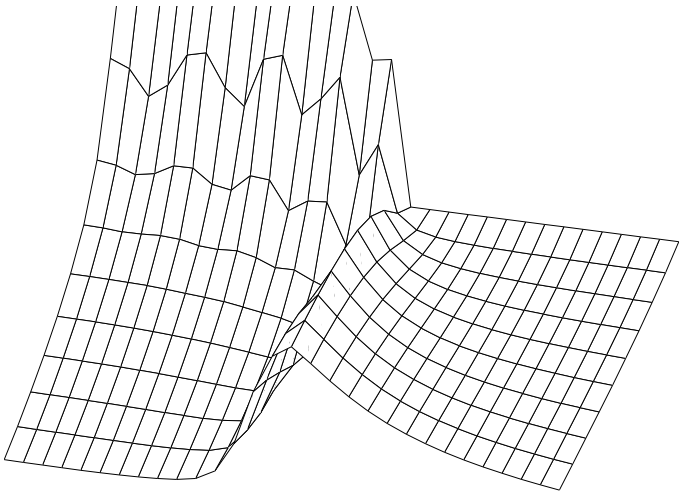
THESIS FOR THE DEGREE OF MASTER OF PHILOSOPHY

von Neumann Entropy of Spin Systems from Exact Diagonalization



HENRIK STEGEBY

Institute of Theoretical Physics
Chalmers University of Technology and Göteborg University
Göteborg, Sweden 2004

Acknowledgments

Without the encouragement, patience, and sincere support of Henrik Johannesson this work would not have been possible.

Abstract

This thesis explores the connection between quantum entanglement, entropy and quantum phase transitions in many body spin-$\frac{1}{2}$ systems. We calculate the entropy for 1-dimensional spin-chain systems using MATLAB for the Ising model and the XY model. Particular interest is given to whether we can find any precursor of critical behavior for systems with few particles. Comparisons with known results are made.

Contents

Chapter 1

Introduction

The total energy of the universe does not change. This is a fundamental law of physics. However, the form of energy does change and from the laws of thermodynamics we know that this process is governed by the increase of entropy. In other words, the universe (i.e. all systems) tends to the greatest degree of randomization. To understand how entropy works for systems on the atomic scale we need to turn to quantum physics.

The *spin* of a particle is a property that can't be explained within the framework of classical physics. A spin can–in some pictorial way–be thought of as the intrinsic rotation of a particle. This rotation contributes to the total angular momentum of the particle. In many-particle systems the orientations of the spins may depend on each other in a quite peculiar way. The study of how these spins depend on each other is closely related to the study of *entanglement*. Entanglement is a term used in quantum theory to describe how particles of energy and matter can become correlated to predictably interact with each other regardless of how far apart they are.

In many quantum-physical systems, the properties of the system depends strongly upon the orientation of the individual spins, in particular at low temperatures. The way the individual spins order themselves dictates the structure of the ground state. The ground state can be simple, with the spins aligned in the same direction, or it can have a complicated structure where entanglement pervades the ordering of the spins. In fact, entanglement appears naturally in low-temperature quantum physics. Entanglement is at the core of many quantum physical phenomena, such as the quantum Hall effect, super-conductivity and the mysterious criticality in quantum phase transitions. Entanglement is also realized to be a crucial resource to process and send information, for example in the areas of cryptography and quantum computers.

Near the absolute zero temperature, matter can switch from being ferromagnetic to paramagnetic through a very small change in an external parameter. One such parameter is the intensity of an applied magnetic field. If the majority of the spins point in the same direction they amplify the magnetic properties of the system. When the properties of a system radically changes because of a small change in a parameter, the system displays criticality. The study of criticality in the extreme environment where the temperature is close to the absolute zero is also

of importance for the understanding of phase transitions. In a way, the study of spin systems is a shortcut to understanding more general systems with a temperature away from the absolute zero. This thesis explores the possibility of studying systems with few particles as a means of understanding critical behavior.

The way the spins are ordered play a crucial role for the energy levels of the system and with that, it also determines its entropy. The entropy of a system is–in a thermodynamic view–a measure of how much order we have in the system. For a quantum dynamical spin system the degree of order depends on how many possible configurations of the orientations of the spins we can find for each state. Since the spins affect each other because of entanglement the study of entropy and entanglement go hand in hand in quantum physics, and in this thesis the study of entropy and entanglement is the central subject, together with quantum criticality.

The concepts of entropy and entanglement are intrinsically very interesting. It is not hard to understand that the notion of quantum entanglement attracts science-fiction writers, and that this sort of interest is what makes physics popular outside the more educated group of scientists. One mind boggling idea is that our conscious mind, our brain, could be compared with quantum computers, where entanglement would play a crucial role. This idea has been used in the discussion about what could happen after death, attempting to explain "after death experiences" where our consciousness seems to be something more than our physical mind. Maybe this might lead to speculations about a global subconscious where "connected" minds could be the result of entangled particles in our brains? These subjects are of course pure speculations so far and this thesis will only deal with scientific facts. The area of entanglement and entropy is a very "fresh" subject where lots of undiscovered territory lies ahead, and it has attracted the interest of leading physicists all over the world.

To help us in our task of understanding how criticality arises in small systems we must first define and understand quantum entanglement, entropy and quantum criticality. Chapter two and three are devoted to this noble cause. I then use these definitions to calculate the entropy for small spin systems using exact diagonalization. In chapter four I show explicitly how the calculations are carried out for a given Hamiltonian and I also explain how the program I constructed for MATLAB works. At the end of chapter five I explain the different Hamiltonians used to model simple spin chain systems such as the Ising model, the Hamiltonian and the XY Hamiltonian. In chapter five I present my results and conclusions.

Chapter 2

Entropy

"Just as the constant increase of entropy is the basic law of the universe, so it is the basic law of life to be ever more highly structured and to struggle against entropy" – Vaclav Havel

What is entropy? The basic thermodynamic definition tells us that entropy has to do with order. In short, entropy measures how disordered something is. The more order we have in a system, the less is the entropy. Information theory tells us that entropy is to be seen as some sort of uncertainty level, how much uncertainty there is in a state. A more precise statement about entropy- coming from statistical physics - is that it has to do with the level of degeneracy in a macroscopic state, i.e., how many microscopical states there are given a macroscopic state. Needless to say, the concept of entropy is complex. This chapter is devoted to build up the reader's intuition about entropy and present the von Neumann definition of entropy, the most important definition of entropy for this thesis. As we shall see, the von Neumann entropy also measures the degree of quantum entanglement in a pure state, and therefore it is of particular interest to us.

2.1 Entropy in thermodynamics

An ensemble is an imaginary collection of systems, each of which is a replica, in terms of macroscopic variables, of the system of interest. A microcanonical ensemble is an ensemble in which the systems may be in different states, but where they all are isolated systems. For a microcanonical ensemble, the entropy is given by

$$S = k \log W, \tag{2.1}$$

where W is the number of states and k is the Boltzmann constant. In this example, entropy only has to do with how many states there are.

In order to generalize the definition of entropy into taking thermal fluctuations into account, we need to learn about the *partition function*, which is given by the equation:

$$Z = \sum_j e^{-E_j/k_BT}, \tag{2.2}$$

where E_j is the energy of a state with index j. Z is an abbreviation of the German word 'Zustandssumme' which means sum-over-states [1]. When we calculate the partition function that is exactly what we do, we sum over states. The classical probability that a system is in a quantum state ψ_i is equal to the number of quantum states associated with ψ_i divided by the total number of states:

$$p_i = \frac{e^{-E_i/k_BT}}{\sum_j e^{-E_j/k_BT}}. \tag{2.3}$$

The denominator in the above equation is, as you can see, the partition function. It may seem as if the partition function is just some normalization constant needed to make the sum of the probabilities equal to one. Considering that for a microcanonical ensemble, all we need to know in order to calculate the entropy is the number of states, we understand that the partition function is much more important than that. From the partition function we can make direct connections between the quantum states of the system and its thermodynamic properties, such as the free energy, the pressure and the entropy. All this can be calculated from the partition function!

Now, with the probabilities given by eqn (2.3), eqn (2.1) leads to the formula:

$$S = -k_B \sum_i p_i \ln(p_i), \tag{2.4}$$

for calculating the entropy in a *canonical ensemble*. By writing

$$\ln(p_i) = -E_i/k_BT - \ln(Z) \tag{2.5}$$

and substituting $\ln(p_i)$ in eqn (2.4) we get

$$S = k_B \sum_i p_i(\frac{E_i}{k_BT} + \ln(Z)). \tag{2.6}$$

The sum over quantum states in eqn (2.6) has one part due to $\ln(Z)$ and another part containing E_i/k_BT which involves the mean or average energy

$$U = \sum_i p_i E_i. \tag{2.7}$$

By substituting the equation for the average energy into eqn (2.6) we get:

$$S = \frac{U}{T} - F \tag{2.8}$$

where the free energy F is related to the partition function by

$$F = -k_B T \ln(Z). \tag{2.9}$$

So, one way of calculating the entropy of a system in a *canonical ensemble* [1] is by calculating the partition function. By understanding how entropy arises in thermodynamics, I hope the reader has been gifted with some intuition as to what entropy is. We now continue to more abstract areas such as information theory.

2.2 Shannon entropy

The key concept of classical information theory is the *Shannon entropy*. Shannon entropy can be viewed as either a measure of our uncertainty *before* we learn about a random variable X, or as a measure of how much information we have gained *after* we have learned the value of X [2]. Intuitively, the information content of a random variable should not depend on the labels attached to the different values that may be taken by X. For example, we expect that a random variable taking the values ”alive” and ”dead”, as in the Schröedinger cat example, with respective probabilities $\frac{1}{4}$ and $\frac{3}{4}$ contains the same amount of information as a random variable that takes the values 1 and 0 with the same respective probabilities. Because of this, the entropy of a random variable is defined to be a function of the probabilities of the different values the random variable takes, and is not influenced by the labels used for those values. We often write the entropy as a function of a probability distribution $p_1, ..., p_n$. The Shannon entropy associated with this probability distribution is defined by

$$H(X) \equiv H(p_1, ..., p_n) \equiv -\sum_x p_x \log_2 p_x. \tag{2.10}$$

Now, the main task in this section is to understand why it is defined in this way, because the *Shannon entropy* is very similar to the *von Neumann entropy* in quantum physics, and that definition of entropy is of most importance to this thesis. The difference between the Shannon entropy and von Neumann entropy is that the classical probabilities p_i in eqn (2.10) are exchanged with operators ρ_i, and the sum is replaced by a trace. The von Neumann definition is the definition that I use when I calculate the entropy in MATLAB for systems with few particles.

2.3 Intuitive justification for the definition of the Shannon entropy

The best reason for the Shannon definition of entropy, eqn (2.10), is that it can be used to *quantify the resources needed to store information* [2]. This justification is a bit hard to fully understand, so to make things easier we instead ask ourselves what properties we want our entropy function to have:

(1) We want our function to be a function of the probabilities of our outcomes only.

(2) We want our function to be smooth.

(3) The information gained from two independent events that occur with individual probabilities p and q should be the sum of the information gained from each event alone, i.e. $I(pq) = I(p) + I(q)$.

A function that fulfills these conditions must be of the form $I(p) = k \log p$, for some constant k [2]. It follows that the average information gain when one of a mutually exclusive set of events with probabilities $p_1, ..., p_n$ occurs is $k \sum_x p_x \log p_x$ [3]. This is just the Shannon entropy, up to a constant factor.

2.4 Probabilistic justification of the Shannon entropy

Now, it is seldom enough to have a fairly good intuition about things in science, we also need to understand more precisely how things works. For this reason a derivation of the definition of the Shannon entropy is in order:

Consider a message written with letters chosen from an alphabet consisting of k numbers of letters:

$$\eta = [a_1, a_2, ..., a_k]. \tag{2.11}$$

Now, suppose that each letter in the message is statistically independent of the other, and that the letters a_x occurs with an *a priori* probability $p(a_x)$, where $\sum_{x=1}^{k} p(a_x) = 1$.

Claude Shannon asked himself: *Is it possible to compress the message to a shorter string of letters that conveys essentially the same information?*

For the number of letters k large, let us write $k = n$ in order to remember that k is large. With a binary alphabet where letter 0 occurs with probability $1 - p$ and letter 1 occurs with probability p, the law of large numbers tells us that *typical* strings will contain about $n(1-p)$ 0's and about np 1's. The number of distinct strings of this form is of order the binomial coefficient n over np, and from the Stirling approximation:

$$\begin{aligned} \log \left(\begin{array}{c} n \\ np \end{array} \right) &= \log(\frac{n!}{(np)![n(1-p)]!}) \cong \\ &\cong n \log n - n - [np \log np - np + n(1-p) \log n(1-p) - n(1-p)] = \\ &= n H(p), \end{aligned} \tag{2.12}$$

where

$$H(p) = -p \log p - (1-p) \log(1-p), \tag{2.13}$$

is the *entropy* function. Hence, the number of typical strings is of order $2^{H(p)}$. To convey essentially all the information carried by a string of n bits, *it suffices to choose a block code that assigns a positive integer to each of the typical strings.* Since this block code has about $2^{H(p)}$ letters, which is less than the original number of letters (for $p \neq \frac{1}{2}$), we have successfully reduced the number of letters needed to send the information.

This is Shannon's result. The key idea is that we only need a code word for every *typical* sequence of letters, instead of all possible sequences of letters [2]. The probability that the actual message is atypical becomes negligible asymptotically, i.e., in the limit $n \to \infty$.

This reasoning is valid even for the case of n letters, with an alphabet where letter x occurs with probability $p(x)$. We don't need to use a binary alphabet [1]. In a string of n letters, x typically occurs about $np(x)$ times, and by once again using the Stirling approximation, the number of typical strings is of order

$$\frac{n!}{\Pi_x (np(x))!} \simeq 2^{-nH(X)}, \tag{2.14}$$

where X is the distribution from where each of the n letters is drawn from, and

$$H(X) = \sum -p(x) \log p(x). \tag{2.15}$$

This is the definition of the *Shannon entropy* of the ensemble $X = \{x, p(x)\}$.

Here, I would like to stress the fact that the derivation is done for a large number of letters, $k >> 1$, in order to be able to use the Stirling approximation and to reduce the probability that the actual message is atypical. Thus, the Shannon entropy should not be very accurate for a small number of letters.

2.5 von Neumann entropy

The difference between quantum and classical information theory lies in the dependence amongst the letters that are drawn. In classical information theory each letter can be drawn independently from an ensemble $X = [x, p(x)]$, whereas in quantum information theory each letter is chosen from an ensemble of quantum *states* p_x, each occurring with a specified *a priori* probability p_x. In quantum theory, the probability of any outcome of any measurement of a letter chosen from this ensemble (where the observer has no knowledge about which letter was prepared), can be completely characterized by the *density* matrix

$$\rho = \sum_x p_x \rho_x, \tag{2.16}$$

[1] See chapter 5 for a discussion about this.

where $\rho_x = |x\rangle\langle x|$ is a projection operator onto state $|x\rangle$ (using the Dirac notation [2]). For any density matrix, we may define the *von Neumann* entropy as:

$$S(\rho) = -tr(\rho \log \rho), \tag{2.17}$$

where we trace over one of the subsystems A or B, i.e.

$$S(A) = -tr(\rho_A \log \rho_A), \tag{2.18}$$

$$S(B) = -tr(\rho_B \log \rho_B). \tag{2.19}$$

If we choose an orthonormal basis $|a\rangle$ that diagonalizes ρ:

$$\rho = \sum_a \lambda_a |a\rangle\langle a|, \tag{2.20}$$

then

$$S(\rho) = H(A), \tag{2.21}$$

where $H(A)$ is the Shannon entropy of the ensemble $A = \{a, \lambda_a\}$.

So, in the case were the signal alphabet consists of mutually orthogonal pure states, the quantum source reduces to a classical one; all of the signal states can be perfectly distinguished since they are independent of each other, and $S(\rho) = H(X)$.

