Entanglement in Finite Spin Systems

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Abstract

In this thesis we investigate the occurrence of entanglement in a number of solid state spin systems. This is done using exact diagonalization. The reason for the interest in the matter is the conjecture that it should exist some connection between entanglement and quantum phase transitions. We also review the most common measures used for comparing entanglement in different systems. A discussion of pros and cons follows. A new measure, Vector Entanglement, is introduced. This measure appears to have some desired properties, such as subadditivity, while being hard to calculate. We review the notion of entanglement of formation and generalize the procedure for calculating this quantity to higher–spin systems. This is used to investigate the entanglement of formation of some spin-1 systems.

Acknowledgements

I would like thank my supervisor, Henrik Johannesson. Without his devotion and strong support this thesis would not have been possible! Also I would like to thank Daniel Larsson for the fun and enlightening time we had when discussing our projects. At last I want to thank my girlfriend and family for believing in me.

Robert Rehammar
Feci quod potui, faciant meliora potentes.

Contents

1 Introduction

The purpose of this thesis it to investigate how, and if, there is any connection between the entanglement in a spin system and the quantum phase transitions that occur in the system. The main problem is to know how the entanglement is to be characterized. At present there is no known general definition of what entanglement is. Instead we know what a "fully" entangled state is and what a "non–entangled" state is. At the time of writing this thesis there is no general *measure* of entanglement for an arbitrary system. There have been different measures of entanglement suggested. Some of these are reviewed and discussed later in this section.

The model most often studied in connection with entanglement is the so called XY model. Therefore we review the procedure of analytically diaonalizing the XY model in section 2. In this section we also see that this diagonalization procedure is rather involved, even for the simple XY model. This is one of the reasons for the desire to work with entanglement in small systems instead (besides the fact that it is very interesting if there is any connections between entanglement and phase transitions). The result in section 2 will be used in later sections. In section 3 we present the theory used for exact diagonalization and in section 4 the main result of the thesis, using the theory from section 3. We begin by introducing spin systems and quantum phase transitions and some other basic stuff.

1.1 Spin Systems

A spin system is something like figure 1.1. There we have a line of spin particles (for example spin–1/2). These systems can exist in any dimension, and the coupling can vary (Coupling means how the spins interact. Classically a spin can be seen as a small bar magnet, thus having a magnetic moment. These magnetic moments can interact.). In figure 1.1 the boxes illustrate coupling to nearest neighbors. This is the most common case, and most of the models considered here will have this property.

When one wants to investigate a spin system the road is: Write down the classical Lagrange function, do a Legrende transform to obtain the classical Hamiltonian and finally quantize this Hamilton function to get the Hamilton operator. For interacting spins the classical Hamilton function can, on tensor form, be written as

$$H = J[g_k{}^{ij} S^k{}_i S^l{}_j d^k_l + B_k{}^i S^k_i + \varepsilon_k{}^i S^k_i]. \tag{1.1}$$

In this equation Einstiens summation convention is employed. J contains the sign which tells if the interaction is ferromagnetic ($J < 0$) or antiferromagnetic ($J > 0$). The first term in the sum represents the interaction between spins in our lattice. The prefactor g^{ij}_k determines the coupling between spins and the dimensionality of the system and S^k is the spin vector. The collective indices, i, j, on S represents the position of the spins, i.e. the lattice site. In a similar manner the second and third term represents interaction with an external field. It would be sufficient in analytical calculations to have the first of these two, but as we will see in section 3, it is convenient to write out the second one when doing numerical calculations. To obtain the Hamilton operator we do a quantization of (1.1), that is, replace the classical variables, S^k, with corresponding operators, σ^k (in this thesis we will set constants like $\hbar$ and k_B equal to 1)

$$H = J[g_k{}^{ij} \sigma^k{}_i \sigma^l{}_j d^k_l + B_k{}^i \sigma^k_i + \varepsilon_k{}^i \sigma^k_i]. \tag{1.2}$$

Here σ^k are the well known Pauli matrices if we are dealing with spin-1/2 systems and higher spin matrices if we are dealing with higher spin systems. From equation (1.2) we can derive some well known special cases, for example the XY model, the Ising model or the Heisenberg spin chain. For example, the ferromagnetic XY model in a transverse field in one dimension is obtained by

putting

$$\begin{aligned} g_k^{ij} &= ((1/2+\gamma)\delta_k{}^x + (1/2-\gamma)\delta_k{}^y)\cdot\delta^{i+1,\,j} \\ d^k_{\ l} &= \delta^k_{\ l} \\ J &= -1/2 \\ \varepsilon &= 0 \\ B_k &= 2B_z, \end{aligned}$$

and we get

$$H = -\frac{1}{2}\sum_{i=1}^{N}((1/2+\gamma)\sigma_i^x\sigma_{i+1}^x + (1/2-\gamma)\sigma_i^y\sigma_{i+1}^y + B\sigma_i^z). \tag{1.3}$$

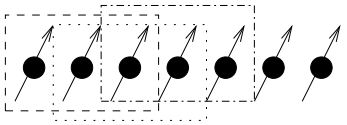


Figure 1.1: A schematic picture of a spin system. The dotted and dashed rectangles represents the interaction length between adjacent spins. We mostly use Hamiltonians with only nearest neighbor interactions.

Often it is useful to write the Hamiltonian on the form

$$H = H_0 + BH_1,$$

where H_0 is the part of the Hamiltonian not coupled to the external field and BH_1 the field–dependent part. In the case of the XX model (i.e. with $\gamma = 0$ in (1.3)) the two parts of the Hamiltonian commute, which means they can be simultaneously diagonalized [3, 8]. For all other XY models

$$[H_0,\ H_1] \neq 0.$$

Thus the XX model has a symmetry different from the other XY models.

It is not always the case that a quantum mechanical system has a classical counterpart. Thus the quantization procedure is not always possible, but one has to start with a quantum mechanical model right away. In this thesis we will take our starting point in equation 1.2, not worrying about weather the model has classical counterparts or not. The analogy with small bar magnets is a pure phenomenological one. By choosing the constants differently, and adding terms which we will motivate later, we will obtain different models which we will study.

The Qubit

In the following discussion we will sometimes treat the two terms *qubit* and *spin* as equivalent. A qubit in quantum information theory is defined as a system that can be in a superposition of two orthogonal states. We often label these states 0 and 1, + and −, or ↑ and ↓. Here the fist convention is often used in quantum informations theory. In quantum information theory your primary concern is not what type of physical realisation you have, but rather the mathematical and information theoretical structure of the system. The other labels with signs and arrows come from the fact that a spin 1/2–system realizes a qubit. But this is not the only system that can be used as a qubit, other two level systems are polarized light or superconducting circuits. In this thesis we focus on spin systems and will use the two terms spin and qubit equivalently.

On the Naming of the XYZ Models

In the literature one often sees names of models like XXY model or XYZ model. These names all refer to spin models. The letters describe how many interacting terms one has. The first position in the list of XYZs is the x–interaction, the second one the y– and the third one the z–interaction.

If one thus writes "XX model" one means a model where we have interactions in the x– and the y–direction, and with the same coupling constant. The XY model on the other hand has coupling in x and y, but with different couplings in each direction. The Ising model is the same as the X model in a transverse field and the anisotropic Heisenberg model is the same as the XYZ model.

1.2 Phase Transitions

A phase transition is a fundamental change in the state of a system. Classically a phase transition is driven by some parameter such as temperature or pressure. Examples of phase transitions are water going from liquid to steam or iron going from a ferro– to a paramagnetic state.

Phase transitions are divided into two different classes: Those with a latent energy, and those without. The transition of water from liquid to steam is a transition with latent heat (energy). That means that when water boils at 100° C this temperature is constant despite the fact that we feed in energy in the form of heat into the system. The temperature will not rise above 100° C until all of the water is gas. This is not the case with magnetic iron. When the temperature increases the magnetization decreases until, at some threshold, it is zero. Then it stays zero for larger temperatures.

Quantum phase transitions

A quantum phase transition is a phase transition in the same way as a classical phase transition, but with the difference that it occurs at zero temperature. This means that the temperature can not drive the phase transition. Many quantum systems exhibit quantum phase transitions, QPT, for different driving parameters, like a magnetic field. Lately it has been conjectured [15, 22, 23, 24] that entanglement, or properties related to entanglement, can be used as a diagnostic tool for these QPT's. The main purpose of this theses is to try to extend the understanding of how this relation between QPT's and entanglement is manifested.

In [7] a quantum phase transition is defined as a nonalyticity in the ground state energy (eigenvalue) of a system. These nonanalyticities can come from two things. Either it is a level crossing in the ground state. These level crossings occur already in finite lattices. The other possibility is the limit of an, in the finite lattice, avoided level crossing.

Phase transitions are closely related to the concept of *universality*. That is, near a phase transition properties of a system behaves universal in the sense that they are independent of the microscopic details of the system. Properties like susceptibility, energy gap and correlation functions behave very simple, depending only on a few universal exponents. For example the energy gap behaves as

$$\Delta \sim |B - B_c|^{z\nu}$$

where Δ is the energy gap, B is a magnetic field driving the QPT, B_c is the critical field at which the transition occurs and $z\nu$ are universal constants [7].

Since absolutely zero temperature cannot be reached in reality one may think that the study of QPT's is a pure theoretical exercise. However, the QPT creates a region of very special behavior which spreads up to finite temperatures. This region is very interesting and is highly dependent on the behavior at the QPT at zero temperature.

Included here for later reference is the phase diagram, figure 1.2, of the ferromagnetic XY model from equation (1.3).

