The quantum advantage to charging electron spin qubit batteries

Bachelor thesis

by

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Abstract

Quantum thermodynamics takes over from classical thermodynamics when systems are of the scale of single particles and quantum fluctuations have a noticeable effect. An interesting topic of research of this relatively new field is the quantum battery, which in this thesis consists of an array of N identical electron spin qubits. In an article by Binder et al. [4], it is proven that in theory, an N-times decrease in charging time of the battery is achieved when global operations on qubits are permitted. This thesis investigates if a similar advantage can be achieved by using a local qubit-qubit interaction operator on a one-dimensional chain of exchange-coupled electron spin qubits that are driven by microwave radiation in the presence of decoherence. This system is described by a density matrix in order to include the presence of external influences. The time-evolution of the state of the system is calculated by solving the Von-Neumann equation both analytically and numerically, which is then used to calculate the extractable work. It is shown that exchange interaction does not have a direct effect on the extractable work, since it creates entanglement between two states of the same energy level and the operator commutes with the Hamiltonian of the system. The effect of the CNOT gate on the state of the system is then investigated. While it does have an effect on the extractable work, it did not achieve a decrease in charging time. These results are only relevant for the specific system used in this thesis. For other methods and systems, exchange interaction could lead to faster charging.

Contents

Chapter 1

Introduction

The theory of quantum thermodynamics is a very new and active field of research. Whereas classical thermodynamics describes macroscopic systems, quantum thermodynamics describes very small systems where quantum effects have a noticeable influence. In the classical situation, a macroscopic system is described by its average quantities, such as temperature or extractable work. However, as the size of a system becomes smaller and smaller, the approximations become less accurate. The quantities will fluctuate around the average due to thermal motion. Stochastic thermodynamics is used to describe this behaviour. Unfortunately, even stochastic thermodynamics fails when the fluctuations start to have a quantum origin. Consequently, the field of quantum thermodynamics was created to investigate these developments. In an article published by Millen in 2016 [3], there is an interesting overview of the current developments in this field and an outlook towards the future of quantum thermodynamics.

An interesting concept of this new field is the quantum battery. The definition of a battery is a physical system that stores energy. In a quantum system, energy can be stored in the populations and coherences of an electron qubit system. When this energy is extracted, this results in an amount of work. Since this system has a quantum nature, there are effects that would not be possible in a classical system and cannot be described as such. In the article by Binder [4], a method is described to charge quantum batteries with more power when a global entangling operator is used. In this thesis, we will look at the possibility of achieving similar advantages in charging time and charging power when using qubit-qubit interaction operators. Specifically, we will investigate the charging of a one-dimensional chain of exchange-coupled electron spin qubits that are driven by microwave radiation in the presence of decoherence; dissipation and dephasing.

In this research, we will gain understanding of the behaviour of electron spin qubits by solving the Von Neumann equation analytically and numerically under the influence of different operators. We describe the system with a density matrix to include external influences, for which the standard wave function is not suitable. The effect of time-dependent entangling operators will be investigated numerically. An important goal of this research is to describe the system realistically and we make use of operators that can be created experimentally.

The theory required to describe our system is given in chapter 2, which is followed by the analytical solutions in chapter 3. The numerical calculations and predictions for optimal charging are made in chapter 4 and the results will be discussed in chapter 5. In the final chapter we draw a conclusion and take a look at possible further research in this area.

Chapter 2

Theory

This chapter introduces the theory required for this thesis. It describes the mathematical representation of the electron spin qubits, including the operators acting on the system and the equations that describe the time dependent state of the system. The power and extractable work of the battery are defined, which can be calculated from the state of the system.

2.1 Pauli matrices

The Pauli matrices act on the 2-dimensional complex Hilbert space [2]. They represent the component of the electron spin along the $\hat{x}, \hat{y}, \hat{z}$-axis respectively.

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{2.1}$$

$$\hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{2.2}$$

$$\hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.3}$$

2.2 Density matrix

When we are dealing with an isolated quantum system, the wave function is a complete representation of the system state. In this thesis, however, the system is no longer isolated and can only be described by a set of quantum states. Therefore, we introduce the density operator, which is the optimal specification for the system. The density operator is defined as [2]:

$$\hat{\rho} = \sum_i p_i \left|\varphi_i\right\rangle \left\langle\varphi_i\right| \tag{2.4}$$

where p_i is the probability for the system to be in the state $|\varphi_i\rangle$. The states are normalised, which means that $\langle\varphi_i \mid \varphi_i\rangle = 1$. Of course, the sum of the probabilities should equal one, since the system always has to be in one of the possible states. Mathematically this is equal to $\sum_i p_i = 1$. The density operator is advantageous when calculating the expectation value of an operator. It uses the trace (tr) operator, which sums the terms on the diagonal of a matrix. In other words, the trace of an n-by-n square matrix $\hat{A}$ is defined as:

$$tr(\hat{A}) = a_{11} + a_{22} + ... + a_{nn} = \sum_{i=1}^{n} a_{ii} \tag{2.5}$$

with respect to an orthonormal basis. The expected value of an operator in state (2.4), is then given by the expression:

$$\langle \hat{A} \rangle = tr(\hat{\rho}\hat{A}) = \sum_{i=1}^{n} p_i \; tr(|\varphi_i\rangle \langle \varphi_i| \, \hat{A}) = \sum_{i=1}^{n} p_i \langle \varphi_i| \, \hat{A} \, |\varphi_i\rangle \tag{2.6}$$

This is just the average of the expectation values for pure quantum states $|\varphi_i\rangle$.

2.3 Evolution of the density matrix in time

Since we are interested in the time dependent state of the system we are investigating, we need to find an expression that describes the time-evolution of the quantum state in terms of the density matrix. We start with the Schrödinger equation that describes the time-evolution of the wave function of the system [2]:

$$i\hbar \frac{\partial}{\partial t} |\varphi(t)\rangle = \hat{H} \, |\varphi(t)\rangle \tag{2.7}$$

The Schrödinger equation is equivalent to the Von Neumann equation, which describes the time-evolution of the density matrix :

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] \tag{2.8}$$

2.4 Electron spin qubit

In this report, we will work with arrays of electron spin qubits. This qubit consists of an electron confined to a quantum dot, a small island in a semiconductor heterostructure, in an external magnetic field $\vec{B}_z$. The field induces Zeeman splitting, such that the two basis state of the qubit, $|0\rangle = |\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, have a difference in energy level of E_z. As mentioned earlier, the state of a system of electron spin qubits is described by a density matrix. Every system has basis states. If we take a system of one qubit as an example, we find the basis states as mentioned above. The diagonal elements of the density matrix describe the probability to be in the corresponding state, which are called the populations. The off-diagonal elements describe the coherence between two of the basis states. Accordingly, they are called the coherences.
A useful way of visualising an electron spin qubit is the Bloch sphere.

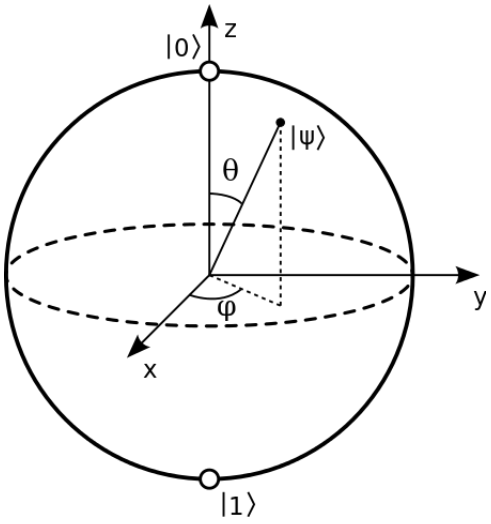

Figure 2.1: The Bloch sphere: a 3D visualisation of the states of an electron spin qubit.

The two basis states are identified with the north and south pole. The surface of the sphere describes the pure states of the qubit. This is seen if we decompose the density matrix $\hat{\rho}$ in its cartesian composition $\mathbf{a} = (a^x, a^y, a^z)^T$ with respect to the Pauli matrices, such that:

$$\hat{\rho} = \frac{1}{2}(I + \mathbf{a} \cdot \boldsymbol{\sigma}) \tag{2.9}$$

where I is the 2×2 identity matrix. A pure density matrix is characterised by the fact that $\hat{\rho}^2 = \hat{\rho}$.

$$\hat{\rho}^2 = \frac{1}{4}(I + 2\mathbf{a} \cdot \boldsymbol{\sigma} + (\mathbf{a} \cdot \boldsymbol{\sigma})^2) = \frac{1}{4}(I + 2\mathbf{a} \cdot \boldsymbol{\sigma} + \mathbf{a}^2) \tag{2.10}$$

This is equal to $\hat{\rho}$ if $\mathbf{a}^2 = 1$ or in other words, if $|\mathbf{a}| = 1$.

The Hamiltonian of an electron spin in a quantum dot in an external magnetic field in the $\hat{z}$-direction is defined as:

$$\hat{H_0} = \frac{1}{2} g^* \mu_b B_z \hat{\sigma}_z \tag{2.11}$$

where $\vec{B}_z$ is defined as the magnetic field applied along the $\hat{z}$-axis, μ_b as the Bohr magneton, g^* as the g-factor and $\hat{\sigma}_z$ as the Pauli spin $\hat{z}$-matrix. If we now define $E_z \equiv |g^* \mu_b B_z|$ as the Zeeman energy splitting, then the Hamiltonian in matrix form is given by:

$$\hat{H}_0 = \begin{bmatrix} -\frac{1}{2}E_z & 0 \\ 0 & \frac{1}{2}E_z \end{bmatrix} \tag{2.12}$$

We observe that this system has two different energy levels, in other words we are dealing with a simple battery that is either charged or not charged. Finally, an electron spin qubit can spontaneously decay from an excited state to a lower state. This phenomenon is described by the projection operator:

$$\hat{S}_\downarrow = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{2.13}$$

The effect of decay of a pure state $|\chi\rangle$ to the ground state is given by:

$$|\chi\rangle \rightarrow \frac{\hat{S}\,|\chi\rangle}{\sqrt{\langle\chi|\,\hat{S}^\dagger \hat{S}\,|\chi\rangle}} \tag{2.14}$$

or in the density matrix form:

$$\hat{\rho} \to \frac{\hat{S}\hat{\rho}\hat{S}^\dagger}{tr(\hat{S}\hat{\rho}\hat{S}^\dagger)} \tag{2.15}$$

For one spin this implies: $|\chi\rangle \to |\uparrow\rangle$ or $\hat{\rho} \to |\uparrow\rangle\langle\uparrow|$.