Now, once again, I would like to point out that the von Neumann entropy might not be very accurate for a small number of letters k, since the Shannon entropy is not accurate for a small number of letters, and the two definitions are analogies of each other. However, the von Neumann definition must not necessarily be derived from the Shannon entropy[3].

The von Neumann entropy quantifies not only the *quantum* information content per letter of the ensemble (the minimum number of qubits per letter needed to reliably encode the information) but also its *classical* information content (the maximum amount of information per letter - in bits, not qubits - that we can gain about the preparation by making the best possible measurement). For a deeper study in quantum information theory I refer the interested reader to [2, 3, 5].

The von Neumann definition of entropy enters quantum information theory in yet a third way, the most important one for this thesis: It quantifies the entanglement of a bipartite *pure* state. This is why quantum information is so largely concerned with the interpretation and uses of the von Neumann entropy.

As a simple example of how the von Neumann entropy works, let us consider a *pure* two-particle spin-$\frac{1}{2}$ system, where if one particle is in a spin up state, the other one must be in a spin

[2] See chapter 4.

[3] I will present a stronger argument for the validity of the von Neumann entropy of entanglement in section 3.3.

down state and vice versa, to preserve the total angular momentum. Each particle has the same probability of being in the spin up state as in the spin down state, and we can write the state as:

$$\psi = \cos(\theta)|\uparrow_1\downarrow_2\rangle + \sin(\theta)|\downarrow_1\uparrow_2\rangle. \tag{2.22}$$

Now, the total density matrix is given by

$$\rho = |\psi\rangle\langle\psi| = (\cos(\theta)|\uparrow_1\downarrow_2\rangle + \sin(\theta)|\downarrow_1\uparrow_2\rangle)(\cos(\theta)\langle\uparrow_1\downarrow_2| + \sin(\theta)\langle\downarrow_1\uparrow_2|). \tag{2.23}$$

Now, with

$$|\uparrow\rangle = |1\rangle, \tag{2.24}$$

$$|\downarrow\rangle = |0\rangle, \tag{2.25}$$

the above equation reduces to

$$\rho = (\cos(\theta)|1_1 0_2\rangle + \sin(\theta)|0_1 1_2\rangle) \times (\cos(\theta)\langle 1_1 0_2| + \sin(\theta)\langle 0_1 1_2|), \tag{2.26}$$

which equals

$$\begin{aligned} \rho &= \cos(\theta)^2|1_1 0_2\rangle\langle 1_1 0_2| + \sin(\theta)\cos(\theta)|1_1 0_2\rangle\langle 0_1 1_2| + \\ &\quad + \sin(\theta)\cos(\theta)|0_1 1_2\rangle\langle 1_1 0_2| + \sin(\theta)^2|0_1 1_2\rangle\langle 0_1 1_2|. \end{aligned} \tag{2.27}$$

Now, we use the definition of the von Neumann entropy and trace over the states of one of the particles, for example particle no. 2 (P_2) to get:

$$\begin{aligned} \rho_1 &= tr_2(|\rho\rangle\langle\rho|) = \sum_{P_2=0,1} \langle P_2|\rho\rangle\langle\rho|P_2\rangle = \\ &= \langle 0_2|\Big[\cos(\theta)^2|1_1 0_2\rangle\langle 1_1 0_2| + \sin(\theta)\cos(\theta)|1_1 0_2\rangle\langle 0_1 1_2| + \\ &\quad + \sin(\theta)\cos(\theta)|0_1 1_2\rangle\langle 1_1 0_2| + \sin(\theta)^2|0_1 1_2\rangle\langle 0_1 1_2|\Big]|0_2\rangle + \\ &\quad + \langle 1_2|\Big[\cos(\theta)^2|1_1 0_2\rangle\langle 1_1 0_2| + \sin(\theta)\cos(\theta)|1_1 0_2\rangle\langle 0_1 1_2| + \\ &\quad + \sin(\theta)\cos(\theta)|0_1 1_2\rangle\langle 1_1 0_2| + \sin(\theta)^2|0_1 1_2\rangle\langle 0_1 1_2|\Big]|1_2\rangle, \end{aligned} \tag{2.28}$$

which gives [4]

$$\rho_1 = \sin(\theta)^2|1\rangle\langle 1| + \cos(\theta)^2|0\rangle\langle 0| \ . \tag{2.29}$$

In matrix form this can be written as

$$\rho_1 = \begin{pmatrix} \sin(\theta)^2 & 0 \\ 0 & \cos(\theta)^2 \end{pmatrix}. \tag{2.30}$$

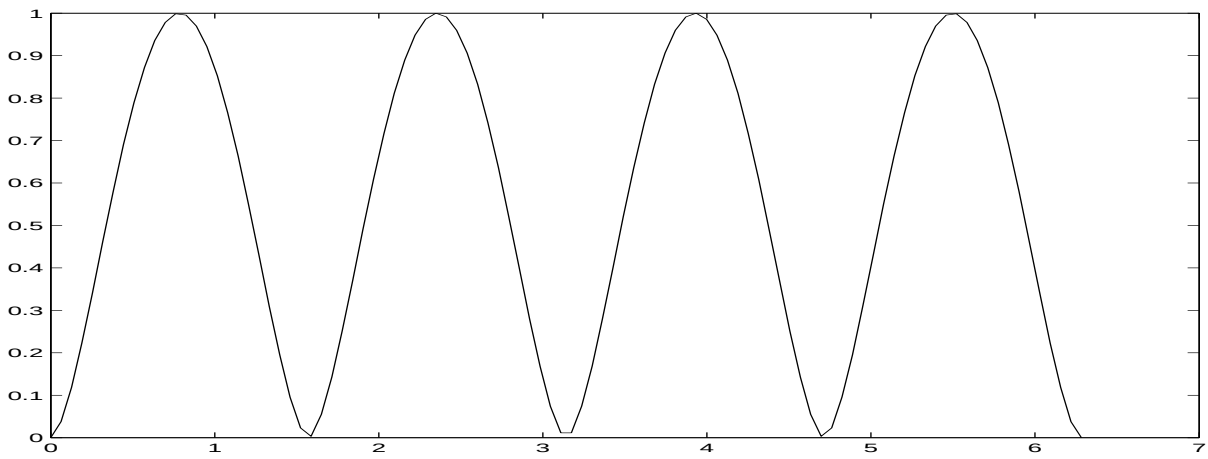


Figure 2.1: von Neumann entropy for a pure two-particle system. The x-axis is the theta axis, the y-axis is the entropy.

Now, inserting this matrix in MATLAB for the von Neumann entropy, eqn (2.18), gives us the plot seen in fig 2.1. Here, the maximum entropy is for $\cos(\theta) = \sin(\theta)$, i.e. for $\theta = \pi/4 + 2n\pi$. This means that the entropy is at a maximum when both configurations are equally probable, where neither one of the configurations are dominant, which means that the "uncertainty" of the system is at a maximum. This is exactly the result we want from a definition of entropy, so the von Neumann entropy seems to be a good one! [5]

The degree of entanglement is in a way a measure of how much the individual particles affect each other. By knowing the degree of entanglement in a system we know how much order we got in the system, its entropy. Because of this, entanglement can be used to calculate the entropy of the system, and vice versa.

[4] See chapter 4 for a more detailed explanation of how tracing works.

[5] It may seem strange that the von Neumann definition of entropy seems to work for this example where we, in the classical analogy, would have a binary alphabet (spin up or spin down) with only two letters ($|10\rangle$ or $|01\rangle$). See chapter 5 for a deeper discussion about this subject.

Chapter 3

Entanglement and quantum phase transitions

Quantum phase transitions have attracted research activities from various fields of physics. Unlike classical phase transitions, which are driven by thermal fluctuations, quantum transitions are induced by a parameter which enhances quantum fluctuations at zero temperature [6]. Entanglement and the understanding of quantum phase transitions go hand in hand. When a system is close to a critical point the correlations become long-ranged and entanglement governs the behavior of the system. This is why quantum phase transitions are of great importance, not only in itself, but also for the understanding of entanglement.

3.1 The degree of entanglement

Particles affect each other through their individual spin orientation. If the net angular momentum of a system is zero, and if all the contributions to the angular momentum comes from the individual particles spins, then the sum of the individual spins of the particles must add up to zero. This means that if we have two particles, with one of the particles having spin "up", then the other must have spin "down". In other words; if we know the spin of one of the two particles, we know the spin of the other one with certainty. This is an example of a maximally quantum entangled system [7].

In a way, the degree of entanglement should be the degree of how "far away" the system is from being able to be written as a *product state*, i.e. an unentangled state. A product state is a state that can be written as

$$\Psi = \psi_1 \otimes \psi_2 \otimes ... \otimes \psi_n \ , \tag{3.1}$$

where each ψ_i corresponds to particle $i's$ state. A measure of how "far away" a system is of being able to be written as a product state may then perhaps be compared with how many terms we need to use in order to write the state as a sum of all possible spin-configurations. As it turns out, the complexity of measuring entanglement is higher than this [12, 8, 9, 17]. The degree of

entanglement is more linked to the form of the resulting reduced density matrices. The reduced density matrices are linked to ”how much” of a product state the system is in, since the ground state that builds up the matrices can be compared to ”how close” it is from being able to be written as a product state. By using different transformations with adherent parameters it is possible to determine how ”far away” the state is from a product state

Characterizing entanglement is about identifying a reduced subset of parameters that are particularly relevant from a physical or computational point of view [4]. Exactly how to do this is not clear, since what is of relevance in one situation might not be the same as in another situation. Because of this, we have many different definitions of entanglement and, therefore, since entropy conveniently measures entanglement, *entropies of entanglement*. The most important one for this thesis is the one for *pure* ensembles, which is the von Neumann entropy, but other definitions of importance are the so called *localizable entanglement* [8, 10], *entanglement of formation* [8] and *concurrence* [12]. First, we need to set things clear about mixed and pure ensembles.

3.2 Entanglement in mixed and pure ensembles

When every particle in an ensemble can be characterized by the same state ket $|\alpha\rangle$ the ensemble is said to be a *pure* ensemble. Conversely, when this is not true, the ensemble is a *mixed* ensemble. As an example, a beam of silver atoms which has gone through a selective Stern-Gerlach-type measurement [7] will be a pure ensemble since all the particles can be characterized by the same state ket. Before the particles go through any apparatus, the ensemble is mixed. In a more precise manner, a pure ensemble and a complete random ensemble can be regarded as the extremes of what is known as a mixed ensemble. In a mixed ensemble a certain fraction - for example, 70% of the members are characterized by a state ket $|\alpha\rangle$, the remaining 30% by $|\beta\rangle$. For a pure ensemble, this fraction is 100% and 0%, respectively.

So, when we try to define entropy of entanglement, we should do it for a mixed ensemble in order to be able to use it on every type of ensemble. However, because of the problems mentioned above, what relevant parameters to identify entanglement with is not universal. In contrast, for a pure ensemble there is no need to complicate matters with transformations and adherent parameters in order to characterize entanglement, and the von Neumann entropy is as of today indisputably a good one. Note, however, that with saying that it is a good one, I am not saying that it is without problems or that it cannot be improved upon. For example, the system needs to be a bipartite system in order to be able to apply the definition of the von Neumann entropy. We would like to have a definition that can be applied to multipartite systems. In addition, it seems to me that it is quite possible that the apparent approximations made in the derivation of the Shannon entropy, together with applying the von Neumann entropy for systems with few particles, should result in an approximation and not in an exact evaluation of the entropy of the system.

3.3 Why is the von Neumann entropy a good measure of entanglement?

Well, first off, it is only a good measurement of entanglement for *pure* states. For mixed states the distinction between entangled and unentangled states are not as sharp as for pure states: *a pure state is entangled or nonlocal if and only if its state vector cannot be expressed as a product $\psi_1 \otimes \psi_2$ of pure states ψ_1 and ψ_2* [7]. This is the core of entanglement.

If we look at the von Neumann definition of entropy, eqn (2.18), from a mathematical point of view, we notice that when we have a maximum of the entropy, the reduced density matrix reduces to a multiple of the identity matrix [13]. Conversely, the entropy reaches a minimum when the reduced density matrix has equal entries in all positions, or when the matrix in other ways is as "far away" from being a multiple of the identity matrix. This minimum happens for product states, as can be understood by writing out a product state and look at its density matrix. From this view, it is clear that the von Neumann entropy "does its job" in the respect of finding maximum and minimum. The definition reflects "how much" of a product state the state is in. But a good definition also needs to fulfill a set of other properties [8, 18]:

- The entanglement, which we shall denote E, of independent systems is additive.
- E is conserved under local unitary operations, i.e., under any unitary transformation U that can be expressed as a product $U = U_A \otimes U_B$ of unitary operators on the separate subsystems.
- The expectation of E cannot be increased by local non-unitary operations: if a bipartite pure state $|\psi\rangle$ is subjected to a local non-unitary operation (e.g. a measurement) resulting in residual pure states $|\psi_j\rangle$ with respective probabilities p_j, then the expected entanglement of the final states $\sum_j p_j E(\psi_j)$ is no greater, but may be less, than the original entanglement $E(\psi)$ [9].
- Entanglement can be concentrated and diluted with unit asymptotic efficiency [**?**], in the sense that for any two bipartite pure states $|\psi\rangle$ and $|\psi'\rangle$, where in the "Alice and Bob example"[1], Alice and Bob are given a supply of n identical systems in a state $|\Psi\rangle = |\psi\rangle^n$. They can use local actions and one-way classical communication to prepare m identical systems in state $|\Psi'\rangle \approx |\psi'\rangle^n$, with the yield m/n approaching $E(|\psi\rangle)/E(|\psi'\rangle)$, the fidelity $|\langle\Psi'|(\psi')^m\rangle|^2$ approaching 1, and probability of failure approaching zero in the limit of large n.
- With regard to entanglement, a pure bipartite state $|\psi\rangle$ is thus completely parameterized by $E(\psi)$, with $E(\psi)$, being a measure of both the asymptotic number of standard singlets

[1] Alice and Bob share an entangled state, see [1].

required to locally prepare a system in state $|\psi\rangle$ – its "entanglement of formation" – and the asymptotic number of standard singlets that can be prepared from a system in state $|\psi\rangle$ by local operations – its "distillable entanglement" [8].

This is a good argument to why the von Neumann definition is a powerful one. However, one might want to understand the details in the definition, and where they come from without looking at the analogy with the Shannon entropy. This would be useful since our doubts about the accuracy of the Shannon entropy for systems with a small number of letters would decrease.

For this purpose, we start by asking ourselves: Can we use partially entangled pure states to characterize entanglement? In other words, can we use pairs of particles in the state

$$|\psi\rangle = \cos\theta|1_1\rangle \otimes |0_2\rangle + \sin\theta|0_1\rangle|1_2\rangle \tag{3.2}$$

to supply entanglement? If so, how many such pairs to substitute for one maximally entangled pair, such as pairs of particles in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|1_1\rangle \otimes |0_2\rangle + |0_1\rangle \otimes |1_2\rangle) \tag{3.3}$$

would be needed? By using the so called *"Schmidt decomposition"* and absorbing phases into the definitions of the basic states, any entangled state can be represented by a biorthogonal expression of this form with positive and real coefficients [9]

$$\Psi(A,B) = \sum_{i=1}^{d} c_i|\alpha_i\rangle \otimes |\beta_i\rangle, \tag{3.4}$$

where $|\alpha_1\rangle, |\alpha_2\rangle, ..., |\alpha_n\rangle$ and $|\beta_1\rangle, |\beta_2\rangle, ..., |\beta_n\rangle$ are orthonormal states of subsystem A and B, respectively, and the coefficients c_i are real and positive. Now, for either observer, an entangled state is described by a density matrix obtained by tracing over the degrees of freedom of the other observer. The density matrices are diagonal in the Schmidt basis:

$$\rho_A = Tr_B|\Psi(A,B)\rangle\langle\Psi(A,B)| = \sum_i c_i|\alpha_i\rangle\langle\alpha_i|, \tag{3.5}$$

and similarly for ρ_B. The entanglement of a partly entangled pure state can now be parameterized by its entropy of entanglement, defined as the von Neumann entropy of either ρ_A or ρ_B, or equivalently as the Shannon entropy of the squares of the Schmidt coefficients.

$$E = -Tr(\rho_A \log_2 \rho_A) = -Tr(\rho_B \log_2 \rho_B) = -\sum_B c_i^2 \log_2 c_i^2. \tag{3.6}$$

The square of the Schmidt coefficients is what we know of as the probability of the possible outcomes p_i in the Shannon entropy.

