Electron Localization and Spin Polarization in a Quantum Circle

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Localization and magnetic properties of electrons in a thin, cyclic quasi one-dimensional GaAs wire with a central potential barrier were studied using the Hartree-Fock and LSDA (Local Spin Density Approximation, exchange only) and compared to more time consuming Quantum Monte-Carlo calculations. Within LSDA, evidence of true localization was found as well as evidence for the existence of both ferromagnetic as well as anti-ferromagnetic states. Also signs of two-dimensional spin localization was found, without associated localized electrons.

Spin polarization, electron localization
To my Mother and Father
Abstract

Localization and magnetic properties of electrons in a thin, cyclic quasi one-dimensional GaAs wire with a central potential barrier were studied using the Hartree-Fock and LSDA (Local Spin Density Approximation, exchange only) and compared to more time consuming Quantum Monte-Carlo calculations. Within LSDA, evidence of true localization was found as well as evidence for the existence of both ferromagnetic as well as anti-ferromagnetic states. Also signs of two-dimensional spin localization was found, without associated localized electrons.
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Chapter 1

Introduction

In recent time low-dimensional semiconductor systems have gained an increased attention and developed into an important part of the nanotechnology as well as spintronics. By low-dimensional one normally refers to two-dimensional, quasi one-dimensional or even true one-dimensional systems with only one degree of freedom, which are often known as quantum well, wires or point contacts. The fabrication of voltage controlled electron density structures \[1\] allows properties such as conductance and to some degree localization to be experimentally investigated. Although experiments are the source, or at least confirmation, of true knowledge it is difficult to investigate spin-polarization and electron-localization properties. This would be of importance if the theory were to be used in quantum computing or spintronics since both utilize spin properties rather than charge properties.

In order to utilize spin properties, localized electrons would offer completely new possibilities over an ensemble-average approach. Recent papers on experiments \[2\] and on simulations \[3\] indeed claim to have observed spatial ordering of otherwise free electrons, commonly referred to as a Wigner crystal. A number of questions still remain unanswered though:

1. Are the observed electron density peaks individual, spatially ordered electrons or a collective phenomena?

2. If the electrons turn out to be localized, are the states then truly antiferromagnetic in all situations considered?

In experiments only the total electron density can be observed. In simulations it would be possible, at least theoretically, to study individual orbitals thus determine whether the ordering truly is Wigner crystallization or a collective behaviour. This would in turn also provide an answer to the question about magnetic properties as well as answering whether the observed density peaks in experiments and other simulations correspond to localized electrons.

It is the aim of this diploma work to analyze the different situations on an orbit-spin density level in order to find answers to the above posed questions. In
the process other interesting features such as two-dimensional Wigner crystals, multiple subband localization etc also will be considered as they do or do not appear. Figure 1.1 provides an overview over the project and some of its key elements.
Chapter 2

The quasi one-dimensional system

This diploma work considers electrons in a narrow channel residing on the surface of a cylinder. A related system is studied in [3] using Quantum Monte Carlo calculations and hence a comparison between findings is possible. The system typically has a circumference of 1.57\textmu m and in theory extends infinitely in the $y$ direction. For practical reasons the system is limited to about 80 nm in the $y$ direction, which neglects only about 8 ppm of the orbital density (see Appendix A). Because of the huge difference in scale between extension in $x$ and $y$, for lower chemical potentials all electrons are found in the first subband, thus in practice the system possesses one-dimensional properties, hence the name quasi one-dimensional. The whole system is thought to exist in a GaAs environment, and for this reason the effective mass of the electron, $m^* \approx 0.067m_e$ is used rather than the free electron mass. For practical reasons the system can easily be regarded as a two-dimensional box with cyclic boundary condition in one dimension, instead of the cylindrical one. The actual size of the simulated system will be changed if needed to incorporate more than one subband.

$$x = R \cdot \theta$$

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{system}
\caption{The system described as a cyclic two-dimensional box}
\end{figure}

Furthermore, the electrons are confined in $y$-direction by a harmonic potential which depend on the parameter $\omega$ to define the width of the wire, see Fig. 2.2(a) and also experience a potential barrier $f(\theta) = \tanh [s(\theta + \theta_0)] - \tanh [s(\theta - \theta_0)]$
The quasi one-dimensional system

which depends on the steepness parameter, $s$, see Fig. 2.2(b).

(a) The harmonic confinement potential and its dependence on the harmonic parameter, $\omega$

(b) The potential barrier and its dependence on the steepness parameter, $s$

Figure 2.2. Population in the barrier for a 3$\mu$m wire

Using the effective Hartree units, with a length scale of $a_0^* = \hbar^2/m^*e^2 \approx 9.8$nm and an energy unit $H^* = e^2/ea_0^* \approx 11.9$meV for GaAs the time independent Schrödinger equation for one orbital can be written:

$$-\frac{1}{2}\nabla^2\Psi_k + \frac{1}{2}\omega^2 y^2\Psi_k + V_g \cdot f(x)\Psi_k + V(\rho)\Psi_k = E\Psi_k$$  \hspace{1cm} (2.1)

$$\Psi_k(x + 2\pi R) = \Psi_k(x)$$  \hspace{1cm} (2.2)

$$\frac{\partial\Psi_k}{\partial x} \bigg|_{x+2\pi R} = \frac{\partial\Psi_k}{\partial x} \bigg|_x$$  \hspace{1cm} (2.3)

where

$$f(x) = \tanh [s(x/R + \theta_0)] - \tanh [s(x/R - \theta_0)]$$  \hspace{1cm} (2.4)

and $x = R\theta$ with the accompanying steepness parameter, $s$, introduced above. $V(\rho)$ is the very important potential arising from electron-electron interaction, here depending on the charge density $\rho$. $\Psi_k$ is real and in the absence of interaction between electrons the solutions will be even or odd. This will also be considered in Chapter 4.
2.1 Analytical solutions

Equation (2.1) is only numerically solvable, however, for simplified systems analytical solutions can be found. In this diploma work, the analytical solutions are primarily used to test the numerical solver. They also serve in identifying critical parameters without simulations. Although the considered system can be described as a many-body problem, no known analytical solutions exist and hence a general restriction for all analytical solutions are found without any kind of interaction between the electrons, i.e. $V(\rho) = 0, \forall \mathbf{x}$.

No gate potential

A first solution is found by letting $V_g = 0$ which gives the equation

$$\frac{1}{2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi_k + \frac{1}{2} \omega^2 y^2 \Psi_k = E \Psi_k$$

(2.5)

Separating the variables, i.e. $\Psi = X \cdot Y$ the equation is transformed into

$$-\frac{1}{2} \frac{d^2 X}{dx^2} = E_x X$$

(2.6)

$$-\frac{1}{2} \frac{d^2 Y}{dy^2} + \frac{1}{2} \omega^2 y^2 Y = E_y Y$$

(2.7)

which both have known solutions. One quickly obtains $E_y = \omega (n_y + \frac{1}{2})$ and $E_x = \frac{n_x^2}{R^2}$. In this system $R \approx 0.25 \mu m \approx 25.51 a_0^*$ and so $E_x = \frac{n_x^2}{2.26 a_0^*} \cdot H^* \approx n_x^2 \cdot 9.14 \mu eV$ whereas $E_y = 0.6 \cdot (n_y + 0.5) \cdot H^* \approx 3.6 \text{ meV} + 7.1 \cdot n_y \text{ meV}$. The energy from the harmonic potential outweights the sinusoidal energy by a factor roughly 777 which means there will be bands populated with about $\sqrt{777} \approx 28$ electrons each. For a small number of electrons, the huge difference in the scale between $x$ and $y$ causes all electrons to exist only in the first state in $y$ making the system practically quasi one dimensional.

To test the non-interacting solver, the first energy level for one electron was calculated to $E_c \approx 3.62 \text{ meV}$ which seems to agree very well with the theoretical $E_t \approx 3.6 \text{ meV}$.