2.5 Electron spin resonance (ESR)

In order to coherently rotate the electron spin, we make use of externally applied microwave radiation, generated by an additional time-dependent cyclic magnetic field $B(t)$ perpendicular to the $\hat{z}$-axis. This process is called Electron Spin Resonance (ESR). If we then take the field along the $\hat{x}$-axis, the corresponding interaction term in the Hamiltonian is given by:

$$\hat{V}(t) = \frac{1}{2} g^* \mu_b B \cos(\omega t)\hat{\sigma}_x \tag{2.16}$$

Here ω is the driving frequency.

2.6 Tensor product

The tensor product is needed for describing a system with multiple particles using product spaces. The product $U \otimes V$ of two vector spaces U and V gives a new vector space and an operation $\otimes$. The operation is defined as sending ordered pairs in the Cartesian product $U \times V$ into $U \otimes V$ [2]. Since we are only concerned with two-level systems, it suffices to introduce the tensor product for a 2×2 matrix. If we have two matrices A and B defined as:

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix}$$

$$B = \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix}$$

Then we define their tensor product as:

$$A \otimes B = \begin{bmatrix} a_{1,1}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{1,2}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \\ a_{2,1}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{2,2}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_{1,1}b_{1,1} & a_{1,1}b_{1,2} & a_{1,2}b_{1,1} & a_{1,2}b_{1,2} \\ a_{1,1}b_{2,1} & a_{1,1}b_{2,2} & a_{1,2}b_{2,1} & a_{1,2}b_{2,2} \\ a_{2,1}b_{1,1} & a_{2,1}b_{1,2} & a_{2,2}b_{1,1} & a_{2,2}b_{1,2} \\ a_{2,1}b_{2,1} & a_{2,1}b_{2,2} & a_{2,2}b_{2,1} & a_{2,2}b_{2,2} \end{bmatrix} \tag{2.17}$$

2.7 Two electron spin system

Most of the calculations in this report are done on a two electron spin system. The basis states for this system are given by:

$$|\uparrow\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad |\downarrow\uparrow\rangle = |\uparrow\rangle \otimes |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \tag{2.18}$$

$$|\uparrow\downarrow\rangle = |\downarrow\rangle \otimes |\uparrow\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad |\downarrow\downarrow\rangle = |\downarrow\rangle \otimes |\downarrow\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Now it is straightfoward to verify that:

$$(A \otimes B) \left|\uparrow\uparrow\right\rangle = A \left|\uparrow\right\rangle \otimes B \left|\uparrow\right\rangle$$

2.8 Exchange interaction

Nearby electron spins feel an effective interaction due to the Pauli exclusion principle. This states that identical fermions cannot be in the same state at the same time. The electrons do not feel this effect if the potential barriers separating them are high enough, however if the potential barrier is lowered, they feel exchange interaction and the qubits become entangled.

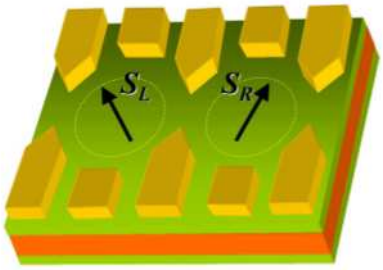

Figure 2.2: Two electron spin qubits in neighbouring quantom dots [8]

The interaction term in the Hamiltonian for this effect is given by:

$$\hat{H}_{ex}(t) = J(t)\vec{\boldsymbol{\sigma}}_1 \otimes \vec{\boldsymbol{\sigma}}_2 \tag{2.19}$$

$$= J(t) \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{2.20}$$

with $\vec{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ the Pauli spin matrix vector and $\vec{\boldsymbol{\sigma}}_i$ acting on qubit i, with $i = 1, 2$. The time-dependence of this operator is modelled by the function $J(t)$. The strength of J can be controlled by changing the height of the potential barriers. Throughout this model, we assume that there is only nearest-neighbour interaction. In other words, there is no exchange possible between electron spin qubits that have another spin qubit between them.

2.9 CNOT gate

The controlled NOT gate (or CNOT gate) is a unitary operation that can be used to entangle and disentangle states of a 2 qubit system. The gate flips the target qubit if and only if the control qubit is in the down state. It can be represented by the matrix form:

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{2.21}$$

The gate then has the following effect: $\hat{\rho} \rightarrow U\hat{\rho}\, U^{\dagger}$.

2.10 Extending operators to N electron spin qubits

In order to extend our calculations to an array of N electron spin qubits, the operators need to be expanded so they act in the larger Hilbert space. Taking the initial 2×2 operator P, we want to describe the operator acting solely on the k^{th} qubit. This is achieved by taking the tensor product of N matrices of which the k^{th} is the operator and the rest are simply identity matrices:

$$P(k) = I \otimes I \otimes ... \otimes P \otimes ... \otimes I \tag{2.22}$$

The operator that describes the array is then simply the sum of all the individual operators:

$$P_N = \sum_{k=1}^{N} P(k) \tag{2.23}$$

2.11 The Lindblad superoperator

In order to describe the decoherence of the electron spin qubits, we make use of the Lindblad superoperator [2]. The projection operator $\hat{S}_i$, acting on the i^{th} electron spin qubit, is achieved by applying the method described in section 2.10 on equation (2.13). The Lindblad operator is then given by:

$$\hat{L}[\hat{\rho}] = \hat{S}_i \hat{\rho} \hat{S}_i^\dagger - \frac{1}{2} \hat{S}_i^\dagger \hat{S}_i \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{S}_i^\dagger \hat{S}_i \tag{2.24}$$

This operator describes the dissipation of energy into the surroundings. Since the system consists of N particles, the operator acting on all particles is described by:

$$\hat{L}_N[\hat{\rho}] = \sum_{i=1}^{N} \hat{S}_i \hat{\rho} \hat{S}_i^\dagger - \frac{1}{2} \hat{S}_i^\dagger \hat{S}_i \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{S}_i^\dagger \hat{S}_i \tag{2.25}$$

2.12 Ergotropy and power of a quantum battery

Ergotropy, $\mathcal{W}$, is defined as the maximum work that can be extracted unitarily from a quantum state $\hat{\rho}$ with respect to a Hamiltonian $\hat{H}_0$ [4]. In order to express the ergotropy of a quantum battery, the internal energy of our system is required. This is given by $tr[\hat{\rho}\hat{H}_0]$, where in this case $\hat{\rho}$ is the state of the battery and $\hat{H}_0$ its internal Hamiltonian. The lowest energy state is called a passive state and the highest energy state a maximally active state, denoted by $\hat{\pi}$ and $\hat{\omega}$. Consequently, the ergotropy is defined as:

$$\mathcal{W} = tr[\hat{\rho}\hat{H}_0] - tr[\hat{\pi}\hat{H}_0] \tag{2.26}$$

The maximal ergotropy is therefore $tr[\hat{\omega}\hat{H}_0] - tr[\hat{\pi}\hat{H}_0]$. Since we are mostly interested in charging a battery, it is useful to consider the average power of a process, which is given by:

$$\langle P \rangle = \frac{\langle W \rangle}{T} \tag{2.27}$$

where T is the time for the process to take place and $\langle W \rangle$ is the average work done in the process.

We define what it means to charge and decharge a battery. Charging a battery means to change its state from $\hat{\rho}$ to a higher energetic state $\hat{\rho}'$ such that $tr[(\hat{\rho}' - \hat{\rho})\hat{H}_0] \geq 0$. On the other hand, extracting energy from a battery changes it to a lower energetic state $\hat{\rho}''$ such that $tr[(\hat{\rho}'' - \hat{\rho})\hat{H}_0] \leq 0$ [4].

For example, if we have a qubit in a general eigenstate $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$, with $|\alpha|^2 + |\beta|^2 = 1$, we can construct the density matrix as:

$$\hat{\rho} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \begin{bmatrix} \alpha^* & \beta^* \end{bmatrix} = \begin{bmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{bmatrix} \tag{2.28}$$

The ergotropy is given by:

$$\mathcal{W} = tr[(\hat{\rho} - \hat{\pi})\hat{H}_0]$$

Here we take $\hat{H}_0$ as equation (2.12) and $\hat{\pi} = |\uparrow\rangle\langle\uparrow|$ as the density matrix of the ground state of a system with one qubit. This leads to the following ergotropy:

$$\mathcal{W} = \frac{1}{2}E_z(|\beta|^2 - |\alpha|^2 + 1) = |\beta|^2 E_z \tag{2.29}$$

This result is logical since if the state is completely in the up state ($\beta = 0$), there is no extractable work in the system. When the system is completely in the down state ($\beta = 1$), we have the maximum amount of ergotropy in the system.

Chapter 3

Analytical solutions

The goal of this chapter is to gain understanding of the dynamic behaviour of electron spin qubits by solving the Schrödinger equation and the Von Neumann equation analytically, which also shows how quickly it becomes more difficult to solve these equations if the system is more complex. This chapter also reproduces the optimal charging protocol as described by Binder et al. [4].