3.4 Entanglement in quantum phase transitions

When the system is in a gap-less (critical) environment, the correlations are long-ranged and entanglement is believed to strongly influence the behavior of the system. The spin at one lattice site may affect another spin from a very great distance. The internal structure in a material becomes secondary to its macroscopic dimensions. This phenomena, when the macroscopic properties of a material becomes dominant, is called *universality*, and it is a contributor to the entanglement of the system and its entropy. The study of this phenomenon involves the study of order parameters and scaling with uses of the *renormalization group* [17, 11].

One phenomenon of particular interest to this thesis is the quantum magnetic order-disorder transition: in the ordered phase the average spin direction (magnetization) along a given direction is nonzero, while in the disordered phase it is zero. This phase transition is believed to be associated with a particular behavior of the quantum entanglement of the system. What this means for the Ising and XY model is the topic of this thesis.

3.5 Critical parameters and magnetization

For a spin lattice system the critical parameter at zero temperature is the intensity of the external magnetic field g [2]. There are conjectures that the quantum entanglement (or the rate of change of the entanglement as a function of g) typically shows a maximum at a quantum critical point. This conjecture raises a number of questions: “Does the scenario *always* happen for *any* model?”, “Is it independent of the particular definition of entanglement that is being used?”, “How does this property show up for small systems, with a finite number of spins?”. These are some of the questions that we address in chapters 4 and 5.

For the spin models that we use at zero temperature, the essential quantum phase transition that happens is that they go from being ferromagnetic to paramagnetic. For this reason it is of interest to calculate the magnetization of a spin system.

The magnetization of the system is given by [9]

$$M = \langle S_i \rangle = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^z \tag{3.7}$$

where N is the number of spins in the system.

I have implemented the calculation of the magnetization into my MATLAB program and the result is shown, together with results for the von Neumann entropy, in the graphs in chapter 5.

[2] An external magnetic field is usually denoted H in physics texts. However, in the context of quantum critical models, like the Ising and XY models, the standard notation is g.

Chapter 4

Calculations

Calculating the entropy of a quantum spin system may seem simple when "seen from a distance". The detailed implementation, however, is a completely different story, and requires quite a bit of work. To illustrate the exact diagonalization method for calculating the entropy for a 1-dimensional spin system with nearest neighbor coupling and a transverse magnetic field, I use, at first, an Ising spin chain consisting of only three lattice spins. I then continue with a chain of five particles. From these simple cases it is possible to understand how to carry out the calculation for more particles. The actual calculation, however, is very time consuming (even for a computer) as the dimensions of the matrices grow quadratically for each added particle.

4.1 The analytical approach as seen from a distance

For a 1-dimensional Ising spin chain with an external transverse magnetic field of magnitude g the Hamiltonian is given by

$$H = \sum_{<i,j>}^{n} J(\sigma_i^x \sigma_j^x + g\sigma_i^z), \tag{4.1}$$

where σ^x and σ^z are the Dirac spin matrices

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \tag{4.2}$$

and J is a coupling constant and g is the intensity of the external magnetic field.

In order to calculate the ground state vector (we are only interested in the ground state for the von Neumann definition of entropy of entanglement) we need to diagonalize the Hamiltonian. From the eigenstate matrix, we select the vector corresponding to the lowest eigenvalue, which, by definition, corresponds to the ground state. Formally, we represent the diagonalization procedure by

$$diag(H) \rightarrow X, D \quad , \tag{4.3}$$

were X is the eigenstate matrix and D is the diagonal matrix with the corresponding eigenvalues. Now, the ground state is given by the vector corresponding to the lowest eigenvalue, which for MATLAB is the vector in the first column:

$$\psi = X(:, 1). \tag{4.4}$$

Our next step is to calculate the density matrix from the state vector ψ for the whole system AB, were A and B are the two subsystems that we have divided our system into in order to get a *bipartite* system. This is given by

$$\rho_{AB} = \psi \times \psi^T. \tag{4.5}$$

Now we need to construct the *reduced* density matrices ρ_A and ρ_B. They are labeled *reduced* because when, for example, we construct ρ_A we trace over the particles corresponding to subsystem B. i.e.

$$\rho_A = tr_B(\rho_{AB}), \tag{4.6}$$

$$\rho_B = tr_A(\rho_{AB}). \tag{4.7}$$

How this tracing is done explicitly will be explained in detail in the next section. The entropy for each subsystem is now, as given by the von Neumann definition

$$S_A = tr(\rho_A \log_2 \rho_A), \tag{4.8}$$

$$S_B = tr(\rho_B \log_2 \rho_B). \tag{4.9}$$

Since the von Neumann definition in a way measures the entropy of entanglement "between" the two subsystems A and B, the total entropy for the whole system AB is equal to the entropy of each subsystem A and B:

$$S_{AB} = S_A = S_B. \tag{4.10}$$

In order to perform these calculations explicitly, I need to switch over to a more convenient notation, the *Dirac notation*.

4.2 Dirac notation

Paul Dirac invented a very clever way of writing quantum states. Instead of using wave functions to describe every possible property of a system this notation allows us to write, for example, a *spin up* property as $|1\rangle$ and a *spin down* property as $|0\rangle$. When there are many qubits in a row, the first qubit corresponds to particle no. 1, the next qubit corresponds to particle no. 2, and so on, and the notation can be simplified to:

$$|0\rangle|1\rangle|0\rangle|1\rangle...|1\rangle|1\rangle = |0101...11\rangle. \tag{4.11}$$

In vector form, spin up and spin down is written as

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{4.12}$$

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{4.13}$$

respectively. For a system with three particles where all particles have spin up, the state would be written as

$$|1\rangle \otimes |1\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0. \end{pmatrix}, \tag{4.14}$$

where it is understood that we are dealing with direct products, i.e. *Kronecker multiplication*:

$$|1\rangle|1\rangle|1\rangle = |1\rangle \otimes |1\rangle \otimes |1\rangle. \tag{4.15}$$

Now it is easy to see that any vector can be written as a sum over spin-configurations, so we can write our ground state as a sum over all possible spin configurations,

$$|\psi\rangle = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_{2^n-1} \\ y_{2^n} \end{pmatrix} = y_1|11...11\rangle + y_2|11...10\rangle + ... + y_{2^n-1}|00...01\rangle + y_{2^n}|00...00\rangle. \tag{4.16}$$

It follows that our density matrix for the whole system AB reads:

$$\begin{aligned} \rho_{AB} &= \psi \times \psi^T = \\ &= (y_1|11...11\rangle + y_2|11...10\rangle + ... + y_{2^n-1}|00...01\rangle + y_{2^n}|00...00\rangle) \times \\ &\times (y_1|11...11\rangle + y_2|11...10\rangle + ... + y_{2^n-1}|00...01\rangle + y_{2^n}|00...00\rangle)^T \\ &= y_1y_1|11..1\rangle\langle 11..1| + y_1y_2|11..1\rangle\langle 1..10| + ... + y_ny_n|00..0\rangle\langle 00..0|. \end{aligned} \tag{4.17}$$

We can write the trace over each subsystem explicitly as

$$\rho_A = tr_B(\rho_{AB}) = \sum_\beta \langle\beta|\rho_{AB}|\beta\rangle =$$
$$= \sum_\beta \langle\beta|(y_1y_1|11..1\rangle\langle 11..1| + y_1y_2|11..1\rangle\langle 1..10| + ... + y_ny_n|0..00\rangle\langle 0..00|)|\beta\rangle \ , \quad (4.18)$$

and

$$\rho_B = tr_A(\rho_{AB}) = \sum_\alpha \langle\alpha|\rho_{AB}|\alpha\rangle =$$
$$= \sum_\alpha \langle\alpha|(y_1y_1|11..1\rangle\langle 11..1| + y_1y_2|11..1\rangle\langle 1..10| + ... + y_ny_n|0..00\rangle\langle 0..00|)|\alpha\rangle \ , \quad (4.19)$$

where $|\beta\rangle$ and $|\alpha\rangle$ are the qubits corresponding to the particles in subsystem B and A respectively.

4.3 Block vectors and particle numbering

In order to use the von Neumann definition to measure the entropy we need to split our system into two subsystems, block A and B. This resulting system is called a *bipartite* system [9]. In our case the undivided original system consists of a chain of particles, each with spin one half. This is called a spin chain. Now, we give each particle a number from 1 to n, were n is the total number of particles, and we let the particles keep this number after we have divided the system into this bipartite system. This is necessary later on in order to keep a clear head about how to trace over each subsystem when we calculate the reduced density matrices.

To help us understand how the final summation for our density matrices are affected by the number of particles and how we split our spin chain into a bipartite system, let us calculate the density matrix for a system consisting of three particles on a spin chain, where we let subsystem A consist of the two leftmost particles and subsystem B to consist of the third particle. For starters, let's have a look at how exactly the corresponding block vectors arise. We can write our ground state vector as:

$$\psi_{AB} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{pmatrix} = y_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + y_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + ... + y_7 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + y_8 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} . \quad (4.20)$$

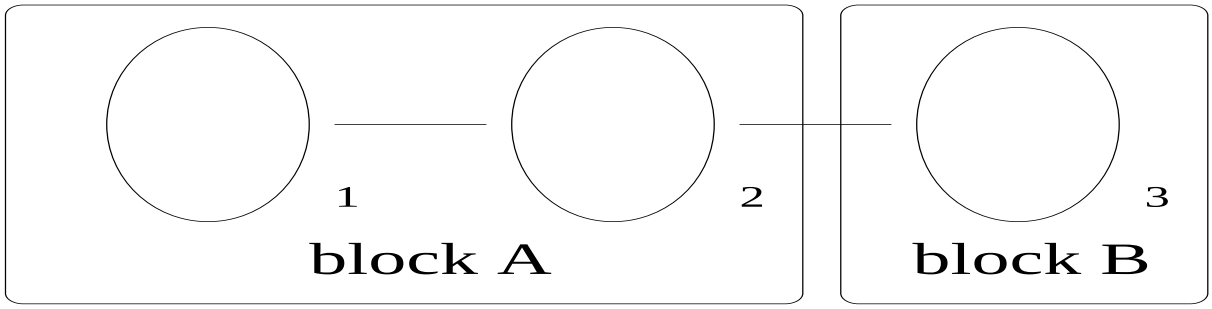


Figure 4.1: A spin graph over 3 particles. Block A consist of the two leftmost particles, block B of the third particle.

As we have seen, this can be written as a sum over configurations in Dirac notation as

$$\begin{aligned} |\psi_{AB}\rangle &= y_1|111\rangle + y_2|110\rangle + y_3|101\rangle + y_4|100\rangle \\ &+ y_5|011\rangle + y_6|010\rangle + y_7|001\rangle + y_8|000\rangle. \end{aligned} \tag{4.21}$$

Now we split our system into block A and block B, where we let block A consist of particle no. 1 and 2, and block B consists of particle no. 3. Here, we rewrite the ground state as

$$\begin{aligned} |\psi_A\rangle &= y_1|11\rangle_A \otimes |1\rangle_B + y_2|11\rangle_A \otimes |0\rangle_B + y_3|10\rangle_A \otimes |1\rangle_B + y_4|10\rangle_A \otimes |0\rangle_B \\ &+ y_5|01\rangle_A \otimes |1\rangle_B + y_6|01\rangle_A \otimes |0\rangle_B + y_7|00\rangle_A \otimes |1\rangle_B + y_8|00\rangle_A \otimes |0\rangle_B. \end{aligned} \tag{4.22}$$

which in the language of linear algebra equals

$$\psi_{AB} = y_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}_A \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_B + y_2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}_A \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_B + \ldots + y_8 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}_A \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_B . \tag{4.23}$$

When we trace over one subsystem, we, in layman terms, *ignore* that subsystem. If we were to "trace" this ground state over block B, our resulting subsystem would become

$$\psi_A = tr_B(\psi_{AB}) = y_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}_A + y_2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}_A + \ldots + y_8 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}_A . \tag{4.24}$$

This is not a trace in the mathematical sense since a trace is defined to operate on matrices. In this example the "trace" is operating on a vector, as a mere illustration of the main idea of

tracing. Now, let us consider a particular configuration of spins and calculate its density matrix by tracing over the two blocks. For example, take the case with a spin chain of five particles, where we have divided our system so that block A consists of the first three particles, and block B of the last two (see fig 4.2):

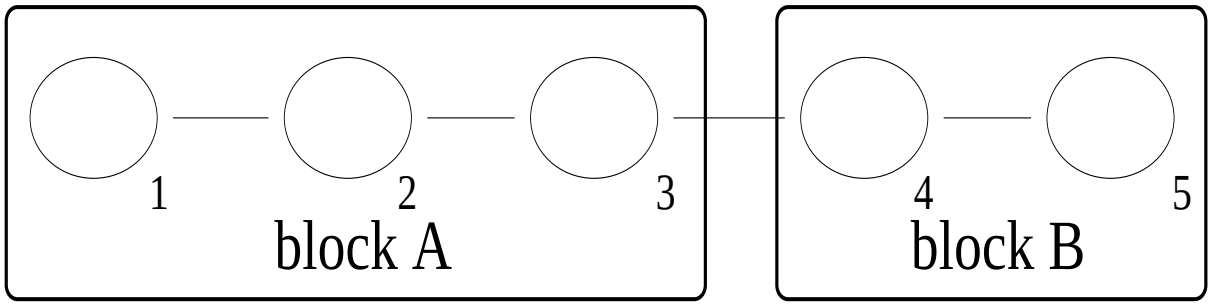


Figure 4.2: A spin chain of 5 particles. Block A consists of particle 1, 2 and 3 and block B of particle 4 and 5.

Here, we choose our state to be the particular configuration

$$|\psi_{AB}\rangle = |101\rangle_A \otimes |01\rangle_B = |101\rangle_A|01\rangle_B = |101_A 01_B\rangle. \tag{4.25}$$

Thus, our density matrix for the whole system becomes

$$\rho_{AB} = \psi_{AB} \times \psi_{AB}^T = |101_A 01_B\rangle\langle 101_A 01_B|, \tag{4.26}$$

with the density matrices for each block given by

$$\rho_A = tr_B(\psi_{AB} \times \psi_{AB}^T) = |101_A\rangle\langle 101_A| = |101\rangle\langle 101| \tag{4.27}$$

$$\rho_B = tr_A(\psi_{AB} \times \psi_{AB}^T) = |01_B\rangle\langle 01_B| = |01\rangle\langle 01|. \tag{4.28}$$

Notice that for this single configuration, we have no summation in the final step.