Simplified gate potential

Since the set of equations (2.1) - (2.3) with the gate potential described by eq. (2.4) fail to have a known analytical solution a simple potential step is studied instead, which is defined by

$$f'(\theta) = \begin{cases} 
2V_0 & |\theta| < \theta_0 \\
0 & \text{otherwise}
\end{cases}$$

(2.8)

on the interval $-\pi \leq \theta < \pi$ and repeated with the periodicity of $2\pi$. The solution

\footnote{See Appendix \ref{appendixA} for details}
for $Y$ remains the same, but the Schrödinger equation for $X$ is split into a system of two equations:

$$-\frac{\hbar^2}{2m^* R^2} \frac{d^2}{d\theta^2} X + 2V_g X = E X \text{ for } |\theta| < \theta_0 \quad (2.9)$$

$$-\frac{\hbar^2}{2m^* R^2} \frac{d^2}{d\theta^2} X = E X \text{ otherwise} \quad (2.10)$$

Letting $b_0^* = \hbar^2/2R^2m^*, \epsilon = E/b_0^*$ and $\beta = V_g/b_0^*$, eq. 2.10 has the solution

$$X(\theta) = A \sin \sqrt{\epsilon} \theta + B \cos \sqrt{\epsilon} \theta \quad (2.11)$$

For eq. 2.9 two cases need to be considered: $\beta < \epsilon$ and $\beta > \epsilon$. The former has the solution

$$X(\theta) = C \sin \sqrt{\epsilon - \beta} \theta + D \cos \sqrt{\epsilon - \beta} \theta \quad (2.12)$$

setting $\kappa = \sqrt{\epsilon}, \omega = \sqrt{\epsilon - \beta}$ differentiating and demanding continuity at $\theta = \theta_0$ the following is obtained

$$A \sin \kappa \theta_0 + B \cos \kappa \theta_0 = C \sin \omega \theta_0 + D \cos \omega \theta_0 \quad (2.13)$$

$$\kappa A \cos \kappa \theta_0 - \kappa B \sin \kappa \theta_0 = \omega C \cos \omega \theta_0 - \omega D \sin \omega \theta_0 \quad (2.14)$$

Treated as a linear vector space, letting $\mathbf{x} = (A, B)^T$, $\mathbf{y} = (C, D)^T$, $\mathbf{z} = (E, F)^T$

$$\mathbf{R}_\varphi = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \quad \mathbf{S}_\alpha = \begin{pmatrix} \alpha & 0 \\ 0 & 1 \end{pmatrix}$$

the above equation can be written

$$\mathbf{S}_\alpha \mathbf{R}_{\kappa \theta_0} \mathbf{x} = \mathbf{S}_\alpha \mathbf{R}_{-\omega \theta_0} \mathbf{y} \iff \mathbf{y} = \mathbf{R}_{-\omega \theta_0} \mathbf{S}_\kappa/\omega \mathbf{R}_{\kappa \theta_0} \mathbf{x} \quad (2.15)$$

where $\mathbf{R}_\varphi$ is a counterclockwise rotation $\varphi$ and $\mathbf{S}_\alpha$ is a discriminating scaling. Applying the same conditioning at $\theta = -\theta_0$ leads to the same equation, but clockwise.

$$\mathbf{S}_\alpha \mathbf{R}_{-\kappa \theta_0} \mathbf{z} = \mathbf{S}_\alpha \mathbf{R}_{-\omega \theta_0} \mathbf{y} \iff \mathbf{y} = \mathbf{R}_{\omega \theta_0} \mathbf{S}_\kappa/\omega \mathbf{R}_{-\kappa \theta_0} \mathbf{z} \quad (2.16)$$
2.1 Analytical solutions

At $\theta = \pm \pi$ the wave function also must match so

$$ R_{\kappa \pi} x = R_{-\kappa \pi} z \iff z = R_{2\kappa \pi} x \quad (2.17) $$

$y$ and $z$ can now be excluded and the following equation for $x$ is obtained

$$ R_{-\omega \theta_0} S_{\kappa/\omega} R_{\kappa \theta_0} x = R_{\omega \theta_0} S_{\kappa/\omega} R_{\kappa (2\pi - \theta_0)} x \iff (S_{\kappa/\omega} R_{\kappa \theta_0} - R_{2\omega \theta_0} S_{\kappa/\omega} R_{\kappa (2\pi - \theta_0)}) x = 0 \quad (2.18) $$

which is an eigenvector problem with the known null eigenvalue. For this to have nontrivial solutions the determinant must vanish, i.e.

$$ \det Q = 0 \quad (2.20) $$

Figure 2.4. The determinant of the transfer matrix for $\theta_0 = 1.5, \beta = 8$

As can be seen in Fig. 2.4 the determinant vanishes more or less periodically. For high values of $\kappa$ the solutions should be similar to particle in a ring, i.e. without the barrier. For that case $E = \frac{n^2 h^2}{2 R^2 m^*} = n^2 h_0^2$ and $\kappa = n$ which means that $\det Q \to A \sin(2\kappa \pi + \varphi_0)$ for some constants $A$ and $\varphi_0$. The solutions of eq. 2.20 will give a set of possible values for $\kappa$ from which the energy can be retrieved. This can be used to test the numerical solver as will be done in Chapter 3.1. Having an expression for the available energies it is also possible to estimate the number of electrons in each subband. Calculations reveal that there are theoretically 51 electrons (for each spin) in the first subband having energy lower than the lowest second subband orbital.
The quasi one-dimensional system
Chapter 3

Simulation and computational techniques

Most of the equations do not have a known analytical solutions which means numerical methods have to be employed. The wave functions need to be expressed in a computer-manageable manner, i.e. in a suitable base. In this paper the spatial base is chosen, although it means the continuous functions have to be discretized. The first step is to use the finite difference approximation. A set of spatial sample points is introduced that can be parameterized by \((\Delta x, \Delta y)\). It is then possible to express the partial derivatives by the following central approximation \[4\]

\[
\frac{\partial^2 \Psi}{\partial x^2} \approx \frac{\Psi(x + \Delta x, y) - 2\Psi(x, y) + \Psi(x - \Delta x, y)}{\Delta x^2} \quad (3.1)
\]

\[
\frac{\partial^2 \Psi}{\partial y^2} \approx \frac{\Psi(x, y + \Delta y) - 2\Psi(x, y) + \Psi(x, y - \Delta y)}{\Delta y^2} \quad (3.2)
\]

The sample points are enumerated as \((x_i, y_j)\) \(\equiv (i \cdot \Delta x, j \cdot \Delta y)\), \(i, j \in \mathbb{N}\) which immediately gives the following equivalent expressions

\[
\Psi_{xx}(x_i, y_j) \approx \frac{\Psi(x_{i+1}, y_j) - 2\Psi(x_i, y_j) + \Psi(x_{i-1}, y_j)}{\Delta x^2} \quad (3.3)
\]

\[
\Psi_{yy}(x_i, y_j) \approx \frac{\Psi(x_i, y_{j+1}) - 2\Psi(x_i, y_j) + \Psi(x_i, y_{j-1})}{\Delta y^2} \quad (3.4)
\]

Analogously a discrete set of function sample points are defined as \(\Psi_{ij} \equiv \Psi(x_i, y_j)\).

