ENTANGLEMENT IN NANO SYSTEMS

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Abstract

This bachelor thesis on entanglement in nano systems includes a short presentation of the history of quantum mechanics before entanglement takes the spot light. A definition of entanglement will be stated as well as a prescription to quantify it for a pure system. The knowledge will then be used to quantify the entanglement for the ground state of few particle systems containing 2, 3 and 4 particles. The model that will be used is chosen to be as simple as possible, but it can still give a feeling of how the entropy behaves in these small systems. The few-particle systems can be compared to atoms in a molecule or quantum dots in a nano system.

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Chapter 1

Introduction

Entanglement is a concept of quantum mechanics that has puzzled the world of science for almost a century. Quantum mechanics was developed in the 1920's and 1930's, and the theory contradicts the importance of common sense when developing physical theories. Niels Bohr even claims that "Anybody who is not shocked by quantum theory has not understood it". [1]

It is not possible to write about entanglement without mentioning the contradiction to classical physics that has shaken the view of the world that the scientists nearly believed to be complete. When Albert Einstein, Nathan Rosen and Boris Podolsky tried to convince the world that quantum mechanics is not a complete theory of nature, they argued for a few "elements of physical reality" that they asserted every physical theory must represent. [2] The EPR-paradox (1935) showed that quantum mechanics violates the element of locality. Realism is a fundamental principle in classical physics, which at can seem like an obvious assumption, but seems to be violated by quantum mechanics as well. These two arguments of common sense states [3]

  (i) There is no action-at-a-distance in nature.

 (ii) There exist an external reality with definite properties, whether or not these properties are observed.

Quantum mechanics violates the state of realism (ii) by suggesting that a system can be a superposition of many different states, and that a certain property can have different outcomes, that is randomized proportionally to the probability of each possible value. A certain value is only determined at the point when the property is measured. According to quantum mechanics, measuring the system could not only give different results, but also collapse the system to that certain state which goes together with the value. Hence, simply measuring or "observing" a property of the system could always put the system into an irreversible state. To make this contradiction with common sense clearer, this can be thought of as saying that the moon only exists in its orbit with certainty when looking at it, since one is somehow observing its position. Not looking at the moon, one can never be certain that the moon is in a determined place in its orbit, or if there even has a position after all, until you observe it again.

That our moon suddenly appears in a galaxy far far away is of course not a probable outcome even in the perspective of quantum mechanics, since the

moon is a macroscopic object that constantly interacts (i.e. gets measured) with the universe. But for sure, how can anyone be certain of the state of a system without interacting with it?

Many attempts has been made to find loopholes in the quantum theory, but even up till the experimental attempts in 2013, the quantum theory seems to agree with nature.

Entanglement is the concept in quantum mechanics that violates the argument of locality (i). If the entanglement is not broken between two subsystems through further operations on the system, the correlation still exists even if the particles are moved 150 kilometres away from each other, (this was experimentally proved with polarization-entangled photon pairs, that were separated to the islands of La Palma and Tenerife 2010 [4]). If their system is collapsed by operating on one of the subsystems, experiments seem to agree that the other subsystem instantly collapses accordingly with the first. This points to an instant connection (or at least a connection faster than the speed of light) that acts independently on the distance between the subsystems.

These results of distance-independent connection might wake dreams about instant information transfer and even teleportation, since the locality, and hence common sense, seems to be broken. In recent years, it has come to knowledge that teleportation *is* possible, but this only includes teleportation of states (i.e. a state of a system can be teleported to another system). Teleporting matter on the other hand still seems to be an unsolved question, and even though states can be teleported, there seems to be no way of achieving information by this without an classical exchange of information as well. In recent years it has been realized that entanglement constitutes a resource for quantum information processing [1]. The prospect of scaling and interfacing quantum devices with conventional electrons has sporred interest in entanglement in nano systems.

Nano systems are small enough systems to be able to behave quantum mechanically (with entanglement as an important application area), but large enough to be included in larger systems such as processors. This is hence a way of being able to use quantum phenomena in our macroscopic world. With the definition of entanglement known in chapter 2, a model will be used to, in the simplest possible way, determine the entanglement quantity of three small nano systems of 2, 3 and 4 $\frac{1}{2}$-spin particles in chapter 4. As it will be mentioned, these small clusters can both be compared with atoms of a trimer molecule, or coupled quantum dots in a nano system.

Chapter 2

Entanglement

Entanglement represents a correlation between two subsystems that goes beyond their individual properties. A definition of entanglement can be stated as "[...], two spatially separated particles are entangled if their state can not be prepared from a product state by operating locally on each particle[...]. [5] This will now be explained mathematically: Consider two subsystems A and B, described by the wave functions $|\psi_A\rangle$ and $|\psi_B\rangle$ respectively. Bringing the two systems together into one system $|\psi\rangle$, would in quantum mechanics be represented by a product state of the two subsystems

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle. \tag{2.1}$$

But, if the two subsystems are prepared together, the total system can end up in a state that do not consist of two individual states, but also has terms that entangle the two subsystems. If the state of the system can not be represented as a product state of two individual subsystems, the system is defined to be entangled. A common entangled state in nature is the spin singlet state for two $\frac{1}{2}$-spin particles:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_A \otimes |\downarrow\rangle_B - |\downarrow\rangle_A \otimes |\uparrow\rangle_B). \tag{2.2}$$

As can be shown, this state can not be achieved from a product state of the two individual states $|\psi_A\rangle = (\alpha_A |\uparrow\rangle_A + \beta_A |\downarrow\rangle_A)$ and $|\psi_B\rangle = (\alpha_B |\uparrow\rangle_B + \beta_B |\downarrow\rangle_B)$ and is hence an entangled state, which can be found in a great part of the electron pairs in nature.