3.1 Analytical solution using ESR

We calculate the time-dependent state of an electron spin qubit, when applying the ESR operator (2.16), without Zeeman splitting. This is equivalent to solving the Schrödinger equation (2.7) with Hamiltonian $\hat{H} = \hat{V}$ for the state $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{bmatrix}\alpha\\ \beta\end{bmatrix}$:

$$i\hbar \begin{bmatrix}\dot{\alpha}\\ \dot{\beta}\end{bmatrix} = \begin{bmatrix}0 & \frac{1}{2}g^*\mu_B B\cos(\omega t)\\ \frac{1}{2}g^*\mu_B B\cos(\omega t) & 0\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} \tag{3.1}$$

which we then simplify into:

$$\begin{bmatrix}\dot{\alpha}\\ \dot{\beta}\end{bmatrix} = \begin{bmatrix}0 & ia\cos(\omega t)\\ ia\cos(\omega t) & 0\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = A\begin{bmatrix}\alpha\\ \beta\end{bmatrix}$$

with $a = -\frac{g^*\mu_B B}{2\hbar}$. We rewrite our matrix A as PDP^{-1}, where P consists of the eigenvectors of A and D is a diagonal matrix with the eigenvalues of A. This gives us the equation $|\dot{\psi}\rangle = PDP^{-1}|\psi\rangle$. We multiply by P^{-1} to get $P^{-1}|\dot{\psi}\rangle = DP^{-1}|\psi\rangle$. Finally, we substitute $Q = P^{-1}|\psi\rangle$ to achieve a simpler differential equation $\dot{Q} = DQ$. The eigenvectors of matrix A are given by: $v_1 = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix}$ and $v_2 = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ -1\end{bmatrix}$ with corresponding eigenvalues $\lambda_1 = ia\cos(\omega t)$ and $\lambda_2 = -ia\cos(\omega t)$. This leads to the following definition of P and D:

$$P = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix},\ D = \begin{bmatrix}ia\cos(\omega t) & 0\\ 0 & -ia\cos(\omega t)\end{bmatrix} \tag{3.2}$$

This gives us the following differential equations:

$$\dot{q_1} = ia\cos(\omega t)q_1,\ \dot{q_2} = -ia\cos(\omega t)q_2 \tag{3.3}$$

which are easily solved and lead to:

$$q_1 = c_1 e^{\frac{ia\sin\omega t}{\omega}},\ q_2 = c_2 e^{\frac{-ia\sin\omega t}{\omega}} \tag{3.4}$$

We multiply equation (3.4) with matrix P to find the solution of the original equation:

$$\begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}c_1 e^{\frac{ia\sin\omega t}{\omega}} + c_2 e^{-\frac{ia\sin\omega t}{\omega}}\\ c_1 e^{\frac{ia\sin\omega t}{\omega}} - c_2 e^{-\frac{ia\sin\omega t}{\omega}}\end{bmatrix} \tag{3.5}$$

The constants $c_1,\ c_2$ can be found by using the initial conditions of the system and are given by:

$$c_1 = \frac{1}{\sqrt{2}}(\alpha(0)+\beta(0)),\ c_2 = \frac{1}{\sqrt{2}}(\alpha(0)-\beta(0)) \tag{3.6}$$

Substituting these values gives the solution:

$$\begin{bmatrix}\alpha(t)\\ \beta(t)\end{bmatrix} = \begin{bmatrix}\alpha(0)\cos(a\frac{\sin\omega t}{\omega}) + \beta(0)i\sin(a\frac{\sin\omega t}{\omega})\\ \alpha(0)i\sin(a\frac{\sin\omega t}{\omega}) + \beta(0)\cos(a\frac{\sin\omega t}{\omega})\end{bmatrix} \tag{3.7}$$

The solution gives the following figure:

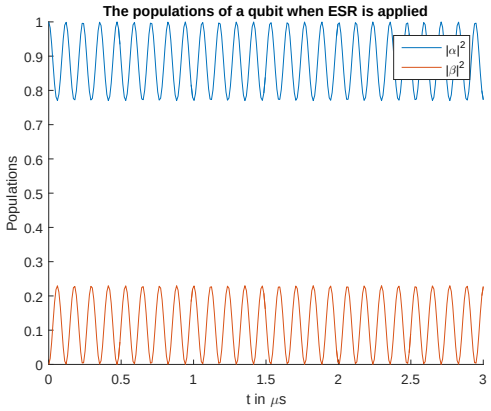

Figure 3.1: The absolute squared populations of a single electron spin qubit rotated by ESR, where the initial state is the up-state.

In order to describe ESR for a system of electron spin qubits with Zeeman splitting we use numerical methods, this can be found in chapter 4.1.

3.2 Analytical solution of the wave equation with exchange interaction

Moving forward from the Von Neumann equations (2.8), the general form of an evolution equation for the density operator $\hat{\rho}$ is the master equation:

$$\frac{\partial\hat{\rho}}{\partial t} = \frac{-i}{\hbar}[\hat{H},\hat{\rho}] + \Gamma\hat{L}\hat{\rho} \tag{3.8}$$

where $\hat{H}$ is the total Hamiltonian, Γ is the decay rate and $\hat{L}$ is the Lindblad superoperator as defined in equations (3.9) and (3.10). Note that $\hat{L}$ is not a matrix. In our system for N particles $\hat{H}$ is of the form: $\hat{H} = \hat{H_0} + \hat{V} + \hat{H_{ex}}$.

In order to solve this equation, we split the master equation into the differential equations for the

populations and coherences respectively

$$\frac{d}{dt}\hat{\rho}_{nn}(t) = -\frac{i}{\hbar}[\hat{H}_0 + \hat{V}(t) + \hat{H}_{ex}(t), \hat{\rho}(t)]_{nn} + W(\hat{L}_N[\hat{\rho}])_{nn} \tag{3.9}$$

$$\frac{d}{dt}\hat{\rho}_{nm}(t) = -\frac{i}{\hbar}[\hat{H}_0 + \hat{V}(t) + \hat{H}_{ex}(t), \hat{\rho}(t)]_{nm} + W(\hat{L}_N[\hat{\rho}])_{nm} - V\hat{\rho}_{nm} \tag{3.10}$$

where $W = 1/\delta_1$ and $V = 1/\delta_2$ and δ_1, δ_2 are the single-spin decay time and single-spin dephasing time, respectively. Throughout this report we will assume that the decay and dephasing time is the same for each energy level. We will now solve the master equation for two electron spin qubits in two situations.

3.2.1 Natural decoherence: dephasing and spontanenous emission

We solve the Von Neumann equation if there is no driving and no interaction, but only the natural decoherence of the system. Therefore we take $\hat{H} = O$ in equation (3.8). We assume that the dephasing rate (W) is the same for all the populations and the emission rate (V) is the same for all the coherences. Furthermore, we assume only one particle may dephase at a time. We leave out the operator sign from here on to increase the readability of this report. For two electrons, ρ is a 4×4 matrix. This gives the following differential equations for n $\neq$ m:

$$\begin{aligned}
\dot{\rho}_{11} &= W\rho_{22} + W\rho_{33} \\
\dot{\rho}_{22} &= W\rho_{44} - W\rho_{22} \\
\dot{\rho}_{33} &= W\rho_{44} - W\rho_{33} \\
\dot{\rho}_{44} &= -2W\rho_{44} \\
\dot{\rho}_{nm} &= -V\rho_{nm}
\end{aligned}$$

The differential equation belonging to the coherences is easily solved: $\rho_{nm}(t) = \rho_{nm}(0)e^{-Vt}$. It is slightly more challenging to solve the coupled system for the populations. We substitute the solution $\rho_{44}(t) = \rho_{44}(0)e^{-2Wt}$. Then by making use of an integrating factor we get

$$\begin{aligned}
\rho_{22}(t) &= -\rho_{44}(0)e^{-2Wt} + (\rho_{22}(0) + \rho_{44}(0))e^{-Wt} \\
\rho_{33}(t) &= -\rho_{44}(0)e^{-2Wt} + (\rho_{33}(0) + \rho_{44}(0))e^{-Wt}
\end{aligned}$$

And finally we use these solutions to get:

$$\rho_{11}(t) = \rho_{44}(0)e^{-2Wt} - (\rho_{22}(0) + \rho_{33}(0) + 2\rho_{44}(0))e^{-Wt} + \rho_{11}(0) + \rho_{44}(0) + \rho_{33}(0)) + \rho_{22}(0))$$

3.2.2 Natural decoherence and exchange interaction

Now we expand the system to include only exchange interaction and decay. We use equation (3.8) with $\hat{H} = \hat{H}_0 + \hat{H}_{ex}$. This gives us the following set of differential equations:

$$\begin{aligned}
\begin{bmatrix} \dot{\rho}_{11} & \dot{\rho}_{12} & \dot{\rho}_{13} & \dot{\rho}_{14} \\ \dot{\rho}_{21} & \dot{\rho}_{22} & \dot{\rho}_{23} & \dot{\rho}_{24} \\ \dot{\rho}_{31} & \dot{\rho}_{32} & \dot{\rho}_{33} & \dot{\rho}_{34} \\ \dot{\rho}_{41} & \dot{\rho}_{42} & \dot{\rho}_{43} & \dot{\rho}_{44} \end{bmatrix} &= -i\kappa \begin{bmatrix} 0 & 2\rho_{12} - 2\rho_{13} & 2\rho_{13} - 2\rho_{12} & 0 \\ 2\rho_{31} - 2\rho_{21} & 2\rho_{32} - 2\rho_{23} & 2\rho_{33} - 2\rho_{22} & 2\rho_{34} - 2\rho_{24} \\ 2\rho_{21} - 2\rho_{31} & 2\rho_{22} - 2\rho_{33} & 2\rho_{23} - 2\rho_{32} & 2\rho_{24} - 2\rho_{34} \\ 0 & 2\rho_{42} - 2\rho_{43} & 2\rho_{43} - 2\rho_{42} & 0 \end{bmatrix} \\
&\quad - \begin{bmatrix} -W\rho_{22} - W\rho_{33} & V\rho_{12} & V\rho_{13} & V\rho_{14} \\ V\rho_{21} & -W\rho_{44} + W\rho_{22} & V\rho_{23} & V\rho_{24} \\ V\rho_{31} & V\rho_{32} & -W\rho_{44} + W\rho_{33} & V\rho_{34} \\ V\rho_{41} & V\rho_{42} & V\rho_{43} & 2W\rho_{44} \end{bmatrix}
\end{aligned} \tag{3.11}$$

where $J(t)$ is taken to be constant in time as $J = \hbar\kappa$. V and W are assumed to be the same for all n,m. We observe that most of these equations do not depend on more than one other equation. There is a large amount of symmetry in the system, which significantly simplifies the solution. We start by solving one of the smaller sets of differential equations:

$$\begin{bmatrix}\dot{\rho}_{12}\\ \dot{\rho}_{13}\end{bmatrix} = \begin{bmatrix}-2i\kappa - V & 2i\kappa\\ 2i\kappa & -2i\kappa - V\end{bmatrix}\begin{bmatrix}\rho_{12}\\ \rho_{13}\end{bmatrix} \tag{3.12}$$