### 3.1 One particle in a rectangular box

Considering a \(L_x \times L_y\) infinitely deep well the Schrödinger equation,

\[
\frac{-\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} \right) = \epsilon \Psi(x, y) \quad (3.5)
\]

\[
\Psi(x, y) \equiv 0 \text{ outside the box} \quad (3.6)
\]
\[ \Psi_{i+1,j} + \Psi_{i,j+1} - 4\Psi_{ij} + \Psi_{i-1,j} + \Psi_{i,j-1} = \lambda \Psi_{ij} \quad (3.7) \]

\[ \lambda = -\frac{2m}{\hbar^2} \Delta^2 \epsilon \quad (3.8) \]

where \( \Delta_x = \Delta_y = \Delta \) Define \( L_x = N_x \cdot \Delta, L_y = N_y \cdot \Delta \). A discrete state vector is now introduced as \( \Psi = (\Psi_{00}, \Psi_{10}, \ldots, \Psi_{N_x 0}, \Psi_{01}, \Psi_{11}, \ldots, \Psi_{N_x N_y})^T \) A matrix representation of the Hamiltonian is now formed as a band matrix having the fundamental line \((1, 0_{N_x-1}, 1, 4, 1, 0_{N_y-1}, 1)\) which gives the following matrix

\[
\hat{H} = \begin{pmatrix}
1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 & \cdots & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1
\end{pmatrix} \quad (3.9)
\]

This matrix has the wrong dimension for an eigenvalue problem. Because of the simply boundary condition all function ghost points are set to 0 and a quadratic form is obtained simply by truncating, shown by the dashed lines above. However, one has to be careful and note that the box is actually larger than it appears. From the infinite potential it is known that the wave function vanishes at the boundary. However the boundary is not explicitly represented by the matrix, making the box one step larger in each direction. From this one obtains the following equation for \( \Delta x \):

\[
\frac{L_x - 2\Delta x}{N_x - 1} = \Delta x \iff \Delta x = \frac{L_x}{N_x - 1} \quad (3.10)
\]

For a grid of \( 3 \times 3 \) points the Hamiltonian has the following matrix

\[
\hat{H} = \begin{pmatrix}
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
-1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{pmatrix} \quad (3.11)
\]

from which its eigenvectors can be calculated. Comparing to [5] the dimensions of the box is set to \( L_x = L_y = 8 \mu m \). If the number of grid points is increased a higher accuracy is achieved and for a \( 20 \times 20 \) the second state would look like depicted in Fig. 3.1.

The numerical solutions of the one-particle problem can also be tested against the analytical ones. The orbital energies was numerically calculated for electrons in an infinitely steep potential barrier, as for the simplified gate potential in Chapter
3.1 One particle in a rectangular box

Figure 3.1. Plot of the first excited state, i.e. $n_x + n_y = 3$.

Comparing to the ones predicted by the analytical solutions, as Fig. 3.2 shows, it is found that the results agree very well, which serves as a nice confirmation that the numerical solver works. In fact, the accuracy is so high that one can safely draw the conclusion that any errors must originate from the used model of the physical system or the iterative algorithm in which the solver is used (to be discussed below), but not the solver itself.
Figure 3.2. Comparison between energies from the analytical and numerical solutions for a sharp barrier.
3.2 Multiple particles in a box

The complexity increases as more than one electrons are included in the model. First of all a formal treatment of a many-body problem is required. In this diploma work a method similar to Hartree-Fock is chosen, with a local exchange energy taken from the LSDA. The general matrix formulation of the many-body problem looks like

\[ H = H_0 + V(\rho) + \mu(x, \sigma) \]  

(3.12)

where \( V(\rho) \) is the diagonal matrix describing the interaction between electrons and \( \mu \) is an additional term necessary to break symmetries discussed further in Chapter 3.3. This cannot be solved in the same manner as the single particle problem since the Hamiltonian depends on the density which is supposed to be calculated. To come around this an iterative approach is adapted. Starting with an initial density the first orbitals are calculated. Specifying what orbitals are to be populated the charge density can be calculated. This is then used to form the second Hamiltonian and so on until so-called self-consistency is reached. This is the method used for most of the calculations in this paper.

3.3 Breaking the symmetries

Using the Hartree-Fock method proper orbitals need to be calculated and populated. However if the lowest orbitals is simply chosen dogmatically there is a high probability that the found solution will be unstable. This originates from the fact that the solver will perform exactly the same calculations for both spin-up and spin-down. This is not physically stable.

Several of methods were tested to break this spin symmetry and other hidden symmetries. Following are short descriptions of some of them.

**Zeeman term**

One very widely used method is to add a small general potential difference between the different spins. This can be considered to originate from a magnetic field. This has the consequence that a certain spin orientation is preferred to the other thus breaking the symmetry. This method was tested but not used.

**Spatial selection**

This method aims to break the spatial symmetry by introducing a small potential depending on both spin and spatial coordinates. The advantage was that if the same magnitude of potential is used for both spin up and spin down the spin populations are not explicitly modified. One problem, however, is that more subtle symmetries may go totally unnoticed. This was the strongest argument for not using this method.

**Random potential**
One way of addressing the problem with hidden symmetries is to introduce a small pseudo-random potential that varies from iteration to iteration. This has the obvious advantage of not introducing a preferred direction, neither in spin nor space. The disadvantage is that calculations have to be repeated in order to ensure that the results are stable and not found by chance. Mathematically the random potential should have the form $V_{\text{random}} = X(x) \cdot a_n$ where $X(x)$ is a stochastic variable, $n$ is a iteration counter and $a_n \rightarrow 0$ whenever $n \rightarrow \infty$. This method was used throughout all the coming calculations with the special case of $(a_n) = (1, 0, 0, \ldots)$.

Gradually introduced potential

In order to find special solutions it might be necessary to introduce part of the external potential gradually. Otherwise the solver may fail to find interesting local energy minima. This was tested but found unnecessary.

Inertia of solutions

In each iteration new orbitals are calculated and populated. The new electron density can then be calculated from the new orbitals. However, this might lock the solver in an astable flip-flop mode, pending between two states. One way to come around this is to choose a convex combination of the new and old density, such that

$$\rho^{n+1} = (1 - \alpha) \rho^n + \alpha \sum_{N} \Psi_k^\dagger \Psi_k$$

where $\alpha$ is the so-called mixing parameter. This way the densities should converge to a stable state. There may, however, be a risk that a combination of two states is found instead. This technique turned out to be indispensable in order to ensure convergence. Without it, the algorithm almost always failed to find any solution at all.

Fixed total spin polarization

Normally the number of electrons having spin up and spin down is determined in by the solver by choosing the lowest energies. However, since the solutions if found by iteration, this number may change from iteration to iteration. In some cases this causes the solver to find a hybrid solution. A way around this is to fixate the number of electrons at start. This requires that more than one configuration have to be tried in order to find a global minimum. For some initial attempts this method was used, but since it is physically unrealistic it was abandoned as the final results were to be calculated.

3.4 A computational scheme

With the considerations from Chapter 3.3 in mind it is at this stage possible to reproduce a scheme for computing the orbitals. This scheme will later be implemented in all simulations with or without minor modifications.
3.5 Implementation

1. Let $\rho^\uparrow(x_i) = a \cdot X_i, \rho^\downarrow(x_i) = a \cdot Y_i$ where $X, Y \in U(0, 1)$ and $\langle \rho^\uparrow \rangle = \langle \rho^\downarrow \rangle = 1$
   Set the system energy to some dummy value such as $E = 1000$.

2. Numerically solve the orbital Schrödinger equation (2.1-2.3) and find $\Psi_k$ for all $k$ needed.

3. Assign the temporary $\rho'^\uparrow$ and $\rho'^\downarrow$ to reflect the new densities, i.e. $\rho'^\uparrow = \sum_{E_k < \mu} \Psi_k^\dagger \Psi_k$ if a fixed chemical potential is considered or $\rho'^\downarrow = \sum_{k < N} \Psi_k^\dagger \Psi_k$ if a fixed number of electron is considered, etc.

4. Construct the new density from $\rho = (1 - \alpha) \rho + \alpha \rho'$. In this paper a typical value of $\alpha$ would be $\alpha = 1\%$.

5. Assign a temporary new energy, $E' = \sum_k E_k$ and store the relative energy error, $\Delta E = \frac{|E - E'|}{E}$, somewhere. Let $E = E'$.

6. Investigate the latest $n$ relative energy errors. If they all fulfill $\Delta E_i < r$ for some $r$, then convergence is assumed and the calculations are completed. Otherwise, continue from step 2.

3.5 Implementation

Several of different implementations were tried as an attempt to achieve a high resolution at a short running time. Of course there is a trade-off between the two above mentioned parameters, but it turned out also to depend on a third parameter - programming time.

The first attempt was to use Octave/Matlab which made the programming part fast and easy. However, it soon was clear that the running time was high, and in addition, the working memory was not enough to describe the system with high resolution.

The second attempt was to use Lapack routines called from a C-program. Of course programming time was higher, but performance of the running program was greatly improved. The program could now handle much larger problems which it solved relatively quickly.