2.0.1 Quantifying entanglement - the von Neumann entropy

There exist different ways of quantifying the entanglement, and different measurements might be used in different areas of the field, but the quantity that has been most successful for determining the entanglement of pure systems (which with a simplification can be considered as isolated systems) is the von Neumann entropy. This is hence the entropy that will be used to quantify the entanglement of the following chapters, since the calculations mostly consist of pure systems. The von Neumann entropy quantifies the entanglement by measuring
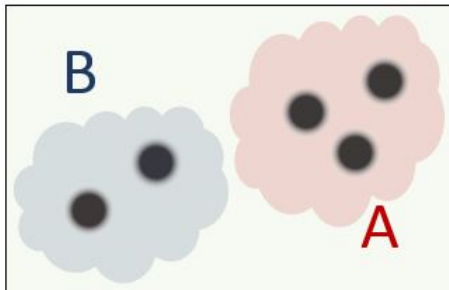
Figure 2.1: An isolated system including two subsystems, A and B. The correlation between the subsystems gives a value for the von Neumann entropy.

the available information between the subsystems A and B. Since the entanglement occurs *between* two participants, the entropy value is independent on whether the calculations are considering the entropy calculated from the perspective of the subsystem A or B. This is quite neat as it drastically reduces the amount of possible subsystem configurations when looking at a symmetric system, as will be noticed in the following chapters.

Once the state of the pure system is known, the *density matrix* needs to be calculated. The density matrix is generally a very useful operator when a system is an ensemble of states or even a mixed system. From the density matrix, the reduced density matrix can be calculated, considering only the subsystem A. The density matrix ρ for a pure state is defined by

$$\rho = |\psi\rangle \langle\psi| \tag{2.3}$$

and the reduced density matrix is then

$$\rho_A = tr_B(\rho) \tag{2.4}$$

The partial trace tr_B is additive, and as the system is divided into the subsystems A and B, each element of the density matrix is calculated according to

$$tr_B(|a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2|) \equiv |a_1\rangle \langle a_2| \, tr(|b_1\rangle \langle b_2|). \tag{2.5}$$

The von Neumann entropy then measures the amount of available information that is shared between the subsystems A and B with the use of the reduced density matrix. The von Neumann entropy is calculated with its definition [1]

$$S(\rho_A) \equiv -tr(\rho_A \log \rho_A) = -\sum_x \lambda_x \log \lambda_x \tag{2.6}$$

where $\{\lambda_x\}$ are the eigenvalues of ρ_A. To calculate the entanglement entropies for simple systems is now a straight forward action.

Chapter 3

The model

To be able to quantify the entanglement for a system of $\frac{1}{2}$-spin particles (which will be done in Chapter 4), the Hamiltonian of the total system have to be calculated. Each particle has two possible spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, which will in the following text be referred to as $|0\rangle$ and $|1\rangle$ respectively.

The Hamiltonian will here be considered in the simplest possible way in these very first calculations of the entanglement. Assume that the Hamiltonian of an isolated system of $\frac{1}{2}$-spin particles consists of two terms

$$H = H_S + H_I \tag{3.1}$$

where H_S represents the Hamiltonian as a result of the individual particle energy contributions to the total system and H_I is the added Hamiltonian that is a result of the interaction between the particles.

The H_S term for a single spin particle in e.g. a magnetic field can be generalized as

$$H_S = \epsilon_\uparrow |0\rangle \langle 0| + \epsilon_\downarrow |1\rangle \langle 1|$$

and further rewritten as

$$H_S = \frac{\epsilon_\uparrow + \epsilon_\downarrow}{2}(|0\rangle \langle 0| + |1\rangle \langle 1|) + \frac{\epsilon_\uparrow - \epsilon_\downarrow}{2}(|0\rangle \langle 0| - |1\rangle \langle 1|)$$

$$\doteq \frac{\epsilon_\uparrow + \epsilon_\downarrow}{2}\mathbb{1} + \frac{\epsilon_\uparrow - \epsilon_\downarrow}{2}\sigma^z \tag{3.2}$$

with $\sigma^z = |0\rangle \langle 0| - |1\rangle \langle 1|$. A constant energy contribution in the Hamiltonian does not have any physical relevance (since the energies in a measurement are already relative energies), therefore, only the second term in expression 3.2 will be considered. We define

$$H_S = \epsilon\sigma^z$$

where $\epsilon = \frac{\epsilon_\uparrow - \epsilon_\downarrow}{2}$ is the deviation from the mean value of the two energy values, here defined to be real and positive, $0 \leq \epsilon \in \mathbb{R}$. For N inseparable spin-particles in equal potential, this term will be the sum of the individual particle energies

$$H_S = \sum_{i=1}^{N} \epsilon\sigma_i^z. \tag{3.3}$$

To simplify the system further, the system is said to follow the Heisenberg XXZ-model, where the interaction in the X and Y directions are taken the same. For simplicity, the interaction in the Z-direction is put to zero. Doing this, and letting a particle interact pairwise with its nearest neighbours only, the interaction term of the Hamiltonian will have the following form

$$H_I = \sum_{i,j=1}^{N} J_{ij}(\sigma_i^x \otimes \sigma_j^x + \sigma_i^y \otimes \sigma_j^y) \tag{3.4}$$

where $\sigma^x = |0\rangle\langle 1| + |1\rangle\langle 0|$, $\sigma^y = i(|0\rangle\langle 1| - |1\rangle\langle 0|)$ and J_{ij} is J if i and j are nearest neighbours, and 0 otherwise. In the calculations in Chapter 4, the particles are always at equal distance to each other and hence, no particle interaction will be neglected. J is the factor that determines the strength of the interaction between the particle pair, here defined to be real, $J \in \mathbb{R}$.

With the Hamiltonian known, the states with their corresponding eigenvalue can now be calculated for the systems that will be considered in the following chapter.

