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Interacting Electrons in a Quantum Dot

Bachelor's thesis in Physics
Supervisor: Prof. Jeroen Danon
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ABSTRACT

We present in this thesis a straightforward way of diagonalising the two-dimensional Hamiltonian of an electron in an elliptically confined harmonic potential in the xy -plane with a constant magnetic field perpendicular to this plane, while motion in the z -direction is restricted. The diagonalisation involves deriving bosonic creation and annihilation operators for the system, for which we utilise a canonical transformation of coordinates and momenta, a scaling transformation, and a rotation of coordinate systems. Such transformations are simple to perform and intuitive to understand, and they produce an elegant way of expressing the creation and annihilation operators. We develop this theory in order to simplify future calculations of pairwise interactions of electrons in the same system. Such calculations would further allow us to investigate the dynamics of a four electron system which may serve as a candidate for a spin-0 semiconductor spin qubit.

ABSTRAKT

Vi presenterer i denne oppgaven en relativt ukomplisert måte å diagonalisere den todimensjonale Hamiltonianen til et elektron i et elliptisk avgrenset, harmonisk brønnpotensial i xy -planet med et konstant magnetfelt vinkelrett på dette planet. Elektronets bevegelse i z -retning er begrenset. Diagonaliseringen involverer å utlede bosoniske kreasjons- og annihileringsoperatorer. Dette gjøres ved hjelp av en kanonisk transformasjon av posisjons- og impulsoperatorer og en skaleringstransformasjon av akser, samt en rotasjon av koordinatsystemer. Slike transformasjoner er intuitive å forstå og resulterer i en elegant måte å uttrykke de utleddede kreasjons- og annihileringsoperatorene. Vi utvikler denne teorien for å simplifisere fremtidige beregninger av parvise interaksjoner mellom elektroner i samme potensialbrønn. Slike kalkulasjoner vil videre tillate oss å undersøke dynamikken til fire elektroner i ett brønnpotensial, da et slikt system kan være en kandidat for en spinn-0 halvleder spinn-qubit.

PREFACE

I extend my sincerest gratitude to my supervisor Prof. Jeroen Danon for presenting me with the opportunity to write this thesis, and for his help and support throughout the process of writing it. Not only has it been tremendously fun to work on the thesis itself, you have also given me experience in individual work and great insights into the world of academics. I will always be grateful for what you have done for me this semester and it has been a pleasure and an honour to work with such an excellent professor.

Additionally I would like to thank my girlfriend, family and friends for all their support and motivation throughout the writing of this thesis. You make my work much more enjoyable, and I am thankful that I get to share my passion with you. I hope to have every one of you along every step of the way.

Lastly I wish to dedicate my work here to my grandfather. His love and excitement for physics sparked a lifelong quest and a dream for knowledge in me, and I take great pride in continuing the legacy his circumstances did not allow himself to follow. Had he been here today with the same opportunities that I have, I am certain he would accomplish great things for physics. Rest well.

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ABBREVIATIONS

List of all abbreviations in alphabetic order:

- **PDE** Partial differential equation
- **QD** Quantum dot
- **Qubit** Quantum bit
- **2D** Two-dimensional

CHAPTER
ONE

INTRODUCTION

As the technological obstacles that humanity faces become too complex for classical supercomputers, one is forced to develop new and perhaps more powerful computational tools. A promising direction that has emerged is the invention of quantum computers and the development of quantum computing. In quantum computers, classical bits of memory are replaced by "quantum bits" or "qubits" for short. The strength of quantum computers comes from the ability of qubits to exist in a superposition of their possible states and to entangle with other qubits to form a large coherent quantum system. In this way the memory and computational power of such computers grow exponentially in accordance to the amount of qubits in the system.

A qubit is a two-level system where the levels are two arbitrary orthogonal states of the qubit system $|0\rangle$ and $|1\rangle$. For the purpose of quantum computation one should be able to reliably prepare states of qubits and maintain control of the qubits so that they do not decohere. One should also be able to predict how the qubits will behave over time, and be able to measure sufficient information about the system at the end of computations [1]. When constructing qubits these criteria must be kept in mind. It turns out that so called semiconductor spin qubits are one platform that fulfills the criteria. A semiconductor spin qubit is a qubit located inside a semiconductor and which encodes its basis states in spin. This might seem natural as the spin of a spin-1/2 particle such as an electron is a two-level system. Semiconductors are attractive as qubit hosts as the scale and advancements of the semiconductor industry could give rise to large scale production and precision manufacturing [2]. The main drawback of quantum computing architectures based upon semiconductors is however that semiconductor environments are noisy [3]. This poses a problem when working with sensitive quantum systems such as qubits. In regards to this sensitivity, an immediate positive about spin defining the two states is that spin-exchange occurs at short range, and is thus somewhat isolated from the environment. This does however result in challenges when attempting to attain control of the qubit. Charge-based qubits are the direct opposite: attaining control does not pose a challenge, but this in turn results in a predisposition for the qubit to be disturbed by its environment. One would ideally be able to construct a qubit which combines the positives of charge- and spin-based qubits while mitigating the negatives. The resulting qubit would be

easy to control and would couple weakly to its environment. An example of such a qubit was proposed by Kyriakidis and Burkard (2007) [4]. This qubit proposition has been central for the work I intend to present in this thesis.

1.1 Motivation

Kyriakidis and Burkard (2007) [4] proposed a qubit which consists of three electrons inside a single quantum dot (QD). The QD they presented was a two-dimensional (2D) elliptically confined harmonic potential with a perpendicular constant magnetic field. Similar to this proposition, one can imagine a qubit which consists of four electrons in the same QD. For such a system there exist two orthogonal states with identical charge density and orbital occupation, as well as a total spin of zero. In this way, the coupling of the qubit to the environment is alike in both qubit basis states, which might in turn decrease the decoherence rate of the qubit; since the two states respond similarly to disturbances. In addition, since the two qubit states will have zero spin, the qubit will be insensitive to disturbances that couple to its spin. This is the main difference between our qubit and the one proposed by Kyriakidis and Burkard (2007), as they propose a spin-1/2 semiconductor spin qubit. One chooses the QD to specifically be elliptically confined because it allows control of the qubit to be attained by tuning the shape of the confinement. Such a qubit seems then to be controllable and somewhat robust against noise and decoherence, making it beneficial to investigate it further

In order to construct and investigate such a qubit, we must first derive expressions for the dynamics of each particle, and the pairwise interactions between them. The calculation of the pairwise interactions become considerably easier to perform if one can use creation and annihilation operators, which one can derive from the single particle Hamiltonian of the system. Such operators have been derived before (see e.g. [5]), but we will in this thesis follow a different approach. We diagonalise this Hamiltonian by deriving purely algebraic expressions for bosonic annihilation and creation operators for the system using a canonical transformation, a scaling transformation, and a rotation of coordinate systems. This method is intuitive to understand and produces elegant expressions for the creation and annihilation operators of the system, such that we find it worthwhile to document the method in a detailed manner. We will furthermore derive expressions for the stationary eigenstates of the system using the ladder operators we derive.

CHAPTER
TWO

THEORY

For later calculations it will be necessary to derive the Hamiltonian of the system we are working in and to present the algebraic method for diagonalising the Hamiltonian of a simple harmonic oscillator.

We derive our Hamiltonian classically and substitute position and momentum by the quantum mechanical position and momentum operators. This is done because we will later diagonalise this Hamiltonian.

The Hamiltonian for the simple harmonic oscillator will be diagonalised by introducing bosonic creation and annihilation operators. We do this in order to introduce the notion of creation and annihilation operators, and because the expressions from this diagonalisation will further be used to construct operators for the Hamiltonian mentioned above.

2.1 Hamiltonian of a Particle in an Electric Potential and Magnetic Field

It will be necessary to construct the Hamiltonian of a particle moving in an electric potential and with a magnetic field. We will follow the method used by Griffiths (2017) [6]. It is firstly done classically by finding a Lagrangian L which yields the Lorentz force when plugged into the Lagrange equations. From the Lagrangian we derive an expression for the classical Hamiltonian H in terms of position \mathbf{r} and momentum \mathbf{p} . Lastly, we go from a classical Hamiltonian H to the corresponding quantum mechanical Hamiltonian operator \hat{H} by substituting position and momentum by position and momentum operators $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$.

The Lorentz force is given as

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (2.1.1)$$

and the Lagrange equation for the i -th coordinate as

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{r}_i} \right) = \frac{\partial L}{\partial r_i} \quad (2.1.2)$$

We will do an educated guess and propose the Lagrangian

$$L = \frac{1}{2} m \dot{r}^2 + q(\dot{\mathbf{r}} \cdot \mathbf{A}) - q\varphi \quad (2.1.3)$$

where $V = V(\mathbf{r}, t)$ is an electric potential and $\mathbf{A} = \mathbf{A}(\mathbf{r}, t)$ is a magnetic vector potential. We then want to insert this Lagrangian into the Lagrange equations and check that the resulting expression is indeed the Lorentz force. Separate equation (2.1.3) into its components and plug the expressions into equation (2.1.2). The expressions can then be manipulated into the form

$$m\ddot{\mathbf{r}} = -q \left(\nabla\varphi + \frac{\partial \mathbf{A}}{\partial t} \right) + q(\dot{\mathbf{r}} \times (\nabla \times \mathbf{A})) \quad (2.1.4)$$

By using $\ddot{\mathbf{r}} = \mathbf{a}$, $\dot{\mathbf{r}} = \mathbf{v}$, $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$, $\mathbf{B} = \nabla \times \mathbf{A}$, and Newton's second law such that $\mathbf{F} = m\mathbf{a}$, one can see that our proposed Lagrangian indeed has yielded the expression for the Lorentz force.