1.3 The Concept of Entanglement

In quantum mechanics we represent a physical system with a state vector in a linear vector space of Hilbert type. A qubit is a vector in a two dimensional Hilbert space. If we have two qubits, say A and B in Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, we can create one larger system containing both qubits. This is done with the tensor product, and we get $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, containing both qubits. With the same symbol, $\otimes$, we represent the product of vectors and operators. That is, we get $O = O_A \otimes O_B$ and $|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$ for operators and vectors respectively. How these operations

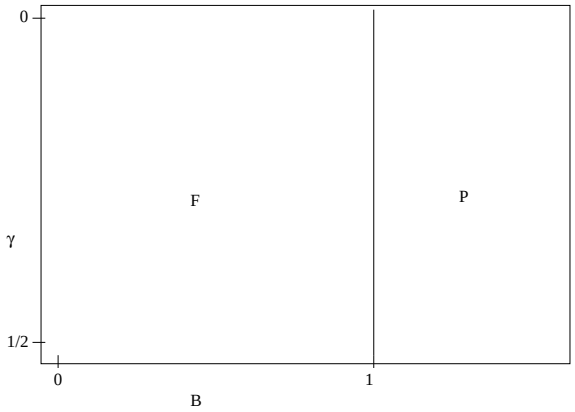


Figure 1.2: The phase diagram of the XY model. γ is the anisotropy parameter found in equation (1.3) and B is the magnetic field, also found in (1.3), F = ferromagnetic, P = paramagnetic. This figure is extracted from [10].

are implemented and behave is discussed in section 3.1. This tensor product is fundamental in quantum mechanics. Yet, it is a very complicated thing. I would say that understanding fully the tensor product is almost the same as understanding entanglement. Before we start discussing in more detail what entanglement is we need to define and introduce a few concepts.

1.3.1 Some Definitions

The *density matrix* is defined as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

where p_i denotes classical probabilities for the state $|\psi_i\rangle$[1]. In this sense the density matrix is the quantum mechanical version of the distribution function in classical thermodynamics [1]. The density matrix is a generalisation in the way that is contains two types of probabilities; first the classical probabilities p_i for different states. In addition it encodes quantum mechanical probabilities for how a measurement may collapse the wave function into an eigenstate of the measurement operator. This dual role of the density operator will turn out to be a bit problematic.

The *reduced density matrix* is the density matrix appropriate for describing a subsystem where some of the degrees of freedom are not accounted for. For a system AB with density matrix ρ the reduced density matrix for system A is

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

where tr_B means "the trace over all B's degrees of freedom multiplied with the rest". For two systems A and B in a pure product state we have:

$$\begin{aligned} &\rho = |AB\rangle\langle AB| \Rightarrow \\ &\rho_A = tr_B(|AB\rangle\langle AB|) = |A\rangle\langle A| \cdot tr(|B\rangle\langle B|) = |A\rangle\langle A| \cdot \langle B|B\rangle. \end{aligned} \tag{1.4}$$

In a more formal notation

$$\rho_{\mathcal{H}_B} = tr_{\mathcal{H}_B}(\rho) = \sum_{|\phi\rangle,|\phi'\rangle \in B_{\mathcal{H}_A}} |\phi\rangle\Big(\sum_{|\psi\rangle \in B_{\mathcal{H}_B}} \langle\phi,\psi|\rho|\phi',\psi\rangle\Big)\langle\phi'|. \tag{1.5}$$

Here $B_{\mathcal{H}_{B/A}}$ are the bases spanning Hilbert spaces A and B respectively [6]. It is not immediately obvious that the reduced density matrix defined in this fashion gives the correct dynamics for the subsystem. See [8] fore further details.

[1] It can be proved that ρ can be calculated via (1.6), see for example [3].

To be precis we here state what we mean by mixture and pure states and product and non–product states.[2]
A *pure state*, ψ is an (infinite) ensemble of the exact same state ket, $|\psi\rangle$ (Not that standard quantum mechanics is formulated in terms of pure states).
A *mixture ensemble* is an (again infinite) ensemble of state kets. This time each ket $|\psi_i\rangle$ occurs with a classical probability p_i giving the ensemble

$$\{p_i,\ |\psi_i\rangle\}.$$

A *non–product state* is a state $|\psi\rangle$ which can not be written as a tensor product of the states describing its constituent systems A, B, ...: $|\psi\rangle \neq |A\rangle \otimes |B\rangle \otimes ....$
A *product state* is a state that can be written as a product of its parts. Here a note should be added. Of course one can always find a basis so that the state is a product state. Just choose the state itself, and you get a product state. But the problem is that this basis may be "non–local"; that is, its base vectors will not represent the local physical objects (e.g. spin 1/2–particles) so the basis itself will be nonlocal. When we say that a state is a product state we mean in some natural basis. In this thesis it will always be the spin basis. As an example of a nonlocal basis take the base vectors of equation (1.7). Since entanglement is all about nonlocal stuff it is a bad idea to introduce a nonlocal basis. Thus it becomes obvious that entanglement is a basis dependent property.
A *mixed state* is a state A to which the density matrix, ρ, is known, but not the ensemble making up the density matrix. Here we can not write $\{p_i,\ |\psi_i\rangle\}$ since this ensemble is not unique. It is in the language of mixed states that statistical quantum mechanics is formulated. There we have that

$$\rho = e^{-\beta H}/Z,\ Z = tr(e^{-\beta H}) \tag{1.6}$$

or some other ensemble which might or might not be canonical, and it is in this sense that the mixture ensemble is unknown (we do not have the explicit expressions for $\{p_i,\ |\psi_i\rangle\}$). The problem of choosing ensemble will be discussed later.

To emphasize the difference between mixture ensemble and mixed state look at the following two mixture ensembles:
1. $A = \{\frac{1}{4},\ |i\rangle\}$, where $|i\rangle$ is one of the Bell states

$$\begin{aligned} |I\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |II\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \\ |III\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |IV\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \end{aligned} \tag{1.7}$$

2. $B = \{\frac{1}{4},\ |n\rangle\}$, where $|n\rangle$ is one of the product states

$$\begin{matrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{matrix}$$

A simple calculation shows that both of these two mixture ensembles have the same density matrix, namely, in the $\{|00\rangle,\ |01\rangle,\ |10\rangle,\ |11\rangle\}$–basis:

$$\rho = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

[2]These definitions vary somewhat in the literature, and for clarity we state here exactly what we mean in this thesis.

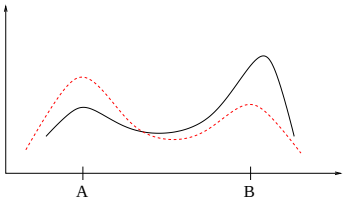


Figure 1.3: Visualization of the wave functions for an entangled pair of particles. The solid line represents the particle A and the dashed line the particle B. Note that this is just a sketch.

All Ensembles Corresponding to a Given Density Matrix In [12] it was proven that all ensembles compatible with a given density matrix, ρ, in a Hilbert space of size N, can be obtained via the transformation

$$|\psi_i\rangle = \sum_{j=1}^{N} U_{ij}|e_j\rangle$$

where $\{|e_j\rangle\}$ is a so called *eigenensemble* of ρ, and U is a matrix built up from orthonormal $\mathbb{C}^n$ vectors ($n \geq N$). An eigenensemble is an ensemble which has the property that $\langle e_i|e_j\rangle = \delta_{ij}\lambda_i$, with λ_i an eigenvalue of ρ. We note that $|e_i\rangle$ is not a standard quantum mechanical state vector since it is not normalized to unity. Also $\{|e_i\rangle\}$ is a trivial ρ–ensemble (that is, it is compatible with the density matrix ρ).

1.3.2 Entanglement

Loosely speaking entanglement is the potential of a quantum state to exhibit correlations that can not be accounted for classically [16]. It was long thought that entanglement was equivalent to violating some Bell type inequality[3]. This is not true however since there are entangled states that do not violate *any* Bell inequality [17].

A pure state[4] is called entangled if it is unfactorisable, that is it can not be written as a product state[4]. A mixed state[4] is entangled if it can not be written as a mixture of factorisable states.

In terms of wave functions these statements can be illustrated as: If we have two entangled particles, A and B, with wave functions $\psi_A(x)$ and $\psi_B(x)$ associated to them, the composite wave function of both particles cannot be written as a simple product $\psi_A(x_A) \cdot \psi_B(x_B)$ but must be written as a linear combination of such, say

$$\psi_A(x_A)\psi_B(x_B) \pm \psi_A(x_B)\psi_B(x_A). \tag{1.8}$$

If we instead express this in bras and kets we get that we need to write $|AB\rangle \pm |BA\rangle$, where $|AB\rangle$ is shorthand for $|A\rangle \otimes |B\rangle$, our product state. For the wave functions this can be visualized pictorially as in figure 1.3.

As I see it, entanglement is a direct consequence of the two quantum mechanical principles (1) superposition and (2) the tensor product prescription for extending Hilbert space. It is these two principles that allow a composite system to be written as a superposition in its extended Hilbert space of both subsystems, allowing nonlocal wave functions of the form (1.8).

We cannot present a more precise definition of how much a general system is entangled. The reason for this is that there is no measure generally accepted. A key part of this thesis will be to discuss some of the measures that look most promising at the moment.

For a system defined on a lattice of some sort we can have entanglement on different length scales. If we are dealing with a spin chain like the one in equation (1.3) and figure 1.1 we can have nearest–neighbor entanglement. This means that only nearest neighbors get entangled. Often this entanglement spreads so that spins next to nearest neighbors get entangled. This phenomenon

[3] See for example [3] for a description of what a Bell inequality is.
[4] Here we use these terms in the way they were defined in section 1.3.1

naturally leads to the concept of *entanglement length*. It has been suggested [23] that the entanglement length should diverge when we approach a quantum phase transition in a similar manner as a classical correlation length diverges. Because of this, one desirable property of an entanglement measure would be to take into account the entanglement length, or allow for a natural definition of entanglement length belonging to the entanglement measure.