Chapter 4

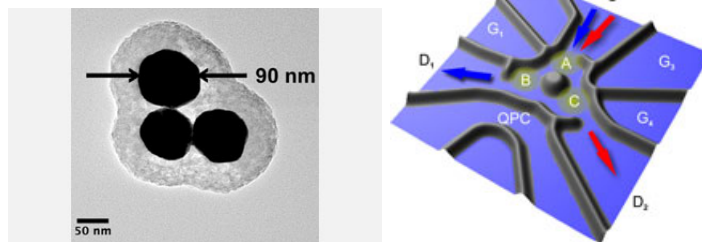# The von Neumann entropy for few-particle systems

Figure 4.1: Examples of possible three $\frac{1}{2}$-spin particle systems. Left: Gold nano particles from Van Duyne Group, Northwestern University. Right: Quantum dots [6].

The entanglement in systems of a few interacting $\frac{1}{2}$-spin particles will now be quantified. These particles could be e.g. magnetically impure metallic nano particles or electrons in quantum dots in a nano system, see figure 4.1. Even though assumptions and simplifications were made in the model that will be used, the results will give some idea of how these kinds of systems behave.

To begin, a small system consisting of two localized $\frac{1}{2}$-spin particles will be considered, to further expand the system to three and even four particles. In all these systems, the entanglement entropy of the ground state (which depends on different rates of J/ϵ) will be calculated. The ground state will be considered because this is the state which is most likely to find a system in when considering nano systems in thermal equilibrium at low temperature. Also, as the number of particles in a system is increased to N, the eigenstates of the Hamiltonian of the system increases to 2^N, which quickly becomes a large number. A lot of symmetries can though be found which minimize the amount of calculations that needs to be done. For larger system, the states are easier to be calculated numerically in a program.
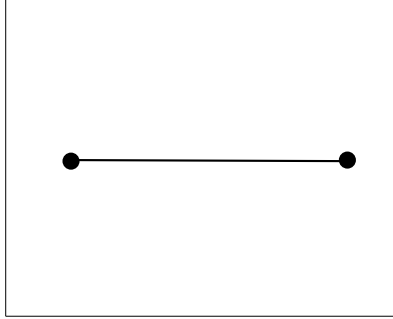
4.1   2 particles

Figure 4.2: Two particles in an isolated system.

According to equation 3.3, the H_S-term in the Hamiltonian for two particles will be

$$H_S = \epsilon(\sigma_1^z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_2^z) \tag{4.1}$$

which means

$$H_S = \epsilon[(|0\rangle\langle 0| - |1\rangle\langle 1|) \otimes (|0\rangle\langle 0| + |1\rangle\langle 1|) + (|0\rangle\langle 0| + |1\rangle\langle 1|) \otimes ((|0\rangle\langle 0| - |1\rangle\langle 1|)]. \tag{4.2}$$

Particle 1 and 2 are chosen to individually be independent of each other and hence commuting. Equation 4.2 can then be easily be simplified by letting $|0_1\rangle\langle 0_1| \otimes |0_2\rangle\langle 0_2|$ be denoted as $|0_1 0_2\rangle\langle 0_1 0_2|$, and further simplified to $|00\rangle\langle 00|$ by letting particle 1 be consistently denoted to the left and particle 2 to the right. The expression of H_S will then become

$$H_S = 2\epsilon(|00\rangle\langle 00| - |11\rangle\langle 11|). \tag{4.3}$$

As can be seen in equation 4.3, the cases where the two particles are of opposite spins, the sum of the individual energies adds to zero.

The term that is a result of the interaction between the two particles will look like

$$H_I = J(\sigma_1^x \otimes \sigma_2^x + \sigma_1^y \otimes \sigma_2^y)$$

which is equal to

$$H_I = J[(|0\rangle\langle 1| + |1\rangle\langle 0|) \otimes (|0\rangle\langle 1| + |1\rangle\langle 0|) + i^2(|0\rangle\langle 1| - |1\rangle\langle 0|) \otimes (|0\rangle\langle 1| - |1\rangle\langle 0|)].$$

Here, one can see that in this model, interaction only occurs when the two particles are of opposite spins. With the new denotation it will be

$$H_I = 2J(|10\rangle\langle 01| + |01\rangle\langle 10|). \tag{4.4}$$

With both terms determined, the Hamiltonian for two $\frac{1}{2}$-spin particles in the chosen model will be the sum of these and the matrix will look like

$$H = \begin{pmatrix} 2\epsilon & 0 & 0 & 0 \\ 0 & 0 & 2J & 0 \\ 0 & 2J & 0 & 0 \\ 0 & 0 & 0 & -2\epsilon \end{pmatrix} \tag{4.5}$$

with matrix denotations in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

Solving the eigenvalues $\{\lambda_i\}$ by diagonalizing the matrix, and with the equation $H|\psi_i\rangle = \lambda_i |\psi_i\rangle$ calculating the eigenstates, the possible eigenstates for the system with their eigenvalues will be

1. $|\psi_1\rangle = |00\rangle$ with eigenvalue 2ϵ
2. $|\psi_2\rangle = |11\rangle$ with eigenvalue -2ϵ
3. $|\psi_3\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$ with eigenvalue $2J$
4. $|\psi_4\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$ with eigenvalue $-2J$