The third way was a parallelization of the C-program. For this, Scalapack was implemented to boost calculation speed. However, although the performance was improved, the complexity at the programming stage increased dramatically. Also contributing to the complexity was that although more memory was available it was distributed over several of processor. This increased level of complexity lead to abandoning parallel computing, at least in the experimental stage.

To summarize, the following table gives a qualitative measure of the different methods
A typical run-time was 5 h on an Intel® Pentium® 4, 3.40 GHz processor for the Lapack case, which refers to about 70 iterations and one set of parameters ($\mu, s, V_g$, etc).

The conclusion was that at an experimental stage, the Lapack method was preferred since a lot of changes were made at all time in the simulation program, which meant the total time spent actually increased by using ScaLapack.
Chapter 4

Recreating and expanding

4.1 The common model

In order to find common ground and comparable results described in [3] the system was simulated using the Thomas-Fermi approximation and local-spin density approximation. This gives a Hamiltonian described by Yakimenko, Bychkov and Berggren [6] (here in units of $H^*$):

$$\left( -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + U_c + U_H + U_x^\sigma \right) \Psi_k^\sigma = E_k \Psi_k^\sigma$$

(4.1)

where $U_c = \omega^2 y^2 / 2 + V_g \cdot f(x)$ is the confinement and barrier potential, $U_H$ is the Hartree potential given by (also in units of $H^*$ and as before $x = R\theta$)

$$U_H = \int \frac{n(r')dr'}{|r-r'|} = \int \frac{n(x',y')dx' dy'}{\sqrt{(y-y')^2 + 2R^2 (1 - \cos(\theta - \theta'))}}$$

(4.2)

and $U_x^\sigma = -4a_0^\sigma \cdot \sqrt{n^\sigma / \pi}$ is the exchange potential. The denominator in Eq. 4.2 is not the standard metric function but is calculated in Appendix C.

4.2 The populating mechanism

It is of great interest to acquire a greater understanding in by what means the electrons populate the barrier. The most studied observable is the barrier population function:

$$n_b^\theta (V_g) = \int_{|\sigma| < \theta_0} n_{\sigma}^{V_g, \theta_0}(x)dx$$

(4.3)

Using the model described in Chapter 4.1, the gate voltage was swept between $0.5H^*$ and $2H^*$ while the total number of electrons was kept constant at 31. As can be seen in Fig. 4.1, the number of electrons inside the barrier is always close to an integer one.
As can be observed in Fig. 4.1, the barrier is populated in a very distinct step-wise manner. This situation is, however, corresponds to controlling the number of electrons directly. An easier and perhaps more common way would be to fixate a chemical potential and consider the system to be in contact with an infinitely large
buffer. Hence the gate potential was swept at different fixed chemical potentials, the first one taken as the Fermi energy of the fixed number of electron system. As Fig. 4.2 shows, the barrier population function, $n_b$, is more stable. Thus indicates that it would also be physically stable. The distinct steps are related to a Coulomb blockade.

### 4.3 The dependence on chemical potential

The fact that a change in chemical potential only seems to translate $n_b$ suggests that there should exist a map $f(\Delta \mu) : n_b(V_g) \rightarrow n_b(V_g + g(\Delta \mu))$ where $g$ is some monotonic function. The exact form of $g$ was left for future studies but the existence of the map $f$ should in turn give rise to another form of discrete populating mechanism, i.e. for a fixed gate potential but with varying chemical potential. This can also be observed in Fig. 4.3 where the gate potential is kept fixed at $V_g = 0.8$ and the chemical potential is varied. As suspected, the barrier is once again populated in a discrete manner. For high chemical potentials, another interesting feature reveals itself, namely a kind of breakdown when the barrier is completely overrun.

**Figure 4.3.** Electron population in the barrier for different chemical potentials, all with $V_g = 0.8$
4.4 Barrier steepness

The barrier considered in Chapter 4.2 and Chapter 4.3 is very close to a classical finite box due to its distinct boundaries. A natural question that arises is what would happen if the barrier were more diffuse. Would the population still increase stepwise? It would probably mean the loss of electrons in integer numbers simply due to the lack a clearly defined border. However, could it also cause the electrons to populate the barrier more continuously?

In order to find an answer, the gate potential was kept constant at $V_g = 0.8$ and the chemical potential $\mu = 30.3$ meV while the steepness parameters, $s$, was swept. As revealed something occurs at approximately $s = 6$. For $s > 6$ the population still remains integer (binary, in this case), but for $s < 6$ there is a high degree of penetration into the barrier. This causes the barrier populating function to assume non-integer values.

![Figure 4.4](image)

**Figure 4.4.** Electron population in the barrier for different steepness parameters, all at $V$. Note especially the almost digital appearance for higher values of $s$.

This can also be observed in the density functions depicted in Fig. 4.5 which confirms that the surrounding electrons penetrate into the barrier for low values of $s$. What is, however, further interesting is that for higher steepnesses of the barrier boundary, there are oscillations outside the barrier, claimed to be Friedel oscillations in ???. These vanish for a smoother barrier. For really high steepnesses the density peaks at the border, similar to Gibbs phenomena, see for instance Fig. ?? If the gate potential is swept for different steepness parameters the population function, $n_b$ becomes less discrete for smaller values of $s$. As can be seen in Fig. ?? there is a greater degree of tunneling that gives rise to non-integer population numbers. For the case $s = 2$, $n_b$ decreases almost linearly on the interval $(0.88, 1.00)$. 


Figure 4.5. Different steepness parameters, \( s \)
Figure 4.6. Electron population in the barrier for different gate potentials and steepnesses.
4.5 Barrier length

A third form of (quasi) discrete transitions is found if the length of the barrier is swept, as Fig. 4.7 shows. Noticeable is also yet another phenomena, namely the non-integer fluctuation that occurs at each integer level. This is believed to be a form of tunneling resonance. Up to a certain degree tunneling can occur until it would be energetically more favourable to employ another number of electrons instead. This property is not yet fully investigated.

![Figure 4.7. Electron population in the barrier for different barrier lengths.](image)

4.6 Multiple subbands

One could ask what would happen when the chemical potential were to be increased. The second subband most certainly also would be populated, but what about the barrier population function? If simply increased the result would look like in Fig. 4.8. As can be seen, some degree of integer population remains, but otherwise there is little evidence of any stepwise increase in population.

If, however, only electrons from the second subband were to be considered, would they populate the barrier in the same manner as for the first subband, only at a different chemical potential? The answer is no, they will not, as can be seen in Fig. 4.9. Although some terraces seem to be present they show a more complex structure as the first subband electrons.

The reason for this difference is the extra first subband electrons, not explicitly represented in Fig. 4.9. They, also undergo a complex transition process. For each electron in the second subband there are also first subband candidates. This
One could still pose another question, however. Do the second subband electrons show any localization? The answer is yes, they do, but not as clear as for the first subband. As can be seen in Fig. 4.10 there is a spatial difference (black indicates spin-up and white spin-down). Without the colors clarifying, one could easily have mistaken the situation for two electrons sharing the same spatial density which is not the case. The reason for the decrease in localization is the contribution from the first subband electrons. The total number of electrons in this case is 138 (compared to typically 32 for two localized first subband electrons) and hence there will already be a barrier population as well as an increased potential from outside the barrier. This forces the second subband electrons to be located close together and even have overlapping wave functions.

Finally, one can find that the first subband can be filled with 39 electrons of each spin before the second subband becomes populated. This is comparable to the predicted 51 in Chapter 2.1. It should be noted that the analytical estimation was for a system without any electron-electron interaction, which explains the difference.
4.6 Multiple subbands

Figure 4.9. Electrons from the second subband in the barrier.

Figure 4.10. Electrons in the second subband showing some degree of localization. Black indicates a spin-up density surplus and white indicates a spin-down density surplus. Here $\mu = 112.6\text{meV}$.
4.7 A $3\mu$m wire

In a longer wire with the same potential barrier new phenomena emerge. For instance, a $3\mu$m long wire would have a populating function as shown in Fig. 4.11.