1.3.3 General Requirements on a Measure of Entanglement

There are a number of requirements that should be fulfiled for a quantity for it to be a good measure of entanglement. Here we will list the most important ones according to my understanding. For further discussion of this see for example [13, 14, 15, 16, 17, 19, 21, 22, 23, 24].

- The measure should be additive. That is, it should have the property: $E(\rho\otimes\sigma) = E(\rho)+E(\sigma)$, with ρ and σ being density matrices. (Or, as will be the case of vector entanglement, the measure introduced by me in section 1.4, additive on something else describing the state of a system, for example the state vector.)
- It should be monotone under local operations. That is, as long as only operations performed on a local part of the system are allowed, the measure should nondecrease or nonincrease.
- It should in some sense classify entanglement as a resource. For example if you have m qubits, each of entanglement E you can, by local operations and classical communication, concentrate this total entanglement, mE to n fully entangled qubits. If this is done, the yield from such an operation should be $n/m = E/E_{max}$, where E_{max} is the maximal entanglement according to your measure.
- The measure should in a natural way introduce, or take account of, entanglement spread.
- The measure should have a connection to correlations functions.
- The measure should have a connection to QPT.

The last three items are important for us when studying entanglement in solid state, while the second and third are of most interest for someone doing quantum information. The first item is the most natural requirement one can have on a measure in general and an entanglement measure should always, by all means, satisfy this.

1.3.4 Different Entanglement Measures

Here we will define some of the measures of entanglement. A whole plethora of measures of entanglement have been suggested. The reason for this variety is the failure to fulfil all reasonable criterion for an entanglement measure there are. For simple pure states the von Neumann entanglement is a suitable measure. This is however not the case for more complex systems involving mixtures of states.

von Neumann entropy The traditional measure of entanglement is the von Neumann entropy[5]. It is a quantum generalisation of the classical information theoretical concept of entropy introduced by Shannon. We start by defining the von Neumann entropy on pure states only. On functional form we have for a state with density matrix ρ the von Neumann entropy

$$E = -tr(\rho \log_2 \rho). \tag{1.9}$$

Thus if we want to calculate the entanglement between two subsystems, A and B say, we use the reduced density matrix ρ_A or ρ_B. It can be proved that $E(\rho_A) = E(\rho_B)$ always. If ρ represent a bipartite system (that is, a system consisting of two parts) one often speaks of E_A as the

[5]The von Neumann entropy is often referred to as local entanglement or entropy of entanglement. We shall most frequently use the later.

entanglement of the system. Since ρ represents a pure state $E(\rho) = 0$ and as the system is bipartite the von Neumann entropy of one of its subsystems is a natural entanglement measure.

We have seen that for a pure bipartite system we can assign the whole system the entanglement equal to the von Neumann entropy of one of its parts. Since both parts have the same von Neumann entropy there is no doubt. Now if the system is, say, tripartite we have three possible partitions of the system; AB and C, A and BC and CA and B. We know that $E(\rho_{AB}) = E(\rho_C)$ and so on, but it is not in general true that $E(\rho_{AB}) = E(\rho_{CA})$. So which entanglement should we assign out who system? There is no general way to tell. This is the first problem with the entropy of entanglement.

Now we turn to mixed ensembles. We only consider bipartite systems for simplicity. When von Neumann introduced his entropy generalisation of the Shannon entropy it was with measurements in mind. It is easily shown [3] that the expectation value of an observable A, $[A]$, equals $tr(\rho A)$ for a systems with density matrix ρ. What von Neumann here achieves is to capture two things in one operator. To begin with we have classical probabilities in a distribution, the second is that we have quantum mechanical probabilities from quantum superposition. This dual role of the density matrix makes it badly suited as a basis for a measure of entanglement since these two phenomena might "interfere".[6] As an example consider the two ensembles given on page 5. They result in the same density matrix. Thus they have the same von Neumann entropy. However, it is obvious that case 1 has a lot of entanglement, even maximally since it is a mixture ensemble of Bell states, while case 2 is not entangled what so ever.

This said about the cons of the von Neumann Entropy, it is still in some cases a good measure of entanglement. Especially in bipartite systems. One of the strongest pros of the von Neumann entropy was given by Bennett *et al.* in [14] where it is proved that if one wants to convert m partly entangled pairs of qubits to n fully entangled pairs using local unitary operations and classical communication then the ratio of success n/m will approach the entropy of entanglement for the partly entangled qubits (this is criteria 3 on the list in section 1.3.3 of aspects to fulfil for an entanglement measure).

Being a generalisation of the Shannon entropy, the von Neumann entropy shares many properties with it, not all though. We will not try to list them all here but rather refer to texts on quantum information [6, 8, 28]. Two important properties that we will discuss are
1) Maximum of the entropy
2) Subadditivity
1) In a d–dimensional Hilbertspace the entropy is maximally $\log_2 d$. This value is reached for a completly mixed state $\rho = I/d$.
2) It can be proved that E fulfils the subadditivity property

$$E(A_1 \otimes A_2) \leq E(A_1) + E(A_2). \tag{1.10}$$

Entanglement Monotones In [21] Vidal argues that the only *a priori* requirement for an entanglement measure is monotonicity under local transforms. He makes the definition

> Every magnitude $\mu(\rho)$ that does not, on average, increase under local transformations (or local quantum operations) we call an *entanglement monotone, EM.*

Vidal argues that viewing entanglement as a nonlocal resource implies that the only reasonable requirement of a measure is monotonicity. That we can satisfy with local quantum operations[7] (LQ), without classical communication (CC), is due to the fact that monotonicity under LQ implies monotonicity under LQCC. The reason why this is a reasonable requirement is of course that it is impossible to increase nonlocal correlations via local operations.

[6] It should be noted that this is not a critique of the concept of the von Neumann entropy in principle, but only for measuring entanglement in certain situations. It should be remembered that von Neumann did not introduce his entropy with entanglement in mind, but rather with statistical quantum mechanics.

[7] If a systems consists in two parts, say A and B, spatially separated, a local operation on subsystem A is an operation $O_A \otimes I_B$, where $I_B \in \mathcal{H}_B$ is the identity operator and $O_A \in \mathcal{H}_A$ is any operator acting in Hilbert space A.

Vidal's article on entanglement monotones was published in 2000 with quantum information and computation as its primary target. For quantum phase transitions the monotonicity requirement might not be sufficient. In [23] Osborn and Nielsen argue that an entanglement measure should take into account the spread of entanglement in the system under considerations. They emphasize the importance of the entanglement length as a property of entanglement. This requirement is naturally not very interesting if the two parts of a bipartite system are not fixed, as is in general the case for quantum computations. In spin systems however, the parts of the system are typically fixed and how the entanglement spreads is of great interest.

Entanglement of Formation Entanglement of formation was first introduced in [14]. We will repeat the definition here for completeness and as it will be used later. It is made up of three steps.

1. The entanglement of formation of a bipartite pure state Y is the von Neumann entropy $E(Y) = S(tr_A(\rho))$ of one of the parts of the system.

2. The entanglement of formation $E_F(A)$ of a bipartite mixture ensemble (in [14] this is called an ensemble of pure bipartite states) $A = \{p_i, Y_i\}$ is the ensemble average, $E_F(A) = \sum_i p_i E(Y_i)$, of the entanglement of formation of each pure state in the ensemble.

3. The entanglement of formation $E_F(M)$ of a bipartite mixed state M is the minimum of $E_F(A)$ over ensembles A making up the mixed state, that is $E_F(M) = \min_A\{E_F(A)\}$.

In [18] it is proved that the entanglement of formation can be calculated directly from the reduced density operator without having to do any optimization procedure. The equations for doing this are found in section 3.3.

One thing that I find strange with the entanglement of formation is the fact that in step 3 we create a certain ensemble to belong to our density matrix. But this might not be possible since if we have a reduced density operator the very definitions of entangled means that there is *no* ensemble belonging to the density matrix. From the definition this is not a problem as the measure is only defined for bipartite systems. But this is not the way in which the measure is used. Often one starts with a multipartite state and then obtains the reduced density matrix of two subsystems (tracing away the rest). After the reduced density matrix is obtained the procedure of optimization is executed.

Entanglement of Assistance The entanglement of assistance is dual to the entanglement of formation. It is defined in Ref. [19]. For the first two cases above the definitions coincide. In the third case, when we deal with a mixed state, the minimum over ensembles realizing the density matrix is replaced by the maximum, that is:
The *entanglement of assistance* for a mixed state M is $E_A(M) = \max_A\{E_A(A)\}$.

In [26] it is shown how the entanglement of assistance can be calculated exactly from the reduced density matrix of two spins without having to do any optimization procedure.

Localisable Entanglement In 2003 Veratraeta *et al.* [24] suggested a new measure of entanglement. The motivation for this was that these authors felt a lack of a measure satisfying the two criteria (i) entanglement should be treated as a physical resource, and (ii) the measure should establish a close connection to correlation functions. (i) has been increasingly important since there has been a shift in view later towards considering entanglement a physical resource for e.g. quantum teleportation, see later in this section. (ii) is also highly motivated since entanglement is a form of correlation between particles. The measures mentioned earlier fail to satisfy one or both of these conditions.

The definition of localisable entanglement is as follows: Every (local) measurement basis specifies a mixed ensemble $\mathcal{E} = \{p_k,\ |\psi_k>\}$ consisting of at least 2^{N-2} elements, where N is the number of spins. The localisable entanglement, E_L is then defined as:

$$E_L = \max_{\mathcal{E}} \sum_k p_k E(|\psi_k\rangle)$$

where $E(|\psi_k\rangle)$ denotes the entanglement of $|\psi_k\rangle$. As we here talk of pure states $|\psi\rangle$, any measure E is ok, since they all are essentially equivalent.