The energy ratio between the interaction energy and the individual energy, J/ϵ, may differ due to circumstances of the system. Plotting the energy ratios $\{\lambda_i/\epsilon\}_{i=1}^4$ to the ratio J/ϵ, the ground state at different ratios can easily be found, see figure 4.3. As mentioned in chapter 3, ϵ is defined to be real and positive, and J is defined to be a real. As can be seen in figure 4.3, in region **I**,
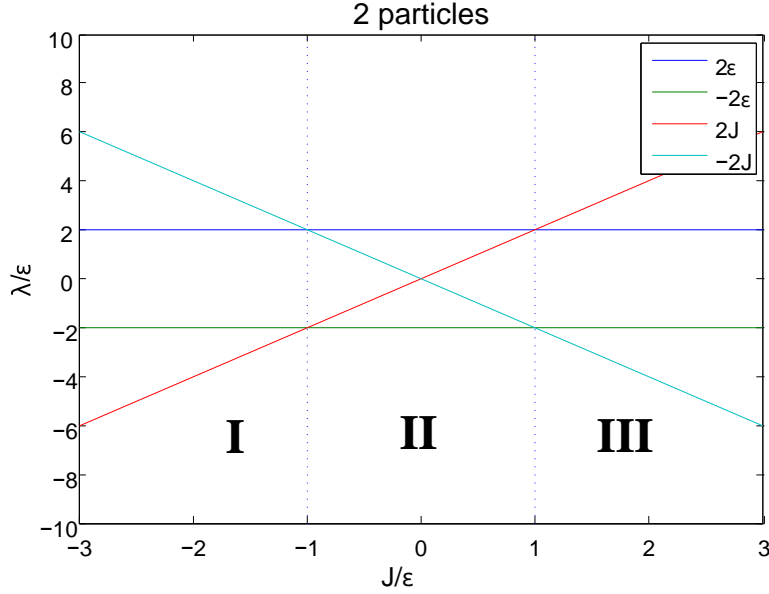

Figure 4.3: The energy ratios for the eigenvalues, $\{\lambda_i/\epsilon\}_{i=1}^4$, plotted to the ratio for the interaction strength J/ϵ for a system of two spin-particles. The plot is divided into three regions, I, II and III, with different ground states.

where $J < -\epsilon$, the ground state is

- $|\psi_g^1\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$

and in region **II**, where $|J| < \epsilon$, the ground state is

- $|\psi_g^2\rangle = |11\rangle$.

In region **III**, where $J > \epsilon$, the ground state is

- $|\psi_g^3\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$.

It is seen that as the absolute value of the interaction strength of the particles increases, it is prefarable for the systems to be in a state that is a superposition of different spin configurations. For a positive J, the singlet state is favored as the ground state of the system. By simply rewriting the H_I-part of the Hamiltonian, it can be shown that the energies of H_I is given a positive contribution from the total spin of the system. Hence, the singlet state with the total spin $S_S = 0$, will be favored as the ground state, compared to the triplet state with the total spin $S_T = 1$. The difference in energy for the triplet and singlet state $|\psi_2\rangle$ and $|\psi_4\rangle$ with spin configurations $|S = 1, M_S = 1\rangle$ and $|S = 0, M_S = 0\rangle$ respectively, is a result of the exchange interaction [7]. The exchange energy X is given by $\lambda_2 - \lambda_4 = -2X = -2(\epsilon + J)$ which with the insert of λ_2 and λ_4 yields $X = \epsilon + J$ for this two-particle system.

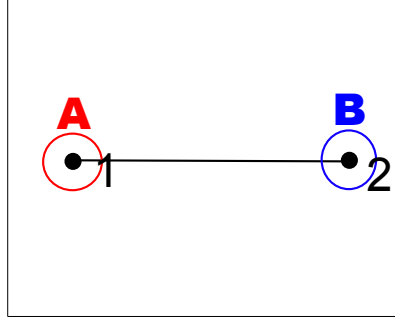### 4.1.1   The von Neumann entropy

Figure 4.4: Two particles in an isolated system where the von Neumann entropy is calculated between the subsystems A and B.

The von Neumann entropy is first calculated for region **I** of figure 4.3, with the ground state $|\psi_g^1\rangle$. Following the steps in section 2.0.1, the density matrix is first determined according to equation 2.3

$$\rho = |\psi\rangle\langle\psi|$$

$\Rightarrow$

$$\rho = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The reduced density matrix for the subsystem A is calculated according to equation 2.4

$$\rho_A = tr_B(\rho)$$

where the calculations for the reduced trace operator is defined in equation 2.5, and the new denotation of the commuting states give the expression

$$tr_B(|a_1 b_1\rangle\langle a_2 b_2|) = |a_1\rangle\langle a_2|\langle b_2|b_1\rangle$$

for each element of the density matrix. For the state $\left|\psi_g^1\right\rangle$ with the density matrix seen above, the reduced density matrix is

$$\rho_A = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.6}$$

With this diagonalized matrix, the von Neumann entropy is simply calculated according to equation 2.6, where

$$S(\rho_A) = -\sum_x \lambda_x \log \lambda_x.$$

The von Neumann entropy for ground state $\left|\psi_g^1\right\rangle$ is

- $S_1 = \log 2 \approx 0.301$.

This is a maximally entangled state for a 2-particle system!

Since the ground state in the second region is not a superposition of different possible states, there can not exist any entanglement. Calculating the reduced density matrix for this state results in a one dimension-matrix $\rho_A = \left|1\right\rangle\left\langle 1\right|$ and the entropy for this state is accordingly

- $S_2 = \log 1 = 0$.

For the third region, where the ground state is $\left|\psi_g^3\right\rangle$, the density matrix is calculated in the same way as above to be

$$\rho = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

This gives a reduced density matrix equal to 4.6 and accordingly the same entropy

- $S_3 = \log 2 \approx 0.301$.

It seems like there is a connection between the strength of the interaction and the entanglement of the ground state. With $|J| > \epsilon$, the entanglement in this system is maximized while for $|J| < \epsilon$, there is no entanglement in the ground state at all.