![Electron population in a barrier](image)

(a) Population in the barrier for a $3\mu$m wire

(b) Population in the barrier for a $3\mu$m wire

**Figure 4.11.** Population in the barrier for a $3\mu$m wire, high resolution of the chemical potential

At first glance (Fig. 4.11(a)) it would appear that electrons no longer populate the barrier one-by-one but rather two at a time. If increasing the resolution on the chemical potential (Fig. 4.11(b)) one discovers that there are in fact states with odd number of electrons, but these are rare compared to the even numbers. As a general rule, the barrier is populated in steps of two electrons.

There still is a degree of localized electrons but the increased pressure from the surrounding electrons forces the electrons inside the barrier to be closer to the middle and to each other as can be seen in Fig. 4.12.

Considering the second subband, one can see from Fig. 4.13 that the picture is more complex than for first subband, but possible simpler than for the shorter wire. In the long wire case there seems to be more clearly defined integer plateaus. As well as for the short wire case, there are second subband (compressed) localization with spin polarization.
Figure 4.12. Two electrons forced close together inside the barrier.

Figure 4.13. Second subband population in the barrier for a 3μm wire.
4.8 Two-dimensional lattice

Of great interest would be to find two-dimensional ordering of localized electrons. One might suspect that this could be done by lowering the confinement steepness ($\omega$) thus making the channel wider. The simulations, however, reveal a more complicated picture.

As can be seen in Fig. 4.14 there are indeed spin peaks coinciding with density peaks. However, if dissected, the individual orbitals reveal that there are no actual electron localization occurring. Instead, a new form of ordering is found, a spatial spin order.

![Figure 4.14](image)

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![Figure 4.15](image)

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**Figure 4.14.** Top-view of spin polarization peaks in two dimensions. White and black color indicates a surplus of spin-up and spin-down respectively. Here $\omega = 0.05, \mu = 28.5$ meV.

**Figure 4.15.** A wide wire without any barrier. As can be seen there are signs of spatial spin ordering. White indicates spin-up and black indicates spin-down. Here $\omega = 0.05, \mu = 15.5$ meV.
4.8 Two-dimensional lattice

If the barrier is removed the spatial spin localization still appears as can be seen in Fig. 4.15. It should still be noted that this is strictly a collective behaviour in the sense that the density peaks do not correspond to single electrons. Thereby this cannot be regarded as a Wigner crystal.
4.9 An attempt to use $\delta$-interaction

Although the approximation used in Chapter 4 produces reasonable results it is of interest to investigate alternative approximations. Lassl et al. [7] have shown promising results by replacing the traditional Coulomb force with a weighted Dirac distribution, $V(x, x') = \gamma \delta(x - x')$ where $\gamma \approx \frac{\hbar^2}{2m}$ is found to be reasonable. This was integrated into the Hartree-Fock model and tested in this paper. Taking a standard expression for the Hartree-Fock approximation [8] it follows

\[
H^{(1)}(1)\Psi_k + \sum_{j=1}^{N} \int \Psi_j^{\dagger}(2) H^{(2)}(1, 2) \Psi_k(1) \Psi_j(2) d(2)
- \sum_{j=1}^{N} \int \Psi_j^{\dagger}(2) H^{(2)}(1, 2) \Psi_j(1) \Psi_k(2) d(2) = E_k \Psi_k
\]  

(4.4)

Considering $\sigma \in \Sigma = \{\frac{1}{2}, -\frac{1}{2}\}$ to be the spin variable in spin space and letting $N_{\sigma}$ be then number of electrons having spin $\sigma$ one arrives at

\[
H_{\text{H}} = \sum_{\sigma \in \Sigma} \sum_{j=1}^{N_{\sigma}} \int \Psi_j^{\dagger}(x') \gamma \delta(x - x') \Psi_k(x) \Psi_j(x') dx' = \sum_{j=1}^{N_{1/2}} \gamma |\Psi_j(x)|^2 \Psi_k(x) + \sum_{j=1}^{N_{-1/2}} \gamma |\Psi_j(x)|^2 \Psi_k(x)
\]

(4.5)

\[
H_{\text{Xc}} = \sum_{j=1}^{N_{\sigma_k}} \int \Psi_j^{\dagger}(x') \gamma \delta(x - x') \Psi_j(x) \Psi_k(x') dx' = \sum_{j=1}^{N_{\sigma_k}} \gamma |\Psi_j(x)|^2 \Psi_k(x) = \gamma \rho_{\sigma_k}(x) \Psi_k(x)
\]

(4.6)

Now adding them as in the sum above

\[
H_{\text{H}} - H_{\text{Xc}} = \gamma \rho_{1/2}(x) \Psi_k(x) + \rho_{-1/2}(x) \Psi_k(x) - \gamma \rho_{\sigma_k}(x) \Psi_k(x) = \gamma \rho_{-\sigma_k}(x) \Psi_k(x)
\]

(4.7)

This means that the Hartree energy is cancelled from the exchange energy for parallel spins and unaffected by opposite spins leaving exactly the opposite-spin part. The external confinement potential is also included as before.

The special equation in this case would be

\[
\left(-\frac{\hbar^2}{2m} \nabla^2 + V(x) + \gamma \rho_{-\sigma_k}(x) \right) \Psi_k(x) = \epsilon_k \Psi_k(x)
\]

(4.8)

where $V$ is the sum of the confinement potential and the gate potential mentioned above.

The numerical results, however, do not even vaguely resemble the results produced by the Thomas-Fermi approximation. As can be seen in Fig. 140 besides the absence of any electrons inside the barrier, the electron density is importantly different from the Coulombic counterpart outside the barrier. This jagged pattern
4.9 An attempt to use $\delta$-interaction

Figure 4.16. The spin up density of the system using a $\delta$-interaction and $V_g = 0.75H^*$. Is thought to be the source of the inability to induce electrons to reside inside the barrier and arises from the fact that the Coulomb interaction is a true force acting over distance thus giving a smoother potential. This behaviour cannot be countered by increasing the $\gamma$-parameter. As can be seen in Fig. 4.17, there are really no electrons inside the barrier and the actual number arises from (pseudo-)noise and tunneling effects. It seems the different values are more noise from the pseudo-random potential than of any physical significance.

Figure 4.17. Electron density inside the barrier for different values of $\gamma$. Note the scale.

If the gate potential is swept over another interval it is clearly seen that the populating process starts at much lower gate potentials, roughly at $0.2H^*$. Also notable is that the population is not as distinct as for the Coulomb case. This
is believed to be a higher degree of tunneling arising from the lower potential. A final comment would be that the electrons do not seem to enter the barrier in a strict order. This suggests that there are other processes involved. The conclusion must hence be, that the $\delta$-interaction cannot be used to model the physics of this system adequately enough.

Figure 4.18. Electrons start populating the barrier with $\delta$-interaction at $0.2H^*$. 
Chapter 5

Results

Two questions were posed in Chapter 1:

1. Are there truly localized electrons?

2. Are the states in which the localized electrons appear ferromagnetic or antiferromagnetic?

After studying the different simulations presented in Chapter 4 it is now possible to give answers to the questions.

5.1 The localization

![Figure 5.1. A gate potential $V_g = 0.74H^*$](image)

Considering the standard wire (length 1.57μm, $\omega = 0.6$ and $s = 15$, a number of conclusions can be drawn. The case $V_g = 0.74$ with $\mu = 30.8$ meV results in a total of 30 electrons. A study of the total electron density shows two peaks inside
the barrier. As can be seen in Fig. 5.2, the orbital wave functions of the electrons having the highest energy do not extend outside the barrier. Furthermore, they only marginally overlap other and thus it is concluded that they represent localized electrons. In this sense, it is not a collective phenomena.

\[ n(x, y) \mu m^2 \]

\[ n(x, y) \mu m^2 \]

(a) The density of the highest spin-up orbital

(b) The density of the highest spin-down orbital

Figure 5.2. The highest spin-up and spin-down orbital densities for the case of \( V_g = 0.74H^* \)
5.1 The localization

(a) Potential without the localized electrons

(b) Experienced potential for a spin-up electron

(c) Experienced potential for a spin-down electron

Figure 5.3. The effective potential for electrons with respect to $x$ for the case of $V_0 = 0.74H^*$

Studying the effective potential gives a hint about the populating mechanism.
In Fig. 5.3(a), the potential for a spin-up electron arising from the localized electrons have been removed and a box structure presents itself.