When this is written (January 2005) there is no known method to calculate the localisable entanglement exactly in general. However in [24] it is given rather tight upper and lower bounds. An obvious upper bound to the localisable entanglement is the entanglement of assistance. These two would coincide if global measurements were allowed for E_L. The E_A can be exact calculated (see section on E_A). A lower bound on E_L is in [24] proven to be the (classical) correlation function. The two bounds thus show that the two criteria (i) and (ii) are satisfied.

1.3.5 The Concept of Concurrence

The concurrence is, as the name suggests, a dual to some entanglement measure. There are different concurrence measures corresponding to different entanglement measures. Since the relations between the entanglement measures defined above and a concurrence is bijective it is reasonable to call also the concurrence an entanglement measure. In particular the concurrence corresponding to the entanglement of formation is of great value as it provides a general way to carry out the optimization procedure, i.e. a functional relation, to calculate the entanglement of formation given the density matrix ρ.

The "von Neumann concurrence" The Bell states (note the special phases)

$$\begin{aligned} |e_1\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |e_2\rangle &= \frac{i}{\sqrt{2}}(|00\rangle - |11\rangle) \\ |e_3\rangle &= \frac{i}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |e_4\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \end{aligned} \tag{1.11}$$

form a basis (the so called "magic basis") for a two–qubit system. For a (pure bipartite) state $|\psi\rangle = \sum_i a_i|e_i\rangle$ expressed in this basis the entanglement (von Neumann entropy) can be written as

$$E(\psi) = f(C(\psi))$$

where $f(C)$ is the function

$$f(C) = H(\frac{1}{2} + \frac{1}{2}\sqrt{1 - C^2}) \tag{1.12}$$

and H the binary entropy function. C is called the (von Neumann) concurrence and is defined [16] by

$$C(\psi) = \left|\sum_i a_i^2\right|. \tag{1.13}$$

Note that this equation only holds when the state is expressed in the basis (1.11). Since the relation between E_E and C is one–to–one it is justified to talk of the concurrence as a measure of the entanglement in the same sense as the entropy of entanglement.

Concurrence of Formation, or Generalised Concurrence In [16] and [18] a close connection between the entanglement of formations and the so called generalised concurrence is made. This connection highly motivates the name generalised concurrence since it proves that the relation between concurrence and entanglement of formation is the same as that between (von Neumann) concurrence and von Neumann entropy.

The set of density matrices that are real when expressed in the basis (1.11) is the same as the set of density matrices describing mixtures of Bell states. This allows us to form the matrix[8] $R = \sqrt{\sqrt{\rho}\rho^*\sqrt{\rho}}$. $tr\ R$ ranges from 0 to 1 and is a measure of the degree of equality between ρ and ρ^*, see [16] and Ref. [11] therein. Since ρ is real for a mixture of Bell states (1.11) the difference between ρ and ρ^* makes $tr\ R$ a measure of entanglement. The function

$$c = \max\{0, 2\lambda_{max} - tr\ R\}$$

where λ_{max} is the largest eigenvalue of R, is then called the concurrence of a mixed state, or the concurrence of formation. This name is justified since it reduces to the regular concurrence in equation (1.13) when the state is pure [16] and because the entanglement of formation of a density matrix ρ is given by[9]

$$E_F(\rho) = f(c)$$

where $f(c)$ is the function in (1.12).[10] For a proof, see [16, 18].

1.3.6 An Entanglement Calculation Example

In this section we do a few calculations on a state to see what results the different entanglement definitions above gives. We test the pure state of two (A and B) 1/2–spins

$$|\psi\rangle = \cos\theta|01\rangle + \sin\theta|10\rangle. \tag{1.14}$$

It is easy to see that this state is normalized for all θ. For $\theta = 0,\ \pi/2$ we have one of the pure states $|01\rangle$ or $|10\rangle$, and for $\theta = \pi/4$ we have a maximally entangled state, a so called Bell state. The density matrix for the whole system is

$$\begin{aligned} \rho &= (\cos\theta|01\rangle + \sin\theta|10\rangle)(\langle 01|\cos\theta + \langle 10|\sin\theta) = \\ &= \cos^2\theta|01\rangle\langle 01| + \sin^2\theta|10\rangle\langle 10| + \cos\theta\sin\theta(|01\rangle\langle 10| + |10\rangle\langle 01|) \equiv \\ &\equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \cos^2\theta & \cos\theta\sin\theta & 0 \\ 0 & \cos\theta\sin\theta & \sin^2\theta & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{1.15}$$

The trace of ρ is 1 as it should be. The matrix representation of the density operator in the last line in (1.15) is in the representation where $|0\rangle \equiv (1\ 0)^T$ and $|1\rangle \equiv (0\ 1)^T$.

The reduced density matrix for spin A is

$$\begin{aligned} \rho_A = tr_B(\rho) &= \cos^2\theta|0\rangle\langle 0|\langle 1|1\rangle + \sin^2\theta|1\rangle\langle 1|\langle 0|0\rangle + \\ &\quad \sin\theta\cos\theta(|0\rangle\langle 1|\langle 1|0\rangle + |1\rangle\langle 0|\langle 0|1\rangle) \equiv \\ &\equiv \begin{pmatrix} \cos^2\theta & 0 \\ 0 & \sin^2\theta \end{pmatrix} \end{aligned} \tag{1.16}$$

In the same way for B we have

$$\rho_B \equiv \begin{pmatrix} \sin^2\theta & 0 \\ 0 & \cos^2\theta \end{pmatrix}$$

The von Neumann entropy is now easily calculated as

$$E = -tr(\rho_A \log_2 \rho_A) = 2\cos^2\theta \log_2\cos\theta + 2\sin^2\theta\log_2\sin\theta.$$

For θ varying from 0 to $\pi/2$ we get the result shown in figure 1.4.

[8] I suspect it to be something rather important physical with this equation. The time-reversed density matrix, ρ^*, can be used to do optimization. That should say something about the relation between time reversal and entanglement!? What happens to entanglement if we reverse time?

[9] It is important to note that the entanglement of formation we get here is the entanglement between spin i and j if ρ is the reduced density matrix for spin i and j. This is in contrast to the entropy of entanglement where $E(\rho)$ means the entanglement of the subsystem described by ρ and the rest of the system.

[10] It should be noted that these equations only are valid when our state is expressed in the "magic basis". Similar equations exist when the system is expressed in the standard spin–up/spin–down basis.

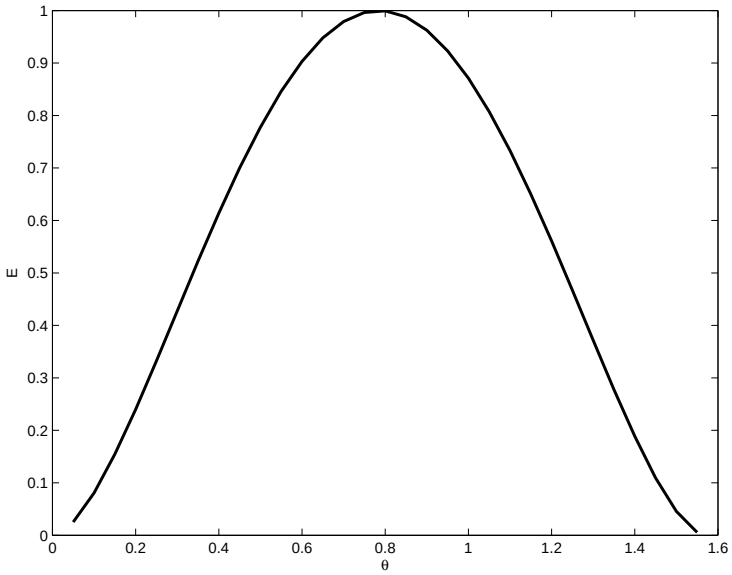


Figure 1.4: The von Neumann entropy for our test state with θ varying from 0 to $\pi/2$.

As for E_F and E_A, the results coincide with E since we deal with a pure ensemble. As for E_L we know that E_A is an upper bound. Alice can measure in the $\{|\rightarrow\rangle, |\leftarrow\rangle\}$ basis creating a singlet if $\theta = \pi/4$. This is a lower bound, and it is the same as the higher bound making also E_L coincide with E for $\theta = \pi/4$.

1.3.7 Entanglement as a Resource

Lately there has been a shift in the view of entanglement towards a more "positive attitude". When first encountered, entanglement was seen as a monster creation of quantum mechanics, while today we like to think of it as a physical resource. A resource that we can put to use in a similar manner as e.g. energy.

In Ref. [14] the term *ebit* is defined. This is a parallel to the term qubit. An ebit is the amount of entanglement in a maximally entangled pair of spin–1/2 particles. That is, an ebit is the amount of entanglement in a singlet.

It is important to note the physical difference between a qubit and an ebit. These two *quantum resources* are resources in different applications. Despite this fact the two terms can in some cases be substituted for one other. In [13] for example it is shown that the transmission of one qubit can be substituted for the use of one ebit and transmission of two classical bits.

If entanglement is truly a physical resource, in my opinion it should be possible to exchange entanglement between different types of systems in the same manner as energy can be exchanged between different forms. I have not seen any discussions on this subject yet.

1.4 Vector Entanglement

This is a measure suggested by me.

1.4.1 Introduction

Traditionally the density matrix, ρ, has been used to calculate entanglement. A variety of measures have been introduced to solve the problems that come with the density matrix approach. In this section we suggest a measure not connected to the density matrix in the usual manner.

In section 1.4.2 we introduce this new measure which we call *vector entanglement*. In section 1.4.3 we present some results, and in section 1.4.4 we briefly discuss pros and cons of this new measure.