The next step is to use our Lagrangian to construct our desired Hamiltonian. We do this by finding canonical momenta $p_i = \frac{\partial L}{\partial \dot{r}_i}$ and expressing \dot{r}_i in terms of p_i . One then substitutes all \dot{r}_i 's by their new expressions in the equation

$$H = \sum_i p_i \dot{r}_i - L \quad (2.1.5)$$

All \dot{r}_i 's in L should also be substituted. The resulting Hamiltonian in our case becomes

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + V \quad (2.1.6)$$

where \mathbf{p} is the momentum of a particle with charge q , \mathbf{A} is the vector potential of the magnetic field \mathbf{B} , and $V = q\varphi$ is the electric potential of the system. We have then derived the classical Hamiltonian of a particle with mass m and charge q moving with momentum \mathbf{p} in an electric potential V and an applied magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$.

Lastly, to get our desired quantum mechanical Hamiltonian operator \hat{H} , we substitute the quantities in equation (2.1.6) by their corresponding quantum mechanical operators. Specifically, $\mathbf{p} \rightarrow \hat{\mathbf{p}}$, $\mathbf{A} \rightarrow \hat{\mathbf{A}}$, and $V \rightarrow \hat{V}$. Our final Hamiltonian operator then becomes

$$\hat{H} = \frac{1}{2m} \left(\hat{\mathbf{p}} - q\hat{\mathbf{A}} \right)^2 + \hat{V} \quad (2.1.7)$$

This is the quantum implementation of the Lorentz force law, and it is sometimes

referred to as the "minimal coupling rule"[6]. In this expression both \hat{V} and $\hat{\mathbf{A}}$ are given, meaning they depend upon the specific problem one is solving.

A note about the magnetic field \mathbf{B} is that it is gauge invariant, meaning it is not uniquely defined by one vector potential $\hat{\mathbf{A}}$. Rather, one must choose between different vector potentials according to the specific problem.

2.2 Diagonalising the Simple Harmonic Oscillator

We summarise the method of diagonalising the one-dimensional Hamiltonian of a particle in a harmonic potential using creation and annihilation operators as described in Griffiths (2017) [6]. This is done to introduce the notion of creation and annihilation operators, and because some of the expressions we present here will be used later when constructing another set of creation and annihilation operators for another Hamiltonian.

A simple harmonic oscillator is one dimensional and consists of a particle with mass m in a harmonic potential¹ $\hat{V} = \frac{1}{2}m\omega^2r^2$. The Hamiltonian of this system is then given as

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2r^2 \quad (2.2.1)$$

The position and momentum operators do not commute, meaning $r_i\hat{p}_i \neq \hat{p}_ir_i$. Products of such operators are related by their commutation relation: $[r_i, \hat{p}_j] = i\hbar\delta_{ij}$. If one ignores for a moment that we are working within an operator algebra, and look at the operators in equation (2.2.1) as though they were normal variables, one might be tempted to factorise equation (2.2.1) as such

$$\hat{H} = \frac{1}{2m}(i\hat{p} + m\omega r)(-i\hat{p} + m\omega r) \quad (2.2.2)$$

Let us use each of the factors in equation (2.2.2) to define two new operators²

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega q) \quad a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega q) \quad (2.2.3)$$

The prefactor in equation (2.2.3) has been chosen in order to simplify the problem, as it ensures that

$$[a, a^\dagger] = 1 \quad (2.2.4)$$

If one now expresses r and \hat{p} in terms of the operators a and a^\dagger and insert these expressions into the Hamiltonian in equation (2.2.1), one can simplify the expression using the commutation relation in equation (2.2.4) and write it as

¹Since $\hat{r}_i = r_i$, we will denote the coordinate operators without a hat.

²We do not put any hats on a and a^\dagger in order to distinguish them from other operators, as they are not Hermitian

$$\hat{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \quad (2.2.5)$$

This is the diagonal form of the Hamiltonian for a simple harmonic oscillator. The next step is to investigate the behaviour of $a^\dagger a$. To do this we introduce a general state of the system $|n\rangle$ and define $a^\dagger a$ to have eigenvalues as such: $a^\dagger a|n\rangle = n|n\rangle$. Using this, one can show that if the Schrödinger equation is satisfied for the state vector $|n\rangle$, meaning $\hat{H}|n\rangle = E|n\rangle$, then the states $a^\dagger|n\rangle$ and $a|n\rangle$ also satisfy the Schrödinger equation with eigenvalues $E + \hbar\omega$ and $E - \hbar\omega$ respectively. It is then apparent that the operators a^\dagger and a , which we shall refer to as "ladder operators" or "creation/annihilation operators", increase and decrease the energy of the system in quanta of $\hbar\omega$. More specifically, a^\dagger is the creation operator which increases the energy of the system, and a is the annihilation operator which decreases the energy of the system.

By imposing that the absolute value of the energy eigenvalue must be greater than or equal to zero, it can be shown that the ground state of the system is $|0\rangle$ and the lowest energy eigenvalue is $E = \frac{1}{2}\hbar\omega$. This implies that $a^\dagger a|0\rangle = 0|0\rangle$. We will refer to the state $|0\rangle$ as "the vacuum". Further, since the eigenvalue n has a lower limit 0 and increases in quanta of $\hbar\omega$ by operating a^\dagger on the state, we deduce that n must be an integer greater than or equal to zero. The resulting energy eigenvalues of the system are then

$$E = \hbar\omega \left(n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots \quad (2.2.6)$$

If one is familiar with the simple harmonic oscillator, one may recognise this as the right answer for the energy eigenvalues. If one investigates the behaviour of a and a^\dagger further, it becomes apparent that the following relations hold

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad (2.2.7)$$

Also important to note is that since $a|0\rangle = 0$, one cannot reach eigenvectors of lower energy than $|0\rangle$. We will refer to the action of operating the annihilation operator on the vacuum as "annihilating the vacuum", which we again stress always gives the eigenvalue 0.

The relations in equation (2.2.7) indicate that one can navigate between basis states of the system using the ladder operators. The introduction of such operators yield then a very useful theoretical framework to work within when performing calculations. It is precisely why we wish to diagonalise the Hamiltonian derived in section 2.1.

CHAPTER
THREE

RESULTS

We will in this section define a Hamiltonian based on the one derived in section 2.1, and diagonalise it to obtain bosonic creation and annihilation operators for the system, as we did for the simple harmonic oscillator in section 2.2. This has been done before, but we will present an alternative way of doing it. The method we utilise is intuitive to understand and produces the results in an elegant way. We derive these results because the Hamiltonian we shall diagonalise describes parts of a system which might be an attractive candidate for a semiconductor spin qubit. In addition, by diagonalising the mentioned Hamiltonian one obtains ladder operators for the system which make further calculations far simpler.

In order to diagonalise the Hamiltonian, we define suitable canonical operators, scale their axes, rotate their corresponding coordinate systems, and construct ladder operators in terms of the canonical operators. The latter step is done in the same way as for the simple harmonic oscillator. Lastly, we transform back to our regular coordinates to obtain ladder operators and a diagonal Hamiltonian in terms of regular coordinate and momentum operators.

3.1 Defining the System

The system we are investigating is that of an electron with mass m and charge $-e$ in an elliptically confined harmonic potential in the xy -plane, with a constant magnetic field in the positive z -direction. We will ignore any terms due to the Zeeman effect in our Hamiltonian as we in this thesis are not interested in any effects relating to the spin of the electron in our system.

The electron's motion is greatly restricted in the z -direction. This can physically be realised if the potential V along z quickly becomes so strong when moving away from the xy -plane that the probability for the electron to move far in the z -direction becomes negligibly small. The engineering of planes one would need for a 2D system can be realised inside semiconductors [7]. If the confinement is narrow enough, the difference in energy between the ground state and the first excited state becomes so large that a transition between the two energy states becomes extremely improbable. These assumptions allow us to ignore the dynamics

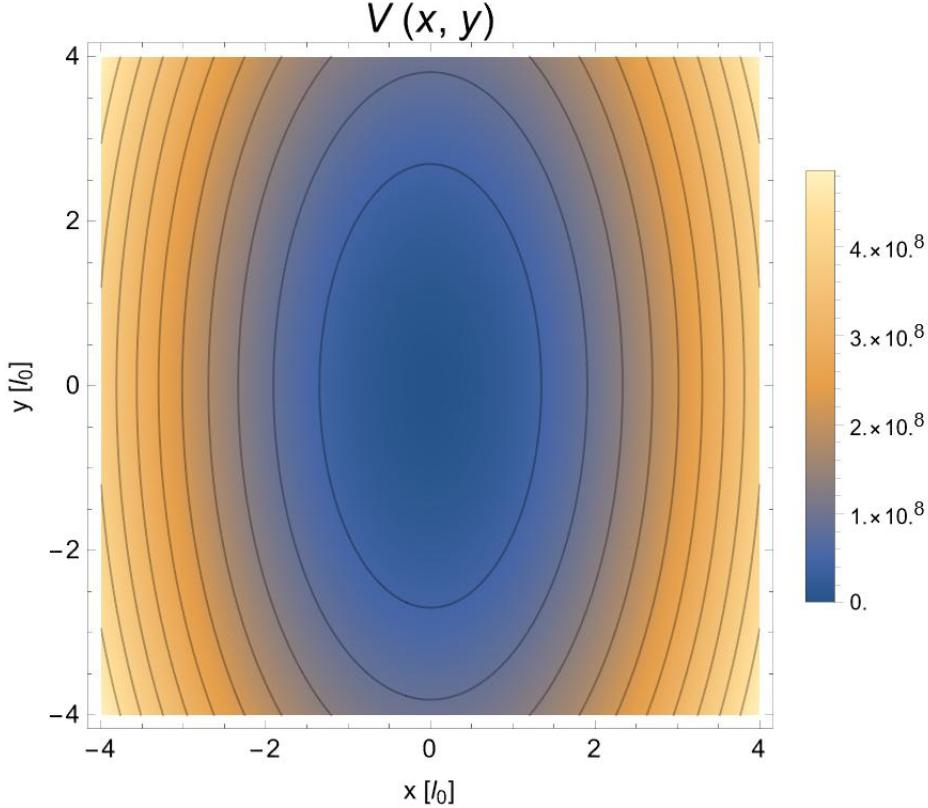


Figure 3.1.1: Example of density plot of the potential $V(x, y)$. The x - and y -axes are both in units of l_0 . We have used $B = 3$ T and parameter ratios $\frac{\omega_c}{\omega_x} = 5$ and $\frac{\omega_y}{\omega_x} = \frac{1}{2}$.

in the z -direction for our calculations.