4.2   3 particles

Now, a system containing three particles will be considered and the von Neumann entropy will be calculated for the ground states. An equilateral triangle is created and the interaction will be calculated pairwise. The H_S-term of the Hamiltonian will now be a sum of three particles

$$H_S = \epsilon(\sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_2^z \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes \sigma_3^z).$$

Computing the term in the same way as for 2 particles gives the result

$$\begin{aligned} H_S = \epsilon[3(\left|000\right\rangle\left\langle 000\right| - \left|111\right\rangle\left\langle 111\right|) + \left|001\right\rangle\left\langle 001\right| + \left|010\right\rangle\left\langle 010\right| + \\ + \left|100\right\rangle\left\langle 100\right| - \left|110\right\rangle\left\langle 110\right| - \left|011\right\rangle\left\langle 011\right| - \left|101\right\rangle\left\langle 101\right|]. \end{aligned}$$
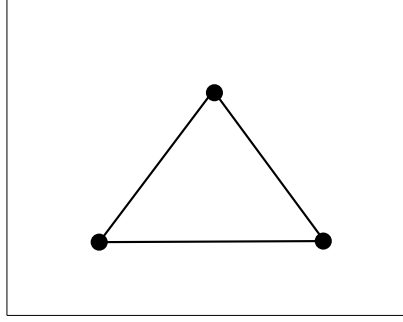
Figure 4.5: Three particles in an isolated system with a symmetric interaction strength between the particles.

This is understood more clearly in matrix form. Let the basis be $\{|000\rangle, |100\rangle, |010\rangle, |001\rangle, |110\rangle, |011\rangle, |101\rangle, |111\rangle\}$. Now, the H_S term can be read as

$$H_S = \epsilon \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}. \tag{4.7}$$

The interaction part for three particles will be

$$H_I = J(\sigma_1^x \otimes \sigma_2^x \otimes \mathbb{1} + \sigma_1^x \otimes \mathbb{1} \otimes \sigma_3^x + \mathbb{1} \otimes \sigma_2^x \otimes \sigma_3^x + \sigma_1^y \otimes \sigma_2^y \otimes \mathbb{1} + \sigma_1^y \otimes \mathbb{1} \otimes \sigma_3^y + \mathbb{1} \otimes \sigma_2^y \otimes \sigma_3^y).$$

Which eventually gives the matrix

$$H_I = 2J \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4.8}$$

The H_S-term and the H_I-term now sum up to the Hamiltonian

$$H = \begin{pmatrix} 3\epsilon & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \epsilon & 2J & 2J & 0 & 0 & 0 & 0 \\ 0 & 2J & \epsilon & 2J & 0 & 0 & 0 & 0 \\ 0 & 2J & 2J & \epsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\epsilon & 2J & 2J & 0 \\ 0 & 0 & 0 & 0 & 2J & -\epsilon & 2J & 0 \\ 0 & 0 & 0 & 0 & 2J & 2J & -\epsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3\epsilon \end{pmatrix} \tag{4.9}$$

according to equation 3.1. The eigenstates and eigenvalues of the block matrices was calculated by hand in the same way as for two particles, and the results were checked in Mathematica. The eigenstates of the Hamiltonian are:

1. $|\psi_1\rangle = |000\rangle$ with eigenvalue 3ϵ
2. $|\psi_2\rangle = |111\rangle$ with eigenvalue -3ϵ
3. $|\psi_3\rangle, |\psi_4\rangle$ are linear combinations of $\alpha_i(|011\rangle - |110\rangle) + \beta_i(|101\rangle - |110\rangle)$ with eigenvalue $(-\epsilon - 2J)$
4. $|\psi_5\rangle, |\psi_6\rangle$ are linear combinations of $\alpha_j(|001\rangle - |100\rangle) + \beta_j(|010\rangle - |100\rangle)$ with eigenvalue $(\epsilon - 2J)$
5. $|\psi_7\rangle = \frac{1}{\sqrt{3}}(|110\rangle + |101\rangle + |011\rangle)$ with eigenvalue $(-\epsilon + 4J)$
6. $|\psi_8\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$ with eigenvalue $(\epsilon + 4J)$
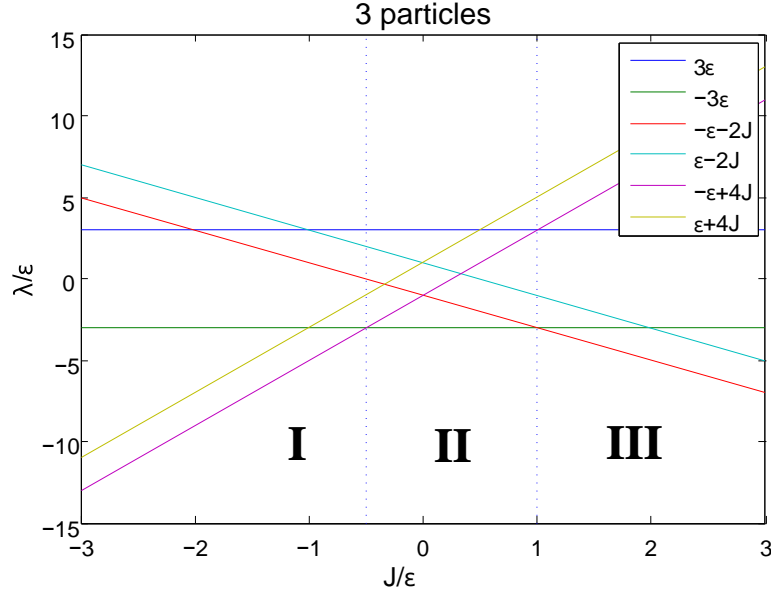

Figure 4.6: The energy ratios for the eigenvalues, $\{\lambda_i/\epsilon\}_{i=1}^8$, plotted to the ratio for the interaction strength J/ϵ for a three particle system.

The energy ratios $\{\lambda_i/\epsilon\}_{i=1}^8$ were plotted against the ratio J/ϵ, as can be seen in figure 4.6. It can be seen that the strongest interaction is found when the three particles are found in a completely symmetric superposition of all possible configurations with the same sum of the spin projections $\sum_{i=1}^3 s_z^{(i)}$. The total spin is not considered. The plot shows that, as for two particles, the ground state depends on the ratio J/ϵ and this ratio can be divided into three regions.