1.4.2 Vector Entanglement

The basic idea is to compare the (ground) state, $|\Psi\rangle$, of a system under consideration with a state not entangled at all. We know what a non-entangled state is. A non-entangled state can be expressed on the form

$$|X\rangle = |A_1\rangle \otimes ...|A_{N-1}\rangle \otimes |A_N\rangle. \tag{1.17}$$

Here $|A_i\rangle$ is subsystem i. This is a physical system in the sense that the basis is local. Using this we define *vector entanglement* by

$$E_V(|\Psi\rangle) = -\max_{|X\rangle} \log(\langle X|\Psi\rangle), \tag{1.18}$$

where $|X\rangle$ is any state vector restricted only by equation (1.17), and the usual normalization condition, that is $\langle X|X\rangle = 1$ This means that we try to approximate the state vector, $|\Psi\rangle$, with a vector, $|X\rangle$, not entangled. How well we succeed with this is a measure of entanglement.

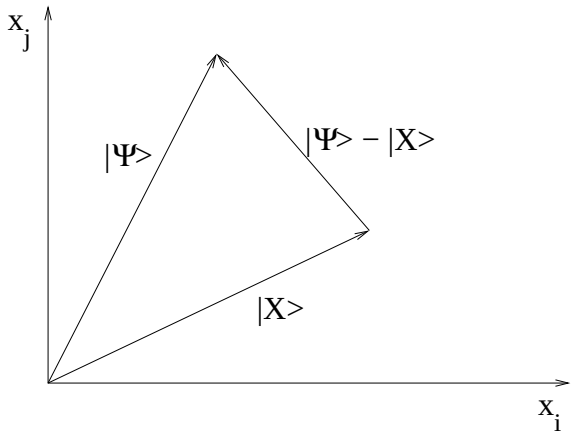


Figure 1.5: The idea of vector entanglement.

Our definition is based on the idea that we want to check how large the difference between $|\Psi\rangle$ and a properly normalised $|X\rangle$ has to be. Therefore we start by constructing $|C\rangle = |\Psi\rangle - |X\rangle$, see figure 1.5. An idea would then be to define the entanglement as $E_V = \min_{|X\rangle}\langle C|C\rangle$. That is, one tries to make $|C\rangle$ as "short" as possible. We note that $\langle C|C\rangle \in [0,\ 2]$. But this will not yield a measure which is additive. Therefore we modify the measure to be

$$E_V(|\Psi\rangle) = \min_{|X\rangle} \left\{ -\log\left(\frac{2 - \langle C|C\rangle}{2}\right)\right\}.$$

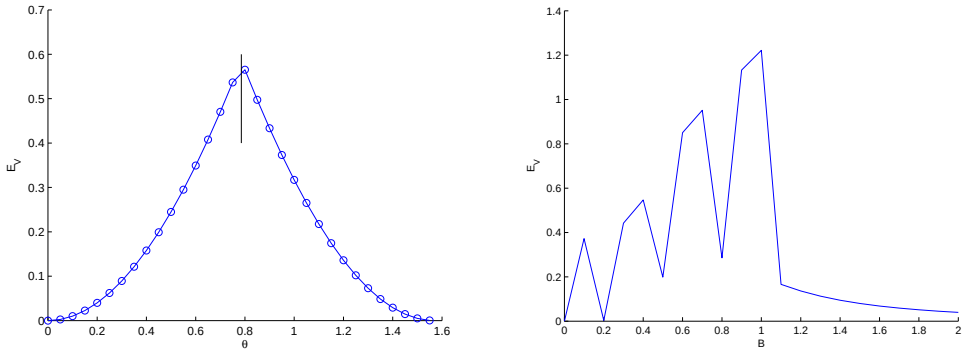
which, by a simple calculation, is seen to be the same as our definition (1.18).[11] As $\langle C|C\rangle \in [0,\ 2]$ it follows that $E_V \in [0,\ \infty]$.

It is easy to see that the definition (1.18) of entanglement is additive, that is, it satisfies

$$E_V(|\Psi\rangle \otimes |\Phi\rangle) = E_V(|\Psi\rangle) + E_V(|\Phi\rangle).$$

However, to have this property we have to require the state vector to be real as above.

[11] This statement is true only for real state vectors. That is, we must require the state vector to be an eigenvector to some hermitian Hamiltonian. Also $|X\rangle$ has to be real. This requirement is not well justified yet, but to introduce a complex phase seems not to improve the match since we assume $|\Psi\rangle$ to be real.



(a) The ϕ–system.

(b) The Ising–system with 4 spin.

Figure 1.6: Vector entanglement for two different systems.

If we assume a spin–1/2 system and parametrise $|X\rangle$ as

$$\begin{aligned} |X\rangle &= (\cos\theta_1|0\rangle + \sin\theta_1|1\rangle) \otimes (\cos\theta_2|0\rangle + \sin\theta_2\|1\rangle) \otimes ... \otimes (\cos\theta_N|0\rangle + \sin\theta_N|1\rangle) \equiv \\ &\equiv \begin{pmatrix} \cos\theta_1 \\ \sin\theta_1 \end{pmatrix} \otimes \begin{pmatrix} \cos\theta_2 \\ \sin\theta_2 \end{pmatrix} \otimes ... \otimes \begin{pmatrix} \cos\theta_N \\ \sin\theta_N \end{pmatrix} \end{aligned} \tag{1.19}$$

we can get a simple expression for E_V. Then the minimisation can be expressed as

$$\nabla_{\theta_i} \langle X|\Psi\rangle = 0. \tag{1.20}$$

Although this expression looks nice and compact, it is not a trivial thing to solve. It is a large nonlinear equation system. Nevertheless it should be possible to find a general solution to it.

1.4.3 Some Results

We have tested our definition (1.18) on two simple cases: (i) The simple two qubit–state

$$|\phi\rangle = \cos\theta|01\rangle + \sin\theta|10\rangle \tag{1.21}$$

which can be tuned by the parameter θ to go from nonentangled ($\theta = 0$) to fully entangled ($\theta = \pi/4$). The result is shown in figure 1.6(a). (ii) An Ising chain with 4 spins. The Ising model in a transverse field is obtained by setting $\gamma = 1/2$ in equation (1.3). The result is shown in figure 1.6(b). When doing the calculations a numerical minimization scheme is implemented. We have not attempted to obtain analytical solutions.

When doing the numerical implementation we use factorized states as in equation (1.17) and a loop over a discrete number of such vectors, choosing the one minimizing as we want it. For the simple system in equation (1.21) we can parametrize the X–vector with two variables only. If we look at the θ–surface it suggests that it might not be as easy as just taking the gradient if we want to find the minimum. This surface does not look continuous.

Already at this primitive stage though, we can see that the results look promising. Both of the two systems tested show a vector entanglement with a qualitative correct behavior (this we know from calculations using the von Neumann entropy). The maximas are located at the right places and the entanglement goes to zero in the appropriate limits.

1.4.4 Discussion

There are many thing to investigate with this new measure. For example:

- How should the measure be generalized to finite temperatures?
- Is there any property similar to the result $m/n = E/E_{max}$ for entropy of entanglement?
- Should the measure be modified somewhat to better represent the physics?
- Algorithms should be developed to calculate E_V.
- How does the entanglement scale with system size? For the von Neumann entropy we have that $E \leq \log(d)$ with d the dimension of the system. Can we find such a criterion also here? It should be possible to find some criterion based on how pure states span in the vector space. Given two product states $|A\rangle$ and $|B\rangle$ their linear combination $\cos\theta|A\rangle + \sin\theta|B\rangle$ is not in general a product state. This is an interesting fact since it vastly restricts the number of states allowed as a product state.
- It has to be better motivated why $|X\rangle$ can always be chosen real. Or, if this is not possible, change the definition so that it can handle the fact that $|X\rangle$ is not real. This is not hard, but will render in a slightly less elegant definition in my opinion.
- In connection to the problem of vector entanglement it should be interesting to investigate what subsets of vectors of $\mathcal{H}$ are spanned by all vectors on the form (1.17). This should be useful for determining how close one can come to an entangled state with an unentangled. It is not obvious that one can not get arbitrary close, making the vector entanglement always equal to zero, and thus nonsense.

The entanglement defined above differs radically from other measures on a number of points. To begin with it does not make use of the density matrix. Another feature is that we get the entanglement contained in a system without looking at its parts. With other measures we have to do some kind of tracing of subsystems to get a subsystem. Then we calculate the entanglement between this remaining part and the rest of the system – the measures are bipartite. With our new entanglement measure in (1.18) we calculate the entanglement *in* a whole system straight away.

As the lengths of $|\Psi\rangle$ and $|X\rangle$ are always 1 it looks as if the definition does not consider system size. This might be a drawback, but also it might not. It should not be to hard to compensate for this. Only scale the entanglement with system size (vector entanglement as we have defined it is an extensive magnitude). In connection with this it should be noted that E_V never reaches ∞ (at least not for finite systems). Every state of a system can be written as a sum of tensor products of its subsystem states:

$$|\Psi\rangle = |A\rangle \otimes |B\rangle \otimes ... \otimes |N\rangle + |A'\rangle \otimes |B'\rangle \otimes ... \otimes |N'\rangle + ... + |A^{(n)}\rangle \otimes |B^{(n)}\rangle \otimes ... \otimes |N^{(n)}\rangle. \quad (1.22)$$

To guarantee that E_V does not reach infinity we have to be able to choose an $|X\rangle$ such that the scalar product $\langle X|\Psi\rangle$ will not become zero. That is, we have to find a vector that is not orthogonal to $|\Psi\rangle$. But this is always possible. Just choose the first term in the sum (1.22). Thus $E_V \in [0, \infty)$. This is a major improvement since it guarantees us that the system scaling prescription given will work, at least for finite systems.

If we look at figure 1.6(a) we see that a maximally entangled system (the Bell state at $\theta = \pi/4$) has a vector entanglement of about 0.55. I can not find an easy physical interpretation of this maximum, it is only the smallest achievable difference between an unentangled state and a maximally entangled one.

A suggestion for a generalization of equation (1.18) to mixture ensembles are

$$E_{V,\ ensemble} = \sum_i p_i E_V(|\Psi\rangle),$$

where p_i are classical probabilities (e.g. a Boltzmann distribution).