An elliptically confined harmonic potential in the xy -plane can be expressed as $\hat{V} = \frac{1}{2}m(\omega_x^2\hat{x}^2 + \omega_y^2\hat{y}^2)$. We have plotted an example of such a potential in Figure 3.1.1. Insert the expression for the potential into equation (2.1.7) to get the Hamiltonian for our system

$$\hat{H} = \frac{1}{2m} \left(\hat{\mathbf{p}} + e\hat{\mathbf{A}} \right)^2 + \frac{1}{2}m (\omega_x^2x^2 + \omega_y^2y^2) \quad (3.1.1)$$

The next step is to choose in what gauge we will work in, so that we can get an expression for the magnetic vector potential $\hat{\mathbf{A}}$. Since our magnetic field \mathbf{B} points along z , we choose to work in the symmetric gauge, meaning

$$\hat{\mathbf{A}} = \frac{B}{2} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} \quad (3.1.2)$$

We define $\hat{\pi} \equiv \hat{\mathbf{p}} + e\hat{\mathbf{A}}$ such that

$$\hat{\pi} = \begin{pmatrix} \hat{\pi}_x \\ \hat{\pi}_y \\ \hat{\pi}_z \end{pmatrix} = \begin{pmatrix} \hat{p}_x - \frac{eB}{2}y \\ \hat{p}_y + \frac{eB}{2}x \\ \hat{p}_z \end{pmatrix} \quad (3.1.3)$$

This is done in order to simplify the process of finding canonical operators later. Further, we introduce the magnetic length $l_B = \sqrt{\frac{\hbar}{eB}}$ and define dimensionless operators

$$\tilde{\mathbf{r}} = \frac{\mathbf{r}}{l_B}, \quad \tilde{\boldsymbol{\pi}} = \frac{\hat{\boldsymbol{\pi}} l_B}{\hbar} \quad (3.1.4)$$

For later convenience, we express the transformation $(\mathbf{r}, \hat{\mathbf{p}}) \rightarrow (\tilde{\mathbf{r}}, \tilde{\boldsymbol{\pi}})$ as

$$\begin{pmatrix} \tilde{\mathbf{r}} \\ \tilde{\boldsymbol{\pi}} \end{pmatrix} = \underline{S} \begin{pmatrix} \mathbf{r} \\ \hat{\mathbf{p}} \end{pmatrix} \quad (3.1.5)$$

Where \underline{S} is the 6×6 matrix

$$\underline{S} = \begin{pmatrix} \frac{1}{l_B} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{l_B} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{l_B} & 0 & 0 & 0 \\ 0 & -\frac{l_B Be}{\hbar^2} & 0 & \frac{l_B}{\hbar} & 0 & 0 \\ \frac{l_B Be}{\hbar^2} & 0 & 0 & 0 & \frac{l_B}{\hbar} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{l_B}{\hbar} \end{pmatrix} \quad (3.1.6)$$

Working with dimensionless operators is beneficial because it simplifies the commutation relations for coordinates and momenta, which in turn simplifies the process of finding canonical operators. The commutation relations for the dimensionless operators are¹

$$[\tilde{r}_i, \tilde{r}_j] = [\tilde{\pi}_i, \tilde{\pi}_z] = 0 \quad [\tilde{r}_i, \tilde{\pi}_j] = i\delta_{ij} \quad [\tilde{\pi}_y, \tilde{\pi}_x] = i \quad (3.1.7)$$

The benefit of dimensionless operators is here apparent as there is no \hbar in the commutator between position and momentum. An important note about these commutation relations is that $\tilde{\pi}_y$ and $\tilde{\pi}_x$ do not commute. This is the main reason why we do not simply diagonalise our Hamiltonian directly: the momentum $\hat{\boldsymbol{\pi}}$ does not behave as $\hat{\mathbf{p}}$.

If we were to write out the Hamiltonian in equation (3.1.1), we would find that there are cross-terms which couple the x -direction to the y -direction, namely one term with $\hat{p}_x y$ and one with $\hat{p}_y x$. These cross terms make it much harder to diagonalise our Hamiltonian. Also, since $\tilde{\pi}_x$ and $\tilde{\pi}_y$ do not commute, one cannot utilise this notation to diagonalise the Hamiltonian as one does for the one-dimensional simple harmonic oscillator; $\tilde{\boldsymbol{\pi}}$ simply does not behave as $\hat{\mathbf{p}}$ does. In order to diagonalise the Hamiltonian it is necessary to work with operators which behave as normal coordinate and momentum operators and which simplify the Hamiltonian such that it does not contain cross-terms between position and momentum operators. For this purpose we introduce canonical operators.

¹Here one should not confuse the index i and the imaginary unit

3.2 Canonical Operators

We wish to define dimensionless canonical operators $\hat{\mathbf{Q}} = (\hat{Q}_x, \hat{Q}_y, \hat{Q}_z)$ and $\hat{\mathbf{P}} = (\hat{P}_x, \hat{P}_y, \hat{P}_z)$, where each component is a linear combinations of the dimensionless operators defined in equation (3.1.4). Each canonical operator should be defined in such a way that there are no cross terms which include components from both $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ when plugged into the Hamiltonian, and the canonical operators must fulfill the commutation relations

$$[\hat{Q}_i, \hat{Q}_j] = [\hat{P}_i, \hat{P}_j] = 0 \quad [\hat{Q}_i, \hat{P}_j] = i\delta_{ij} \quad (3.2.1)$$

If there are no cross-terms we will be able to diagonalise the Hamiltonian, and if the operators obey the above mentioned commutation relations they behave like normal dimensionless coordinate and momentum operators. Such behaviour will later allow use of the theory for the simple harmonic oscillator to construct ladder operators, which is exactly what we want.

The change from $(\tilde{\mathbf{r}}, \tilde{\boldsymbol{\pi}}) \rightarrow (\hat{\mathbf{Q}}, \hat{\mathbf{P}})$ is a canonical transformation defined as

$$\begin{pmatrix} \hat{\mathbf{Q}} \\ \hat{\mathbf{P}} \end{pmatrix} = \underline{C} \begin{pmatrix} \tilde{\mathbf{r}} \\ \tilde{\boldsymbol{\pi}} \end{pmatrix} \quad (3.2.2)$$

where \underline{C} is a 6×6 matrix. In our case we find that the matrix

$$\underline{C} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 1 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (3.2.3)$$

yields a transformation that satisfies our boundary conditions. To get the new Hamiltonian we express operators in real space $(\tilde{\mathbf{r}}, \tilde{\boldsymbol{\pi}})$ in terms of the canonical operators $(\hat{\mathbf{Q}}, \hat{\mathbf{P}})$, and insert these expressions into the Hamiltonian in equation (3.1.1). One can disregard for the time being the terms in our Hamiltonian relating to the z -axis, since it does not couple to the other axes in any way. We collect the xy -terms in the Hamiltonian in such a way that it becomes

$$\hat{H}_{xy} = A_Q \hat{Q}_x^2 + B_Q \hat{Q}_x \hat{Q}_y + C_Q \hat{Q}_y^2 + A_P \hat{P}_x^2 + B_P \hat{P}_x \hat{P}_y + C_P \hat{P}_y^2 \quad (3.2.4)$$

The coefficients are in this case

$$\begin{aligned}
A_Q &= \frac{Be\hbar}{8m} + \frac{m\hbar\omega_x^2}{2Be} \\
B_Q &= \frac{Be\hbar}{4m} \\
C_Q &= \frac{Be\hbar}{8m} \\
A_P &= \frac{Be\hbar}{2m} \\
B_P &= \frac{Be\hbar}{m} \\
C_P &= \frac{Be\hbar}{2m} + \frac{2m\hbar\omega_y^2}{Be}
\end{aligned} \tag{3.2.5}$$

It is now apparent that the canonical transformation we performed has resulted in a Hamiltonian with no cross-terms between \hat{Q} 's and \hat{P} 's, meaning we are one step closer to diagonalising the Hamiltonian. The next step is to transform the canonical operators further such that the last cross terms fall away. We will do this by scaling and rotating the coordinate axes of \hat{Q} and \hat{P} .