This system is solved by finding the eigenfunctions and eigenvalues of the matrix: $v_1 = \begin{bmatrix}-1\\ 1\end{bmatrix}$, $v_2 = \begin{bmatrix}1\\ 1\end{bmatrix}$, with corresponding eigenvalues $\lambda_1 = -V - 4i\kappa$, $\lambda_2 = -V$. The solution is then equal to:

$$\begin{bmatrix}\rho_{12}(t)\\ \rho_{13}(t)\end{bmatrix} = \begin{bmatrix}c_1(V+4i\kappa)e^{-(V+4i\kappa)t} & -c_2Ve^{-Vt}\\ -c_1(V+4i\kappa)e^{-(V+4i\kappa)t} & -c_2Ve^{-Vt}\end{bmatrix} \tag{3.13}$$

The constants are solved by making use of the initial conditions of the density matrix:

$$c_1 = \frac{\rho_{12}(0) - \rho_{13}(0)}{2V + 8i\kappa} \tag{3.14}$$

$$c_2 = \frac{\rho_{12}(0) - \rho_{13}(0)}{2V} \tag{3.15}$$

The solutions for equations ρ_{21} and ρ_{31}, ρ_{24} and ρ_{34} and ρ_{42} and ρ_{43} are similar. The differential equations for ρ_{41}, ρ_{14} and ρ_{44} have already been solved in the previous situation and are given by:

$$\rho_{14}(t) = \rho_{14}(0)e^{-Vt},\ \rho_{41}(t) = \rho_{41}(0)e^{-Vt} \tag{3.16}$$

Finally, we need to solve the more intricate system of six coupled differential equations. Since none of these are time independent, we only need to determine the eigenvectors and eigenvalues of the following matrix:

$$\begin{bmatrix}\dot{\rho_{11}}\\ \dot{\rho_{22}}\\ \dot{\rho_{23}}\\ \dot{\rho_{32}}\\ \dot{\rho_{33}}\\ \dot{\rho_{44}}\end{bmatrix} = \begin{bmatrix}0 & W & 0 & 0 & W & 0\\ 0 & -W & 2i\kappa & -2i\kappa & 0 & W\\ 0 & 2i\kappa & -V & 0 & -2i\kappa & 0\\ 0 & -2i\kappa & 0 & -V & 2i\kappa & 0\\ 0 & 0 & -2i\kappa & 2i\kappa & -W & W\\ 0 & 0 & 0 & 0 & 0 & -2W\end{bmatrix}\begin{bmatrix}\rho_{11}\\ \rho_{22}\\ \rho_{23}\\ \rho_{32}\\ \rho_{33}\\ \rho_{44}\end{bmatrix} \tag{3.17}$$

This gives the following eigenvectors:

$$v_1 = \begin{bmatrix}1\\0\\0\\0\\0\\0\end{bmatrix}\ v_2 = \begin{bmatrix}1\\-1\\0\\0\\-1\\1\end{bmatrix}\ v_3 = \begin{bmatrix}-2\\1\\0\\0\\1\\0\end{bmatrix} \tag{3.18}$$

$$v_4 = \begin{bmatrix}0\\0\\1\\1\\0\\0\end{bmatrix}\ v_5 = \begin{bmatrix}0\\-1\\\frac{8i\kappa}{W-V+\sqrt{W^2+(8i\kappa)^2-2WV+V^2}}\\-\frac{8i\kappa}{W-V+\sqrt{W^2+(8i\kappa)^2-2WV+V^2}}\\1\\0\end{bmatrix}\ v_6 = \begin{bmatrix}0\\-1\\\frac{8i\kappa}{-W+V+\sqrt{W^2+(8i\kappa)^2-2WV+V^2}}\\-\frac{8i\kappa}{-W+V+\sqrt{W^2+(8i\kappa)^2-2WV+V^2}}\\1\\0\end{bmatrix}$$

And the corresponding eigenvalues:

$$\lambda_1 = 0, \lambda_2 = -2W, \lambda_3 = -W, \lambda_4 = -V,$$
$$\lambda_5 = \frac{1}{2}(-\sqrt{W^2 - 2WV + (8i\kappa)^2 + V^2} - W - V)$$
$$\lambda_6 = \frac{1}{2}(\sqrt{W^2 - 2WV + (8i\kappa)^2 + V^2} - W - V)$$

We can then construct the solution as:

$$\begin{bmatrix} \rho_{11}(t) \\ \rho_{22}(t) \\ \rho_{23}(t) \\ \rho_{32}(t) \\ \rho_{33}(t) \\ \rho_{44}(t) \end{bmatrix} = c_1 e^{-\lambda_1 t} v_1 + ... + c_6 e^{-\lambda_6 t} v_6 \tag{3.19}$$

Where $c_1, ..., c_6$ are given by the initial conditions of the system.

3.3 Optimal charging of a single electron spin qubit

It is important to define our view of optimal charging. In this report, we will look at charging the battery in the least amount of time. Ideally, this would mean the time to charge from the ground state to the maximally excited state. This is not so simple, however, since it can be difficult to charge the battery completely. Therefore, we will also investigate charging with maximal power as defined in equation (2.27).

The optimal charging of a quantised particle is described in [4]. Take note, that while this is similar to our system of electron spin qubits, we only work with particles at $T = 0$. This means that thermodynamic constraints are less relevant to investigate as they are in the article. The Hamiltonian we use is shifted such that the ground state has negative energy and the excited state has positive energy compared to the article. It still has the same difference between the levels, up to the constants. We perform similar calculations to see whether we get the same result. If we then ignore the decoherence of the system, the Von Neumann equation for this system is given by:

$$i\hbar \frac{\partial}{\partial t}\hat{\rho}(t) = [\hat{H}_0 + \hat{V}(t), \hat{\rho}(t)] \tag{3.20}$$

If we parametrise $\hat{\rho}(t)$ by its Cartesian decomposition as in section 2.4 and rewrite the Hamiltonian for a single electron spin qubit as $\hat{H}_0 = -\frac{1}{2}E_z\hat{\sigma}_z$, we can rewrite this into the simpler form:

$$i\hbar \frac{\partial}{\partial t}\hat{\rho}(t) = \frac{1}{2}[\mathbf{v}(t) \cdot \hat{\sigma}, (I + \mathbf{a}(t) \cdot \hat{\boldsymbol{\sigma}})] \tag{3.21}$$

Optimal charging is achieved by optimising the derivative of the ergotropy, since this leads to the largest increase in ergotropy and therefore the shortest charging time:

$$\frac{\partial}{\partial t} tr[\hat{\rho}(t)\hat{H}_0] = tr[\frac{\partial}{\partial t}\hat{\rho}(t)\hat{H}_0] = tr[(\frac{\partial}{\partial t}\hat{\rho}(t))\hat{H}_0] \tag{3.22}$$

Therefore, our aim is to find $\mathbf{v}(t)$ such that equation (3.22) is maximal. We achieve this by rewriting the differential equation into two different forms:

$$\frac{\partial}{\partial t}\hat{\rho}(t) = \frac{1}{2}\frac{\partial}{\partial t}(I + \mathbf{a}(t) \cdot \hat{\boldsymbol{\sigma}}) = \frac{1}{2}(\frac{\partial}{\partial t}\mathbf{a}(t)) \cdot \hat{\boldsymbol{\sigma}} \tag{3.23}$$

We also know that:

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = \frac{1}{2}[\mathbf{v}(t)\cdot\hat{\sigma}, (I + \mathbf{a}(t)\cdot\hat{\sigma})] = i(\mathbf{v}(t)\times\mathbf{a}(t))\cdot\hat{\boldsymbol{\sigma}} \tag{3.24}$$

due to the commutation relations of the Pauli matrices. We then compare equations (3.23) and (3.24) and conclude that:

$$\frac{\partial}{\partial t}\mathbf{a}(t) = \frac{2}{\hbar}(\mathbf{v}(t)\times\mathbf{a}(t)) \tag{3.25}$$

We substitute this information into equation (3.22):

$$tr[(\frac{\partial}{\partial t}\hat{\rho}(t))\hat{H}_0] = \frac{1}{\hbar}(\mathbf{v}(t)\times\mathbf{a}(t)\cdot tr[\hat{\boldsymbol{\sigma}}\hat{H}_0] = \frac{1}{\hbar}(\mathbf{v}(t)\times\mathbf{a}(t))\cdot tr\begin{bmatrix} O \\ O \\ -\frac{1}{2}E_z I \end{bmatrix} = \frac{E_z}{\hbar}(v(t)^y a(t)^x - v(t)^x a(t)^y) \tag{3.26}$$

This is the same result as described by [4]. If we now rewrite our Cartesian decomposition of $\hat{\rho}(t)$ into polar coordinates we achieve $\mathbf{a}(t) = r\sin\theta(t)(\sin\theta(t)\cos\phi(t), \sin\theta(t)\sin\phi(t), \cos\theta(t))$, such that:

$$tr[(\frac{\partial}{\partial t}\hat{\rho}(t))\hat{H}_0] = \frac{E_z}{\hbar}(v(t)^y\cos\phi(t) - v(t)^x\sin\phi(t))\ r\sin\theta(t) \tag{3.27}$$

We conclude that the optimal charging conditions are indeed:

$$v(t)^x = -E_{max}\sin\phi(t), \quad v(t)^y = E_{max}\cos\phi(t), \quad v(t)^z = 0 \tag{3.28}$$

with $E_{max} = \frac{1}{2}g^*\mu_B B$ the driving constraint. It is logical that this result corresponds to driving directly along the outside of the Bloch sphere, with constant $\phi(t) = \phi_0$. This gives us the optimal charging operator:

$$\hat{V}_{opt} = E_{max}(\cos\phi_0 - \sin\phi_0) \tag{3.29}$$

Another result of equation (3.25) is that a pure state remains pure when applying the operators mentioned above. Since any evolution is perpendicular to $\mathbf{a}(t)$, any pure state remains on the Bloch sphere and therefore remains pure.