A point that might be interesting is to study the need of the logarithm in equation (1.18). This logarithm is required to make the entanglement additive, or *extensive*, in the same way that we

have to take the logarithm of the state density function in classical statistical physics to get the extensive quantity entropy. Otherwise we will get something which is multiplicative with system size instead. How should this be interpreted? Are we doing something wrong when we believe the world to be additive – is multiplicative a more natural thing?

2 Analytical Diagonalisation of the XY Hamiltonian

To have something to compare the results from exact diagonalisation with we here diagonalise the XY Hamiltonian analytically. We have tried to be explicit in the analysis so to make the derivations easy to follow.

The Hamiltonian for the 1–dimensional (anisotropic ferromagnetic) XY model (XY chain) with N spins has the form

$$H = -\sum_{i=1}^{N} \left((1+\gamma)\sigma_i^x \sigma_{i+1}^x + (1-\gamma)\sigma_i^y \sigma_{i+1}^y + B\sigma_i^z \right). \tag{2.1}$$

In (2.1) γ is the anisotropy term which determines how the spins couple in the x and y directions. B is the magnetic field, here taken in the z–direction.

2.1 Analytical Diagonalisation

Diagonalizing (2.1) requires a number of steps:[12] We perform a series of transformations from the original spin basis to end up with a diagonal Hamiltonian in a free fermionic basis. We first make a switch to the eigenbasis of step operators $\sigma^{\pm}$ [3], with

$$\sigma^+ = \sigma^x + i\sigma^y$$

$$\sigma^- = \sigma^x - i\sigma^y.$$

By adding and subtracting the two sides above one obtains the inverted expressions

$$\begin{array}{rcl} \sigma^x & = & \frac{\sigma^+ + \sigma^-}{2} \\ \sigma^y & = & \frac{\sigma^+ - \sigma^-}{2i} \end{array} \tag{2.2}$$

and, with the commutation relation for σ^i, $[\sigma^x,\ \sigma^y] = (i/2)\sigma^z$, σ^z gets represented by

$$\sigma^z = \sigma^+\sigma^- - \frac{1}{2}.$$

By inserting the new operators, $\sigma^{\pm}$, in (2.1) via (2.2) we obtain:

$$H = -\frac{1}{2}\sum_{i=1}^{N} (\gamma(\sigma_i^+\sigma_{i+1}^+ + \sigma_i^-\sigma_{i+1}^-) + \sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+ + 2B(\sigma_i^+\sigma_i^- - \frac{1}{2})) \tag{2.3}$$

In the next transformation we want to switch to a fermionic basis[13] on which we then make a final transformation to accomplish our goal and get free fermions. The definition of a fermion is that its creation and destruction operators obey the "fermionic relations"

$$\{a_i^\dagger\ a_j\} = \delta_{ij},\ \{a_i,\ a_j\} = \{a_i^\dagger,\ a_j^\dagger\} = 0. \tag{2.4}$$

[12] The procedure to solve (2.1) varies somewhat in different textbooks and articles on the subject. Two different ways of doing the calculations are presented in [5] and [7]. We mostly follow the procedure outlined in [5].

[13] See any book on quantum field theory for an introductions to the concept of fermions, for example [4].

The Jordan–Wigner transformation is a standard scheme to get fermions from spins. The transformation looks like

$$\begin{aligned} \sigma_i^+ &= \exp[i\pi \sum_{k=1}^{i-1} c_k^\dagger c_k] c_i^\dagger, \ \sigma_1^+ = c_1^\dagger \\ \sigma_i^- &= c_i \exp[-i\pi \sum_{k=1}^{i-1} c_k^\dagger c_k], \ \sigma_1^- = c_1 \end{aligned} \tag{2.5}$$

The Jordan–Wigner transform is "the way to go" because the new operators, c_i and $c_i^\dagger$, obey the fermionic anticommutations relations in (2.4) provided that the spin operators, $\sigma_i^\pm$, obey spin commutation relations. (This can readily be checked via an analysis similar to the one contained in equation (2.6) and the discussion following it.) Now we need to replace the σ's in (2.3) via the transformation (2.5). We start by doing an explicit calculation on the first term in (2.3):

$$\begin{aligned} \sigma_i^+ \sigma_{i+1}^+ &= \left(\exp[i\pi \sum_{k=1}^{i-1} c_k^\dagger c_k] c_i^\dagger \right) \left(\exp[i\pi \sum_{k=1}^{i} c_k^\dagger c_k] c_{i+1}^\dagger \right) \\ &= \exp[i\pi \sum_{k=1}^{i-1} c_k^\dagger c_k] \cdot \exp[i\pi \sum_{k=1}^{i-1} c_k^\dagger c_k] \left(c_i^\dagger \exp(i\pi c_i^\dagger c_i) \right) c_{i+1}^\dagger \\ &= \exp[2i\pi \sum_{k=1}^{i-1} c_k^\dagger c_k] c_i^\dagger \exp(0) c_{i+1}^\dagger \\ &= \hat{1} c_i^\dagger \hat{1} c_{i+1}^\dagger = c_i^\dagger c_{i+1}^\dagger. \end{aligned} \tag{2.6}$$

In the derivation the following relations have been used: In the first line we have simply inserted the transformation (2.5). Next, to commute $c_i^\dagger$ with the exponentiated sum we consider the fermionic anticommutation relations (2.4) which say:

$$\{c_i, \ c_j\} = 0 \Leftrightarrow c_i c_j = -c_j c_i$$

$$c_i^\dagger c_j = -c_j c_i^\dagger, \ i \neq j.$$

Using the Taylor expansion (defining the exponential function for operators) of the exponential operator function:

$$\exp(x) = 1 + x + \frac{1}{2!} x^2 + ...$$

we can thus commute $c_i^\dagger$ with all but the last term in the sum. This results in line two. To get line three we use the general algebraic property that

$$c_i^\dagger f(c_i^\dagger c_i) = c_i^\dagger f(0). \tag{2.7}$$

This expression can be motivated by the following: Any operator function f can be written as (again Taylor)

$$f(X) = k_o + k_1 X + k_2 X^2 + ...$$

Now we apply the LHS of (2.7) to a ket $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes ... \otimes |\psi_N\rangle$ and get

$$\begin{gathered} c_i^\dagger f(c_i^\dagger c_i)|\psi\rangle = \\ I \otimes I \otimes ... \otimes c^\dagger \otimes I \otimes ... \otimes I (k_0 + k_1 I \otimes I \otimes ... \otimes c^\dagger c \otimes I \otimes ... \otimes I + ...)|\psi_1\rangle ... \otimes |\psi_N\rangle \equiv \\ c_i^\dagger k_0 |\psi\rangle + 0. \end{gathered}$$

Here the $c_i^\dagger$ is operating on Hilbert space i. When the operator $c_i^\dagger (c_i^\dagger c_i)^n$ operates on a ket in Hilbert space i we must always get the result zero since fermions cannot be created more than one per position (Pauli exclusion principle). This motivates our formula. In similar ways one can derive other identities like

$$c_i f(c_i^\dagger c_i) = c_i f(1).$$

In line three we have also changed the product of two exponentials to a single exponential of a sum. For the last line we note that we get a $2\pi i$ in front of the sum of number operators (number operators count the number of particles in a given state) resulting in a term $\exp(2i\pi(i-1)I)$[14]. The argument for this is similar to the one above for the relation (2.7) where one investigates what happens when the operator acts on a ket. In addition we use the fact that $\exp(2i\pi k) = 1,\ k \in \mathbb{N}$.

Now the other terms in (2.3) can be calculated in a similar manner, and we get for our new Hamiltonian

$$H = -\frac{1}{2}\sum_{i=1}^{N}\Big(c_i^\dagger c_{i+1} + c_{i+1}\dagger c_i + \gamma(c_i^\dagger c_{i+1}^\dagger + c_{i+1}c_i) + B(c_i^\dagger c_i - 1)\Big) + Corr. \tag{2.8}$$

In equation (2.8) the term $Corr.$ represents corrections due to boundary conditions. If one assumes periodic boundary conditions for the spins this results in non–periodic boundary conditions for the fermionic operators; e.g. one readily sees that $\sigma_N^+\sigma_1^- \neq c_N^+ c_1$. The error in doing this approximation is of order $1/N$ [5]. It follows that the new model is periodic in the new variables if we exclude the corrections.[15]

In equation (2.8) we first of all note that the fermions are still coupled to each other; we still have terms like $c_i^\dagger c_{i+1}$. Thus we have not yet achieved our goal to diagonalise the Hamiltonian. To decouple the fermions in the Hamiltonian we make use of the following transformation (the Bogoliubov transformation)[16]:

$$\begin{aligned} \eta_k^\dagger &= \sum_{i=1}^{N}(g_{ki}c_i^\dagger + h_{ki}c_i) \\ \eta_k &= \sum_{i=1}^{N}(g_{ki}c_i + h_{ki}c_i^\dagger). \end{aligned} \tag{2.9}$$

The transformation (2.9) does not in any obvious way do what we want; that the new variables $\eta^\dagger,\ \eta$ will render a diagonal Hamiltonian has to be proved.

At first we want the new variables $\eta^\dagger,\ \eta$ to be fermionic, that is, to obey the fermionic relations (2.4). Secondly we want our Hamiltonian to be diagonal[17] in the new basis, that is

$$H = \sum_{k=1}^{N}\Lambda_k(\eta_k^\dagger\eta_k + const.), \tag{2.10}$$

with Λ_k constants.