3.3 Scaling and Rotation of Coordinate Axes

What is important during the diagonalisation is that only transformations which do not change the commutation relations of the canonical operators are used. By an analogy of ellipses in \hat{Q} - and \hat{P} -space, we show here that by scaling the operators and rotating their coordinate systems, one eliminates the last cross-terms in the Hamiltonian. Scaling and rotation transformations do not alter the commutation relations of the operators involved, meaning the resulting Hamiltonian will be composed of operators which behave as dimensionless real coordinate and momentum operators. What is also beautiful about this method is how intuitive it is to understand what we are doing; one essentially stretches and squeezes, then rotates two ellipses. Also, since a rotation involves trigonometric expressions, they may be manipulated to be written on a purely algebraic form.

The general expression of a rotated ellipse centered at the origin is

$$AX^2 + BXY + CY^2 = F \tag{3.3.1}$$

as we show in Appendix A. Using this, and a little bit of imagination, one can see equation (3.2.4) as the expression of two rotated ellipses in two separate coordinate systems (\hat{Q}_x, \hat{Q}_y) and (\hat{P}_x, \hat{P}_y) . An ellipse on the form given in equation (3.3.1) is rotated by an angle ϕ with respect to the x -axis, where ϕ is given by

$$\phi = \arctan \left(\frac{1}{B} \left(C - A - \sqrt{(A - C)^2 + B^2} \right) \right); \quad B \neq 0 \tag{3.3.2}$$

as stated in equation (A.6) from Appendix A.

In order for us to diagonalise the Hamiltonian, we must eliminate the last cross-terms in equation (3.2.4). To do this we will use our analogy of two separate ellipses to scale the \hat{Q}_x and \hat{P}_x axes by a factor α and $\frac{1}{\alpha}$ respectively, such that the angles ϕ are the same for the ellipses in both the (\hat{Q}_x, \hat{Q}_y) system and the (\hat{P}_x, \hat{P}_y) system. In this way the two ellipses can be rotated by the same angle to eliminate the cross-terms in equation (3.2.4). It is important to scale the axes before we rotate the systems because the coordinates and momenta are interconnected and must be rotated through the same angle.

Why does momentum scale as $\frac{1}{\alpha}$ if position scales as α ? As mentioned above, the commutation relations between the new scaled operators must remain the same as before. One can thus see why the factors must be the inverse of each other from the commutation relation.

We perform the scaling by imposing $\hat{Q}_x \rightarrow \alpha \hat{Q}_x$ and $\hat{P}_x \rightarrow \frac{1}{\alpha} \hat{P}_x$ via the transformation

$$\begin{pmatrix} \tilde{\mathbf{Q}} \\ \tilde{\mathbf{P}} \end{pmatrix} = \underline{A} \begin{pmatrix} \hat{\mathbf{Q}} \\ \hat{\mathbf{P}} \end{pmatrix} \quad (3.3.3)$$

where \underline{A} is the 6×6 matrix

$$\underline{A} = \begin{pmatrix} \frac{1}{\alpha} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (3.3.4)$$

Notice here that we are only scaling \hat{Q}_x and \hat{P}_x . Scaling these two does not alter \hat{Q}_y or \hat{P}_y , and it is not necessary for our purposes to scale all four. Write $(\hat{\mathbf{Q}}, \hat{\mathbf{P}})$ in terms of the scaled operators $(\tilde{\mathbf{Q}}, \tilde{\mathbf{P}})$ and plug this into equation (3.2.4). The effect of this is that

$$\begin{aligned} A_Q &\rightarrow \alpha^2 A_Q \equiv \tilde{A}_Q \\ B_Q &\rightarrow \alpha B_Q \equiv \tilde{B}_Q \\ A_P &\rightarrow \frac{1}{\alpha^2} A_P \equiv \tilde{A}_P \\ B_P &\rightarrow \frac{1}{\alpha} B_P \equiv \tilde{B}_P \end{aligned} \quad (3.3.5)$$

whereas $\tilde{C}_Q = C_Q$ and $\tilde{C}_P = C_P$. We now wish to uncover what α is. To do this we use equation (3.3.2) to set up the equation

$$\frac{1}{\tilde{B}_Q} \left(\tilde{C}_Q - \tilde{A}_Q - \sqrt{(\tilde{A}_Q - \tilde{C}_Q)^2 + \tilde{B}_Q^2} \right) = \frac{1}{\tilde{B}_P} \left(\tilde{C}_P - \tilde{A}_P - \sqrt{(\tilde{A}_P - \tilde{C}_P)^2 + \tilde{B}_P^2} \right) \quad (3.3.6)$$

and solve it for α . There are two solutions to equation (3.3.6). We choose the positive solution, as scaling with a negative factor would flip the direction of the axes and cause our coordinate system to not be right-handed. The resulting scaling factor α is thus given by

$$\alpha = \frac{Be}{\sqrt{B^2e^2 + 2m^2(\omega_x^2 + \omega_y^2)}} \quad (3.3.7)$$

Using this expression for α , the transformation in equation (3.3.3) yields two ellipses which are rotated by the same angle ϕ in their respective coordinate systems.

The canonical transformation we presented made all terms in the Hamiltonian in equation (3.2.4) positive. Thus the two hypothetical ellipses lay parallel after the scaling. Other canonical transformations should also work, though many produce a Hamiltonian in which a scaling will not result in parallel ellipses, but rather perpendicular ones. Such a scenario would require a slightly different equation to solve when calculating the scaling factor α . Specifically, the angles of the two ellipses should not be the same, but rather $\phi_Q = \frac{\pi}{2} - \phi_P$, where ϕ_Q is the angle for the \hat{Q} -space ellipse and ϕ_P the angle for the \hat{P} -space ellipse. Apart from this and a potentially different value for α , the rest of the method would remain the same.

The next step is to rotate the two ellipses. In order to do this, we must first uncover the angle through which the systems should be rotated; ϕ . We do this by inserting the expression for α into equation (3.3.2) for either \hat{Q} 's or \hat{P} 's. The angle ϕ we get in our case is then

$$\begin{aligned} \phi &= \arctan \left[\frac{1}{\tilde{B}_Q} \left(C_Q - \tilde{A}_Q - \sqrt{(\tilde{A}_Q - C_Q)^2 + \tilde{B}_Q^2} \right) \right] \\ &= \arctan \left[-\frac{\omega_-^2 + \Omega^2}{\omega_c \omega_0} \right] \end{aligned} \quad (3.3.8)$$

where we have introduced the cyclotron frequency $\omega_c = \frac{eB}{m}$ and defined

$$\omega_- = \sqrt{\omega_x^2 - \omega_y^2} \quad \omega_0 = \sqrt{\omega_c^2 + 2(\omega_x^2 + \omega_y^2)} \quad \Omega = (\omega_-^4 + \omega_c^2 \omega_0^2)^{\frac{1}{4}} \quad (3.3.9)$$

To ensure that ω_- is real we assume, without loss of generality, that $\omega_x \geq \omega_y$. The introduction of these variables also allows us to rewrite the scaling factor as $\alpha = \frac{\omega_c}{\omega_0}$.

With a suitable angle ϕ , we now rotate both ellipses by ϕ to get rid of the cross-terms in the Hamiltonian from equation (3.2.4). The rotation is expressed by the transformation

$$\begin{pmatrix} \hat{\Theta} \\ \hat{\Pi} \end{pmatrix} = \underline{R} \begin{pmatrix} \tilde{Q} \\ \tilde{P} \end{pmatrix} \quad (3.3.10)$$

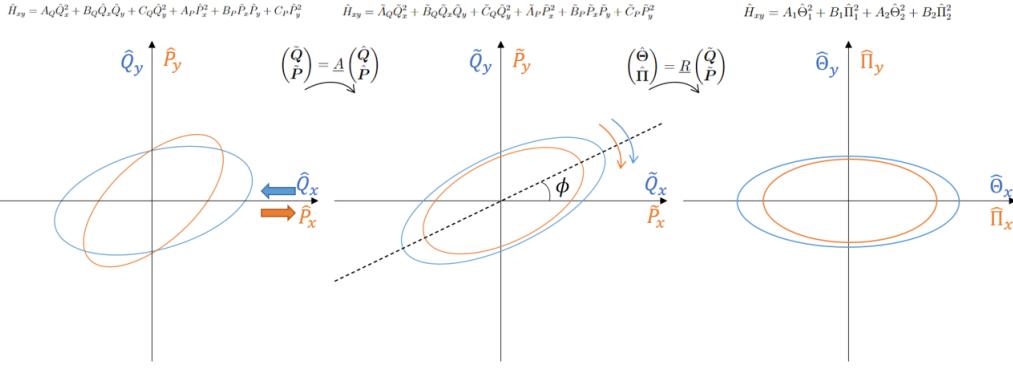


Figure 3.3.1: Schematic which visualises how the Hamiltonian is transformed using the analogy of ellipses in \hat{Q} - and \hat{P} -space

where \underline{R} is the 6×6 rotation matrix

$$\underline{R} = \begin{pmatrix} \cos \phi & \sin \phi & 0 & 0 & 0 & 0 \\ -\sin \phi & \cos \phi & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos \phi & \sin \phi & 0 \\ 0 & 0 & 0 & -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (3.3.11)$$