Chapter 4

Numerical approach

This chapter uses a numerical approach to overcome the issue of increasing complexity in solving the Von Neumann equation. It investigates the general behaviour of electron spin qubits and the effect the exchange operator has on them. After finding that the exchange operator does not have a direct effect on the ergotropy of the system, the CNOT gate is investigated. As seen in the previous chapter, it is possible to solve the Von Neumann equation if our system is simple and small, but it becomes very difficult to solve if it is more complex.

4.1 Numerical solution of realistic system

We will show that applying microwave radiation rotates the spin of the electron spin qubit. We no longer solve this system analytically since the coefficients in the differential equation are time-dependent and the differential equation is too complex. We simulate the time-evolution of equation (3.8) with $\hat{H} = \hat{H}_0 + \hat{V}$.

As seen in figure 4.1, when the system is started in its ground state, the electron spin starts rotating in a cyclic manner from the up-state to the down-state. This confirms what we expected.

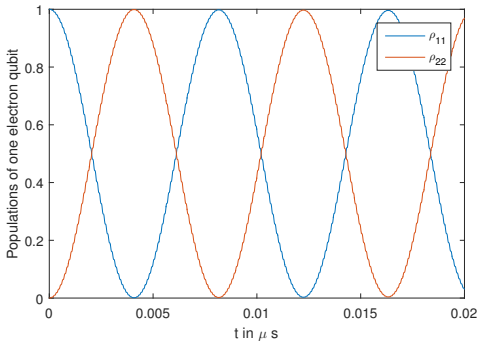

Figure 4.1: The populations of a single electron spin qubit rotated by ESR, where the initial state is the up-state.

4.2 Entanglement caused by exchange interaction

We now check that applying the Hamiltonian (2.19) to the basis states of the two-spin Hilbert space creates entanglement. We solve equation (3.8) for this system with $\hat{H} = \hat{H}_{0,2spins} + \hat{H}_{ex}$ and

$\Gamma = 0$, where $\hat{H}_{0,2spins} = \hat{H}_0 \otimes I_2 + I_2 \otimes \hat{H}_0$ and I_2 is the 2×2 identity matrix. Filling in the known values, gives:

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\begin{bmatrix} -E_Z & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_z \end{bmatrix} + J(t) \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \hat{\rho}] \tag{4.1}$$

We apply this to the basis state $|\uparrow\downarrow\rangle$ and show that the state will start rotating to and from the state $|\downarrow\uparrow\rangle$. In this calculation, J is set to be constantly 1 meV.

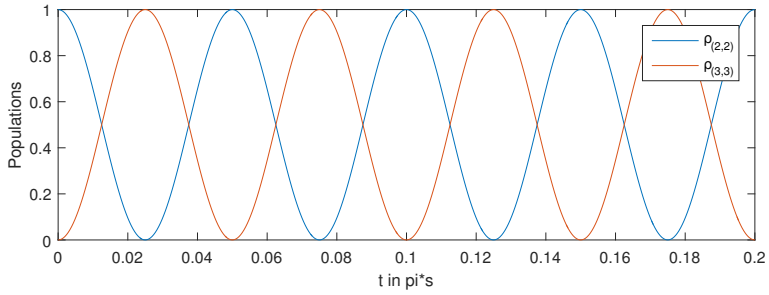

Figure 4.2: The populations of a two electron spin qubit system under the influence of the exchange operator where $J = 1\ meV$. When started in the $|\uparrow\downarrow\rangle$ state, the system starts rotating from $\rho_{22} = 1$ to $\rho_{22} = 0$.

From figure 4.2, we can conclude that the exchange operator rotates the populations such that both states are occupied at the same time and causes exchange between the two population.

4.3 Realistic values of parameters

An important goal for this research is to find charging conditions that could be used, at least partially, in a real experiment. For this reason, we take realistic values for parameters, as observed experimentally in articles [5] and [6].

Table 4.1: Experimental values of relevant parameters.

Parameter	Value	Unit
g^*	0.35	-
μ_B	$5.78 * 10^{-2}$	meV/T
J	0.1	meV
δ_1	5	μs
δ_2	0.5	μs
B	0.050	T
B_z	1	T

4.4 Optimal charging for N electron spin qubits

We investigate the optimal charging for an array of N qubits. The first logical option would be to charge each qubit individually and simultaneously as in the manner described in section 3.3. This is described in [4] as parallel driving with the Hamiltonian $\hat{V}_{opt,N}$, the expanded version of equation (3.29). According to [4], if we apply an entangling, global operator, this leads to an N-times decrease of the process duration. This interaction operator is given by:

$$\hat{V}_{global} = NE_{max}(|1^{(N)}\rangle \langle 0^{(N)}| + |0^{(N)}\rangle \langle 1^{(N)}|) \tag{4.2}$$

where $|0^{(N)}\rangle$ and $|1^{(N)}\rangle$ are the basis states for the ground state and maximally excited state respectively, for N particles. The charging from $|0^{(N)}\rangle$ to $|1^{(N)}\rangle$ is evaluated for both operators. This gives the following results:

Table 4.2: Overview of process duration and average power for global charging compared to parallel charging.

N	1	2	3	4
T_{global} in μs	0.0020	0.0010	6.8037*10^{-4}	5.1028*10^{-4}
$T_{global}/T_{parallel}$	1	0.4995	0.3324	0.2507
$\langle P \rangle$ in $\frac{meV}{\mu s}$	9.9250	39.6999	89.3247	158.7995

We observe the N-times decrease in process duration as prescribed, as well as an N-times increase in average power per particle. This leads to some interesting questions: if we take a very large number of particles, could we make the charging time arbitrarily small? It is outside the scope of this research to put a restraint on this development. Intuitively one can argue that the cost would be a longer process duration in total and that any gain found in the charging process is correlated to the power needed to create the entanglement, as stated in [4]. Nevertheless, this is an extremely interesting result on its own and deserves further research.

4.5 Analysis of simulation for two electrons

In the previous sections, we have seen that the charging time can be decreased by making use of a global operator. We investigate if exchange interaction, which is a qubit-qubit interaction

operator, can speed up the charging process of a two electron spin qubit array from the ground state to the state in which all the qubits are in the fully excited state. Initially, the simulation is started in the ground state and electron spin resonance is applied to both qubits. The evolution of the populations is plotted in figure 4.3. The resulting ergotropy is plotted in figure 4.4.

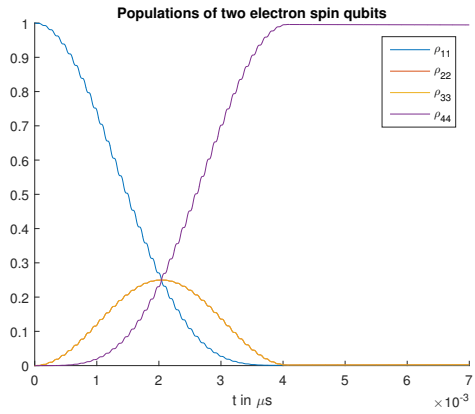

Figure 4.3: The populations of two exchange-coupled electron spin qubits while being rotated simultaneously.

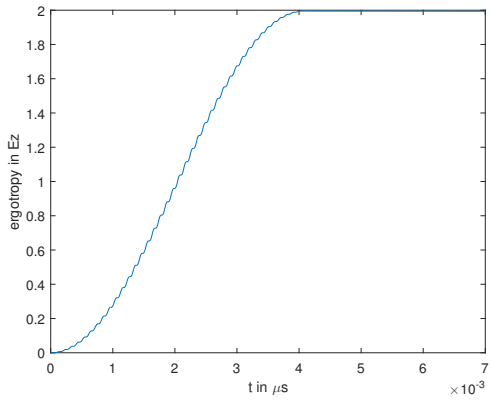

Figure 4.4: The ergotropy of two exchange-coupled electron spin qubits while being rotated simultaneously. In 0.0041 μs the battery is charged.

It takes 0.0041 μs to charge the system completely. The timescale of the rotation is determined by the energy $E = |g^* \mu_B B x|$. It is useful to note that the timescale of emission and dephasing is small compared to the timescale of ESR, such that the battery remains relatively stable after turning off the ESR. We observe that turning on the exchange operator would give the same behaviour, since both qubits are rotated equally. This implies that the coupled states are equally occupied and the exchange would be equally fast in both directions. The smaller oscillation that can be seen is a numerical artefact and shall be discussed later.

In order to let exchange interaction play a role, we only rotate one qubit and turn the exchange interaction on. The following figure shows the ergotropy for different values of J:

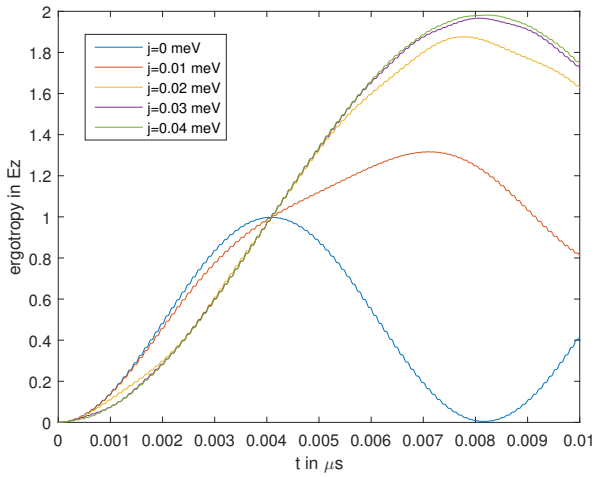

Figure 4.5: The ergotropy of a two spin qubit system for different constant values of j. ESR is applied on only one electron spin qubit.