Now that we understand how tracing over subsystems work, we can go back and calculate the reduced density matrix for the bipartite system of three particles (cf. fig. 5.1). Writing out

the sum in eqn (4.18) explicitly one obtains

$$
\begin{aligned}
\rho_A &= tr_B(\rho_{AB}) = \\
&= \sum_\beta (\langle\beta|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|\beta\rangle) \\
&= \quad \langle 0|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|0\rangle \\
&\quad +\langle 1|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|1\rangle \\
&= \quad y_1y_1|11\rangle\langle 11| + y_1y_3|11\rangle\langle 10| + y_1y_5|11\rangle\langle 01| + y_1y_7|11\rangle\langle 00| \\
&\quad + y_2y_2|11\rangle\langle 11| + y_2y_4|11\rangle\langle 10| + y_2y_6|11\rangle\langle 01| + y_2y_8|11\rangle\langle 00| \\
&\quad + y_3y_1|10\rangle\langle 11| + y_3y_3|10\rangle\langle 10| + y_3y_5|10\rangle\langle 01| + y_3y_7|10\rangle\langle 00| \\
&\quad + y_4y_2|10\rangle\langle 11| + y_4y_4|10\rangle\langle 10| + y_4y_6|10\rangle\langle 01| + y_4y_8|10\rangle\langle 00| \\
&\quad + y_5y_1|01\rangle\langle 11| + y_5y_3|01\rangle\langle 10| + y_5y_5|01\rangle\langle 01| + y_5y_7|01\rangle\langle 00| \\
&\quad + y_6y_2|01\rangle\langle 11| + y_6y_4|01\rangle\langle 10| + y_6y_6|01\rangle\langle 01| + y_6y_8|01\rangle\langle 00| \\
&\quad + y_7y_1|00\rangle\langle 11| + y_7y_3|00\rangle\langle 10| + y_7y_5|00\rangle\langle 01| + y_7y_7|00\rangle\langle 00| \\
&\quad + y_8y_2|00\rangle\langle 11| + y_8y_4|00\rangle\langle 10| + y_8y_6|00\rangle\langle 01| + y_8y_8|00\rangle\langle 00|.
\end{aligned}
\tag{4.29}
$$

which in our chosen basis (cf. eqn (4.12),(4.13)) can be written as a 4×4 matrix

$$
\rho_A = \begin{pmatrix}
(y_1y_1 + y_2y_2) & (y_1y_3 + y_2y_4) & (y_1y_5 + y_2y_6) & (y_1y_7 + y_2y_8) \\
(y_1y_3 + y_2y_4) & (y_3y_3 + y_4y_4) & (y_3y_5 + y_4y_6) & (y_3y_7 + y_4y_8) \\
(y_1y_5 + y_2y_6) & (y_3y_5 + y_4y_6) & (y_5y_5 + y_6y_6) & (y_5y_7 + y_6y_8) \\
(y_1y_7 + y_2y_8) & (y_3y_7 + y_4y_8) & (y_5y_7 + y_6y_8) & (y_7y_7 + y_8y_8)
\end{pmatrix}. \tag{4.30}
$$

Similarly, eqn (4.19) can be written as

$$\begin{aligned}
\rho_B &= tr_A(\rho_{AB}) = \\
&= \sum_\alpha (\langle\alpha|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|\alpha\rangle) \\
&= \quad \langle 00|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|00\rangle \\
&\quad +\langle 01|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|01\rangle \\
&\quad +\langle 10|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|10\rangle \\
&\quad +\langle 11|(y_1y_1|111\rangle\langle 111| + y_1y_2|111\rangle\langle 110| + ... + y_8y_8|000\rangle\langle 000|)|11\rangle \\
&= \quad y_1y_1|1\rangle\langle 1| + y_1y_2|1\rangle\langle 0| + y_2y_2|0\rangle\langle 0| + y_2y_1|0\rangle\langle 1| \\
&\quad + y_3y_3|1\rangle\langle 1| + y_3y_4|1\rangle\langle 0| + y_4y_4|0\rangle\langle 0| + y_4y_3|0\rangle\langle 1| \\
&\quad + y_5y_5|1\rangle\langle 1| + y_5y_6|1\rangle\langle 0| + y_6y_6|0\rangle\langle 0| + y_6y_5|0\rangle\langle 1| \\
&\quad + y_7y_7|1\rangle\langle 1| + y_7y_8|1\rangle\langle 0| + y_8y_8|0\rangle\langle 0| + y_8y_7|0\rangle\langle 1|,
\end{aligned} \tag{4.31}$$

with matrix representation

$$\rho_B = \begin{pmatrix} (y_1^2 + y_3^2 + y_5^2 + y_7^2) & (y_1y_2 + y_3y_4 + y_5y_6 + y_7y_8) \\ \\ (y_2y_1 + y_4y_3 + y_6y_5 + y_8y_7) & (y_2^2 + y_4^2 + y_6^2 + y_6^2) \end{pmatrix}. \tag{4.32}$$

Already for this simple system of only three particles, the resulting sum that needs to be carried out in order to calculate the reduced density matrices looks surprisingly heavy. However, the reader might have noticed that the final step in equations (4.29) and (4.31) suggests some sort of "summation rule" for knowing which entries in the ground state vector that should be multiplied to which "block vector". Indeed, such a rule exists, and our next goal is to understand how it works. For this simple system with three particles the pattern is not hard to see from equation (4.30) and (4.32). When we trace over one particle to get the reduced matrix for block A, the entries in the reduced density matrix are even and odd pairs of the entries in the ground state vector when grouped together from left to right and up to down. This explanation might not have made things clearer, but a careful inspection of the entries in the reduced density matrices (eqn (4.30) and (4.32)) will help the reader understand the details. However, for larger systems where we need to trace over more particles, things are not as easy.

When we trace over a subsystem, the terms that are left in the summation are the terms where the subsystem that is being traced over has the same "sub-configuration" on both sides,

i.e. for both the vector and the row. For example, consider the following trace:

$$\begin{aligned}
&\sum_{\beta=0,1} \langle\beta|\left[|11_B\rangle\langle 10_B| + |10_B\rangle\langle 10_B|\right]|\beta\rangle = \\
&= \langle 1_B|\Big[|11_B\rangle\langle 10_B| + |10_B\rangle\langle 10_B|\Big]|1_B\rangle + \langle 0_B|\Big[|11_B\rangle\langle 10_B| + |10_B\rangle\langle 10_B|\Big]|0_B\rangle = \\
&= |1\rangle\langle 1| \,, \qquad (4.33)
\end{aligned}$$

where only the second term, for $\beta = 0$, in the last step survives.

Similarly, for a system with three particles, we see from the ground state written as in eqn (5.21) that the terms that can be multiplied with each other without disappearing after tracing over block B (cf. fig 5.1) are the ones with the same configuration in the third entry (i.e. the same state for particle no. 3). Thus, the products consist of odd entries multiplied with odd entries and even entries multiplied with even entries. The positions in the resulting 4×4 matrix where these products appear are given by the corresponding configurations to each pivot position in the ground state that are left after "tracing out" the third particle.

The product of terms that survive the tracing over the two particles in block A, and which gives us the reduced density matrix for block B, are the ones with the same configurations in the first two entries (i.e. the state of the first two spins). These configuration pairs are given by pivot position 1 and 2, 3 and 4, 5 and 6 and 7 and 8. The positions in the resulting 2×2 matrix are given by configurations that are left of each term after "tracing out" the first two particles. To see which configuration pairs that survive after any tracing over an arbitrary number of particles it helps to write a graph over the configurations as is done in fig 4.3.

A careful inspection of fig 4.3 allows us to construct an equation that tells us which entries in the ground state vector should be multiplied to which block vector in order to obtain the reduced density matrices. The following sum, with the block vectors A and B, calculates the reduced density matrices for an arbitrary number of particles and subsystem configuration:

$$\rho_A = \sum_{i=1}^{2^n} \sum_{j=a:2^{n-k}}^{2^n} A(i) \times A(j)^T, \qquad (4.34)$$

$$\rho_B = \sum_{t=0}^{2^{k-1}} \sum_{i=t(2^{n-k})+1}^{(t+1)2^{n-k}} \sum_{j=t(2^{n-k})+1}^{(t+1)(2^{n-k})} B(i) \times B(j)^T, \qquad (4.35)$$

where k is the number of particles in block A and s is the number of particles in block B. Here I have also used the notation that is used in matlab where $j = a : 2^{n-k}$ means that j goes from a in steps of 2^{n-k}. The value of a is given by

$$a = \begin{cases} 0, \text{ for } (i)\text{mod}(2^{n-k}) = 0 \\ 2^s, \text{ for } (i)\text{mod}(2^{n-k}) \neq 0 \end{cases} \qquad (4.36)$$

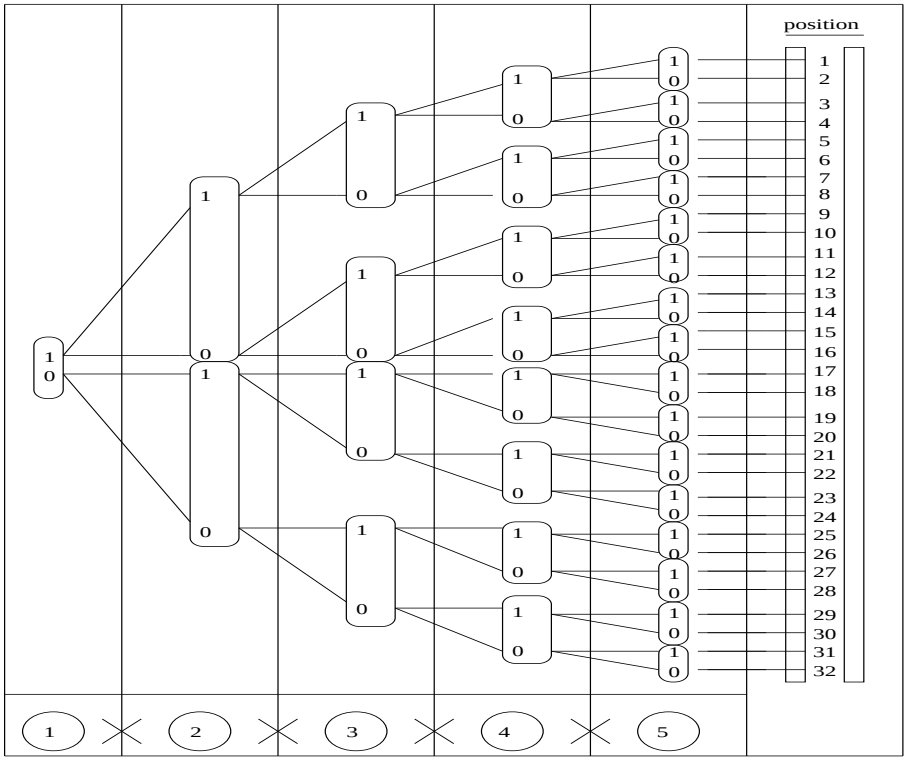


Figure 4.3: A spin graph for five particles. For each pivot-position (to the right) there corresponds a unique configuration of the spins for each particle. This configuration can be seen from the figure by following the lines from the position number at the right to the the numbers to the left.

From the symmetry of the matrices in eqn (4.30) and (4.32), one concludes that there must be more ways of calculating the reduced density matrices. One other such approach is to look at the density matrix for the whole system AB and see which terms in the reduced density matrices that comes from which terms in the total density matrix. One will find simple rules for how to build up the reduced density matrices involving sums of block matrices from the total density matrix.

4.4 Nearest-neighbor summation and boundary conditions

The point of numbering the particles and not simply order them in ”left block” and ”right block”, is because of the periodic boundary conditions that we use. Our spin chain is actually a ”spin-ring”. This is important when we calculate the matrices that builds up the Hamiltonian. These matrices must be calculated as a sum over interactions. The nearest neighbor interaction in the

Hamiltonian is shown when we write the sum explicitly so that a computer may understand it (I is the identity matrix of dimension 2 in the following equation):

$$\Omega_{nearest} = \sum_{i=1}^{n-1} \Big(\bigotimes_{j=1}^{i-1} I_j \otimes \sigma_i^x \otimes \sigma_{i+1}^x \otimes \bigotimes_{k=1}^{n-(i+1)} I_k \Big). \tag{4.37}$$

This sum can be understood with help from the following picture:

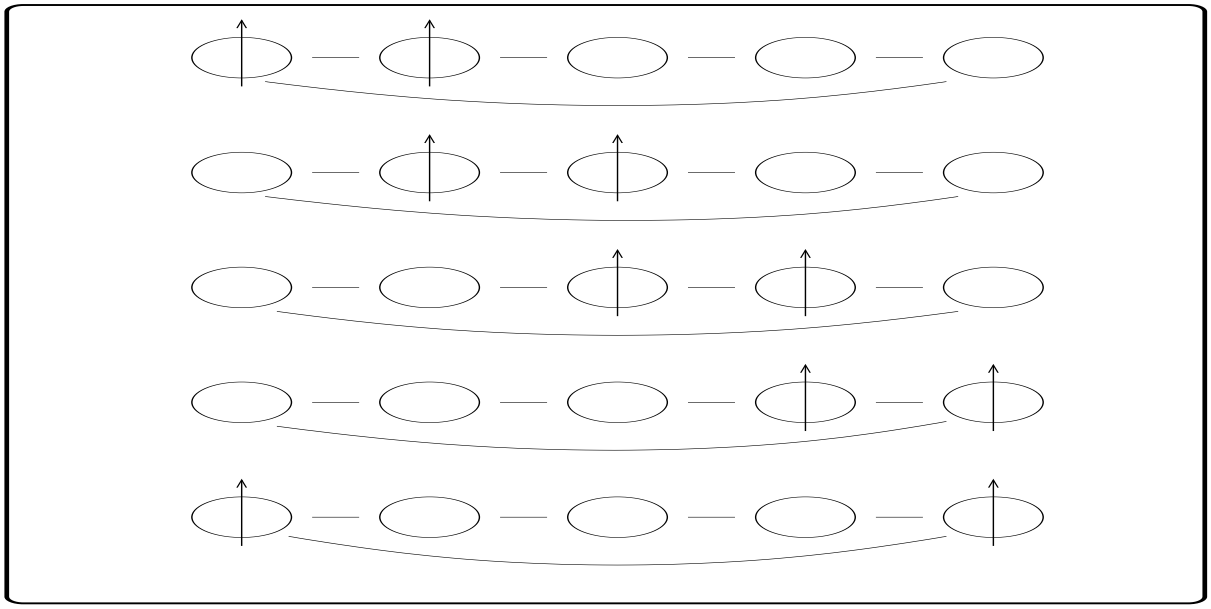


Figure 4.4: A spin chain of 5 particles with periodic boundary conditions. The bottom configuration is not included in the sum so this term must be added explicitly. The arrows correspond to interactions between the particles. Block A consists of particle 1,2 and 3, block B of particle 4 and 5.

The last configuration in figure (4.4) is not included in the sum above so we need to add the term

$$\sigma_1^x \otimes \bigotimes_{j=1}^{n-2} I_j \otimes \sigma_n^x \tag{4.38}$$

explicitly. Now we have the complete formula for how to calculate the Hamiltonian. If we were to add next nearest-neighbors, we would have the case seen in figure (4.5). Here, the sum would then be of the form

$$\Omega_{next} = \sum_{i=1}^{n-1} \Big(\bigotimes_{j=1}^{2(i-1)} I_j \otimes \sigma_i^x \otimes I \otimes \sigma_{i+1}^x \otimes \bigotimes_{k=1}^{2(n-(i+2))} I_k \Big). \tag{4.39}$$

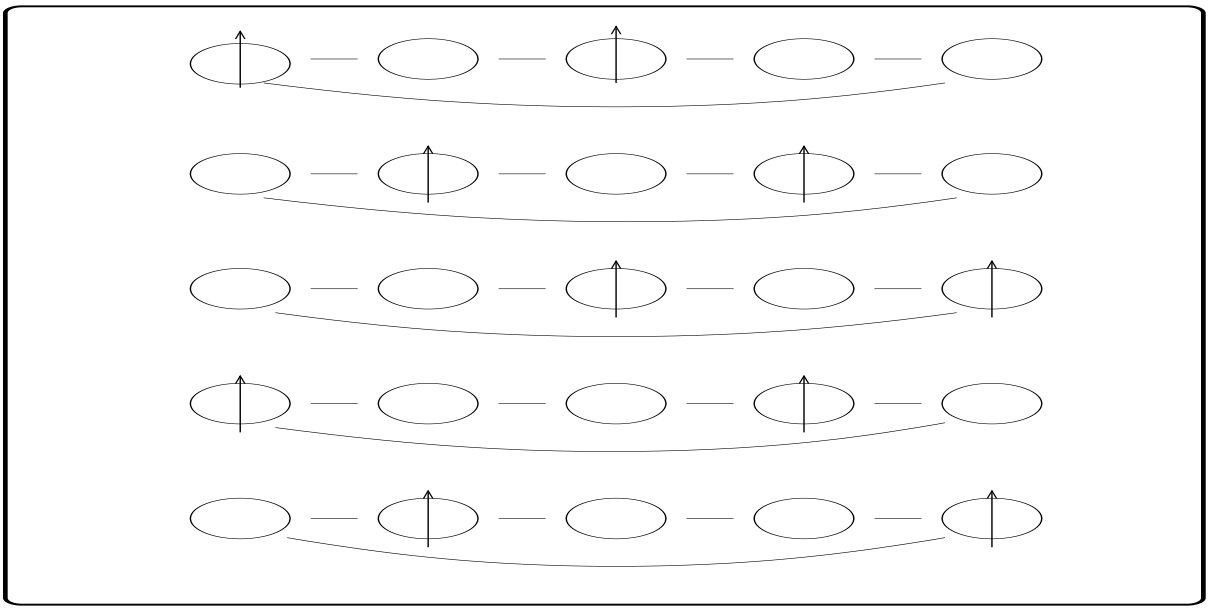


Figure 4.5: A spin chain of 5 particles. Here the last two configurations need to be added explicitly. The arrows correspond to particle pairs with next-nearest correlations. Block A consists of particle 1,2 and 3, block B of particle 4 and 5.