The ground level of the box, however, is actually at a higher energy level than the surroundings. When instead examining Fig. 5.3(b), which shows the potential for a spin-up electron caused by all electrons, a lowering is observed exactly where the localized electron resides. This lowering definitely arises from the exchange term of the Hamiltonian, $U^\sigma_\sigma$, (see Eq. 4.1). When distributing the last electron of each spin, it seems that although the surroundings may appear to have a lower energy, the extra electron would cause a higher total energy for the whole system, if distributed outside the barrier. Thus the only possible solution is to localize it inside the barrier. In this sense the population mechanism is clearly a collective phenomena. At the same time, a peak is observed next to the locally lowered potential. This corresponds to the contribution from the spin-down electron also present in the barrier. If the effective potential were to be considered with respect to a spin-down electron, the picture would look as Fig. 5.3(c), which shows a lowering at the location of the spin-down electron and a peak at the location of the spin-up electron.
The picture, however, does not need to be as simple. If studying another case, for \( V_g = 0.73 \), again two electrons are located inside the barrier. However, in this case, they have the same spin, spin-up. As can be seen in Fig. 5.5, they occupy orbitals similar to the first and second orbital of a two dimensional box. In this case the two peaks observed in Fig. 5.4 are clearly not two localized electrons, but the interference pattern from two electrons having the same spin, closely packed in conventional space. This is a counterexample showing that all peaks need not necessarily be localized electrons.

It should also be noted that these calculations were done using the LSDA (exchange only), and the picture may change if classical Hartree-Fock were fully implemented.
(a) The second highest spin-up orbital

(b) The highest spin-up orbital

Figure 5.5. The two occupied spin-up orbitals in the barrier region for the case of $V_g = 0.73H_*$.
5.2 Magnetic properties

The question about magnetic properties can also be answered by studying the examples discussed in Chapter 5.1. Both are cases with two electrons confined to the barrier. If only the two highest orbitals are considered for \( V_g = 0.73 H^* \) they show an anti-ferromagnetic state as can be seen in Fig. 5.6. If, however, the two highest orbitals for the case \( V_g = 0.74 H^* \) as shown in Fig. 5.7 clearly shows a ferromagnetic one. Thus the answer must be that there can exist ferromagnetic states as well as anti-ferromagnetic ones.

If furthered studied, the total energy of the anti-ferromagnetic state is calculated to be \( E_{0.74} = 892.90 \text{ meV} \) and for the ferromagnetic one, \( E_{0.74} = 892.75 \text{ meV} \). This gives a difference of 0.15 meV, but of that, 0.01 \( H^* \approx 0.119 \text{ meV} \), is explained by the increase in gate potential. This leaves a reconfigurational energy difference of only 31 \( \mu \text{eV} \). Thus it is in fact possible to consider the two states to be (almost) degenerated. From this it should be clear that anti-ferromagnetism needs not to be a property of all gate configurations.

Figure 5.6. Density function of the two highest orbitals for \( V_g = 0.73 H^* \). The colors indicate spin polarization, red spin-up and green spin-down.

Figure 5.7. Density function of the two highest orbitals for \( V_g = 0.74 H^* \). The red color indicates spin-up polarization. In this case there is no spin-down polarization.
5.3 Restoring the (anti-)symmetry

The states shown in Fig. 5.6 and Fig. 5.7 also implicitly define two degenerate states, i.e. states with the same spatial wave-function but inverted spin-functions. From this proper wave-function can be constructed. If considered first the case in Fig. 5.6, this can be mathematically be written:

\[ |\Phi(1, 2)\rangle = |\phi_1(1)\phi_2(2)\rangle \otimes |\alpha\beta\rangle \quad (5.1) \]

where \( |\phi_1(1)\phi_2(2)\rangle \) is the spatial part of the two coordinates 1 and 2. Implicitly defines is also however the state

\[ |\Phi(1, 2)\rangle = |\phi_1(2)\phi_2(1)\rangle \otimes |\beta\alpha\rangle \quad (5.2) \]

If these are combined in the following manner a singlet is obtained:

\[ |\Phi_{00}(1, 2)\rangle = \frac{1}{\sqrt{2}} (|\phi_1(1)\phi_2(2)\rangle + |\phi_1(2)\phi_2(1)\rangle) \otimes |\alpha\beta\rangle \quad (5.3) \]

where the spatial part is symmetric and the spin part is anti-symmetric thus leaving a total anti-symmetric function with spin quantum number \( s = 0 \).

If the spatial part had been anti-symmetric and the spin part symmetric one would instead have a state with \( s = 1 \) which would correspond to the mixed state of a triplet. Taking a leap and calling the functions depicted in Figs. 5.6 and 5.7 to be degenerate the complete triplet can be constructed as

\[ |\Phi_{11}(1, 2)\rangle = |\phi_1(1)\phi_2(2)\rangle - |\phi_1(2)\phi_2(1)\rangle \otimes |\alpha\alpha\rangle \quad (5.4) \]

\[ |\Phi_{10}(1, 2)\rangle = \frac{1}{\sqrt{2}} (|\phi_1(1)\phi_2(2)\rangle - |\phi_1(2)\phi_2(1)\rangle) \otimes |\alpha\beta + \beta\alpha\rangle \quad (5.5) \]

\[ |\Phi_{1-1}(1, 2)\rangle = |\phi_1(1)\phi_2(2)\rangle - |\phi_1(2)\phi_2(1)\rangle \otimes |\beta\beta\rangle \quad (5.6) \]

Of course one could object that the states might not really be degenerate, but at least to the degree of computational accuracy used for these simulations, the energy difference is below the detection limit.
Chapter 6

Summary and conclusions

6.1 The project in short

This work investigated the properties of electrons in a cyclic thin wire with an additional barrier using a simplified Hartree-Fock approximation and LSDA (exchange only). The following results have been found

- It was found that the electrons enter the barrier one at a time, thus making the populating function an integer one.
- Inside the barrier there are truly localized electrons under the right circumstances. There also exist more complicated structures that produce density peaks, but not individually localized electrons.
- There exist both ferromagnetic modes and anti-ferromagnetic ones. In some cases there seem to be degenerate ferromagnetic/anti-ferromagnetic pairs.
- For higher subband electrons there also exists a form of localization, albeit not as distinct as for the first subband electrons.
- From the degenerate states of two localized electrons, proper wave functions can be constructed to produce both singlet and triplet states.
- The $\delta$-interaction was tested but discarded as a substitute for the Coulomb interaction in this particular study.
- A two-dimensional localization was sought but not found. Instead signs of a spatial spin lattice were found.
- A form of resonance was observed when the size of the barrier was varied. This effect has not been investigated.
6.2 Future work

The results found in this paper are interesting but would need further studies to be confirmed. Preferable real experiments should be conducted to confirm the findings. More simulations could also be of interest, for example classical Hartree-Fock (without the LSDA) to investigate whether the results would agree. It would also be necessary to include temperature in order to determine the usefulness in real world applications.

Extensions of these calculation could also be interesting, for instance multiple circular wires close to each other or even overlapping. The search for entangled states is of great interest for the quantum computer research. This would probably have to be performed using a more exact technique than the one used in this paper.