We observe that when exchange is turned off the maximum ergotropy is $1E_z$ as expected. The charging process slows down when exchange is turned on, but reaches a larger amount of ergotropy. Once J reaches approximately 0.040 meV the increase no longer makes a difference. The time required to reach maximum ergotropy is then 0.0082 μs, which is twice as long as with ESR acting on two qubits. This is as expected, since ESR is only applied on one qubit. Our expectation that the power with which the qubits are charged does not increase is confirmed when the average power for different strengths of the entanglement operator is calculated:

Table 4.3: Average power while charging two electron spin qubits compared to different values of the exchange strength.

j in meV	0	0.01	0.02	0.03	0.04
$\langle P \rangle$in meV/s	4.9478	3.7597	4.8684	4.9370	4.8857

Note that although $j = 0.03\ meV$ for the exchange strength gives a higher average power than $j = 0.04\ meV$, this situation does not reach the maximally active state as required. While it is interesting to investigate which exact strength the qubit for the entangling operator gives the perfect charging process, this situation is not beneficial to our goal of decreasing the charging time in general.

We try implementing the exchange at different time points and observe the behaviour of the two qubits. The following figure shows the time-evolution of two qubits, one rotated at half the ESR strength of the second one. We briefly apply exchange, until they are fully entangled. We then continue to charge both particles individually at full strength.

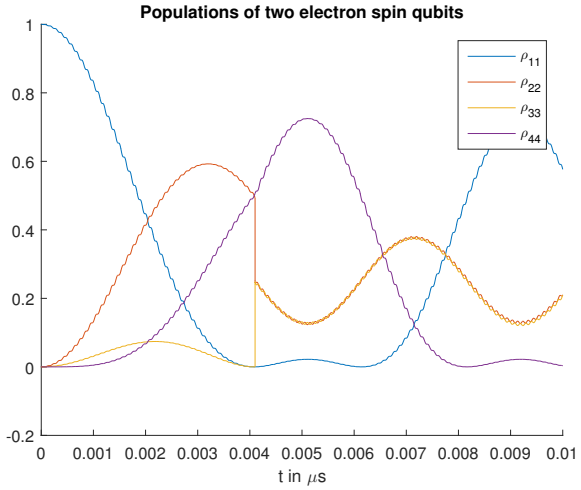

Figure 4.6: Time-evolution of the populations of two qubits: one particle rotated at full speed, one at half, then fully entangled at $t = 0.0041\ \mu s, J = 0.1\ meV$. Finally, both particles are rotated individually at full speed.

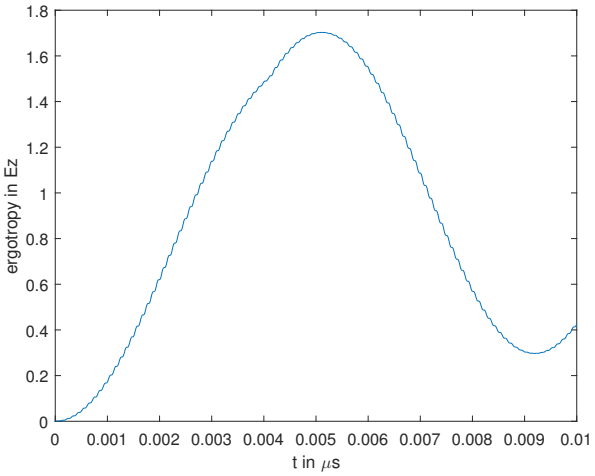

Figure 4.7: Ergotropy corresponding to figure 4.6.

There are two things to note in these figures; Firstly, the steepness of the maximally excited state ρ_{44} is higher after the entangling operation has been switched on, which we also see in the ergotropy. Secondly, the battery is no longer able to be fully charged after the entanglement. For this specific situation, we investigate what happens during the charging process. The scheme below is a representation, which does not account for any phase factors:

$$|\uparrow\uparrow\rangle \Rightarrow |\downarrow\rightarrow\rangle \Rightarrow \frac{1}{\sqrt{2}}(|\downarrow\rightarrow\rangle + |\rightarrow\downarrow\rangle)$$

The $|\rightarrow\rangle$ state is meant to show that the second particle is rotated halfway down on the Bloch sphere. Since ESR is a linear operator, this means that we are constantly rotating a particle down as well as up, such that it will never reach its maximum.

We now investigate if the exchange operator has any influence on the ergotropy. For simple states, such as the ground state and the maximal state, we already know that this will not have an influence, because they are eigenstates of the operator. However, for other two qubit basis states such as $|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$, we also observe that $\frac{\partial}{\partial t} tr(H_0\rho) = 0$. In other words, while the density matrix is certainly influenced by the operator, it seems it does not affect the ergotropy. The following figure further supports this conclusion:

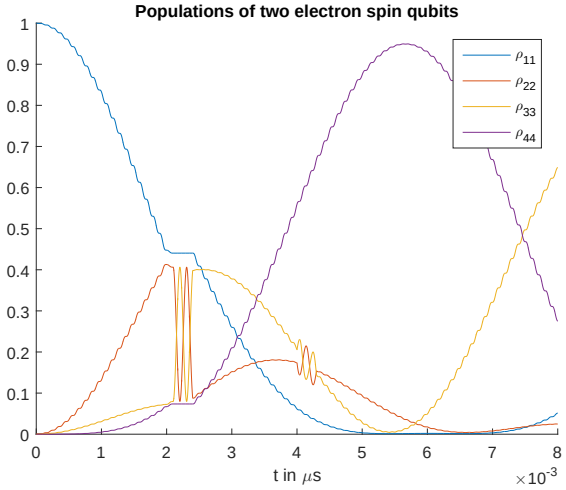

Figure 4.8: Two spin qubit system while being charged, exchange is then applied and ESR turned off. Afterwards charging is continued and exchange is turned on during rotation. $J = 0.01\ meV$.

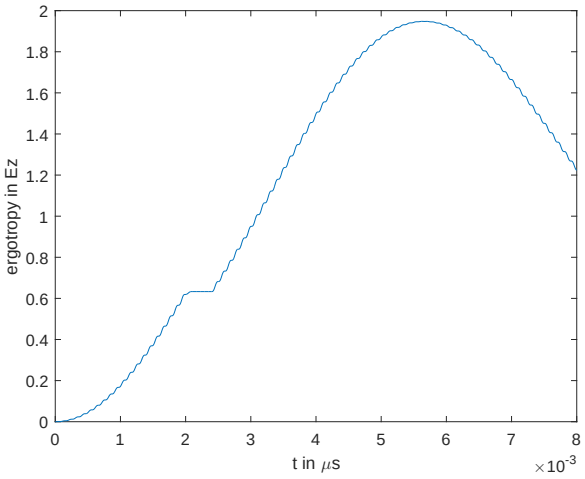

Figure 4.9: Ergotropy corresponding to figure 4.8.

Figure 4.8 shows a two spin qubit system being charged in a similar manner as in figure 4.6. The exchange operator is then applied to the system for 0.0003 μs at 0.002 μs and the rotation is stopped. In order to make the visualisation better, the strength of the exchange operator is $\frac{1}{10}$ of the realistic parameter value given in section 4.3. When this simulation is repeated with the original value, we achieve the same result, only with faster oscillations. We observe that the ergotropy

does not increase during this first time period. The rotation is continued without exchange. The exchange operator is turned on again at 0.004 μs, but the rotation is continued. We observe that while the populations (and coherences) are certainly influenced, the ergotropy continues as before.

After having applied the exchange operator in many possible ways, including for shorter and longer periods, as well as in subsequent bursts, we want to examine the direct effect of H_{ex}. This was done by calculating if the expected value of the ergotropy increases when applying the exchange operator. In other words, if

$$\frac{\partial}{\partial t}\mathcal{W} = \frac{\partial}{\partial t} tr(H_0\rho) = tr(H_0 \frac{\partial}{\partial t}\rho) = tr(H_0 \frac{-i}{\hbar}[H_{ex}, \rho]) \tag{4.3}$$

is larger than 0. This equation was evaluated and tunrned the exchange operator off on all occasions that were implemented, indicating that we might be able to prove that in our simulation there is no direct consequence on the ergotropy due to the exchange operator. In the following section we show this mathematically.

4.6 Indication that the exchange operator does not affect ergotropy

In the previous section, the simulations have shown that in many situations, the exchange operator does not affect the ergotropy of a two electron spin qubit system. In fact, this has been the case as well in every simulation which has not been included in this report. We prove that the derivative of the ergotropy of a two electron spin qubit system is 0 when applying only the exchange operator. In other words, the ergotropy is constant. We derive the useful equivalence that the derivative of the ergotropy is equal to zero if the operator $\hat{A}$ applied to the system commutes with the Hamiltonian of an electron spin qubit:

$$tr[H_0[A, \rho]] = tr[H_0 A\rho] - tr[H_0\rho A] = tr[H_0 A\rho] - tr[AH_0\rho] = tr[[H_0, A]\rho] \tag{4.4}$$

If we compare this to equation (4.3), it is easily verified that the derivative of the ergotropy is 0 if the operator commutes with the Hamiltonian of the system. A simple calculation shows that H_{ex} commutes with H_0 and therefore does not have a direct influence on the ergotropy. However, this does not describe the system of electorn spin qubits completely. We now look at $\frac{\partial}{\partial t}\mathcal{W}$ when the full electron spin Hamiltonian is included.

$$\frac{\partial}{\partial t}\mathcal{W} = tr[H_0 \frac{\partial}{\partial t}\rho] = \frac{-i}{\hbar}\ tr[H_0[H_0 + H_{ex}, \rho]]$$

Then by the properties of the trace operator and the result in equation (4.4), we get the following equation:

$$\frac{\partial}{\partial t}\mathcal{W} = \frac{-i}{\hbar}\ tr[H_0 H_0\rho - H_0\rho H_0] + \frac{-i}{\hbar}\ tr[H_0[H_{ex}, \rho]] = \frac{-i}{\hbar}\ tr[H_0 H_0\rho - H_0 H_0\rho] + 0 = 0$$

This result again indicates that we cannot influence the ergotropy by using only the exchange operator. However, we have only looked at systems consisting of two particles, when perhaps the advantage is to be had in larger systems. The original derivation of this result can be found in appendix C.