This sum would miss out on the two last configurations. The sums defined in eqn (4.37) and (4.39) are the ones I used in my program. The sum missed interactions were added ”by hand”.

However, there is a theoretical problem with adding more interactions than the ones between nearest neighbors. Other interactions should not contribute as much as the nearest neighbor interaction, and the degree of interaction is not as simple as regular forces. Usually forces decays as the square of the distance, but this would not make sense for this interaction because of many reasons [16]:

1) The interaction between next-nearest neighbors is in a way what is ”left of” the interaction between nearest neighbors.

2) Quantum physics don’t work the same way as classical physics.

3) Measuring ”how much” entropy is not the same as labeling ”how much” we have ”left” of a force.

This area is of a very complex nature and is a bit outside the theme of this thesis. For this reason I restrict my calculations to the case of nearest-neighbors interactions.

4.5 Expected numerical problems for a finite number of particles

When we have an infinite number of particles the ground state close to a quantum phase transition becomes infinitely sensitive to disturbances. For an Ising system without external disturbances such as temperature or a magnetic field, the spins order themselves in the same direction, either they are all up, or they are all down. Having spins pointing in opposite directions costs energy since the magnetic field caused by the spins themselves has to "fight against" these irregularities. Both cases, when the spins are all up or all down, have the same lowest energy. This means that the ground state has equal probability to be in a state where all spins point up as in the state where all points down and therefore we have an entangled ground state [11]. In a real spin system there is always some disturbance that forces the ground state to choose one of these states. The ground state is then no longer entangled, since the spins are either all up, or all down. For a system with few particles the situation is quite different. Here a very small disturbance is not enough to throw away all possible entanglement between the particles.

The limitations that follow from exact diagonalization as a numerical approach forces us to work with a finite number of particles. A computer can not handle matrices with infinite dimensions, so an infinitely sensitive system does not come into effect. This leaves us with the problem of an entangled ground state.

Since it is of interest to study the real world and not some strange laboratory environment, we need to add a small disturbance in order to force the system to choose one of the two possible ground states (all spins up *or* all spins down) so as to avoid entanglement when there is no transverse magnetic field present. This is done by adding an extra magnetic field along the spin up-alignment, with a sufficiently small magnitude so that it will not compete with the transverse magnetic field. This extra magnetic field is made to decrease as the system gets closer to the critical point in order to get the correct behavior near the critical point. The behavior of the system near the critical point is what is of most importance for our study, and we therefore have to be very careful of how to treat the critical region.

Adding a small disturbance is done by adding the following term to the Hamiltonian:

$$h_{pert} = \delta \sum_i \sigma_i^x \ , \tag{4.40}$$

where δ is some small number. In order to not affect the critical behavior with our small disturbance, we should choose some function that switches off this disturbance before we get close to the critical region. My choice is the following function:

$$\delta = \frac{a}{100}(1 - \tanh(g))(1 - \text{sign}(b - g)) \ , \tag{4.41}$$

where a and b are varied depending on the number of particles in our system (b is the value where we switch off the disturbance). This function gives a reasonable behavior of the graphs with a

smooth transition towards the critical region. When the function switches off the disturbance it is already close to zero.

Another numerical issue is the notorious problem of round off errors, unavoidable since a computer needs to round off in order to keep all the numbers in its memory. The effects of this is that our results are approximations to the actual behavior. In addition, because the system is finite, the critical behavior becomes somewhat ”damped”. We do not obtain the same graphs as an analytical approach would predict for the thermodynamical limit, simply because our system is finite.

What makes our results interesting is that even for a small number of particles we see the same typical behavior as we would see for an infinite number of particles as predicted by analytical theories. Maybe we don’t need to make things so complex in order to understand criticality?

4.6 The Ising model with a transverse magnetic field

The Ising model with a transverse field is the model we principally study in this thesis. It is a simple model were the spins only affect each others alignment along one direction. The interaction of the spins are modeled by a product of two σ^x matrices in the Hamiltonian and the transverse field is applied in the x-direction with magnitude g by the term $g\sigma^z$. This model has been studied in the context of both entanglement and state transport [20]. It is an intriguing model that is integrable with the use of the Jordan-Wigner transformation [4], where interacting spins are transformed into noninteracting spinless fermions. By using this transformation the Hamiltonian can be transformed into a new one that can be diagonalized for systems with an infinite number of particles [4]. This model has been found relevant to many physical systems, and one of the most important features of this model is the application to quantum phase transitions separating ferromagnetic and paramagnetic phases at zero temperature. Since this is the main topic of this thesis, this model is of particular importance. The advantage of this model compared to other models is its simplicity. The Hamiltonian is given by

$$H = \sum_{\langle i,j \rangle}^{n} J(\sigma_i^x \sigma_j^x + g\sigma_i^z). \tag{4.42}$$

Here, J is a local exchange coupling strength, g is the intensity of the external transversal field and the sum is over nearest neighbors. For $g < 1$, the system is in a ferromagnetic phase with a nonzero expectation value of the S_x component of the total spin, while for $g > 1$ the system is paramagnetic with vanishing S_x spin expectation value, the point $g = 1$ being the quantum critical point. This might be understood from the fact that at $g = 1$ the interaction strength between two spins is equal to the coupling to the external transverse magnetic field.

4.7 The XY model with a transverse magnetic field

The other important model for this thesis is the XY model. The XY Hamiltonian allows spins to interact with each other through the 2-dimensional xy-plane. The advantage with this extension from the Ising model is that it models a real spin system in a more accurate way. In reality spins interact with each other in three dimensions, so this Hamiltonian is naturally a bit closer to the truth. The disadvantage is the added complexity. We want to understand criticality, not chaos theory! The luxury of a model that models reality in a closer way comes at the cost of the added complexity in understanding the results. The heart of criticality might not need a complex model in order to be understood. Then again, it just might.

The XY Hamiltonian is given by

$$H = \sum_{\langle i,j \rangle}^{n} J(\frac{1+\gamma}{2}\sigma_i^x\sigma_j^x + \frac{1-\gamma}{2}\sigma_i^y\sigma_j^y + g\sigma_i^z). \tag{4.43}$$

It is easy to see that when $\gamma = 1$ the XY model reduces to the Ising model. This Hamiltonian produces 3-dimensional graphs with the entropy plotted against both the magnitude of the external magnetic field g and the parameter γ. It should be mentioned that when γ equals zero, we notice that the x and y interactions contribute the same amount to the Hamiltonian. For this case, where $\gamma = 0$, the Hamiltonian is called the Hamiltonian.

Chapter 5

Results

For a system of n spin - $\frac{1}{2}$ particles, the number of different spin configurations is equal to 2^n. This means that the dimension of the state space doubles for each particle we add to the system and accordingly the matrices grow quadratically. For any computer, this is a major problem as the matrices become huge. The computer needs to diagonalize the matrix representing the Hamiltonian for the models we use, that is, calculating the eigenvectors and eigenvalues. This is the time consuming part of the calculations. Although it should be possible to calculate the entropy for any number of particles with the program I have written, a normal home computer can only handle up to eleven particles for the Ising model and only ten particles for the XY Hamiltonian. If we would try to calculate the entropy behavior for even more particles the calculations would take days. Turning to my results, what is particularly interesting is how fast the critical value of the external magnetic field closes in on $g_c = 1$ (which is the exact result in the thermodynamical limit) as one increases the number of particles.

In other words, the exact diagonalization method seems to be a fair approximation to the case with an infinite number of particles, for a system of only eight particles. One can predict the behavior of systems with an infinite number of particles by looking at how the graphs evolve for each added particle. The notorious problem with calculating the resulting matrix for the Hamiltonian by using a mathematical program like MATLAB is the round off errors made when it diagonalizes the Hamiltonian in order to calculate the ground state vector. Because of this, our values for the entropy near the critical value of g are not exact, and the peaks tend to get a bit smoothed out. However, already for ten particles, we see a precursor of an expected sharp peak close to the analytical value of the critical external transverse field.

5.1 The Ising model

For this model my program can calculate up to ten particles on a normal home computer without having to wait for too long. On my computer, a Pentium4 with a 2.4GHz processor and 256mb RAM, the von Neumann entropy for 8, 9, 10 and 11 particles takes approximately 40 seconds,

2 minutes, 20 minutes and 136 minutes, respectively, to plot. The time it uses to calculate the graphs grows rapidly, so we should not have high hopes of being able to calculate the entropy for systems with many more particles than, say, 15-20 particles on a supercomputer. However, time may not be the only factor here, since my computer will not even begin to calculate 12 particles. I suspect there to be some fundamental numerical problem when the matrices become too big. The program I used for calculating is MATLAB, since it is known for handling matrix operations very well. Therefore, I don't think it would help to use some other mathematical program. The possible solutions that I see is to use a more effective algorithm for diagonalizing huge matrices, or to take advantage of the fact that the matrices that sum up the matrix for the Hamiltonian are very sparse. Also, it may be possible to use the symmetry of the matrix for the Hamiltonian or the matrices in my program that sum up the Hamiltonian. Exactly how to go about for solving this problem would take a lot of time and I don't think that it would be a very fulfilling task for a creative mind since the results we get already from 10 particles are sufficient to reveal a distinct pattern. The only outcome of such a research would be to be able to add one or a few more particles, and that would not significantly enhance our understanding of the problem.

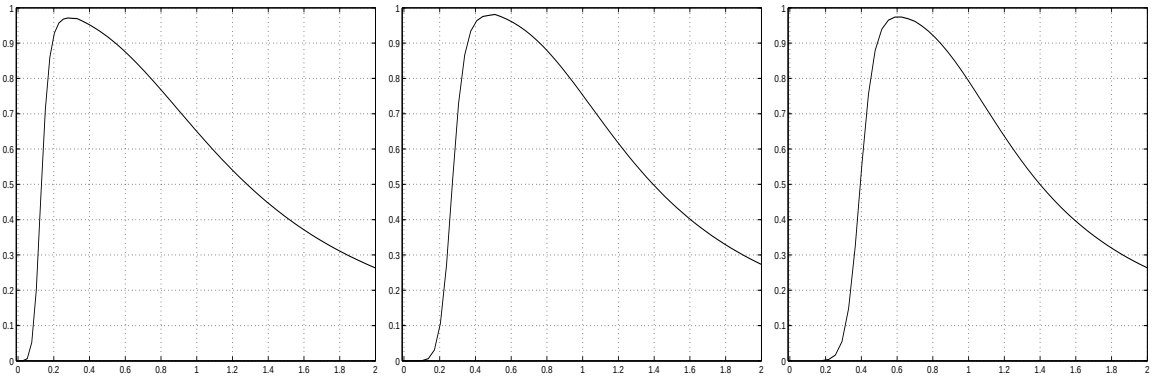


Figure 5.1: A graph over the von Neumann entropy for 3, 4, and 5 particles. Here we see that for few particles the critical value of the external magnetic field g goes from 0.3 for 3 particles to 0.5 and 0.6 for 4 and 5 particles respectively. The peaks are smooth.

For three particles we find the maximum of the entropy around the value of 0.3 for the external magnetic field, which is quite far away from the expected value of $g_c = 1$. However, this can be explained. For a few number of particles the correlations, the entanglement, between the particles are few, the magnitude by which the entanglement "glues" the system together is not as powerful as for a system with more particles. Therefore, an external disturbance such as a magnetic field affects the system more than it would do for a system in a stronger entangled 'bind", and the critical value of g is lower than the expected value for a system with an infinite number of particles.

In this context, let us recall that the definition of the von Neumann entropy can be compared with the classical analogue of the Shannon entropy. If we look at the derivation of the Shannon entropy, we notice that it makes use of the Stirling approximation. The Stirling approximation is not a very good approximation for a small number of letters in the message. The number of letters in the message should be a very big number in order for the approximation to be a good one, and for three particles, the corresponding number of letters is only $2^3 = 8$ for our model. However, this possible weakness of the von Neumann definition does not seem to be very serious when measuring entanglement, as our example with the EPR-pair in chapter four shows us. The reason for this might be the fact that the von Neumann definition of entropy does not need to be derived directly from the Shannon entropy, as can be seen in section 3.3. However, it is interesting to keep this analogy in mind and see what would happen if we changed the definition of the von Neumann entropy.

From the derivation of the Shannon entropy, we see that the end result, the definition of the Shannon entropy is for an alphabet of n different letters. For our models, we have a simpler situation where our alphabet would correspond to a binary one, i.e. we only have two different letters. A direct comparison of the Shannon entropy and the von Neumann entropy would now give us the following definition:

$$H(\rho) = -Tr(\rho \log \rho + (I - \rho) \log(I - \rho)) \tag{5.1}$$

I tested this definition out of curiosity, and it turns out that it produces the same graphs (after dividing the total entropy with two)! This may be understood by knowing that the maximum of the entropy is taken when the reduced density matrices are multiples of the identity matrix, and this experimental definition does not change this since we only affect the multiple, not the structure of the density matrix. From this experiment I concluded that although the von Neumann definition is a good one, it might not be the only good one since we can define new definitions that also display the same maxima and minima for the entropy. The reason why this experimental definition that I tried is not as good as the von Neumann definition, is that the graphs are identical except for this factor of two, and we want the maximum value of the entropy to be one, not two.

When we add more particles to the system the graphs start to look more like the known analytical solution for an infinite number of particles [21]. Already for 8 particles the peak of the graph is found close to the critical value of $g_c = 1$ and it is quite sharp. The peaks would be even sharper if the applied disturbance could be better adjusted without ruining the behavior of the graphs as a whole. Without this disturbance the maximum of the entropy is found in the ground state where we have a maximally entangled state between the two possible configurations of all spins ”up” and all spins ”down”, and it stays in a maximally entangled state until the transverse field is strong enough to ruin this entanglement. In order to know the ”correct” value of the critical value for each number of particles, I switched off this disturbance and looked at where the entropy left its maximum.

When I press my computer for all its worth, I can plot the graph for the system with eleven particles. In order to make it more accurate in the neighborhood of the critical value, I have concentrated the plot points around the peak. Therefore, the "tail" is not included in the figure. This "tail" is not of interest, since it follows the same behavior as the "tails" in the graphs for the systems with fewer particles. This can be seen in figure 5.4.