We have as a formality included elements corresponding to \tilde{Q}_z and \tilde{P}_z that leave them unchanged under the rotation; only x and y terms are rotated. By expressing $(\tilde{\mathbf{Q}}, \tilde{\mathbf{P}})$ in terms of $(\hat{\Theta}, \hat{\Pi})$ and plugging these expressions into equation (3.2.4), the cross-terms disappear and we are left with a Hamiltonian of form

$$\hat{H}_{xy} = A_1 \hat{\Theta}_1^2 + B_1 \hat{\Pi}_1^2 + A_2 \hat{\Theta}_2^2 + B_2 \hat{\Pi}_2^2 \quad (3.3.12)$$

where the resulting coefficients are

$$\begin{aligned} A_1 &= \frac{\hbar \omega_c (\omega_0^2 + \omega_-^2 - \Omega^2)}{8\omega_0^2} \\ B_1 &= \frac{\hbar (\omega_0^2 - \omega_-^2 - \Omega^2)}{2\omega_c} \\ A_2 &= \frac{\hbar \omega_c (\omega_0^2 + \omega_-^2 + \Omega^2)}{8\omega_0^2} \\ B_2 &= \frac{\hbar (\omega_0^2 - \omega_-^2 + \Omega^2)}{2\omega_c} \end{aligned} \quad (3.3.13)$$

We have now successfully eliminated the cross-terms in our Hamiltonian when written in terms of $(\hat{\Theta}, \hat{\Pi})$. To showcase how one could visualise the method in this section, we have included a schematic of the analogy of ellipses in Figure 3.3.1. If we were to reverse our transformations such that $(\hat{\Theta}, \hat{\Pi}) \rightarrow (\mathbf{r}, \hat{\mathbf{p}})$, we would

recover the original Hamiltonian given in equation (3.1.1). However in order to write the Hamiltonian on diagonal form, similar to the Hamiltonian for the simple harmonic oscillator given in equation (2.2.5), we must construct creation and annihilation operators for our current system.

3.4 Construct Ladder Operators

We present here how to use the theory of diagonalising the simple harmonic oscillator to diagonalise the Hamiltonian in equation (3.3.12). We do this by constructing ladder operators $(a_1^\dagger, a_1, a_2^\dagger, a_2)$ for our system in terms of $(\hat{\Theta}, \hat{\Pi})$ and then performing the transformation $(\hat{\Theta}, \hat{\Pi}) \rightarrow (\mathbf{r}, \hat{\mathbf{p}})$ to express our ladder operators in terms of $(\mathbf{r}, \hat{\mathbf{p}})$.

The ladder operators we introduce are on the same form as those of the simple harmonic oscillator. We must however first use our constants A_1, A_2, B_1 , and B_2 to find new constants m_1, m_2, Ω_1 and Ω_2 that fit the form of the Hamiltonian for the simple harmonic oscillator given in equation (2.2.1). In this way, the new constants can simply be substituted into equation (2.2.3) to get our desired ladder operators in terms of $(\hat{\Theta}, \hat{\Pi})$.

We do this by imposing²

$$B_1 = \frac{\hbar}{2m_1} \quad A_1 = \frac{\hbar}{2} m_1 \Omega_1^2 \quad B_2 = \frac{\hbar}{2m_2} \quad A_2 = \frac{\hbar}{2} m_2 \Omega_2^2 \quad (3.4.1)$$

Solve these sets of equations for m_1, m_2, Ω_1 and Ω_2 to get the fitted constants

$$\begin{aligned} m_1 &= \frac{\omega_c}{\omega_0^2 - \omega_-^2 - \Omega^2} \\ m_2 &= \frac{\omega_c}{\omega_0^2 - \omega_-^2 + \Omega^2} \\ \Omega_1 &= \frac{1}{2} \sqrt{\omega_c^2 + \omega_0^2 - 2\Omega^2} \\ \Omega_2 &= \frac{1}{2} \sqrt{\omega_c^2 + \omega_0^2 + 2\Omega^2} \end{aligned} \quad (3.4.2)$$

Construct now our ladder operators for the system in terms of $(\hat{\Theta}, \hat{\Pi})$ by substituting m in equation (2.2.3) by m_1 and m_2 , and ω by Ω_1 and Ω_2 . The ladder operators we get are³

²The \hbar 's show up here but not in the "regular" Hamiltonian in equation (2.2.1) because the latter case is based in a system where $[q, p] = i\hbar$, while we have chosen to work with dimensionless bosonic commutation relations.

³Here the \hbar 's from the "regular" expression fall away; see equation (2.2.3)

$$\begin{aligned}
a_1 &= \frac{1}{\sqrt{2m_1\Omega_1}} \left(i\hat{\Pi}_1 + m_1\Omega_1\hat{\Theta}_1 \right) \\
a_1^\dagger &= \frac{1}{\sqrt{2m_1\Omega_1}} \left(-i\hat{\Pi}_1 + m_1\Omega_1\hat{\Theta}_1 \right) \\
a_2 &= \frac{1}{\sqrt{2m_2\Omega_2}} \left(i\hat{\Pi}_2 + m_2\Omega_2\hat{\Theta}_2 \right) \\
a_2^\dagger &= \frac{1}{\sqrt{2m_2\Omega_2}} \left(-i\hat{\Pi}_2 + m_2\Omega_2\hat{\Theta}_2 \right)
\end{aligned} \tag{3.4.3}$$

The last step is to express our ladder operators in terms of the original coordinates of our system; $(\mathbf{r}, \hat{\mathbf{p}})$. We do this by performing the transformation $(\hat{\Theta}, \hat{\Pi}) \rightarrow (\mathbf{r}, \hat{\mathbf{p}})$ given by

$$\begin{pmatrix} \hat{\Theta} \\ \hat{\Pi} \end{pmatrix} = \underline{R} \underline{A} \underline{C} \underline{S} \begin{pmatrix} \mathbf{r} \\ \hat{\mathbf{p}} \end{pmatrix} \tag{3.4.4}$$

Here we use the transformation matrices given in equations 3.3.11, 3.3.4, 3.2.3, and 3.1.6. Insert the new expressions for $(\hat{\Theta}, \hat{\Pi})$ in terms of $(\mathbf{r}, \hat{\mathbf{p}})$ into equation (3.4.3). Tidy up the expressions to get our final ladder operators

$$\begin{pmatrix} a_1 \\ a_2^\dagger \end{pmatrix} = \underline{X} \underline{Y} \begin{pmatrix} x/2l_0 \\ \hat{p}_y l_0/\hbar \end{pmatrix} + i\underline{X}^{-1} \underline{Y}^T \begin{pmatrix} \hat{p}_x l_0/\hbar \\ y/2l_0 \end{pmatrix} \tag{3.4.5}$$

$$\begin{pmatrix} a_1^\dagger \\ a_2 \end{pmatrix} = \underline{X} \underline{Y} \begin{pmatrix} x/2l_0 \\ \hat{p}_y l_0/\hbar \end{pmatrix} - i\underline{X}^{-1} \underline{Y}^T \begin{pmatrix} \hat{p}_x l_0/\hbar \\ y/2l_0 \end{pmatrix}$$

Since $l_0 = \sqrt{\frac{\hbar}{m\omega_0}}$ naturally comes out of the calculations to make the operators dimensionless, we interpret it to be the characteristic length scale of the system. The matrices above are defined as

$$\underline{X} = \begin{pmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix}, \quad \underline{Y} = \begin{pmatrix} \beta_1 & \beta_2 \\ -\beta_2 & \beta_1 \end{pmatrix} \tag{3.4.6}$$

where the coefficients are given by

$$\begin{aligned}
\alpha_1 &= \sqrt{\frac{2m_1\Omega_1}{\alpha}}, & \alpha_2 &= \sqrt{\frac{2m_2\Omega_2}{\alpha}} \\
\beta_1 &= \cos\phi & \beta_2 &= \sin\phi
\end{aligned} \tag{3.4.7}$$

By algebraic manipulation one can also express these coefficients as such

$$\begin{aligned}
\alpha_1 &= \left(\frac{\omega_0^2 + \omega_-^2 - \Omega^2}{\omega_0^2 - \omega_-^2 - \Omega^2} \right)^{\frac{1}{4}} & \alpha_2 &= \left(\frac{\omega_0^2 + \omega_-^2 + \Omega^2}{\omega_0^2 - \omega_-^2 + \Omega^2} \right)^{\frac{1}{4}} \\
\beta_1 &= \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\omega_-^2}{\Omega^2}} & \beta_2 &= -\frac{1}{\sqrt{2}} \sqrt{1 + \frac{\omega_-^2}{\Omega^2}}
\end{aligned} \tag{3.4.8}$$

These coefficients are essentially the same ones used in reference [8], but with slightly different notation.

One may see from the definition of our variables that when $\omega_x = \omega_y$ we have that $\alpha_1 = \alpha_2 = 1$ and $\beta_1 = -\beta_2 = \frac{1}{\sqrt{2}}$. Thus when the two parametres are equal the ladder operators reduce to those of an isotropic electric potential ($\omega_x = \omega_y$).

Some important properties of the ladder operators are their commutation relations. Analogously to the simple harmonic oscillator, the following commutation relations will hold

$$\begin{aligned} [a_i, a_j] &= [a_i^\dagger, a_j^\dagger] = 0 \\ [a_i, a_j^\dagger] &= \delta_{ij} \end{aligned} \quad (3.4.9)$$

We have hence ensured that the two sets of ladder operators commute with each other, but within each set the operators have the same commutation relation as for the simple harmonic oscillator.