4.7 Using a CNOT gate to assist charging

While we did not prove that the exchange operator could not benefit the ergotropy in any possible situation, the evidence provided by the simulations and the simple proof were enough reason to

look into other operations that might be helpful. As the theory prescribes, the CNOT gate is most effective if the control qubit is completely in the down state and the target qubit is left in the up state. If we then apply the operator, this should result in the maximally excited state for this system. This should obviously have an effect on the ergotropy of the system. The simulation shows the following result:

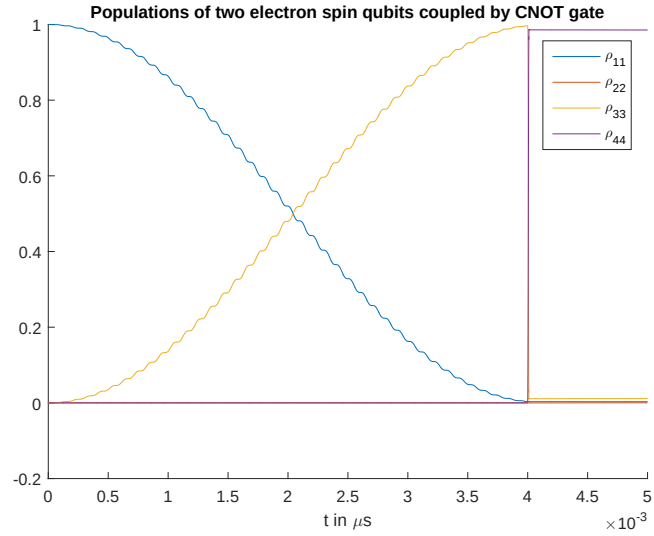

Figure 4.10: Two spin qubit system where control qubit is charged, CNOT is then applied and ESR turned off.

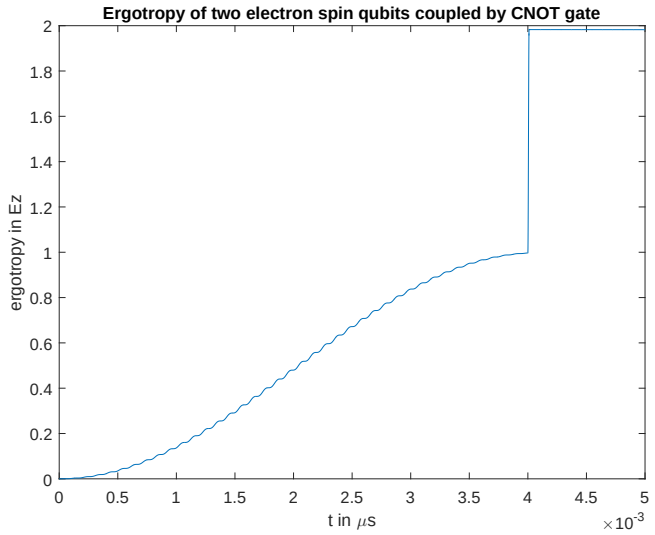

Figure 4.11: Evolution of the ergotropy of two CNOT-coupled electron spin qubits as a function of time.

The ergotropy shows an almost instantaneous increase to maximum ergotropy. This complies with what we expected, but please note that this is only an artificial view of the situation. In order

to describe the CNOT gate accurately, the program should be adapted. This is explained in the discussion. The result does not give an overall decrease in charging time, since only one qubit is being rotated. If we were to rotate both qubits, this would give the same end state in the same amount of time. This means that it does not decrease the charging time of the electron spin qubits, but it may have other useful applications. It would simplify the charging process if only one qubit needs to be rotated by ESR, but the maximum ergotropy for the system can still be reached. This would also decrease the amount of variables in the experiment.

4.8 Numerical methods

In order to investigate the different effects operators can have on the state of our qubit system, we need to solve the Von Neumann equation. As mentioned before, it is much more efficient to do this numerically. This also gives a large array of options on how to apply the operators on our system. Consequently, a large part of the work put into this research has been programming and finding more efficient ways to describe our system numerically.

The basis of the script that was used can be found in the appendices, but this has been adapted to over 30 versions to look into specific situations. The script consists of a general part and a master equation that solves the differential equation. The programming work to solve a differential equations is quite simple, but what made this script far more complex is the fact that all the operators and calculations had to be dependent on the amount of qubits you wanted to include in your calculation. Therefore all the operators had to be generalised. It also had to be possible to turn on any operator on any qubit, while leaving the others unaffected.

When all the variables and initial conditions have been set, the time development of the density matrices is calculated with a simple ode solver. The output is then reshaped into matrices, such that the ergotropy can be calculated and the results can be plotted and analysed. The script has been left as general as possible such that any operator can be inserted instead of the exchange operator, which leaves it open for future research.

Chapter 5

Discussion

Although we have not observed a *direct* effect on the charging time of the qubit systems caused by a qubit-qubit interaction operator, this is no reason to conclude that a decrease in the charging time of a quantum battery cannot be achieved. There may be other ways of implementing the exchange operator and CNOT gate. In this section, we will discuss the limitations of the simulations that have been performed and the suggestions made to improve on them.

While we have shown that the exchange operator does not affect the ergotropy in our simulation by our specific standard that $\frac{\partial \mathcal{W}}{\partial t}$ should be larger than zero, we cannot conclude that there is no possible decrease in charging time due to the exchange operator. In figure 4.7, there is a slight peak after we entangled the qubits. This gives a battery that does not charge to its full capacity, but is quicker to charge to 80% which might be interesting for other purposes. We know that the mathematical reason that $\frac{\partial \mathcal{W}}{\partial t} = 0$ is that the exchange operator commutes with the Hamiltonian, but what does this mean for the qubits? If we look at the matrix form of ρ while exchange is turned on during the simulation for two electrons, we see that only the population terms ρ_{22} and ρ_{33} change. The coherences are affected as well, but they are not relevant for the trace operator in ergotropy. Any increase in ρ_{22} is directly opposite to the decrease in ρ_{33} and vice versa. Since these populations have the same energy level, as can be seen in the Hamiltonian for two electron spin qubits, it is logical that this does not give an increase in ergotropy.

Almost all research in this paper has been done for two electrons. While larger arrays of electrons have been simulated, they gave the same result as with two electrons. Intuitively, this seems logical since the exchange operator only works on two neighbouring electrons, but it is entirely possible that if implemented in another way this can still have an influence on the ergotropy. Further research could be done on sequences of rotations and applying the exchange operator. It would be interesting to look into larger arrays where there is more than only nearest neighbour interaction.

Since our results were found indepent of the assumptions we have made, it is not very relevant to discuss their validity. For example, the dissipation time has been set the same for each energy level, while this is not necessarily true for an experiment. We have also assumed that there is only nearest neighbour interaction and that any operator can be turned on in any way possible. If we did observe an effect on the charging of the qubits, it would be relevant to investigate the maximum possible increase and the validity of these assumptions. However, since this is not the case, it is reasonable to leave them in place. Finally, we need to address the slight oscillation in the simulated results, as can be seen in the figures 4.3 until 4.11. This 'wiggle' shows up independent of the constants and applied operators and therefore it is assumed that this is a numerical error. Changing the time step of the ODE-solver does not affect the oscillation, so it might be useful to look into other ODE-solvers to solve this problem.

The main research goal of this thesis is to investigate the effects of the exchange operator, but when this did not give a decrease in charging time, the CNOT gate was taken into consideration. Due to the different nature of these operations it is not fair to compare them directly. In fact, we cannot represent the CNOT gate as a term in the Hamiltonian as it is. For any proper comparison the CNOT operator should be written as a sequence of Hamiltonians that are subsequently applied to the system. In figure 4.10, it seems strange that an instantaneous jump can be the result of a differential equation. We saw in the simulation that if the CNOT operator was applied continuously, the state jumped back and forth during every time step. If the time steps are made smaller, the jumps start going faster. This means that our simulation can not describe this process accurately. The program should be adapted in order to include the effect of a gate on the system. Further research should be done on this topic in order to draw a conclusion, but for now we leave it as an indication that the CNOT gate can have an effect on the ergotropy of a quantum battery, but when applied with a single ESR rotation it does not give a decrease in charging time for our system.

Chapter 6

Conclusion

In this thesis, research was done on the effects of entanglement on the charging of electron spin qubits. The goal was to find a decrease in charging time i.e. an increase in power per qubit by using an entangling qubit-qubit interaction operator on an array of electron spin qubits. The time evolution of the state was calculated by solving the Von Neumann equation both analytically and numerically and then calculating the extractable work of the system.

6.1 The effect of exchange interaction

The exchange operator has been applied extensively in our simulation, although none of the methods have given a decrease in charging time. Although we did observe the entanglement of the qubits, this did not have influence on the ergotropy of our system. We found that when we rotated only one qubit of our two qubit system and applied the exchange operator, we could still fully charge our battery if the strength of the exchange operator was high enough. This did however double the charging time compared to simply rotating both qubits simultaneously. After observing the lack of effect of the exchange operator on the ergotropy, we optimised the simulation such that it evaluated in each time step if it should apply the exchange operator or not, which constantly turned the operator off. This was evaluated by calculating the time derivative of the ergotropy. This led to an analytical calculation that showed that in our system the derivative would always be zero, due to the commutation of the exchange operator with the Hamiltonian of the qubits. Although the exchange operator did influence the states, it entangled the qubits between two states of the same energy. Further research could look into the effect of also allowing next-nearest neighbour interaction and using sequences of rotations and entangling operators. The code written for this thesis can be used to include these suggestions as well as extending the calculations to larger arrays.