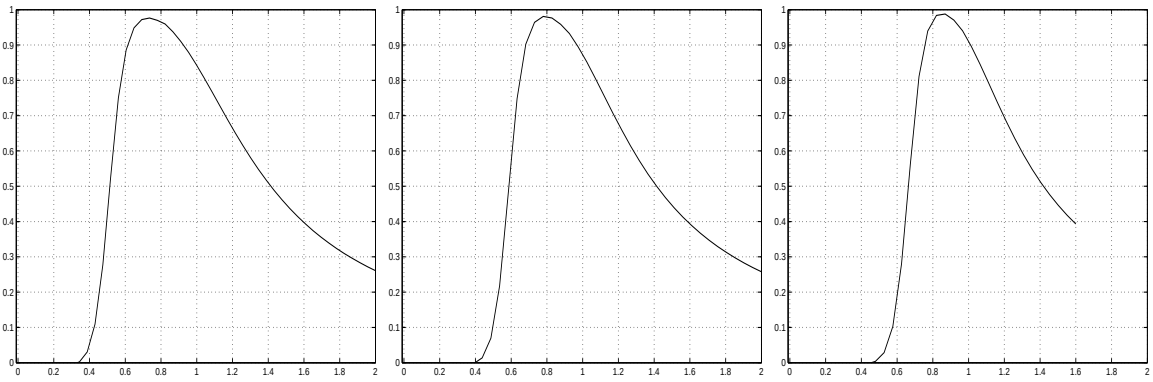


Figure 5.2: The von Neumann entropy for systems with 6, 7 and 8 particles, from left to right. Here we see that the graphs are closing in rapidly on the critical expected value of $g_c = 1$. For six particles we have the value of 0.7, for seven 0.8 and for eight particles the value is 0.87. We can also see that the critical value of the external magnetic field g where the entropy has its maximum closes in on $g_c = 1$ with a rate that decreases for each added particle. This is good since we do not want the critical value to be greater than one. Furthermore, the top is getting sharper as we add more particles to the system, as is to be expected.

In figure 5.5 we see how the difference between the calculated critical value of g and the analytical critical value of g for a system with an infinite number of particle get smaller and smaller for each added particle to our system.

In conclusion, the method of exact diagonalization seems to be a good approximation [1] for calculating the entropy for systems with few particles. This method also displays precursor of critical behavior for these simple systems with few particles, something that might be used in order to pinpoint and study quantum phase transitions. We can guess how the graphs would look if we were able to add an infinite number of particles to the system, and this guess corresponds to the results of the analytical approach involving *majorization* and an exact solution via Jordan-Wigner transformations (see chapter 5) [4].

[1] It is not really an approximation, but due to numerical round off errors and the necessity of an applied disturbance to avoid an entangled ground state, it becomes one.

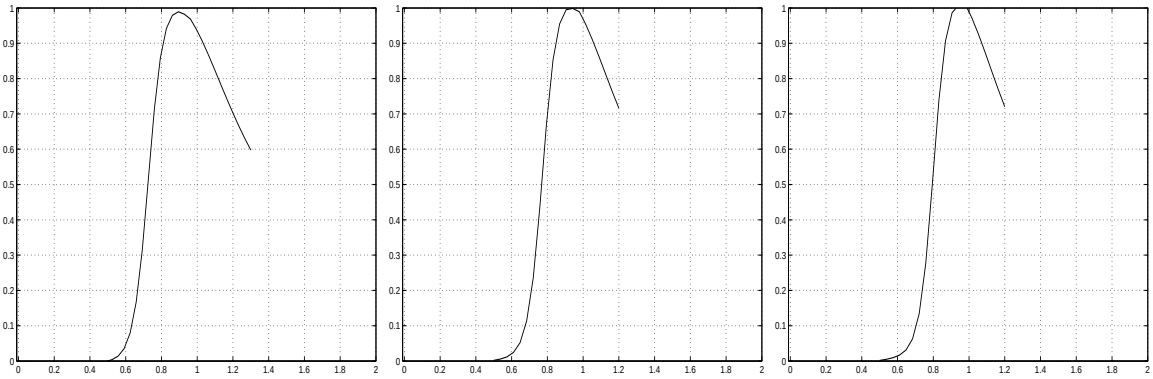


Figure 5.3: The von Neumann entropy for systems with 9, 10 and 11 particles, from left to right. For nine particles we have the value of 0.90, for ten 0.95 and for eleven particles the value is 0.98. We see a precursor of the analytically expected sharp peak. This peak would be even sharper if one would be able to find an even better function for the applied disturbance h_{pert}.

5.2 Magnetization

At the value of g where the magnetization drastically changes and the system goes from being ferromagnetic to paramagnetic we have a quantum phase transition. Where the phase transition occur the magnetization should be zero. In my graphs this occurs roughly around the same point as where the entropy has its maximum.

However, the problem with adding a disturbance in order to avoid an entangled ground state is that the behavior of the magnetization gets affected, and if we look at the graph over the magnetization (cf. fig 5.7) we can see a strange behavior when the magnetization is close to zero, i.e. at the quantum critical point. The disturbance that we add is an external magnetic field applied in the direction of the z-axis, which is the same axis as the one we measure our magnetization. Because of this, the results we get for the magnetization is not to be trusted near the critical value $g = 1$.

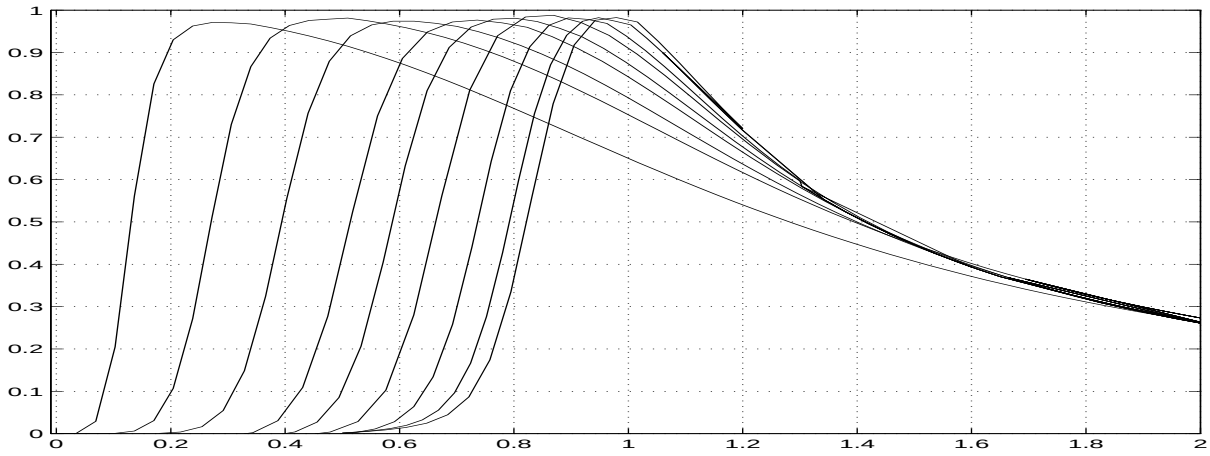


Figure 5.4: The von Neumann entropy for systems ranging from three particles (leftmost graph) to ten particles (rightmost graph). As we add more particles to the system, we see a tendency of the graphs to have a sharper peak, where the peak is closer to the expected analytical value of 1.0 for the external magnetic field g.

In conclusion, we have a quantum phase transition near a critical value of the intensity of the external transverse field. This critical value closes in rapidly on unity as we add more particles to the system, and for eleven particles, it is $g = 0.97$.

5.3 The XY Hamiltonian

A numerical study of the XY Hamiltonian requires a larger effort: there is now one more parameter γ that can be tuned (cf. eqn (4.43)). In my program each plot for this model corresponds to 11 plots for the Ising model, as this number of plots is the largest that my computer can handle in order for MATLAB to use the "mesh-function" for the resulting matrix. In this model the goundstate is entangled for $g < g_c$, even for $N \to \infty$ [19]. Adding a disturbance without ruening the behavior of our graphs will be a more complex problem for this model. Our graphs might not be very accurate for the top left corner in the figures, and as we shall see, we have some strange irregularities on the surface. However, the result for ten particles looks OK, where the graph is quite smooth and the irregularities are small.

Interesting to note is that the criticality occurs for different values of g than in the Ising model. For $\gamma \to 0$ the critical behavior occurs for lower values of g, and as can be seen, when $\gamma = 0$, when the XY model reduces to the XX model, we find critical behavior for g close to zero. How this criticality develops from three to ten particles is also interesting, and we can see a wave-like behavior for the entropy that diminishes as we add more particles. This wave-like

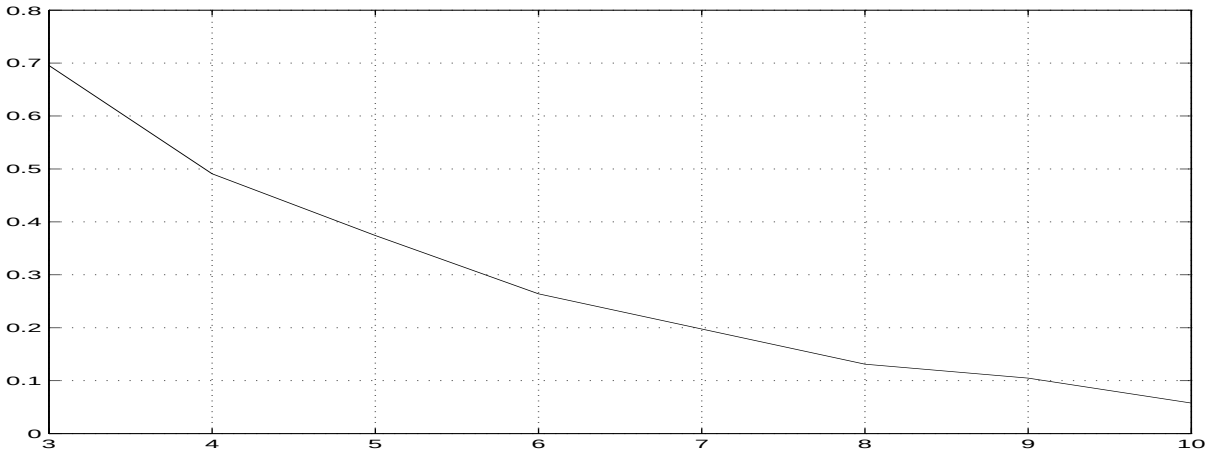


Figure 5.5: A graph over the difference (y-axis) between the calculated critical value of g and the analytical critical value $g = 1$, for systems with n number of particles (x-axis). We see a behavior where the distance tends to zero and the critical value of g does not seem to ever cross the analytical value of unity.

behavior, these “dips” in our surface, might be explained with the mixing between singlet and triplet states, and higher multiplet states [14].

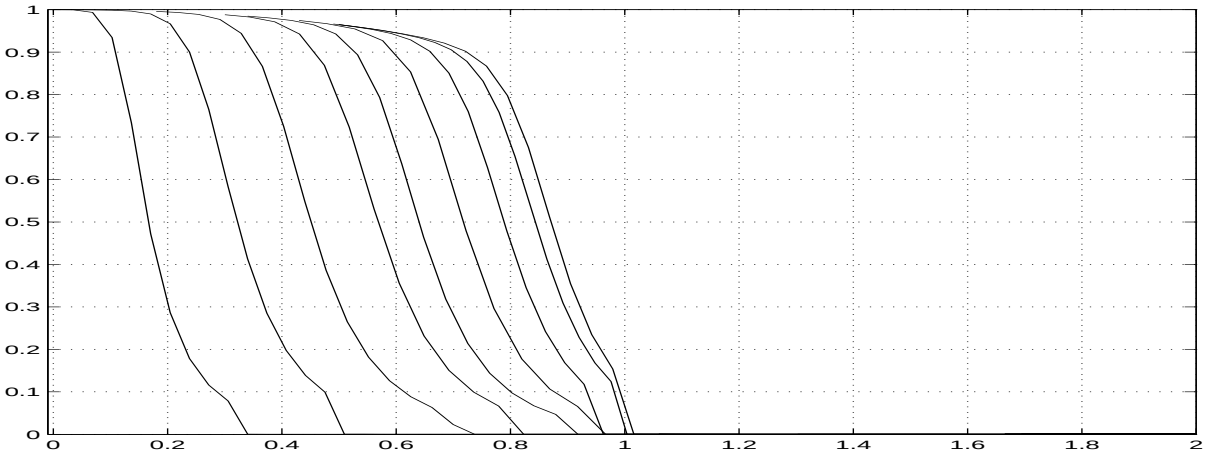


Figure 5.6: Here we see the magnetization for systems with 3, 4, 5, 6, 7, 8, 9, 10 and 11 particles, from left to right. When the magnetization is close to zero we see a strange behavior due to numerical problems with adding the disturbance h_{pert}.

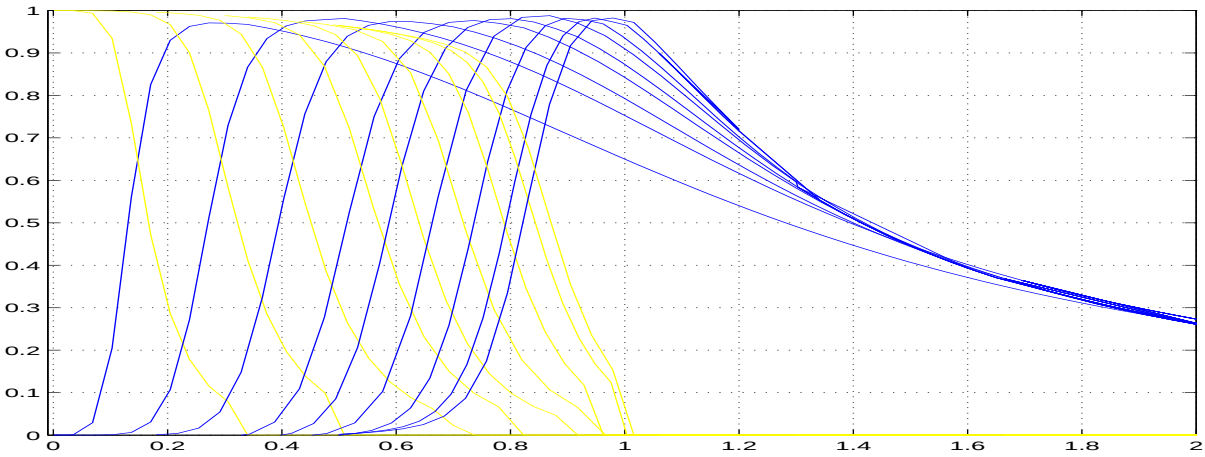


Figure 5.7: Here we see the von Neumann entropy (blue) and the magnetization (yellow) for systems with 3, 4, 5, 6, 7, 8, 9, 10 and 11 particles, from left to right.