In the eigenstates for three particles, there exist degenerated states for the eigenvalues $(-\epsilon - 2J)$ and $(\epsilon - 2J)$, which is a result of the symmetry of our system and/or possible hidden symmetries that are not considered here. The degeneration leads to an existence of an infinite number of eigenstates that is a linear combination of two eigenstates.

In region **I**, where $J < -\frac{1}{2}\epsilon$, the ground state is

- $\left|\psi_g^1\right\rangle = \frac{1}{\sqrt{3}}(\left|110\right\rangle + \left|101\right\rangle + \left|011\right\rangle)$

with the energy $(-\epsilon + 4J)$. In region **II**, where $-\frac{1}{2}\epsilon < J < \epsilon$, the ground state is

- $\left|\psi_g^2\right\rangle = \left|111\right\rangle$.

and in region **III**, where $J > \epsilon$, the ground state is a mixed state of the degenerated states with eigenvalue $(-\epsilon - 2J)$. The states which are chosen to be considered can have different criteria, such as rotational symmetry, but there is no principle that claims that a system prefers one state in front of the other. A trace over degenerated states is basis invariant, so the von Neumann entropy will be calculated, even though it is not as successful for what now is a mixed state. To create an orthonormal base, orthogonalization is done by hand with the Gram-Schmidt and checked with Mathematica. The results are the two states

- $\left|\psi_g^{31}\right\rangle = \frac{1}{\sqrt{2}}(\left|011\right\rangle - \left|110\right\rangle)$
- $\left|\psi_g^{32}\right\rangle = \frac{1}{\sqrt{6}}(-\left|011\right\rangle - \left|110\right\rangle + 2\left|101\right\rangle)$.
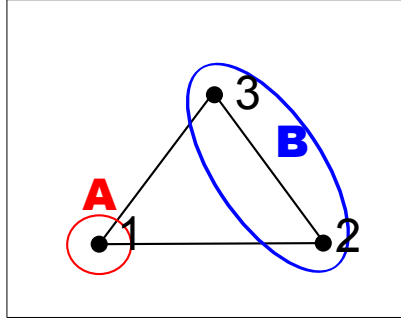
4.2.1 The von Neumann entropy

Figure 4.7: The Neumann entropy calculated between the two subsystems A and B.

In the same way as for two particles, the entropies of the ground states were calculated to be

- $S_1 = -\frac{1}{3}\log 1/3 - \frac{2}{3}\log 2/3 \approx 0.637$
- $S_2 = 0$.

The ground state of the third region consists of degenerated states. Since no principle claims that a system prefers one state in front of the other, the density matrix is calculated with its general definition that includes mixed states [1]

$$\rho \equiv \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| \tag{4.10}$$

where p_i is the probability for the state $\left|\psi_i\right\rangle$. The probability for each state is assumed to be the same, following the argument that no pinciple claims that a system prefers one state in front of the other. With $p_{31} = p_{32} = 1/2$, the density matrix was calculated and the entropy of this mixed state was calculated to be

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- $S_3 = -\frac{1}{3} \log \frac{1}{3} - \frac{2}{3} \log \frac{2}{3} \approx 0.6365$.

Even for three particles, the interaction strength is shown to affect the entanglement of the ground state in the same way as for two particles.

Since there exist symmetries in the system and in the entanglement quantity, and the von Neumann entropy is most suitable for pure systems where all subsystems are included in the calculations, there exists no other way of dividing the subsystems A and B to achieve different entropy values.
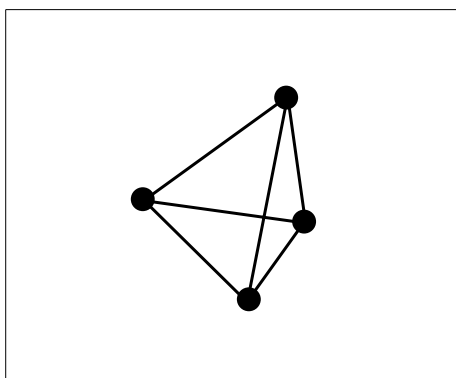
4.3 4 particles

Figure 4.8: A four particle system with equal interaction strength between the particles.

Four particles are placed as a tetrahedron, where each particle pair has the same interaction strength (all pairs are nearest neighbours). The Hamiltonian was calculated by hand in the same way as for two and three particles. The matrix in the chosen basis is

$$H = \begin{pmatrix}
4\epsilon & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2\epsilon & 2J & 2J & 2J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2J & 2\epsilon & 2J & 2J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2J & 2J & 2\epsilon & 2J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2J & 2J & 2J & 2\epsilon & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2J & 0 & 2J & 2J & 2J & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2J & 0 & 2J & 2J & 2J & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2J & 0 & 2J & 2J & 2J & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2J & 2J & 2J & 0 & 0 & 2J & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2J & 2J & 2J & 0 & 0 & 2J & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2J & 0 & 2J & 2J & 2J & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2\epsilon & 2J & 2J & 2J & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2J & -2\epsilon & 2J & 2J & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2J & 2J & -2\epsilon & 2J & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2J & 2J & 2J & -2\epsilon & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4\epsilon
\end{pmatrix}$$

(4.11)

For time saving, Mathematica calculated the eigenstates and eigenvalues of this matrix. The results are:

1. $|\psi_1\rangle = |0000\rangle$ with eigenvalue 4ϵ
2. $|\psi_2\rangle = |1111\rangle$ with eigenvalue -4ϵ
3. $|\psi_3\rangle , |\psi_4\rangle , |\psi_5\rangle$ are linear combinations of $\alpha_i(|1001\rangle - |0110\rangle) + \beta_i(|1010\rangle - |0101\rangle) + \gamma_i(|1100\rangle - |0011\rangle)$ with eigenvalue 0

4. $|\psi_6\rangle = \frac{1}{\sqrt{4}}(|0111\rangle + |1011\rangle + |1101\rangle + |1110\rangle)$ with eigenvalue $-(\epsilon - 3J)$