Our results make it possible to write our original Hamiltonian from equation (3.1.1) on its final diagonal form, analogously to equation (2.2.5) for the simple harmonic oscillator, as

$$\hat{H}_{xy} = \hbar\Omega_1 \left(a_1^\dagger a_1 + \frac{1}{2} \right) + \hbar\Omega_2 \left(a_2^\dagger a_2 + \frac{1}{2} \right) \quad (3.4.10)$$

where we have omitted including $\hat{p}_z^2/2m$. With our results we have accomplished what we set out to do: Diagonalise the Hamiltonian of our system using ladder operators.

3.4.1 Summary of Main Results

For convenience, we choose to summarise the main results of this thesis; the expressions of our ladder operators and the diagonalised Hamiltonian. The ladder operators can be expressed compactly as

$$\begin{pmatrix} a_1 \\ a_2^\dagger \end{pmatrix} = \underline{X} \underline{Y} \begin{pmatrix} x/2l_0 \\ \hat{p}_y l_0 / \hbar \end{pmatrix} + i \underline{X}^{-1} \underline{Y}^T \begin{pmatrix} \hat{p}_x l_0 / \hbar \\ y/2l_0 \end{pmatrix} \quad (3.4.11)$$

where $\begin{pmatrix} a_1 \\ a_2^\dagger \end{pmatrix}$ is found by complex conjugation. The matrices are defined as

$$\underline{X} = \begin{pmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix}, \quad \underline{Y} = \begin{pmatrix} \beta_1 & \beta_2 \\ -\beta_2 & \beta_1 \end{pmatrix} \quad (3.4.12)$$

where we have used

$$\begin{aligned}\alpha_1 &= \left(\frac{\omega_0^2 + \omega_-^2 - \Omega^2}{\omega_0^2 - \omega_-^2 - \Omega^2} \right)^{\frac{1}{4}} & \alpha_2 &= \left(\frac{\omega_0^2 + \omega_-^2 + \Omega^2}{\omega_0^2 - \omega_-^2 + \Omega^2} \right)^{\frac{1}{4}} \\ \beta_1 &= \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\omega_-^2}{\Omega^2}} & \beta_2 &= -\frac{1}{\sqrt{2}} \sqrt{1 + \frac{\omega_-^2}{\Omega^2}}\end{aligned}\quad (3.4.13)$$

and furthermore

$$\begin{aligned}\omega_c &= \frac{eB}{m}, & \omega_- &= \sqrt{\omega_x^2 - \omega_y^2}, & \omega_0 &= \sqrt{\omega_c^2 + 2(\omega_x^2 + \omega_y^2)} \\ l_0 &= \sqrt{\frac{\hbar}{m\omega_0}}, & \Omega &= (\omega_-^4 + \omega_c^2\omega_0^2)^{\frac{1}{4}}\end{aligned}\quad (3.4.14)$$

The presented expressions for α_1 , α_2 , β_1 , and β_2 are arrived at by algebraic manipulation of alternative expressions for the constants, namely

$$\begin{aligned}\alpha_1 &= \sqrt{\frac{2m_1\Omega_1}{\alpha}}, & \alpha_2 &= \sqrt{\frac{2m_2\Omega_2}{\alpha}} \\ \beta_1 &= \cos \phi, & \beta_2 &= \sin \phi\end{aligned}\quad (3.4.15)$$

where we have defined

$$\begin{aligned}m_1 &= \frac{\omega_c}{\omega_0^2 - \omega_-^2 - \Omega^2}, & m_2 &= \frac{\omega_c}{\omega_0^2 - \omega_-^2 + \Omega^2} \\ \Omega_1 &= \frac{1}{2} \sqrt{\omega_c^2 + \omega_0^2 - 2\Omega^2}, & \Omega_2 &= \frac{1}{2} \sqrt{\omega_c^2 + \omega_0^2 + 2\Omega^2}, \\ \alpha &= \frac{\omega_c}{\omega_0}, & \phi &= \arctan \left[-\frac{\omega_-^2 + \Omega^2}{\omega_c\omega_0} \right]\end{aligned}\quad (3.4.16)$$

Using the ladder operators and the defined constants, we can express the diagonal Hamiltonian of the system as

$$\hat{H}_{xy} = \hbar\Omega_1 \left(a_1^\dagger a_1 + \frac{1}{2} \right) + \hbar\Omega_2 \left(a_2^\dagger a_2 + \frac{1}{2} \right) \quad (3.4.17)$$

We look briefly in section 3.5 at how the theory we have developed can be used to further investigate properties about the system by looking at its energy eigenvalues and stationary eigenstates.

3.5 Eigenstates

From the diagonal Hamiltonian in equation (3.4.10) one can easily read off the eigenvalues of the system as

Enm	Energy [yJ]	E/E_{00}
E_{00}	28.9	1.00
E_{10}	30.0	1.04
E_{01}	85.6	2.96
E_{11}	86.6	3.00

Table 3.5.1: Examples of energy eigenvalues of the four lowest energy states of the electron in yoktojoules and relative to the energy of the ground state; energy eigenvalues are defined in equation (3.5.1). We have used $B = 3$ T and parameter ratios $\frac{\omega_c}{\omega_x} = 5$ and $\frac{\omega_y}{\omega_x} = \frac{1}{2}$

$$E_{nm} = \hbar\Omega_1 \left(n + \frac{1}{2} \right) + \hbar\Omega_2 \left(m + \frac{1}{2} \right) \quad (3.5.1)$$

coming from the fact that one can define a single particle state vector $|nm\rangle$ such that $a_1^\dagger a_1 |nm\rangle = n|nm\rangle$ and $a_2^\dagger a_2 |nm\rangle = m|nm\rangle$ where n and m are quantum numbers of the system. We give examples of the four lowest energy eigenvalues in Table 3.5.1. The above properties indicate that the two sets of operators separately alter different quantum numbers. By effectively working in two dimensions we need two quantum numbers to describe the level of the system, and thus two sets of ladder operators to diagonalise the Hamiltonian of the system. Other important relations for the ladder operators are

$$\begin{aligned} a_1|nm\rangle &= \sqrt{n}|(n-1)m\rangle & a_1^\dagger|nm\rangle &= \sqrt{n+1}|(n+1)m\rangle \\ a_2|nm\rangle &= \sqrt{m}|n(m-1)\rangle & a_2^\dagger|nm\rangle &= \sqrt{m+1}|n(m+1)\rangle \end{aligned} \quad (3.5.2)$$

These are important relations for further investigation of the dynamics of our system, since they allow us to move between states in a simple manner. It may also be apparent that these relations are very useful when studying the eigenstates of the system. In order to find the ground state, one simply solves the set of coupled partial differential equations (PDEs)

$$a_1|\psi_{00}\rangle = 0 \quad a_2|\psi_{00}\rangle = 0 \quad (3.5.3)$$

where we are now working in regular position space. These equations will be of form

$$axf(x, y) + byf(x, y) + c\frac{\partial f}{\partial x}(x, y) + d\frac{\partial f}{\partial y} = 0 \quad (3.5.4)$$

where the coefficients are complex and are determined by the coefficients in a_1 and a_2 . The set of PDEs can be solved using the ansatz $|\psi_{00}\rangle = Ce^{ax^2+by^2+cxy}$. Another approach which we followed is to use a superposition of the two annihilation operators a_1 and a_2 such that we are left with two PDEs where each only contains one partial derivative. The two PDEs we are left with are

$$\begin{aligned} \left(\frac{1}{\alpha_1 \beta_2} a_1 - \frac{1}{\alpha_2 \beta_1} a_2 \right) |\psi_{00}\rangle &= 0 \\ \left(\frac{\alpha_1}{\beta_1} a_1 + \frac{\alpha_2}{\beta_2} a_2 \right) |\psi_{00}\rangle &= 0 \end{aligned} \quad (3.5.5)$$

Here, the first PDE only contains a partial derivative in x , and the second PDE only in y . Combining the resulting wavefunctions from the two PDEs and normalizing such that $\iint_{-\infty}^{\infty} dx dy \langle \psi_{00} | \psi_{00} \rangle = 1$, we obtain the eigenfunction for the ground state

$$|\psi_{00}\rangle = \sqrt{\frac{\alpha_1 \alpha_2 (\beta_1^2 + \beta_2^2)}{2\pi l_0^2 (\alpha_1^2 \beta_2^2 + \alpha_2^2 \beta_1^2)}} \exp \left\{ -\frac{ax^2 + by^2 + cxy}{4l_0^2 (\alpha_1^2 \beta_2^2 + \alpha_2^2 \beta_1^2)} \right\} \quad (3.5.6)$$

where we have coefficients

$$a = \alpha_1^2 \alpha_2^2 (\beta_1^2 + \beta_2^2) \quad b = (\beta_1^2 + \beta_2^2) \quad c = 2i \beta_1 \beta_2 (\alpha_1^2 - \alpha_2^2) \quad (3.5.7)$$

Continuing to use the properties of our ladder operators described in equation (3.5.2), one can see that every state can be reached from the ground state by operating the creation operator on it. Thus we can express every eigenstate by

$$|\psi_{nm}\rangle = \frac{1}{n!m!} (a_1^\dagger)^n (a_2^\dagger)^m |\psi_{00}\rangle \quad (3.5.8)$$

Another great benefit of working with ladder operators may now be apparent: they give us simple ways of finding eigenvalues and eigenfunctions of the system. In Figure 3.5.1 we have found the four eigenfunctions with lowest energy and plotted their absolute value squared, $|\langle \psi_{nm} | \psi_{nm} \rangle|^2$, as this corresponds to the probability density of an electron in our system.