If these conditions can be fullfiled we have succeeded with our goal. Now we prove that the transformation (2.9) with the coefficients $g_i,\ h_i$ real really does the job. First of all we want to check what follows from the requirement that the η's are to be fermionic:

$$\begin{aligned} 0 &= \{\eta_k^\dagger,\ \eta_l^\dagger\ \} = \left\{\sum_{i=1}^{N}(g_{ki}c_i^\dagger + h_{ki}c_i),\ \sum_{j=1}^{N}(g_{lj}c_j^\dagger + h_{lj}c_j)\right\} = \\ &= \sum_{i=1}^{N}(g_{ki}c_i^\dagger + h_{ki}c_i)\cdot\sum_{j=1}^{N}(g_{lj}c_j^\dagger + h_{lj}c_j) + \sum_{j=1}^{N}(g_{lj}c_j^\dagger + h_{lj}c_j)\cdot\sum_{i=1}^{N}(g_{ki}c_i^\dagger + h_{ki}c_i) = \\ &= \sum_{i,i}(g_{ki}h_{li}c_i^\dagger c_i + g_{ki}h_{li}c_ic_i^\dagger + g_{li}h_{ki}c_ic_i^\dagger + g_{li}h_{ki}c_i^\dagger c_i) = \\ &= \sum_{i}(g_{ki}h_{li}(c_i^\dagger c_i + c_ic_i^\dagger) + g_{li}h_{ki}(c_ic_i^\dagger + c_i^\dagger c_i)) = \sum_{i}(g_{ki}h_{li} + h_{ki}g_{li}). \end{aligned} \tag{2.11}$$

[14] Note the bad use of i as both the imaginary number $i^2 = -1$ and an index for a Hilbert space.

[15] This is motivated when N is large. For small systems the soundness of this approximations is not obvious and we will address the question further later in the thesis.

[16] This is a kind of generalized Fourier transform where we allow any phase, not just plane waves. The idea behind the transformation is to preserve the anticommutation relations.

[17] Compare normal modes for a harmonic oscillator, see for example Refs. [2] or [3].

In a similar manner,

$$\delta_{kl} = \{\eta_k,\ \eta_l^\dagger\} = \sum_{i=1}^{N}(g_{ki}g_{li} + h_{ki}h_{li}).$$

Here we have used the fact that the c's are fermionic variables and hence anticommute for all but $\{c_i^\dagger, c_i\} = 1$. For the $2 \cdot N^2$ unknown coefficients $g_i,\ h_i$ this gives us $2N^2/2$ equations.

The next step is to use the fact that the fermions are independent (as follows from the Hamiltonian being diagonal). This can be expressed as

$$[H,\ \eta_k^\dagger] = -\Lambda_k \eta_k^\dagger. \tag{2.12}$$

The sign on the right hand side comes from the fact that we are dealing with a ferromagnetic Hamiltonian. By inserting (2.9) and (2.3) into (2.12) we obtain the remaining N^2 equations

$$\begin{aligned} \sum_j C_{ij}(g_{kj} + h_{kj}) &= -\Lambda_k(g_{ki} - h_{ki}) \\ \sum_j D_{ij}(g_{kj} - h_{kj}) &= -\Lambda_k(g_{ki} + h_{ki}),\ i,k = 1,...,N. \end{aligned} \tag{2.13}$$

The two matrices C and D have the form

$$C = \begin{pmatrix} -B & \frac{1}{2}(1+\gamma) & 0 & ... & 0 & \frac{1}{2}(1-\gamma) \\ \frac{1}{2}(1-\gamma) & -B & \frac{1}{2}(1+\gamma) & 0 & ... & 0 \\ \vdots & & \ddots & & & \vdots \\ \frac{1}{2}(1+\gamma) & 0 & ... & 0 & \frac{1}{2}(1-\gamma) & -B \end{pmatrix}$$

$$D = \begin{pmatrix} -B & \frac{1}{2}(1-\gamma) & 0 & ... & 0 & \frac{1}{2}(1+\gamma) \\ \frac{1}{2}(1+\gamma) & -B & \frac{1}{2}(1-\gamma) & 0 & ... & 0 \\ \vdots & & \ddots & & & \vdots \\ \frac{1}{2}(1-\gamma) & 0 & ... & 0 & \frac{1}{2}(1+\gamma) & -B \end{pmatrix}$$

The expressions in (2.13) define a linear equation system, which can be written in matrix form with vectors Φ and Ψ as

$$\begin{aligned} C\Phi &= -\Lambda_k\Psi \\ D\Psi &= -\Lambda_k\Phi \end{aligned} \Leftrightarrow DC\Phi = \Lambda_k^2\Phi,\ CD\Psi = \Lambda_k^2\Psi. \tag{2.14}$$

Equation (2.14) can be readily solved and we refer to [5] or [9, 10] and references therein for this. The solutions give us the eigenvalues

$$\Lambda_k = \sqrt{(\gamma\frac{1}{B}\sin\phi_k)^2 + (1 + \frac{1}{B}\cos\phi_k)^2} \tag{2.15}$$

with $\phi_k = 2\pi k/N$. We also not that these are not the eigenvalues of the XY Hamiltonian, but rather eigenvalues to equation (2.14). The energy eigenvalues of the Hamiltonian are linear combinations of these.

2.2 Density Matrices

Now the one–site density matrix, ρ_1, can be found using

$$\rho_1 = \frac{1}{2}\sum_{\nu=0}^{3}\langle\sigma_i\rangle\sigma_i. \tag{2.16}$$

Note that ρ_1 is site independent as we have cyclic boundary conditions. That this is the correct density matrix can be shown in several ways. It is sufficient to note that for a pure ensemble we have

$$[\sigma_i] = \langle\sigma_i\rangle = tr(\sigma_i\rho)$$

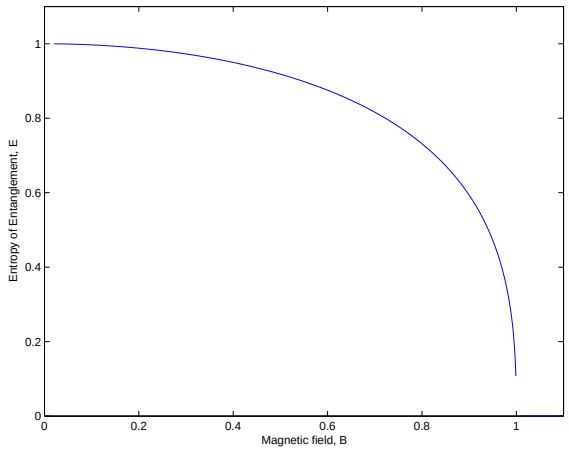


Figure 2.1: Entropy of entanglement from the analytical solution of the infinite XX model ($\gamma = 0$).

where $[\circ]$ and $\langle\circ\rangle$ denote expectation values for mixed and pure ensembles (as we have a pure ensemble the two expectation values coincide). And this is all there is to it. Now according to (2.16) if we can calculate the $\langle\sigma_i\rangle$'s we have the one–site density matrix. If we write the density matrix out explicitly it will be very clear what we do:

$$2\rho \equiv \langle I\rangle \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \langle\sigma_x\rangle \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \langle\sigma_y\rangle \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \langle\sigma_z\rangle \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

First note that $\langle I\rangle$ must be 1 since this is the only element affecting the trace. The trace must equal 1, and hence $\langle I\rangle = 1$. As the Hamiltonian is real it follows from the equation $\rho = \exp(-\beta H)/Z$ that the density matrix must also be real. This makes $\langle\sigma_y\rangle = 0$. As is easily verified the Hamiltonian commutes with σ_z. This makes ρ commute with σ_z. Hence $\langle\sigma_x\rangle$ must also vanish (note that this reasoning requires that we already know that $\langle\sigma_y\rangle = 0$). Now the only coefficient left to calculate is $\langle\sigma_z\rangle$. This is a bit harder, we refer to Ref. [9] for details. The solution reads

$$\langle\sigma_z\rangle = -\frac{1}{\pi}\int_0^\pi d\nu(1 + \frac{1}{B}\cos\nu)\frac{\tanh(\frac{1}{2}\beta\Lambda(\nu))}{\Lambda(\nu)}, \tag{2.17}$$

where $\Lambda(\nu)$ is taken from (2.15) in the limit $N \to \infty,\ \phi_k \to \nu$.

Having obtained the density matrix it is easy to use it to get the entropy of entanglement for a single site. The result for $\gamma = 0$ is shown in figure 2.1.

2.3 Various Comments on the Solution

Ideally one would like to use equation (2.15) to find the eigenstates of the Hamiltonian and then transform these eigenstates back to the original basis via the inverse transformations of the ones used above. If we could do this we would know everything. This is however not a very easy task. The fermions in the solution are complicated nonlocal objects in the spin basis and are very hard to inverse transform. This is the reason for using the limited set of density matrices in section 2.2.

In the form (2.10) the difference between the ferromagnetic and the antiferromagnetic spin chain is quite transparent. The minus sign separating the two models has followed us all the way without being afflicted by the transformations. Thus the ground state of the two models are really opposite – the eigenvalue representing the highest energy in the ferromagnetic case is the lowest energy in the antiferromagnetic one, and vice versa. The eigenstates of the Hamiltonian in the η–basis are kets like

$$\eta^\dagger_{k^1}\cdots\eta^\dagger_{k^{(n)}}|0\rangle,$$

where

$$|0\rangle = |0_1\rangle \otimes |0_2\rangle \otimes ... \otimes |0_N\rangle$$

and $|0_k\rangle$ represents the (Fock–) vacuum state[18] of fermion k (note that $\eta_k^\dagger$ is the creation operator of fermion k). To verify that these states really are eigenstates of (2.10) is trivial.