5. $|\psi_7\rangle, |\psi_8\rangle, |\psi_9\rangle$ are linear combinations of $\alpha_j(|1000\rangle - |0001\rangle) + \beta_j(|0100\rangle - |0001\rangle) + \gamma_j(|0010\rangle - |0001\rangle)$ with eigenvalue $2(\epsilon - J)$

6. $|\psi_{10}\rangle, |\psi_{11}\rangle$ are linear combinations of $\alpha_k(|0110\rangle + |1001\rangle - |0011\rangle - |1100\rangle) + \beta_k(|0101\rangle + |1010\rangle - |0011\rangle - |1100\rangle)$ with eigenvalue $-4J$

7. $|\psi_{12}\rangle = \frac{1}{\sqrt{6}}(|0101\rangle + |1010\rangle + |0011\rangle + |1100\rangle + |0110\rangle + |1001\rangle)$ with eigenvalue $8J$

8. $|\psi_{13}\rangle, |\psi_{14}\rangle, |\psi_{15}\rangle$ are linear combinations of $\alpha_l(|1110\rangle - |0111\rangle) + \beta_l(|1101\rangle - |0111\rangle) + \gamma_l(|1011\rangle - |0111\rangle)$ with eigenvalue $-2(\epsilon + J)$

9. $|\psi_{16}\rangle = \frac{1}{\sqrt{4}}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle)$ with eigenvalue $2(\epsilon + 3J)$.

As for three particles, the strongest interaction occurs when the state is a completely symmetric superposition of all possible configurations with the same and minimized sum of the spin projections $\sum_{i=1}^{4} s_z^{(i)}$. The total spin is not considered. The energy ratios $\{\lambda_i/\epsilon\}_{i=1}^{16}$ against J/ϵ were plotted and since the
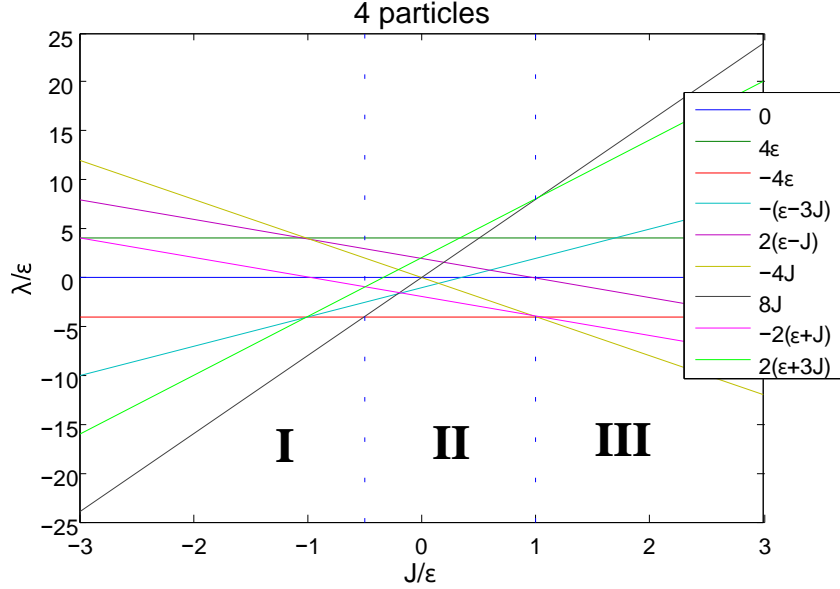

Figure 4.9: The energy ratios for the eigenvalues, $\{\lambda_i/\epsilon\}_{i=1}^{16}$, plotted to the ratio for the interaction strength J/ϵ for a four particle system.

J-dependence of the eigenvalues stays linear as the number of particles increases, there are three different regions to examine.

In region **I**, where $J < -\frac{1}{2}\epsilon$, the ground state is the state

- $\left|\psi_g^1\right\rangle = |\psi_{12}\rangle = \frac{1}{\sqrt{6}}(|0011\rangle + |0110\rangle + |1100\rangle + |0101\rangle + |1010\rangle + |1001\rangle)$.

In region **II**, where $-\frac{1}{2}\epsilon < J < \epsilon$, the ground state is the state

- $\left|\psi_g^2\right\rangle = |\psi_2\rangle = |1111\rangle$

and finally, in the third region, where $J > \epsilon$, the ground states consist of degenerated states with eigenvalue $-4J$. With the same arguments as for three

particles, the density matrix will be calculated for a mixed state constructed from two orthogonal eigenstates with equal probability

- $\left|\psi_g^{31}\right\rangle = \frac{1}{\sqrt{4}}(\left|0110\right\rangle + \left|1001\right\rangle - \left|0011\right\rangle - \left|1100\right\rangle)$
- $\left|\psi_g^{32}\right\rangle = \frac{1}{\sqrt{12}}(2\left|0101\right\rangle + 2\left|1010\right\rangle - \left|0011\right\rangle - \left|1100\right\rangle - \left|0110\right\rangle - \left|1001\right\rangle).$

In figure 4.9, points can be found where the ground state shifts. In this four-particle system, the shift at $J = \epsilon$ also includes a degeneration of the states $\left|\psi_{13}\right\rangle, \left|\psi_{14}\right\rangle, \left|\psi_{15}\right\rangle$, which are not ground states in any of the regions. These states will though not be considered when calculating the entropy for the ground states.

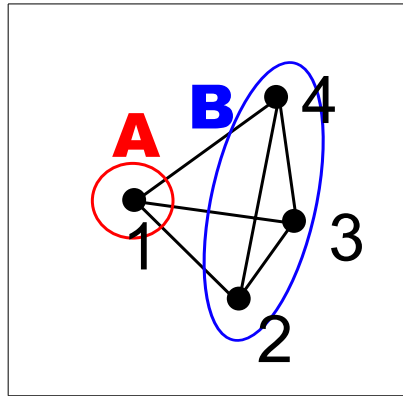### 4.3.1 The von Neumann entropy

Figure 4.10: Division of the subsystems A and B between which the entropy will be calculated.