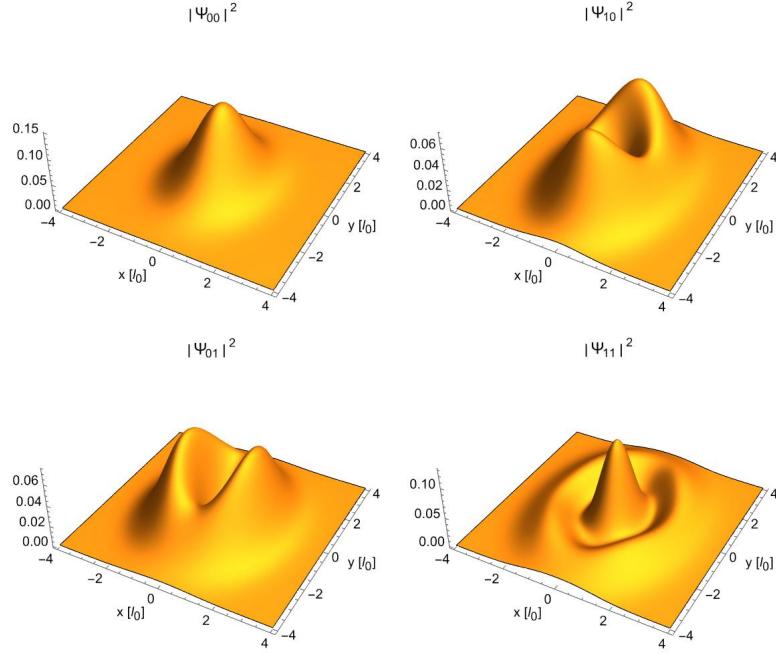


Figure 3.5.1: Examples of 3D-plots for the probability density distributions of the four lowest energy eigenstates in our system. We have used $B = 3$ T, and parameter ratios $\frac{\omega_c}{\omega_x} = 5$ and $\frac{\omega_y}{\omega_x} = \frac{1}{2}$ in both figures. The x - and y -axes are in units of l_0 .

The plots from Figure 3.5.1 show qualitatively the effect of the elliptic potential. The distributions are symmetric or anti-symmetric along the coordinate axes separately, but are not isotropic as they would be if the potential itself was isotropic. We also see the difference between the two first excited states $|\psi_{10}\rangle$ and $|\psi_{01}\rangle$, where the electron is more likely to lie closer to the x -axis or the y -axis respectively. It is also generally apparent that the electron is less likely to move further in the x -direction than the y -direction, due to the stronger electric field in the x -direction. The difference between the two quantum numbers is quantitatively apparent in Table 3.5.1, where we have given examples of eigenvalues for the four eigenstates with lowest energy. Increasing m yields a larger energy increase than if one increases n . This means that the orbitals related to the quantum number m are more energetic than those of n . This too is due to the fact that the electron is less restricted in the y -direction than in the x -direction.

CHAPTER
FOUR

DISCUSSION

4.1 Method

The diagonalisation of the Hamiltonian in equation (3.1.1) has been done before. One example of how to diagonalise this Hamiltonian is to employ Bogoliubov transformations. This method demands one has knowledge of such transformations, and is somewhat more abstract in nature [5]. The method we have showcased is simply a different method, and an intuitive one at that since it is based upon geometric arguments. The results we obtain are however, with some algebra, identical to those of Kyriakidis and Penney (2005) [8], and the elegant way of presenting the results falls very naturally from the calculations. In the paper, Kyriakidis and Penney do not disclose how they arrive at the results they obtain for their diagonalised Hamiltonian, so we cannot be sure if they have employed the same method as we have done. There is of course only one solution to the problem, so the fact that the results are the same is as expected.

It is worthwhile to mention that a canonical transformation might not be necessary in order to follow the method we have showcased. The original Hamiltonian is, when expanded, of form

$$\hat{H}_{xy} = ax^2 + bx\hat{p}_y + c\hat{p}_y^2 + dy^2 + ey\hat{p}_x + f\hat{p}_x^2 \quad (4.1.1)$$

where the coefficients are constants. By again utilising an analogy of ellipses, only this time the two ellipses are in the systems (x, \hat{p}_y) and (y, \hat{p}_x) , it might be possible to simply scale and rotate these systems in the exact same way as we did in section 3.3; scale x and \hat{p}_x by a factor α and rotate both ellipses through the same angle. As the process of finding a suitable canonical transformation was the hardest and most abstract task of developing the method of diagonalisation, skipping this step would simplify the method even further.

An additional note about the method is the importance of working with the symmetric gauge for the magnetic vector potential $\hat{\mathbf{A}}$. A simpler gauge alternative could be the Landau gauge $\hat{\mathbf{A}} = (0, Bx, 0)$. Such a gauge also yields a magnetic field \mathbf{B} in positive z -direction. The resulting Hamiltonian would however not be

of the form of two rotated ellipses. One of the ellipses would not be rotated. In equation (4.1.1) this would correspond to $e = 0$, and in equation (3.2.4) it would correspond to either $B_Q = 0$ or $B_P = 0$. in order to scale a rotated ellipse to align parallel with a non-rotated ellipse, the scaling factor would have to be $\alpha = \infty$. Such a scaling would be nonsensical and would certainly not yield any meaningful results. The symmetric gauge is thus our best alternative, as its corresponding Hamiltonian yields two rotated ellipses.

4.2 Properties of the System

The parameter l_0 occurs in the expressions for the ladder operators in equation (3.4.5), which we briefly mentioned seemed to be the characteristic length scale of the system. This is analogous to the magnetic length l_B , which is the characteristic length scale of the radii of the orbitals of a particle in a magnetic field. If we use $B = 3$ T and the relations $\frac{\omega_c}{\omega_x} = 5$, and $\frac{\omega_y}{\omega_x} = \frac{1}{2}$, we get that $l_B \approx 14.8$ nm and $l_0 \approx 14.4$ nm. For these specific values we see that l_0 is just over 2% smaller than l_B . This in turn can indicate that the orbitals of the elliptically confined electron in general have a slightly smaller radius than those of an electron in just a magnetic field. This is coherent with what one would expect: the harmonic electric potential somewhat restricts how far away from the origin the electron can move, meaning it must orbit with a smaller radius compared to the case with no electric field. From their definitions it is also apparent that l_0 always will be smaller than or equal to l_B , specifically because $\omega_0 \geq \omega_c$.

4.3 Future Work

As mentioned in the introduction, the motivation for diagonalising the Hamiltonian of our system was to construct a theoretical framework to be used in the construction of a spin-0 semiconductor spin qubit. We discuss in this section what work must further be done to construct our desired qubit, and other interesting remarks. Most of the points we bring up about future work is based on the methods of Kyriakidis and Burkard (2007) [4].

In order to further investigate the dynamics of our system we would have to consider electron interactions. We would do this by considering pairwise long-range Coulomb interactions explicitly, and we would utilize our bosonic operators in order to work within the second quantized formalism. In the second quantized formalism the total Hamiltonian of a multi-particle system of identical particles can be expressed as the infinite sum of Hamiltonians

$$\hat{H} = \hat{H}^{(1)} + \hat{H}^{(2)} + \hat{H}^{(3)} + \dots \quad (4.3.1)$$

The first term is the sum of all non-interacting single-particle Hamiltonians, the second term is the sum of all two-particle interactions, the third term is the sum of all three-particle interactions, and so on [9]. The work we have done above has been to diagonalise the first term in the expansion in equation (4.3.1). The

pairwise long-range Coulomb interactions will be governed by the second term of the expansion. The long range Coulomb interaction energy goes as $1/r$, and in the total Hamiltonian of the system the pairwise interactions are expressed as such

$$\hat{H}^{(2)} = \frac{1}{2} \sum V_{ijkl} c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma'} c_{k\sigma} \quad (4.3.2)$$

where all indices $(ijkl\sigma\sigma')$ are summed over, the Latin indices $(ijkl)$ each represent a pair of orbital quantum numbers (n, m) , and the Greek indices represent spin $(\sigma, \sigma' = \pm 1/2)$. To calculate the matrix elements V_{ijkl} , we would perform a two-dimensional Fourier transform as such

$$V_{ijkl} = \int d^2q \frac{e^2}{2\pi q} (m_1 n_1, m_2 n_2 | e^{i\mathbf{q} \cdot (\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2)} | m_3 n_3, m_4 n_4) \quad (4.3.3)$$

It may now be apparent why diagonalising the single-particle Hamiltonian pays off here. To evaluate this integral we express the coordinate $\hat{\mathbf{r}} = (x, y)$ in terms of our bosonic operators defined in equation (3.4.5). We then proceed by inserting these expressions into the integral in equation (4.3.3) and evaluating it explicitly. The exponential will then be expanded as an infinite power series where each term contains of our bosonic ladder operators. The use of ladder operators simplifies of our calculations because the following is true

$$(m_1 n_1, m_2 n_2 | m_3 n_3, m_4 n_4) = \delta_{m_1 m_3} \delta_{n_1 n_3} \delta_{m_2 m_4} \delta_{n_2 n_4} \quad (4.3.4)$$

The implication of this is that the only terms that are non-zero in the integral in equation (4.3.3) are terms where $m_1 = m_3 \wedge n_1 = n_3 \wedge m_2 = m_4 \wedge n_2 = n_4$. Since the ladder operators in each term alter the values of m_3 , n_3 , m_4 , and n_4 , only terms with a specific number of different creation and annihilation operators will contribute to the matrix elements V_{ijkl} . In this way one can eliminate numerous terms that do not contribute and ultimately end up with an explicit expression for V_{ijkl} . These results would then be used further in the construction of our desired qubit.