It would also be interesting to investigate the properties of the two-dimensional spatial spin order described in Chapter 4.8 as well as the resonance effects in Chapter 4.6.
Bibliography


Appendix A

Transformations of the Schrödinger Equation

Often the Schrödinger Equation is not solved in SI Units but in some other units designed to simplify the appearance. For instance the form used in [3] has a length scale

\[ a_0^* = \frac{\hbar^2}{m^* e^2} \approx 9.8 \text{ nm} \]

and an energy

\[ H^* = \frac{e^2}{ea_0^*} \]

The original equation has the form

\[
-\frac{\hbar^2}{2m^*} \nabla^2 \Psi(r) + \frac{1}{2m^*} \epsilon \frac{\partial^2 \Psi}{\partial r^2} + \frac{e^2 \Psi(r)}{\epsilon r} + f(\theta) \Psi(r) = E \Psi(r)
\] (A.1)

where summation over particles has been ignored. The first modification is

\[ a_0^* r' = r \]

which gives

\[
-\frac{\hbar^2}{2m^*} \nabla^2 \Psi(r) + \frac{1}{2m^*} \epsilon \frac{\partial^2 \Psi}{\partial r'^2} + \frac{e^2 m^* \Psi(r)}{\hbar^2 e^2 r^2} + f(\theta) \Psi(r) = E \Psi(r)
\] (A.2)

further a wave function \( \Psi'(r') \equiv \Psi(r) \) along with the new differential operator \( \nabla' \equiv \nabla/a_0^* \) is introduced and the equation takes the form

\[
-\frac{1}{2} \nabla'^2 \Psi'(r') + \frac{1}{2} \frac{\omega^2 r^2 \Psi'(r')}{r'} + \frac{1}{2} \frac{\Psi'(r)}{r'} + f'(\theta) \Psi'(r') = \frac{1}{H^*} E \Psi'(r')
\] (A.3)

which is the form found in [3].

In this paper similar transformations are performed leading to the equation used

\[
-\frac{1}{2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi + \frac{1}{2} \omega^2 y^2 \Psi + V(\rho) \Psi + f'(\theta) \Psi = \frac{1}{H^*} E \Psi
\] (A.4)

The analytical solution for the harmonic part in Chapter 2.1 is found from the following manner. The standard form of a harmonic oscillator is

\[
-\frac{\hbar^2}{2m^*} \frac{d^2}{dy^2} \Psi + \frac{1}{2} m^* \Omega^2 y^2 \Psi = E \Psi
\] (A.5)
and has the energies $E_n = \hbar \Omega (n + 1/2)$. After transforming Eq. A.5 in a similar way as for Eq. A.3 the equation looks like

$$-\frac{\hbar^2}{2m^*} \frac{1}{a_0^2} \frac{d^2}{dy^2} \Psi' + \frac{1}{2} m^* \Omega^2 a_0^2 y^2 \Psi' = E \Psi'$$  \hspace{1cm} (A.6)$$

But the equation describes exactly the same system, so the energies must be the same. An equation for $\omega$ can now be found by identification of coefficients in Eq. A.5.

$$\omega = m^* \Omega^2 a^2 \cdot \frac{m^* a^2}{\hbar^2} = \frac{m^* \Omega^2 a_0^4}{\hbar^2} \implies \Omega \pm \frac{\omega \hbar}{m^* a_0^2}$$  \hspace{1cm} (A.7)$$

Still the same system is described so the energies must be

$$E_n = \frac{\omega \hbar^2}{m^* a_0^2} \left( n + \frac{1}{2} \right) = \omega \left( n + \frac{1}{2} \right) \cdot H^*$$  \hspace{1cm} (A.8)$$

and the wave function is

$$\Psi(y) = \left( \frac{\omega}{\pi a_0^2} \right)^{1/4} e^{-\frac{\omega y^2}{2 m^* a_0^2}}$$  \hspace{1cm} (A.9)$$

This explicit form allows calculating how large part of the orbital that would fit within the truncation as

$$\int_{-L_y/2}^{+L_y/2} |\Psi|^2 dy$$  \hspace{1cm} (A.10)$$

which, if evaluated using Mathematica 6.0, would compute to be 0.999992 for a $L_y = 80$ nm as for the standard size. This means that only 8 ppm of the orbitals is neglected by this restriction.
Appendix B

An analytical analysis of the possible energies

Equation 2.20 of the vanishing determinant is not trivial to solve. In its full it
looks like
\[
\frac{4\kappa\omega + (\kappa - \omega)^2 \cos^2 [2(\kappa\pi - \kappa\theta_0 - \omega\theta_0)] - (\kappa + \omega)^2 \cos^2 [2(\kappa\pi - \kappa\theta_0 + \omega\theta_0)]}{2\omega^2} = 0
\]  
(B.1)

In fact, generally, this equation can only be solved numerically, but it can still be useful to study it analytically in order to determine existence of solutions. This can later be used to construct a numerical algorithm to find all energies within a certain interval.

At first the case \( \beta < \kappa^2 \) is considered. A new variable is introduced in order to simplify the calculations.

\[
\sigma = \kappa + \sqrt{\kappa^2 - \beta}
\]

\[
\kappa = \frac{\sigma^2 + \beta}{2\sigma}
\]  
(B.2)

Noting that \( \omega > 0 \) only the numerator is considered

\[
0 = \sigma^2 - \frac{\beta^2}{\sigma^2} + \frac{\beta^2}{\sigma^2} \cos 2\left(\frac{\sigma + \frac{\beta}{2}}{\sigma} - \sigma\theta_0\right) - \sigma^2 \cos 2\left(\frac{\sigma + \frac{\beta}{2}}{\sigma} - \frac{\beta}{\sigma}\theta_0\right) = (B.3)
\]

\[
= -2\frac{\beta^2}{\sigma^2} \sin^2\left(\frac{\sigma + \frac{\beta}{2}}{\sigma} - \sigma\theta_0\right) + 2\sigma^2 \sin^2\left(\frac{\sigma + \frac{\beta}{2}}{\sigma} - \frac{\beta}{\sigma}\theta_0\right) \iff (B.4)
\]

\[
\iff \frac{\beta^2}{\sigma^2} \sin^2\left(\frac{\sigma + \frac{\beta}{2}}{\sigma} - \sigma\theta_0\right) = \sigma^2 \sin^2\left(\frac{\sigma + \frac{\beta}{2}}{\sigma} - \frac{\beta}{\sigma}\theta_0\right) \iff (B.5)
\]

\[
\iff \sin^2\left(\frac{\sigma^2 + \beta}{2\sigma} - 2\sigma^2\theta_0\right) = \frac{\sigma^4}{\beta^2} \sin^2\left(\frac{\sigma^2 + \beta}{2\sigma} - \frac{\beta}{\sigma}\theta_0\right) (B.6)
\]

Apparently the L.H.S \( \leq 1 \) while the R.H.S has an amplitude \( \geq 1 \). The R.H.S still has zero points, and moreover \( \frac{\partial}{\partial \sigma} \left(\frac{(\sigma^2 + \beta\pi - 2\beta\theta_0)}{2\sigma}\right) = \left(\frac{1}{2} - \frac{\beta}{2\sigma^2}\right) \pi > 0 \), i.e. the argument to the sine function is strictly increasing which, together with the fact that the functions are continuous, means that there must be exactly two solutions to Eq. B.6 for each zero point of the R.H.S:

\[
0 = \sin^2\left(\frac{(\sigma^2 + \beta)\pi - 2\beta\theta_0}{2\sigma}\right) \iff (B.7)
\]

\[
\iff n\pi = \frac{(\sigma^2 + \beta)\pi - 2\beta\theta_0}{2\sigma} \iff (B.8)
\]

\[
\iff 2\sigma n = \sigma^2 + \left(1 - \frac{2\theta_0}{\pi}\right)\beta \iff (B.9)
\]

\[
\iff \sigma = n \pm \sqrt{n^2 + \left(\frac{2\theta_0}{\pi} - 1\right)\beta} (B.10)
\]