In the same way as for two and three particles, the entropies between the subsystems A and B as shown in figure 4.10 was calculated to be

- $S_1 = \log 2 \approx 0.301$
- $S_2 = 0.$

With the density matrix for mixed state defined in equation 4.10, with $p_1 = p_2 = 1/2$, the von Neumann entropy was calculated to be

- $S_3 = \log 2 \approx 0.301.$

These entropy values of $\log 2$ are the same as the values calculated for two particles. This is notable since the subsystems are here divided with 1 and 3 particles respectively.

This pattern may suggest that all systems with an even number of particles, and with one subsystems containing one particle only, gives these results, but this statement needs to be further examined.

The calculated von Neumann results quantifies the entanglement between the subsystems A, with one particle, and B, with three particles. For this pure four
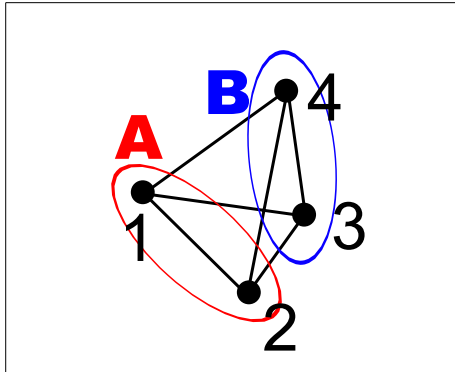
Figure 4.11: Division of the subsystems A and B, containing two particles each.

particle system, there is also another way of dividing the subsystems to calculate the entanglement. Dividing the particles two and two, as can be seen in figure 4.11, might give a different result.

Calculating the reduced density matrices with this division gives the following result of the entropies for the ground states of the system:

- $S_1 = -\frac{2}{6}\log\frac{1}{6} - \frac{4}{6}\log\frac{4}{6} \approx 0.868$
- $S_2 = 0,$

and for the mixed state

- $S_3 = -\frac{3}{6}\log\frac{1}{6} - \frac{3}{6}\log\frac{3}{6} \approx 1.2425.$

Dividing the system like this results in the largest entropy values that has been calculated so far. Even though S_3 is is not fully considered as it is a mixed state, S_1 still reaches the tops of the calculated entropies.

Consistently, the results have shown that the entropy is at its largest value when the ground state is a superpositioned state that is as symmetric as possible, with a the sum of the spin projections $\sum_{i=1}^{N} s_z^{(i)}$ of each superpositioned state as small as possible.

Chapter 5

Outlook

Even if the model in these calculations are as simplified as possible, the results give a feeling of how the entropy behaves in few interacting $\frac{1}{2}$-spin particle systems. With a strong interaction between the particles, the entanglement seems to exist in the ground state. The pattern that have occured for the pure state, that the strongest interaction occurs for a completely symmetric superposition would be interesting to further examine for larger systems. To give a better grasp of the behaviour of the entropy, it would also be interesting to calculate the entropy for the states which superpositioned states are not minimized in the sum of the spin projections. The total spin of the system was only considered for the two-particle systems, but it would be interesting to consider the total spin in the states of the systems of 3 and 4 particles.

With a better grasp of the phenomena with these possible patterns, the quantification could be made more systematic for larger systems. Comparing mixed states with pure states are not to prefer, since different methods are prefered in the entanglement quantification of these systems. Degenerate states can be avoided by considering systems with less symmetry, but then the approximation of nearest neighbour-interaction will result in a quantification that is more approximated than the symmetrized systems that has been considered here. With a system consisting of more than 4 particles though, the symmetry must be broken, since the dimension of space needed for equal distance of the particles is already maximized in the 4-particle case. To be able to create these kinds of system in a laboratory, the importance of the simplifications that have been made need to be considered.

The field of quantum mechanics and entanglement is in a historical sense a new field, that is still developing and explored with curiosity. The limits of what could be achieved with the new gained knowledge have not yet been reached, and how to quantify entanglement and other new properties in a useful way is still a question with an unclear answer. Nano systems might though, as mentioned earlier, be a way to connect quantum mechanical phenomena with the macroscopic world. Knowledge is good, but knowledge is even better if it can be applied. The areas where entanglement is potentially useful are, so far, superdense coding, quantum teleportation, interferometry and quantum cryptography. The future with applications of entanglement might not be far away.

Chapter 6

Self-reflection

During this work, I have gained a lot of knowledge and experienced personal growth. I have learned to use programs that are used in the daily work for many mathematical physicists. Both Latex and Mathematica were unknown softwares to me before I started, but now I can not imagine writing a thesis without them. Before I started my thesis I had already heard about entanglement and gained curiosity about the subject, but not fully known the area and its capabilities. I now feel that I have gained more knowledge about the history of quantum mechanics and entanglement, which has been very interesting as this is an area which is really up to date and which possibilities are still examined. I have learned terminology about the subject which deepens my understanding of it and I too, as I believe every person that learn about the subject, have gone through a lot of thinking and discussions to come to the point where I at least think that I know enough about the subject to be able to figure out what it is possible, and what it is not.

I have really enjoyed working with entanglement, since this is the part of the world of physics which has really captured my interest. I hope and believe that my future studies will keep focusing on the world of quantum mechanics.

I also feel that I have grown personally during these months. To work with a thesis together with a supervisor for a whole semester, and now have the result in my hands feel like a great achievement that strengthens my self-confidence that will help my future studies and master thesis. Overall, it has been really fun to do my bachelor thesis and I am so happy that I was able to work in the subject of physics which I am most interested in, with Peter Samuelsson as my supervisor.

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Figures

Figure 4.1 (left) was found from the source *http://www.ineffableisland.com/2011/04/nanotechnology-to-aid-art-restoration.html*.

All other figures was made by the author.