A qubit is a two-level system, meaning it can always be described by the Hamiltonian of a spin-1/2 particle in a pseudomagnetic field

$$\hat{H} = b_x \sigma_x + b_y \sigma_y + b_z \sigma_z \quad (4.3.5)$$

where the matrices σ_i are the Pauli spin matrices and $\mathbf{b} = (b_x, b_y, b_z)$ is the pseudomagnetic field. The more general Hamiltonian would include a term with the identity matrix I , but this term does not alter the dynamics of the system, so we ignore it here. By pseudomagnetic field we mean an effective magnetic field with which the system "is affected by". The field is not physically present, but the system behaves as if it was. The picture of a spin-1/2 particle is used to make it easier to think about the behaviour of our arbitrary two-level system.

For a system of four electrons in a single quantum dot we would be able to construct the two levels $|0\rangle$ and $|1\rangle$ of a qubit to have the same orbital occupation, the same charge density, and both with a total spin of zero. The Hamiltonian of the qubit could then be expressed on the form in equation (4.3.5) by projecting the total Hamiltonian of the system onto the subspace spanned by the two basis states we choose for the qubit, and then mapping the Hamiltonian to the spin-1/2 particle Hamiltonian in equation (4.3.5). If one wants an exact Hamiltonian for the qubit one would need to compute all terms in equation (4.3.1)s, but the two first terms would potentially be enough to sufficiently describe the behaviour of the qubit.

It might seem counter intuitive that we have defined a qubit with zero spin which behaves as a pseudospin-1/2 particle in a pseudomagnetic field, but this is just a simple and intuitive way to imagine the dynamics of a two-level system. The general theory is identical for any two-level system, and thus one can think of a spin-1/2 particle precessing about a magnetic field when working with an arbitrary two-level system in order to get an intuitive sense of how the system behaves.

When constructing the system of our qubit we insisted there be a constant magnetic field perpendicular to the xy -plane in which the electric field lies. Why do we insist there be a magnetic field? It turns out that we need two tunable parameters in our electric potential to control the qubit.¹ An ellipse is the simplest such shape, but asymmetric potentials would also work. Altering these parameters would directly affect the pseudomagnetic field \mathbf{b} of our qubit. The two parameters of the electric potential are however not enough to control the qubit. In [4] it is found that the pseudomagnetic field of their three-electron qubit depends upon the two ratios $\frac{\omega_y}{\omega_x}$ and $\frac{\omega_c}{\omega_x}$. The magnetic field is included in the second ratio, and it seems therefore a physical magnetic field must be present to control the qubit. It is however important to note that the two ratios can be completely determined by ω_x and ω_y . The magnetic field need only be present, but it can be left constant. This is a huge advantage as altering and controlling the magnetic field is a relatively harder task than altering the electric potential.

The critical effect of being able to control the pseudomagnetic field by tuning the eccentricity of the confinement potential is that it allows us to control the qubit even if the spin of the qubit is zero. If the qubit is spinless, it does not couple at all to its environment through spin channels. This fact does implicate that one cannot control the qubit through spin channels. Even though the total spin of the qubit is zero, the individual electron spins vary between the two qubit basis states. One must therefore physically alter the spin of the electrons when rotating the qubit between states. This would seem to pose a problem, since it appears one needs to alter spin of a system with total spin zero. This is however not a problem, specifically because the system can be controlled by tuning the electric potential. In this way, tuning of the potential omits the problem of spin channels and allows us to keep the monumental positive of having a spinless qubit.

As we now have discussed how a single qubit would look and work, we will now

¹A circular confinement would therefore not suffice, seeing it has one tunable parameter.

turn our attention to how we would manipulate the entanglement between two qubits. The entanglement between qubits is what gives quantum computers their computational edge relative to classical computers, and controlling this is critical. Control in the context of our qubit would be attained by lowering the magnitude of the potential between the two qubits in question. In this way one can write the total Hamiltonian of a system containing two of our qubits as

$$\hat{H} = \hat{H}_{dot1} + \hat{H}_{dot2} + \hat{H}_{coupling} \quad (4.3.6)$$

where \hat{H}_{dot1} and \hat{H}_{dot2} are Hamiltonians for the two qubits, and $\hat{H}_{coupling}$ is the Hamiltonian for altering of the potential wall between qubits. By lowering the potential wall, one can control to what degree the different orbitals in each qubit couple. One can for example lower the wall just enough in such a way that coupling between the qubits is dominated by coupling between the single-particle orbital occupation with the highest energy. This occupation will couple first because it is highest in energy, meaning it overcomes the gap between qubits first when the potential is lowered, and because the orbital is located closer to the edge of the qubit potential.

CHAPTER
FIVE

CONCLUSIONS

We have presented in this thesis an intuitive and elegant way of diagonalising the Hamiltonian for an electron in an elliptically confined harmonic potential in the xy -plane, and a constant magnetic field that points in the positive z -direction. We did this by deriving creation and annihilation operators for the system. The method we presented involved a canonical transformation of dimensionless coordinate and canonical momentum operators, followed by a scaling and a rotation of the coordinate systems. We then acquired canonical operators for which the corresponding Hamiltonian is diagonal. The scaling and rotation we performed utilised an analogy of scaling and rotating ellipses, as the form of the Hamiltonian matched the general expressions of rotated ellipses centered at the origin. By use of such an analogy we are able to visualise and intuitively understand the diagonalisation process. Further, we used theory about ladder operators for the simple harmonic oscillator to construct our final ladder operators. This was done by mapping our diagonal Hamiltonian onto the expression for ladder operators for the simple harmonic oscillator. To finalise our ladder operators, we reversed our transformations. The expressions for the ladder operators can be expressed using purely algebraic expressions. Lastly we looked at how to derive the eigenstates of the system using our ladder operators. This was done by obtaining a partial differential equation by annihilating the vacuum. One then solves this partial differential equation to obtain a wavefunction for the stationary ground state. Lastly one can obtain any stationary eigenstate by iterative operations of the creation operators on the ground state. The resulting probability densities show clearly the influence of an elliptic potential, as they all exhibit the same symmetries as an ellipse. In addition, the elliptic potential results in two quantum numbers n and m that are needed to describe a state of the system. By assessing energy eigenvalues of the system it is apparent that the energy increase corresponding to an increase in either n or m is not equal; again iterating the influence of an elliptic potential.

The purpose of deriving the ladder operators we obtained is to document the intuitive way in which we did so. Additionally, we derived the ladder operators in order to simplify further calculations. We hypothesise that one could construct a spin-0 semiconductor spin qubit by having four electrons in the elliptic quantum dot we have described. Theory about how the electrons will interact would then be needed, and the ladder operators we have derived would simplify such calcu-

lations considerably. To construct such a qubit could be worthwhile as a spin-0 semiconductor spin qubit is insensitive to noise from the environment which couples to the spin of the qubit. Additionally, the two basis states of the qubit would have the same charge density and orbital occupation, meaning the two states react similarly to disturbances. This in turn could counteract decoherence of the qubit significantly. In order to control the qubit one would simply need to tune the eccentricity of the electric confinement of the dot. We would then be able to reliably control the qubit whilst keeping the magnetic field constant. Entanglement between qubits would be manipulated by altering of the electric potential. The combination of controlling the qubit by manipulating the electric potential, the two basis states of the qubit being similar and of spin-0, and the possibility of keeping a constant magnetic field, makes for an attractive proposal for a qubit.

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APPENDICES

A - ROTATED ELLIPSE

In our calculations we need an expression for the angle of a rotated ellipse using the coefficients in the equation of the ellipse. We derive such an expression in this appendix.

The equation of a non-rotated ellipse centered at the origin is

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad (\text{A.1})$$

In order to get the expression for a rotated ellipse, we rotate our coordinate system by an angle ϕ . This is done using the substitutions $x = X \cos \phi + Y \sin \phi$ and $y = -X \sin \phi + Y \cos \phi$. By plugging this into equation (A.1) and rearranging a bit, one gets the general equation for a rotated ellipse centered at the origin

$$AX^2 + BXY + CY^2 = F \quad (\text{A.2})$$

where the coefficients can be found to be

$$\begin{aligned} A &= a^2 \sin^2 \phi + b^2 \cos^2 \phi \\ B &= 2 \sin \phi \cos \phi (b^2 - a^2) \\ C &= a^2 \cos^2 \phi + b^2 \sin^2 \phi \\ F &= a^2 b^2 \end{aligned} \quad (\text{A.3})$$

In equation (A.3) we would like to solve for ϕ . We do so by assessing

$$\begin{aligned} A - C &= \cos^2 \phi (b^2 - a^2) - \sin^2 \phi (b^2 - a^2) \\ \frac{B}{2 \sin \phi \cos \phi} &= b^2 - a^2 \end{aligned} \quad (\text{A.4})$$

Combine these two equations to get the quadratic equation

$$\frac{B}{2} \tan^2 \phi + (A - C) \tan \phi - \frac{B}{2} = 0 \quad (\text{A.5})$$

This has two solutions from which we chose the smallest one, since the other

solution does not correspond to the angle in which we are interested. The resulting expression for the angle of a rotated ellipse centered at the origin then becomes

$$\phi = \arctan \left(\frac{1}{B} \left(C - A - \sqrt{(A - C)^2 + B^2} \right) \right) \quad (\text{A.6})$$