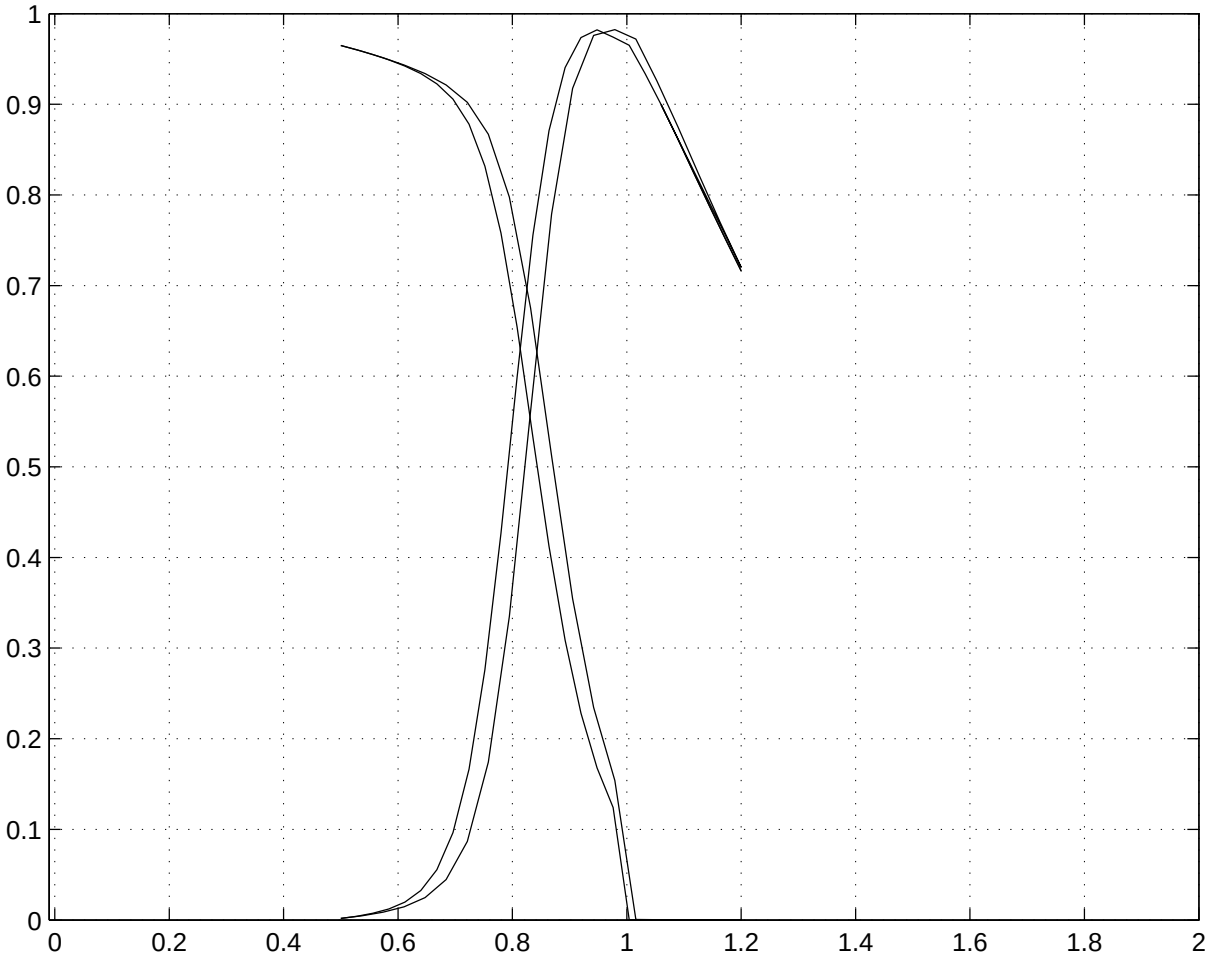


Figure 5.8: The entropy (the graphs with a maximum close to $g = 1$) and the magnetization (the graphs with a minimum close to $g = 1$) for systems with 10 and 11 particles, from left to right. The system behaves very close to the case with an infinite number of particles. Because of the numerical problem with adding a disturbance h_{pert}, the actual zero value of the magnetization is found at about the same value for g as where the entropy has its maximum. One expects the behavior near the zero value of the magnetization to be a little more smooth, with a more long-lived "tail", than the graphs shows us.

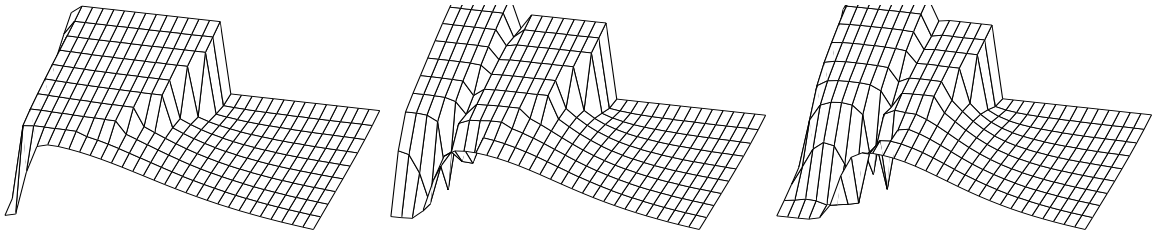


Figure 5.9: The von Neumann entropy for the XY model for systems with 3, 4, and 5 particles. The front most axis is the g-axis (x-axis), the y-axis is the value of γ from $\gamma = 1$ as closest to us to $\gamma = 0$. The front most part of the surface is the Ising model, the part of the surface that is furthest away from us in the figure plots the XX model. Here we see the strange wave-like behavior of the entropy as we add more particles.

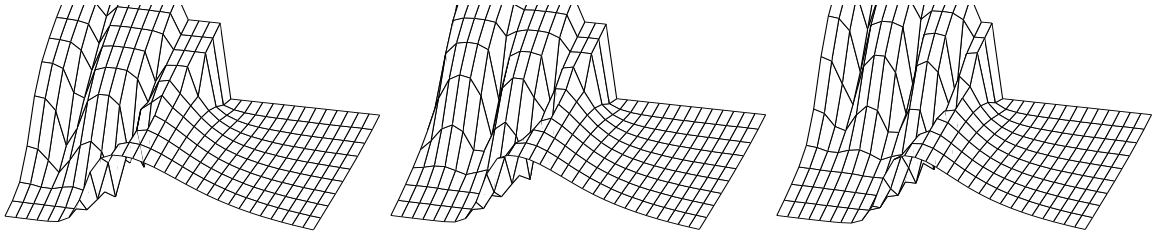


Figure 5.10: The von Neumann entropy for the XY model for systems with 6, 7, and 8 particles. The front most axis is the g-axis (x-axis), the y-axis is the value of γ from $\gamma = 1$ as closest to us to $\gamma = 0$. The front most part of the surface is the Ising model, the part of the surface that is furthest away from us plots the XX model. The "dips" are smoother than for fewer particles as can be compared with the previous plots.

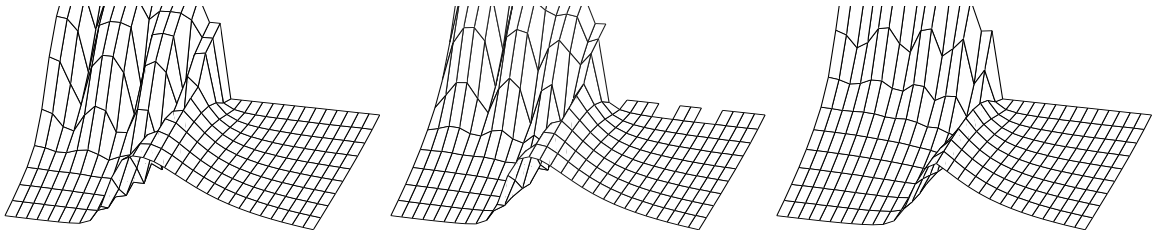


Figure 5.11: The von Neumann entropy for the XY model for systems with 8, 9, and 10 particles. The front most axis is the g-axis (x-axis), the y-axis is the value of γ from $\gamma = 1$ as closest to us to $\gamma = 0$. The front most part of the surface is the Ising model, the part of the surface that is furthest away from us plots the XX model. The top left corner of the graphs is "pushed" upwards and the strange wave-like behavior is diminishing and our surface starts to look more smooth.

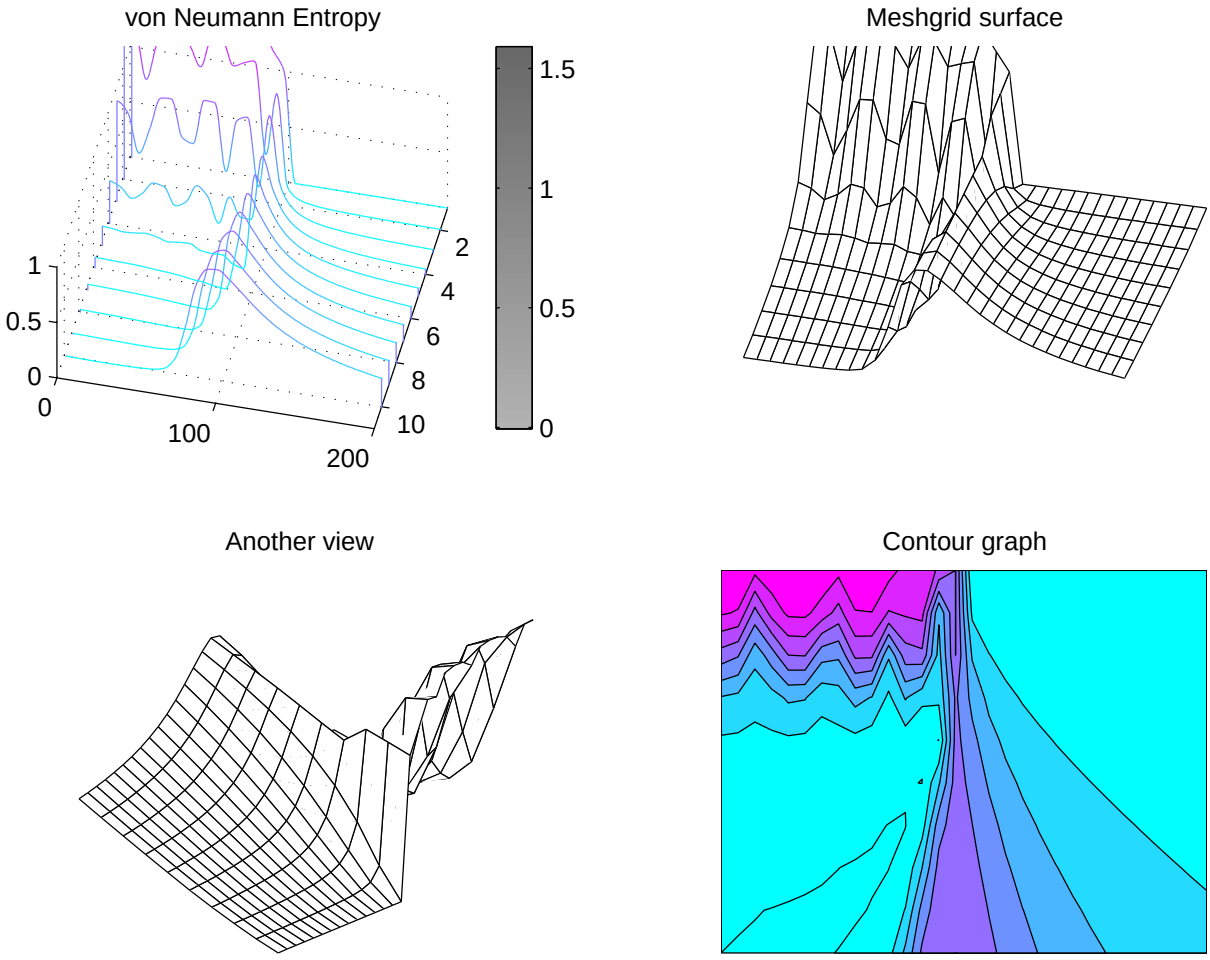


Figure 5.12: The von Neumann entropy for the XY model for ten particles. The top left graph is made with the ”waterfall”-function in MATLAB, the top right and the bottom left graphs are made with the ”mesh”-function. The bottom right graph is a contour plot.

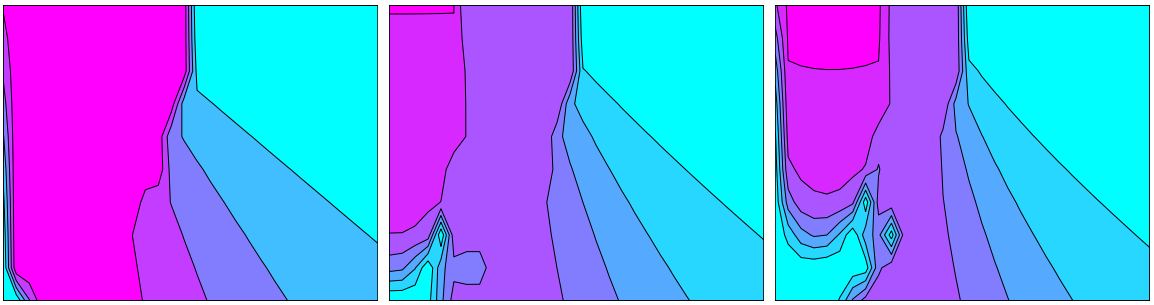


Figure 5.13: A contour plot of the von Neumann entropy for the XY model for systems with 3, 4, and 5 particles. The x-axis is the g-axis (x-axis), the y-axis is the value of γ from $\gamma = 1$ to $\gamma = 0$.

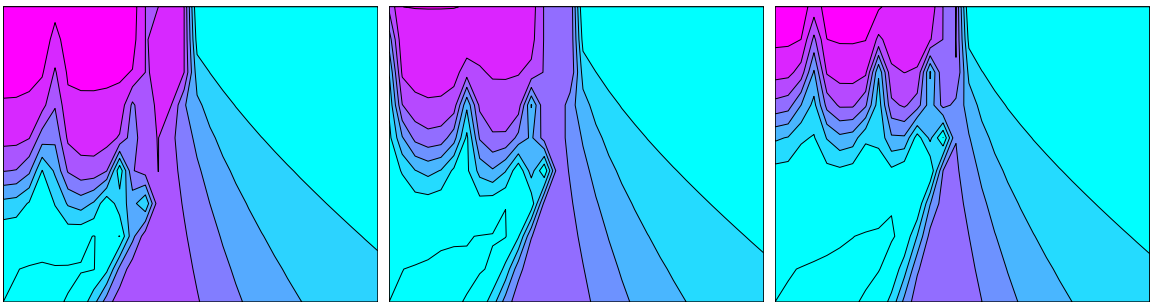


Figure 5.14: Same as fig 5.13, now with 6, 7 and 8 particles.

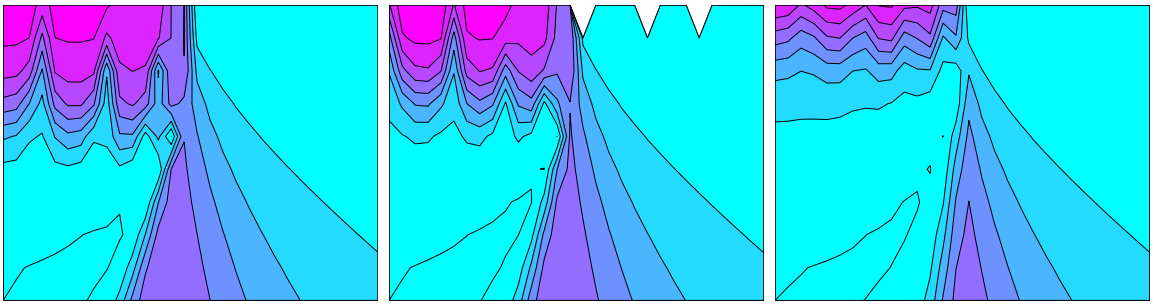


Figure 5.15: Same as fig 5.13, now with 8, 9 and 10 particles.

