( r_0 \) is increased. Using the same type of illustration as in section 3.1.1, figure 3.5 visualizes this.

The energy of the \( m_l \) states decrease, resulting in the filling of states with higher angular momenta before the states with a different radial distribution. This will result in an increased level of degeneracy in the many-body states, which is a potential problem when using our perturbative methods since the energy difference appears in the denominator. To counteract this, an extended model space needs to be used, including all degenerate and nearly degenerate interacting states in the model space. Special measures need to be taken when using an extended model space, the details of which will not be included in this work.
3.2.1 Concentric Rings

Recently more complex ring-like structures have been experimentally created, such as the concentric rings by Mano, [8]. Concentric rings are several QR:s that share the same center. The rings created by Mano are Double Concentric Quantum Rings (DCQR), and have been modeled as two bell-curves rotated around the z-dimension in other theoretical studies of the system, [33]. Using such a model, the potential will be:

\[
V(r) = V_i \exp \left[ -\left( \frac{r - R_i}{W_i} \right)^2 \right] + V_o \exp \left[ -\left( \frac{r - R_o}{W_o} \right)^2 \right],
\]

(3.4)

where \(V_i, R_i, W_i\) and \(V_o, R_o, W_o\) are the potential depth, ring radius and ring width of the inner and outer rings. These parameters have been determined for the experimental system, but can for the sake of modeling be set freely. Figure 3.6 shows an illustration of such concentric ring potential.

Filling the rings with electrons is a complicated process. Whether the outer or inner ring is the favorable, or if the electron wave function will be distributed in both rings is dependent on the ring parameters and the number of electrons. The outer ring distributes the electrons over a larger area, reducing the importance of the electron-electron interaction, but angular momentum is higher. While the smaller ring has the opposite properties. So every electron added must be distributed favorable between the rings to minimize the energy. The high variability of the system can allow the shell structure of the electrons to be engineered in various ways as well as creating highly correlated few
electron states, with a potential of being used when constructing quantum computing qubits. But as in the case of the single QR this implies degeneracy or near degeneracy of several states, that will require the use of an extended model space when perturbation theory is used.
Chapter 4

Outlook

4.1 Outlook

Some work on the elliptical two electron quantum dot remains, the experimental data still purposes a larger angle than found when using the harmonic oscillator, and a larger radius for the hard wall case. New results are pointing in the right direction and some further fitting of the parameters will hopefully be able to give better agreement with the experiment. After confirming that theory and experimental results match, a scheme for determining the oscillator ellipticity for an experimental dot will be worked on. Given the different results in different azimuthal angles, one should be able to determine in what direction and by how much a dot is elliptic by applying a rotating magnetic field to it.

The rings and concentric rings have a good one-electron basis developed, and solving the many-body problem for two electrons is possible with existing code. To go beyond this CCSD with an extended model space needs to be implemented. With a many body solution there are many interesting properties to be investigated; shell-structure, coherent states and excited state lifetimes to name a few. Thanks to the methods ability to give the many-body energies and wave functions with a high accuracy, these properties can all be determined and compared to experimental data for validation.
I would like to start of by thanking the everyone at the atomic physics division for the nice working environment and all the good fredagsfika.

Special thanks go to my co-workers Marcus and Tor for our joint effort in learning many-body physics and Fortran programing, as well as the fun game/beer/sausage-evenings. Also my predecessor Erik Waltersson deserves some extra thanks for laying the groundwork for what i continued on.

And lots of thanks to my supervisor Eva for teaching us all the physics and Fortran skills needed to get any of this work done and the great opportunity to become acquainted to the entire ”Nordforsk group”.

Thanks to Esa Räsänen and his group to for all the nano-knowledge and the many great visits to Finland. Also big thanks to Jan-Petter Hansen and the Bergen group for the collaboration on paper 2 and the great time at the Jukola relay.

Lots of thanks to my family and friends for everything. And finally $\infty$-thanks to Cecilia (+1) for all the support and love needed and supplied, always!
Bibliography