Of the two solutions, only the positively signed is valid, which can be realized
from
\[ \beta \leq \sigma = n - \sqrt{n^2 + \left( \frac{2\theta_0}{\pi} - 1 \right) \beta} \leq n \] (B.11)

\[ \beta \leq n - \sqrt{n^2 + \left( \frac{2\theta_0}{\pi} - 1 \right) \beta} \leq n^2 \] (B.12)

\[ \iff n^2 + \left( \frac{2\theta_0}{\pi} - 1 \right) \beta \leq n^2 - 2n\sqrt{\beta} + \beta \]

\[ \iff n \leq \left( 1 - \frac{\theta_0}{\pi} \right) \sqrt{\beta} \leq \beta \]

where it is clear that Eqs. B.11 and B.12 contradict each other. Furthermore only positive \( n \) meeting certain criteria are allowed as shown by:

\[ \sqrt{\beta} \leq n + \sqrt{n^2 + \left( \frac{2\theta_0}{\pi} - 1 \right) \beta} \]

\[ \implies \beta - 2n\sqrt{\beta} + n^2 \leq n^2 + \left( \frac{2\theta_0}{\pi} - 1 \right) \beta \]

\[ \iff n \geq \left( 1 - \frac{\theta_0}{\pi} \right) \sqrt{\beta} \] (B.13)

The map \( \kappa \to \sigma \) is injective so Eq. B.9 defines a \( \kappa \) for each \( n \in \mathbb{N} \) Furthermore between two adjacent solutions of Eq. B.9 there are two solutions to 2.20

One could of course object that the L.H.S and the R.H.S of Eq. B.6 might be zero simultaneously. However this cannot be the case, since suppose \( \exists n, m \in \mathbb{Z} \):

\[
\begin{cases}
\sigma + \frac{\beta}{\pi} - \sigma \theta_0 = n\pi \\
\sigma + \frac{\beta}{\pi} - \beta \theta_0 = m\pi
\end{cases}
\] (B.14)

then \( \sigma \theta_0 - \frac{\beta}{\pi} \theta_0 = l\pi = 2\theta_0 \sqrt{\kappa^2 - \beta} \) for some \( l \in \mathbb{Z} \) and \( \kappa = \sqrt{\frac{\Omega^2 \theta_0^2}{4 \theta_0} + \beta} \) but inserted in the original equation this produces a contradiction:

\[ \sqrt{\frac{\Omega^2 \theta_0^2}{4 \theta_0} + \beta} \pi - \sqrt{\frac{\Omega^2 \theta_0^2}{4 \theta_0} + \beta \theta_0} - \frac{|l|\pi}{2} = n\pi \] (B.15)

unless \( l \) is even and \( \theta_0 = \pi \) which is uninteresting.

For the case \( \kappa^2 < \beta \), one could theoretically solve it using the same technique, but one quickly run into numerical issues. For instance if \( \omega = \Omega \) then \( \cosh \Omega \theta_0 - \sinh \Omega \theta_0 = e^{-\Omega \theta_0} \), but evaluated on a standard computer for \( \Omega \theta_0 = 19 \) the approximation \( \cosh 19 - \sinh 19 \approx -1.4901 \cdot 10^{-8} \) is clearly useless since it is supposed to be a positive number. The way go come around this is to embrace
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the hyperbolic trigonometric functions in the first place and return to the original equations:

\[
\begin{align*}
A \sin \kappa \theta_0 + B \cos \kappa \theta_0 &= C \sinh \Omega \theta_0 + D \cosh \Omega \theta_0 \\
A \kappa \cos \kappa \theta_0 - B \kappa \sin \kappa \theta_0 &= C \Omega \cosh \Omega \theta_0 + D \Omega \sinh \Omega \theta_0 \\
- E \sin \kappa \theta_0 + F \cos \kappa \theta_0 &= -C \sin \Omega \theta_0 + D \cosh \Omega \theta_0 \\
E \kappa \cos \kappa \theta_0 + F \kappa \cos \kappa \theta_0 &= C \Omega \sinh \Omega \theta_0 - D \Omega \cosh \Omega \theta_0 \\
\end{align*}
\]

(B.16)

where \( \Omega = \sqrt{\beta - \kappa^2} \). Once again introducing vectors \( x = (A, B)^T \), \( y = (C, D)^T \), \( z = (E, F)^T \) and adding and subtracting the equations in Eq. (B.16) the following is obtained:

\[
\begin{align*}
S_\kappa (R_{-\kappa \theta_0} x + R_{\kappa \theta_0} z) &= 2 \cosh \Omega \theta_0 S_\Omega y \\
S_\kappa (R_{-\kappa \theta_0} x - R_{-\kappa \theta_0} z) &= 2 \sinh \Omega \theta_0 S_\Omega Ny
\end{align*}
\]

(B.17)

where \( N = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \) is the row exchange operator. Once again making use of the relation \( z = R_{2\pi \kappa} \), \( y \) can be excluded and the following equation is found:

\[
\begin{align*}
sinh \Omega \theta_0 S_\kappa / \Omega (R_{-\kappa \theta_0} + R_{\kappa (2\pi - \theta_0)}) x &= \cosh \Omega \theta_0 N S_\kappa / \Omega (R_{-\kappa \theta_0} - R_{\kappa (2\pi - \theta_0)}) x \\
&\iff \left( \tanh \Omega \theta_0 S_\kappa / \Omega (R_{-\kappa \theta_0} + R_{\kappa (2\pi - \theta_0)}) - N S_\kappa / \Omega (R_{-\kappa \theta_0} - R_{\kappa (2\pi - \theta_0)}) \right) x = 0
\end{align*}
\]

(B.18)

The determinant equation can now be written:

\[
\begin{align*}
\kappa \Omega (\cos^2(\pi - \theta_0) \kappa \tanh^2 \Omega \theta_0 - \sin^2(\pi - \theta_0) \kappa) + (\kappa^2 - \Omega^2) \sin 2(\pi - \theta_0) \kappa \tanh \Omega \theta_0 &= 0 \\
\kappa \Omega (\tan(\pi - \theta_0) \kappa - \cot(\pi - \theta_0) \kappa \tanh^2 \Omega \theta_0) &= (\kappa^2 - \Omega^2) \tanh \Omega \theta_0
\end{align*}
\]

(B.19)

from which it can be seen that there must be one solution every \( \pi/2 \) of \( (\pi - \theta_0) \kappa \). This means that there will exist \( \left\lfloor \frac{2 \sqrt{\beta - \theta_0}}{\pi} \right\rfloor \) or \( \left\lceil \frac{2 \sqrt{\beta - \theta_0}}{\pi} \right\rceil \) solutions having energy lower than \( \beta \).
Appendix C

The metric function

The are two spatial coordinates to each point considered. When Coulomb interaction is included, a metric is necessary. This, however, turn out not to be the common one. The reason for this lies in the fact that the system is supposed to by cyclic in \( x \), and thus a difference arises as can be realized from the following:

\[
d(x, y) = \sqrt{\sum_n |x_i - y_i|^2}
\]

**Figure C.1.** A standard cartesian system

A standard cartesian space could easily be turned into a metric space by equipping it with the conventional metric function. If considered instead a cylindrical system with valid spatial points only on the surface of a fixed \( R \) the three-dimensional metric of \( \mathbb{R}^3 \) also defines a metric for the two-dimensional limitation as:

\[
d_3(x, y) = \sqrt{|x_1^c - y_1^c|^2 + |x_2^c - y_2^c|^2 + |x_3^c - y_3^c|^2} = \quad (C.1)
\]

\[
= \sqrt{R^2 \cdot |\cos \varphi_x - \cos \varphi_y|^2 + R^2 \cdot |\sin \varphi_x - \sin \varphi_y|^2 + |x_2 - y_2|^2} = \quad (C.2)
\]

\[
= \sqrt{2R^2 - 2R^2 \cdot (\cos \varphi_x \cos \varphi_y + \sin \varphi_x \sin \varphi_y) + |x_2 - y_2|^2} = \quad (C.3)
\]

\[
= \sqrt{2R^2 - 2R^2 \cos(\varphi_x - \varphi_y) + |x_2 - y_2|^2} \quad (C.4)
\]
The metric function

\[ d(x, y) = \sqrt{(x^2_2 - x^2_2)^2 + 2R^2 (1 - \cos(\varphi_x - \varphi_y))} \]

**Figure C.2.** A cylindrical surface. The system only resides on the surface, but the distance is thought to be the three-dimensional shortest route.

where it also should be noted that the coordinates \(x^1, x^2, x^3\) refers to the standard cartesian coordinates of \(\mathbb{R}^3\).