Appendix A

A.1 The MATLAB program for the Ising model

```
disp(' ')
disp('                        ********************************************')
disp('                        *                 WELCOME                  *')
disp('                        *  to my von Neumann entropy of entanglement  *')
disp('                        *  for the Ising model calculating program!   *')
disp('                        *                                           *')
disp('                        ********************************************')
disp(' ')
clf
clear all
u=input('How many graphs do you want to plot?: ');
for p=1:u
n=input('Number of spinparticles?: ');
if n==3
    plotp=60;
    off=0.31;
    intensity=0.0002;
    min=0.001;
    max=2;
elseif n==4
    plotp=60;
    off=0.5;
    intensity=0.00035;
    min=0.001;
    max=2;
elseif n==5
    plotp=50;
    off=0.7;
    intensity=0.0005;
    min=0.18;
    max=2;
elseif n==6
    plotp=40;
    off=0.8;
    intensity=0.0008;
    min=0.3;
    max=2;
elseif n==7
    plotp =35;
    off=0.88;
    intensity=0.0009;
    min=0.34;
```

```
    max=1.65;
elseif n==8
    plotp=25;
    off=0.95;
    intensity=0.0013;
    min=0.43;
    max=1.6;
elseif n==9
    plotp=25;
    off=0.95;
    intensity=0.002;
    min=0.49;
    max=1.3;
elseif n==10
    plotp=26;
    off=0.99;
    intensity=0.0028;
    min=0.5;
    max=1.2;
else plotp=20;
    off=0.99;
    intensity=0.003;
    min=0.5;
    max=1.2;
end
k=input('How many of those spinparticles are in the largest block?: ');
tic
J=1;
sigmaX=[0 1;1 0];
sigmaY=[0 -i;i 0];
sigmaZ=[1 0;0 -1];
AX=zeros(2^n);   %These lines below creates the matrices of the form ~ I*sigmaX*I
for i=1:n
AAX=kron(eye(2^(i-1)),kron(sigmaX,eye(2^(n-i))));
AX=AAX+AX;
end
AZ=zeros(2^n);   %These lines below creates the matrices of the form ~ I*sigmaZ*I
for i=1:n
AAZ=kron(eye(2^(i-1)),kron(sigmaZ,eye(2^(n-i))));
AZ=AAZ+AZ;
end
                %These lines creates the matrices of the
                %form ~ I*sigmaX*sigmaX*I needed for the
                %nearest neighbours
BX=zeros(2^n);
for i=0:n-2
    BBX=kron(kron(eye(2^(i)),sigmaX),kron(sigmaX,eye(2^((n-2)-i))));
    BX=BX+BBX;
end
                %This line creates the matrix missing in the
                %sum above ~ sigmaX*I^(2^(n-2))*sigmaX:
CX=kron(kron(sigmaX,eye(2^(n-2))),sigmaX);
BX=CX+BX;
                %These lines creates the matrices of the
                %form ~ I*sigmaY*sigmaY*I needed for the
                %nearest neighbours
BY=zeros(2^n);
for i=0:n-2
    BBY=kron(kron(eye(2^(i)),sigmaY),kron(sigmaY,eye(2^((n-2)-i))));
    BY=BY+BBY;
end
                %This line creates the matrix missing in the
```

```
               %sum above ~ sigmaY*I^(2^(n-2))*sigmaY:
CY=kron(kron(sigmaY,eye(2^(n-2))),sigmaY);
BY=CY+BY;
               %This loop below generates the spinvectors a[1] to a[n]
               %needed to construct the two "blockvectors"
               %for each position j in the groundstate vector y(j)
I=eye(2);
for j=1:2^n
     for i=1:n
         if mod(ceil(j/(2^(i-1))),2)==1
             eval(['a',int2str(i),'=I(:,1)']);
         else
             eval(['a',int2str(i),'=I(:,2)']);
         end
     end
m=n-k+1;
if k==1                          %These rows below constructs the "leftmost" blockvector
    b=eval(['a',num2str(m)]);    %from the spinvectors already calculated above
else
    b=kron((eval(['a',num2str(m+1)])),(eval(['a',num2str(m)])));
end
while m<n-1
    m=m+1;
    b=kron((eval(['a',num2str(m+1)])),b);
end
eval(['A',int2str(j),'=b']);
s=n-k;
if s==1                          %These rows below constructs the "rightmost blockvector"
    c=a1;                        %from the spinvectors already calculated above
else
    c=kron((eval(['a',num2str(s)])),(eval(['a',num2str(s-1)])));
end
while s>2
    s=s-1;
    c=kron(c,(eval(['a',num2str(s-1)])));
end
eval(['B',int2str(j),'=c']);
end
                                 %Now I calculate the groundstate vector and its
                                 %corresponding density matrix in order to
                                 %calculate the entropy and plot it against
                                 %the magnitude of the transversal magnetic field, g.
r=1;
h = waitbar(0,'Please wait...');
for g=linspace(min,max,plotp);
    Hz=abs((1-tanh(g))*(0.99+sign(off-g))*intensity);
                                 %This line below Sums up the matrices calculated
                                 %above to construct the Hamiltonian for the
                                 %1-dimensional XY model which contains both the Ising
                                 %model (gamma=1) and the XX model (gamma = 0).
H=-J*BX-J*(g*AZ+Hz*AX);
[X,D]=eig(H);


y=X(:,1);                        %The groundstate vector!

Magnetization=(1/n)*y'*AX*y;
                                        %Now I construct the density matrix
                                        %for block A
rhoA=zeros(2^k);
for i=1:2^n
        if mod(i,2^(n-k))==0;
```

```
          a=2^s;
        else a=mod(i,2^(n-k));
        end
            for j=a:2^(n-k):2^n
                rhoAA=y(i)*(eval(['A',int2str(i)]))*y(j)*(eval(['A',int2str(j)]))';
                rhoA=rhoA+rhoAA;
            end
end
                                        %Now I construct the density matrix
                                        %for block B
rhoB=zeros(2^(n-k));
for t=0:2^k-1
    for i=t*(2^(n-k))+1:(t+1)*(2^(n-k))
        for j=t*(2^(n-k))+1:(t+1)*(2^(n-k))
            rhoBB=y(i)*(eval(['B',int2str(i)]))*y(j)*(eval(['B',int2str(j)]))';
            rhoB=rhoB+rhoBB;
        end
    end
end

SA=-trace((rhoA)*real(logm(rhoA)/log(2)));     %Entropy for block "A"
SB=-trace((rhoB)*real(logm(rhoB))/log(2));     %Entropy for block "B"
Entropy=(SA+SB)/2;                             %Total entropy, taking the medium value of
                                               %SA and SB to neutralize rounding
                                               %errors made by the computer

eval(['S',num2str(r),'=g']);
eval(['R',num2str(r),'=Entropy']);
S(r,1)=eval(['S',num2str(r)]);
R(r,1)=eval(['R',num2str(r)]);
eval(['M',num2str(r),'=Magnetization']);
M(r,1)=eval(['M',num2str(r)]);
r=r+1;
waitbar(r/plotp,h)
end
close(h)
toc
colordef none
plot(S,R,'b-')
axis([-0.01,2,0,1])
grid on
hold on
plot(S,M)
grid on
end
```

A.2 The MATLAB program for the XY model

```
disp(' ')
disp('                        ****************************************')
disp('                        *                WELCOME                 *')
disp('                        *   to my entropy of entanglement for the  *')
disp('                        *    XY Hamiltonian calculating program!   *')
disp('                        *                                        *')
disp('                        ****************************************')
disp(' ')
clf
clear all
n=input('Number of spinparticles?: ');
if n==3
    off=0.31;
    intensity=0.0002;
```

```
elseif n==4
    off=0.5;
    intensity=0.00035;
elseif n==5
    off=0.7;
    intensity=0.0005;
elseif n==6
    off=0.8;
    intensity=0.0008;
elseif n==7
    off=0.88;
    intensity=0.0009;
elseif n==8
    off=0.95;
    intensity=0.0013;
elseif n==9
    off=0.95;
    intensity=0.0017;
elseif n==10
    off=0.99;
    intensity=0.008;
else off=0.99;
    intensity=0.01;
end
k=input('How many of those spinparticles are in the largest block?: ');
tic
J=1;
sigmaX=[0 1;1 0];
sigmaY=[0 -i;i 0];
sigmaZ=[1 0;0 -1];
AX=zeros(2^n);   %These lines below creates the matrices of the form ~ I*sigmaX*I
for i=1:n
AAX=kron(eye(2^(i-1)),kron(sigmaX,eye(2^(n-i))));
AX=AAX+AX;
end
AZ=zeros(2^n);   %These lines below creates the matrices of the form ~ I*sigmaZ*I
for i=1:n
AAZ=kron(eye(2^(i-1)),kron(sigmaZ,eye(2^(n-i))));
AZ=AAZ+AZ;
end
                %These lines creates the matrices of the
                %form ~ I*sigmaX*sigmaX*I needed for the
                %nearest neighbours
BX=zeros(2^n);
for i=0:n-2
    BBX=kron(kron(eye(2^(i)),sigmaX),kron(sigmaX,eye(2^((n-2)-i))));
    BX=BX+BBX;
end
                %This line creates the matrix missing in the
                %sum above ~ sigmaX*I^(2^(n-2))*sigmaX:
CX=kron(kron(sigmaX,eye(2^(n-2))),sigmaX);
BX=CX+BX;
                %These lines creates the matrices of the
                %form ~ I*sigmaY*sigmaY*I needed for the
                %nearest neighbours
BY=zeros(2^n);
for i=0:n-2
    BBY=kron(kron(eye(2^(i)),sigmaY),kron(sigmaY,eye(2^((n-2)-i))));
    BY=BY+BBY;
end
                %This line creates the matrix missing in the
                %sum above ~ sigmaY*I^(2^(n-2))*sigmaY:
```

```
CY=kron(kron(sigmaY,eye(2^(n-2))),sigmaY);
BY=CY+BY;
               %This loop below generates the spinvectors a[1] to a[n]
               %needed to construct the two "blockvectors"
               %for each position j in the groundstate vector y(j)
I=eye(2);
for j=1:2^n
     for i=1:n
         if mod(ceil(j/(2^(i-1))),2)==1
             eval(['a',int2str(i),'=I(:,1)']);
         else
             eval(['a',int2str(i),'=I(:,2)']);
         end
     end
m=n-k+1;
if k==1                          %These rows below constructs the "leftmost" blockvector
    b=eval(['a',num2str(m)]);    %from the spinvectors already calculated above
else
    b=kron((eval(['a',num2str(m+1)])),(eval(['a',num2str(m)])));
end
while m<n-1
    m=m+1;
    b=kron((eval(['a',num2str(m+1)])),b);
end
eval(['A',int2str(j),'=b']);
s=n-k;
if s==1                          %These rows below constructs the "rightmost blockvector"
    c=a1;                        %from the spinvectors already calculated above
else
    c=kron((eval(['a',num2str(s)])),(eval(['a',num2str(s-1)])));
end
while s>2
    s=s-1;
    c=kron(c,(eval(['a',num2str(s-1)])));
end
eval(['B',int2str(j),'=c']);
end
                                 %Now I calculate the groundstate vector and its
                                 %corresponding density matrix in order to
                                 %calculate the entropy and plot it against
                                 %the magnitude of the transversal magnetic field, g.
R=zeros(30,1);
RRR=zeros(10,200);
TTT=zeros(10,30);
rr=1;
h = waitbar(0,'Please wait...');
for gamma=linspace(0,1,10)
r=1;
for g=linspace(0.001,2,30);
    Hz=abs((1-tanh(g))*(0.99+sign(off-g))*intensity);
                                 %This line below Sums up the matrices calculated
                                 %above to construct the Hamiltonian for the
                                 %1-dimensional XY model which contains both the Ising
                                 %model (gamma=1) and the XX model (gamma = 0).
H=-J*0.5*((1+gamma)*BX+(1-gamma)*BY)-J*(g*AZ+Hz*AX);
[X,D]=eig(H);


y=X(:,1);     %The groundstate vector!
                                        %Now I construct the density matrix
                                        %for block A
rhoA=zeros(2^k);
```

```
for i=1:2^n
        if mod(i,2^(n-k))==0;
           a=2^s;
        else a=mod(i,2^(n-k));
        end
            for j=a:2^(n-k):2^n
                rhoAA=y(i)*(eval(['A',int2str(i)]))*y(j)*(eval(['A',int2str(j)]))';
                rhoA=rhoA+rhoAA;
            end
end
                                        %Now I construct the density matrix
                                        %for block B
rhoB=zeros(2^(n-k));
for t=0:2^k-1
    for i=t*(2^(n-k))+1:(t+1)*(2^(n-k))
        for j=t*(2^(n-k))+1:(t+1)*(2^(n-k))
            rhoBB=y(i)*(eval(['B',int2str(i)]))*y(j)*(eval(['B',int2str(j)]))';
            rhoB=rhoB+rhoBB;
        end
    end
end

SA=-trace((rhoA)*real(logm(rhoA)/log(2)));     %Entropy for block "A"
SB=-trace((rhoB)*real(logm(rhoB)/log(2)));     %Entropy for block "B"
Entropy=(SA+SB)/2;                             %Total entropy, taking the medium value of
                                               %SA and SB to neutralize rounding
                                               %errors made by the computer
eval(['S',num2str(r),'=g']);
eval(['R',num2str(r),'=Entropy']);
S(r,1)=eval(['S',num2str(r)]);
R(r,1)=eval(['R',num2str(r)]);
r=r+1;
end
RR=interp1(S,R,linspace(0.001,2,200),'cubic');
RRR(rr,:)=RR;
TTT(rr,:)=R';
if rr==10
    vv=S
    ww=R
end
waitbar(rr/10,h)
rr=rr+1;
end
close(h)
toc
colordef black
colormap(cool)
mesh(TTT)
axis('ij')
view(13,64)
axis([0,30,1,11,0,1])
axis off
disp('Click on the figure to see the graph, then click any key to see a contour plot over the entropy')
pause
clf
hold off
contourf(TTT)
axis('ij')
colormap(cool)
axis off
```

Bibliography

[1] R. Bowley and M. Sanches, *Introductory Statistical Mechanics* (Oxford Science Publications, Oxford, 2001).

[2] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, (Cambridge University Press, 2003).

[3] J. Prescill, Lecture notes, chapter 4, *Shannon for dummies*, USA, 2002.

[4] J. I. Latorre, E. Rico and G. Vidal, *Groundstate Entanglement in Quantum Spin Chains*, Quantum Information & Computation 4 (1) 48-92 (2004).

[5] J. I. Latorre and R. Orús, *Universality of Entanglement and Quantum Computation Complexity*, Phys. Rev. A**69** (5) 052308 (2004).

[6] T. Stauber and F. Guinea, *Entanglement at the Boundary of Spin Chains near a Quantum Critical Point and in Systems with Boundary Critical Points*, Phys. Rev. A**70** (2) 022313 (2004).

[7] J.J.Sakurai, *Modern Quantum Mechanics* (Addison-Wesley Publishing Company, 1994).

[8] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, *Mixed State Entanglement and Quantum Error Correction*, Phys. Rev. A**54** (5): 3824-3851 (1996).

[9] C. H. Bennett, H. J. Bernstein, S. Popescu, B. Schumacher, *Concentrating Partial Entanglement by Local Operations*, Phys. Rev A**53** (4): 2046-2052 (1996).

[10] B.-Q. Jin and V.E. Korepin, *Localizable Entanglement in Antiferromagnetic Spin Chains*, Phys. Rev. A**69** (5) 062314 (2004).

[11] T. J. Osborne and M. A. Nielsen, *Entanglement, Quantum Phase Transitions, and Density Matrix Renormalization*, Phys. Rev. A**66** (3) 032110 (2002).

[12] O. F. Syljuasen, *Concurrence in the Two-dimensional XXZ- and Transverse Field Ising-models*, Phys. Rev. Lett. **322** (1-2): 25-35 (2004).

[13] F. Verstraete, M. Popp and J.I Cirac, *Entanglement versus Correlations in Spin Systems*, Phys. Rev. Lett. **92** (2) 027901 (2004).

[14] M.C. Arnesen, S. Bose and V. Vedral, *Natural Thermal and Magnetic Entanglement in 1D Heisenberg model*, Phys. Rev. Lett. **87** (1) 017901 (2001).

[15] L. H. Ryder, *Quantum field theory* (Cambridge University Press, 1985).

[16] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, 1999).

[17] J. Gaite, *Entanglement Entropy and the Density Matrix Renormalization Group*, http://www.arxiv.org/pdf/quant-ph/0301120.

[18] N. Linden and A. Winter, *A New Inequality for the von Neumann Entropy*, http://www.arxiv.org/pdf/quant-ph/0406162.

[19] A. Miranowicz and A. Grudka, *Relative Entropy of Entanglement for a given Negativity can be higher for Mixed States than for Pure States*, http://www.arxiv.org/pdf/quant-ph/0409009.

[20] N. Takei, T. Aoki, S. Koike, K. Yoshino, K. Wakui, H. Yonezawa, T. Hiraoka, J. Mizuno, M. Takeoka, M. Ban, and A. Furusawa, *Quantum Teleportation of a Squeezed State*, http://www.arxiv.org/pdf/quant-ph/0311056.

[21] T.-C. Wei, D. Das, S. Mukhopadyay, S. Vishveshwara, and P. M. Goldbart, *Global Entanglement and Quantum Criticality in Spin Chains*, http://www.arxiv.org/pdf/quant-ph/0405162.