6.2 Alternatives to the exchange operator

We have reproduced the increase in power due to a global entangling operator as described by Binder et al. [4] numerically for our system. Since it is currently not possible to carry out this experiment, we looked into other operations. The matrix representing the CNOT gate was promising, since it did not commute with the Hamiltonian of the qubits. When one qubit is rotated to a maximally energetic state, it almost instantaneously flips the second qubit such that the system is fully charged. This does not give an increase in charging time due to the rotation time of the first qubit. Since the CNOT gate is a different form of operator, we do not know enough to compare it to exchange interaction. This result is left as an indication that the CNOT gate does have an effect on the ergotropy of a quantum battery and needs further research.

Appendices

A: Main program

```
% #quantum dots
N=2;

% initial conditions
state  = [1; 0; 0; 0];

%constants
g = 0.35;   %GaAs quantum dots
mu = 5.788*10^(-2);  %Bohrmagneton meV/T
Bx = 0.050; %T
hbar = 6.582*10^(-7); % meV*micros
delta1 = 5; %microseconds
delta2 = 0.5; %microseconds

%parameters
Bz = 1; % Tesla
j = 0.1; %meV, if j = 0, exchange interaction is off
esrswitch = 1; % if 0, esr is off
Tstart = 0;
Tend = pi;
TVstart = 0;
TVend = 5*pi;
T = 0.01;
Pot = ones(N);
Ex = ones(N-1);

%definining constants
Ez = abs(g*mu*Bz);
omega = Ez/hbar;
a = 1/2*g*mu*Bx;

%defining the basis for the operators
ground = zeros(2^N,2^N);
ground(1,1) = 1;
E = [-1/2*Ez 0; 0, 1/2*Ez];
H0 = zeros(2^N,2^N);

%expanding the hamiltonian for N particles
```

```
for kk = 1:N;
    part = zeros(N,1);
    part(kk) =1;
    for ll = 1:N;
    H(:,:,ll) = part(ll)*E + (1-part(ll))*eye(2);
    end
    Hfinal = H(:,:,1);
    for qq = 1:(N-1)
    Hfinal = kron(Hfinal,H(:,:,qq+1));
    end
    H0part(:,:,kk)=Hfinal;
    H0 = H0 + H0part(:,:,kk);
end

%making the start density matrix and reshaping
rhostart = state*state';
rhostart = reshape(rhostart,[2^(2*N),1]);

%defining the options for the ODE solver
options= odeset('Reltol',0.000001,'Stats','on');

% calculating differential equation
[t,rho] = ode45(@(t,rho)Master_equation_final(t,rho,g,mu,Bx,Bz,
   Tstart,Tend,TVstart,TVend,j,N,hbar,delta1,delta2,esrswitch,Pot,
   Ex),[0 T],rhostart,options);

%reshaping the solution into matrices
[m,n] = size(rho);
for i= 1: m
rhom(:,:,i) = reshape(rho(i,:),[2^N,2^N]);
end

%calculating the ergotropy
for dt = 1:length(t)
    ergotropy(dt) = trace(rhom(:,:,dt)*H0-ground*H0);
end
```

B: Master equation

```
function rhop = Master_equation_final(t,rho,g,mu,Bx,Bz,Tstart,Tend,
    TVstart,TVend,j,N,hbar,delta1,delta2,esrswitch,Pot,Ex,H0)


J = j*(heaviside(t-Tstart) - heaviside(t-Tend));
Ez = abs(g*mu*Bz);
omega = Ez/hbar;
a = 1/2*g*mu*Bx;

gamma1 = 1/delta1;
gamma2 = 1/delta2;
sigma1 = [0,1;1,0];
sigma2 = [0,-1i;1i,0];
sigma3 = [1,0;0,-1];


E = [-1/2*Ez, 0; 0, 1/2*Ez];
H0 = E;
Hex1 = sigma1;
Hex2 = sigma2;
Hex3 = sigma3;

I = eye(2);
V = (heaviside(t-TVstart) - heaviside(t-TVend))*a*cos(omega*t)*
    sigma1;

%ESR

for i =1:N
    Vf = zeros(2^N,2^N);
    c = zeros(1,N);
    c(i) = 1;
    for s =1:N
        Vs(:,:,s) = c(s)*V + (1-c(s))*I;
        Vf= Vs(:,:,1);
    end

    for k = 1:N-1
        Vf = kron(Vf,Vs(:,:,k+1));
    end
    Vfinal(:,:,i) = Vf;
end

%exchange interaction
for l =1:(N-1)
    d = zeros(N);
    d(l) = 1;
    d(l+1)= 1;
    for s = 1:N
        h1(:,:,s) = d(s)*sigma1 + (1-d(s))*I;
```

```
        h2(:,:,s) = d(s)*sigma2 + (1-d(s))*I;
        h3(:,:,s) = d(s)*sigma3 + (1-d(s))*I;
    end
    Hf1 = h1(:,:,1);
    Hf2 = h2(:,:,1);
    Hf3 = h3(:,:,1);
    for s=1:N-1
        Hf1 = kron(Hf1,h1(:,:,s+1));
        Hf2 = kron(Hf2,h2(:,:,s+1));
        Hf3 = kron(Hf3,h3(:,:,s+1));
    end
    H1(:,:,l) = Hf1;
    H2(:,:,l) = Hf2;
    H3(:,:,l) = Hf3;
    HEX(:,:,l) = J*(Hf1 + Hf2 + Hf3);
end

rhomatrix = reshape(rho,[2^N,2^N]);
Comex = zeros(2^N,2^N);
Compot = zeros(2^N,2^N);
H0 = zeros(2^N,2^N);

for kk = 1:N;
    part = zeros(N,1);
    part(kk) =1;
    for ll = 1:N;
    H(:,:,ll) = part(ll)*E + (1-part(ll))*eye(2);
    end
    Hfinal = H(:,:,1);
    for qq = 1:(N-1)
    Hfinal = kron(Hfinal,H(:,:,qq+1));
    end
    H0part(:,:,kk)=Hfinal;
    H0 = H0 + H0part(:,:,kk);
end

for m = 1:(N-1);
    Comex = Comex + Ex(m)*HEX(:,:,m);
end
for q = 1:(N);
    Compot = Compot + Pot(q)*Vfinal(:,:,q);
end

if trace(-i*hbar(H0(HEX(:,:,1)*rho - rho*HEX(:,:,1))))> 0;
    j = 1;
else  j = 0;
end

Comex = J*j*Comex ;    %time dependence of exchange
Compot = esrswitch*Compot;

%spontaneous emission
```

```
Semis = [0,1;0,0];

for q = 1:N;
    Sf = zeros(2^N,2^N);
    part = zeros(N);
    part(q)=1;
    for r = 1:N;
        Stemp(:,:,r) = part(r)*Semis + (1-part(r))*eye(2);
        Sf = Stemp(:,:,1);
    end
    for u = 1:(N-1);
       Sf = kron(Sf,Stemp(:,:,u+1));
    end
    Sfinal(:,:,q) = Sf;

end

emission = zeros(2^N,2^N);


commutator = (Comex + Compot + H0)*rhomatrix - rhomatrix*(Comex +
   Compot + H0);
commutator = reshape(commutator,[2^(2*N),1]);
rhop = zeros(2^(2*N),1);



for i = 1:2^(2*N);
    rhop(i) = -1i/(hbar)*commutator(i);
end
rho = reshape(rho,[2^N,2^N]);
rhop = reshape(rhop,[2^N,2^N]);
temp = ones(2^N,2^N)-eye(2^N);
rhop = rhop - gamma2*temp.*rho;

for y = 1:N;
    emission = emission + Sfinal(:,:,y)*rho*Sfinal(:,:,y)' -0.5*
       Sfinal(:,:,y)'*Sfinal(:,:,y)*rho -0.5*rho*Sfinal(:,:,y)'*
       Sfinal(:,:,y);
end

rhop = rhop + gamma1*emission;
rhop = reshape(rhop,[2^(2*N),1]);
```

C: Original derivation that the exchange operator does not influence ergotropy directly

$$\frac{\partial}{\partial t}\mathcal{W} = tr[H_0 \frac{\partial}{\partial t}\rho] = tr[H_0 \frac{-i}{\hbar}(H_{ex}\rho - \rho H_{ex})]$$

$$= tr\big[\frac{-i}{\hbar}H_0 J(t)\big(\begin{bmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{bmatrix}\begin{bmatrix}\rho_{11}&\rho_{12}&\rho_{13}&\rho_{14}\\\rho_{21}&\rho_{22}&\rho_{23}&\rho_{24}\\\rho_{31}&\rho_{32}&\rho_{33}&\rho_{34}\\\rho_{41}&\rho_{42}&\rho_{43}&\rho_{44}\end{bmatrix} - \begin{bmatrix}\rho_{11}&\rho_{12}&\rho_{13}&\rho_{14}\\\rho_{21}&\rho_{22}&\rho_{23}&\rho_{24}\\\rho_{31}&\rho_{32}&\rho_{33}&\rho_{34}\\\rho_{41}&\rho_{42}&\rho_{43}&\rho_{44}\end{bmatrix}\begin{bmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{bmatrix}\big)\big]$$

$$= \frac{-i}{\hbar}E_z J(t)\ tr\big[\begin{bmatrix}-1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{bmatrix}\begin{bmatrix}0&2\rho_{12}-2\rho_{13}&-2\rho_{12}+2\rho_{13}&0\\-2\rho_{21}+2\rho_{31}&-2\rho_{23}+2\rho_{32}&2\rho_{33}-2\rho_{22}&-2\rho_{24}+2\rho_{34}\\2\rho_{21}-2\rho_{31}&2\rho_{22}-2\rho_{33}&2\rho_{23}-2\rho_{32}&2\rho_{24}-2\rho_{34}\\0&2\rho_{42}-2\rho_{43}&-2\rho_{42}+2\rho_{43}&0\end{bmatrix}\big]$$

$$= \frac{-i}{\hbar}E_z J(t)\ tr\begin{bmatrix}0&-2\rho_{12}+2\rho_{13}&2\rho_{12}-2\rho_{13}&0\\0&0&0&0\\0&0&0&0\\0&2\rho_{42}-2\rho_{43}&-2\rho_{42}+2\rho_{43}&0\end{bmatrix} = 0$$

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