Due to the fact that we throw away terms like the ones in equation (2.8) when going from (2.1) to (2.10) our result (2.10) might not be very accurate for small systems. There the boundary conditions might be a significant part of the interaction. It should be interesting to see how well our analytical equation (2.10) approximates the exact finite size result obtained using computers in section 3. A possible way to overcome this problem could be to use a Hamiltonian the form

$$H = \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x + ...$$

or

$$H = \frac{1}{2} \sum_{i=2}^{N-1} \sigma_i^x \sigma_{i+1}^x + \sigma_{i-1}^x \sigma_i^x + ...$$

for a system using N particles. This Hamiltonian should be possible to diagonalise analytically without having to throw away boundary terms since we do not use cyclic boundaries but rather use no interaction at all (which is sometimes called *open boundary conditions*). This type of calculation has been done in [27] and the result is shown to be equivalent to having some type of impurity at the end sites.

3 Background Theory for Exact Diagonalization

To test the hypothesis that it is entanglement that drives a quantum phase transition we have performed numerical exact diagonalisation calculations on a variety of different Hamilton spin operators. Since the number of parameters describing a system grows exponentially with the number of particles in the system this method is quite limited. Despite this limitation it is still a useful exploratory tool. The programs are written in MATLAB and MATLABs routines for finding eigenvalues and such are used.

All algorithms used are implemented in a MATLAB program, Entangle, that can be accessed at `http://www.etek.chalmers.se/~e9ravn/masterThesis/index.html`. At this site an updated version of the thesis will also be available.

3.1 Theory for Exact Diagonalization

The eigenvectors of σ^z are denoted $|0\rangle$ and $|1\rangle$ and are represented as matrices as

$$|0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

This gives the spin operators the following matrix representations

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

[18] The Fock basis is built from the so called vacuum states $|0\rangle$. This state contains no particles. Then we get the rest of the base vectors by applying creation operators to this state: $\eta_i^\dagger |0\rangle = |00...1_i 0...0\rangle$ and so on.

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The tensor product used to extend the Hilbert space is the most general bilinear product. That is, it is linear in each of its arguments. Numerically it can be represented by the Kronecker product on matrices. This product is defined for matrices A and B as follows

$$C = A \otimes B \equiv \begin{pmatrix} a_{11} \cdot B & a_{12} \cdot B & \cdots \\ a_{12} \cdot B & \ddots & \\ \vdots & & \end{pmatrix}$$

where a_{ij} are the matrix element of A If A and B have dimensions $m \times n$ and $m' \times n'$ respectively, then C is $m \cdot m' \times n \cdot n'$.

When extending an operator acting on particle i, e.g. σ_i^z, so that it acts on the full Hilbert space of all spins the operator is tensor multiplied by the identity operators of the other Hilbert spaces. This means that σ_i^x does nothing on Hilbert spaces other than i. So σ_i^x is defined as

$$\sigma_i^x = I \otimes ... \otimes I \otimes \sigma^x \otimes I \otimes ... \otimes I \tag{3.1}$$

and each identity operator has the size of the Hilbert space it belongs to. Since $I_{m\times n} \otimes I_{m'\times n'} = I_{m\cdot m'\times n\cdot n'}$ and the tensor product is associative, equation (3.1) can be written as

$$\mathbf{I} \otimes \sigma^x \otimes \mathbf{I}.$$

This is used in the algorithms.

3.2 Algorithms for Exact Diagonalization

The main algorithm for calculating the entropy of entanglement of the 1–dimensional XY model is algorithm 1. The functions `Si()` and `partialTrace()` are described later in this section. Many

Algorithm 1 Main algorithm for calculating the entropy of entanglement in the 1–dimensional XY model.

1: **function** OneDimensionalXYHamiltonian($systemSize, magneticField, tr$)
2: $\sigma^x \leftarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
3: $\sigma^y \leftarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
4: $\sigma^z \leftarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
5: $H \leftarrow 0$
6: **for** $n \in \{1..systemSize\}$ **do**
7: $H \leftarrow H + \mathrm{Si}(\sigma^x, n, systemSize) \cdot \mathrm{Si}(\sigma^x, n+1, systemSize) + \mathrm{Si}(\sigma^y, n, systemSize) \cdot \mathrm{Si}(\sigma^y, n+1, systemSize) + magneticField \cdot \mathrm{Si}(\sigma^z, n, systemSize)$
8: **end for**
9: $[V\ D] \leftarrow \mathrm{eig}(H)$
10: $\rho \leftarrow V(:,1) \cdot V(:,1)^\dagger$
11: $\rho_R \leftarrow \mathrm{partialTrace}(\rho, tr)$
12: $E \leftarrow trace(\rho_R * \log_2 \rho_R)$ ▷ Matrix logarithm.
13: **return** E
14: **end function**

possible ways exist to do the calculation on line 12 in algorithm 1 (this is the implementation of the entropy of entanglement definition (1.9)), e.g. one could diagonalize the reduced density matrix, ρ_R, and then use the eigenvalues and the Shannon entropy. Sometimes we have added $\epsilon\mathbf{1}$

in the calculations, where ϵ is the machine precision number and $\mathbf{1}$ is the matrix with ones on all positions. The motivation for doing this is that $\log 0$ is not defined. It should not affect the result as $\lim_{x\to 0} x \ln x = 0$ and this addition of ϵ can be seen as the numerical version of this limit.

In MATLAB the Kronecker product is implemented via the command `kron(A, B)`. When extending matrices over the full Hilbert space of N spins, e.g. creating the σ^x matrix (without site index), this is carried out in algorithm 2. Elements like $\sigma_i^x \cdot \sigma_{i+1}^x$ are then obtained by matrix

Algorithm 2 Algorithm to extend the Hilbert space for an operator. The dot in the exponent represents the MATLAB elementwise exponentiation. This algorithm assumes all sites i to have the same size and that the model has cyclic boundary conditions. This last assumption can be seen in the if–statement in the beginning.

function SI(X, k, N)
  if $k == N + 1$ **then**
    $k \leftarrow 1$
  end if
  $I1 \leftarrow eye(size(X)^{\cdot(k-1)})$
  $I2 \leftarrow eye(size(X)^{\cdot(N-k-1)})$
  $S \leftarrow kron(kron(I1, X), I2)$
  return S
end function

multiplication. It is worthwhile to note that this way of doing the calculation is equivalent to that in algorithm 3 since $A \otimes B \equiv A \otimes I_B \cdot I_A \otimes B$; that is, if $\otimes$ represents the Kronecker product, then `kron(A,B) = kron(A,I)·kron(B,A)`. We often write $A \otimes B$ directly. In the literature the notation is often abused and the tensor product $A \otimes B$ is often written $A_A \cdot B_B$ or something similar.

Algorithm 3 Another algorithm to extend a Hilbert space. Here the first part of algorithm 2 taking care of the cyclic boundary conditions is left out, but it is the same here.

function SMN(X, Y, k, l, N)
  $I1 \leftarrow eye(size(X)^{\cdot(k-1)})$
  $I2 \leftarrow eye(size(X)^{\cdot(l-k-1)})$
  $I3 \leftarrow eye(size(X)^{\cdot(N-k-1)})$
  $S \leftarrow kron(kron(kron(kron(I1, X), I2), Y), I3)$
  return S
end function

The partial trace is defined as in equation (1.4) or (1.5). For the matrix representation this definition is used in algorithm 4. This can be visualised as in equation (3.2). If we want to trace away system i, and assume all systems to be of the same 2–dimensional size we get a recursive algorithm so that tracing system i the same as summing "block diagonals" (this is *not* block diagonal in the usual sense). Which block diagonal to choose depends on the subsystem index. As an illustration consider

$$\rho = \begin{pmatrix} \begin{pmatrix} (B_1) & \\ & (B_1') \end{pmatrix} & \begin{matrix} (B_2) & \\ & (B_2') \end{matrix} \\ \begin{matrix} (B_3) & \\ & (B_3') \end{matrix} & \begin{pmatrix} (B_4) & \\ & (B_4') \end{pmatrix} \end{pmatrix} \tag{3.2}$$

where the $B_i^{(')}$'s represent the "second order block diagonal" and the larger parentheses indicate the "first order block diagonal". If ρ came from a state $|\psi\rangle = |A\rangle \otimes |B\rangle \otimes ...$ and we want to trace away A the first block diagonal should be summed. If we want to trace the second system, B, we should sum "block diagonals" B_i to get

$$\rho_R = \begin{pmatrix} B_1 + B_2' & B_2 + B_2' \\ B_3 + B_3' & B_4 + B_4' \end{pmatrix},$$

and so on. This yields the recursive algorithm in 4.

Algorithm 4 The algorithm to perform a partial trace over systems according to the vector tr (this vector contains a list of which systems, numbered from left to right, to trace). ρ is the density matrix of the full system. This algorithm assumes all local sub–Hilbert spaces to be 2–dimensional. In Entangle this algorithm is generalized to handle both spin–1/2 and spin–1 systems, but this generalisation is trivial.

```
function PARTIALTRACE(ρ, tr)
    R ← ρ
    [m n] ← size(R)
    for k ∈ [1 : N] do
        R ← PT(R, tr(k))
        for j ∈ [k + 1 : N] do                          ▷ Correct indices...
            if tr(j) > tr(k) then
                tr(j) ← tr(j) − 1
            end if
        end for
    end for
    function PT(R, subSpace)
        if subSpace = 1 then
            return ρ ← R(1 : m/2, 1 : n/2) + R(m/2 + 1 : m, n/2 + 1 : n)
        else
            return ρ ← [PT(R(1 : m/2, 1 : n/2), subSpace − 1)PT(R(1 : m/2, n/2 + 1 :
                n), subSpace − 1); PT(R(m/2 + 1 : m, 1 : n/2), subSpace − 1)PT(R(m/2 + 1 :
                m, n/2 + 1 : n), subSpace − 1)
        end if
    end function
    return ρ
end function
```

3.3 Entanglement of Formation for Spin-1 Systems (and a Closer Review of the Spin-1/2 Case)

In a number of papers [12, 14, 18] it is proved that the entanglement of formation, $E_F(\rho)$, has a simple functional relation to the density matrix, ρ, in the case of spin–1/2 systems. In this section we will generalize this relation to hold for a spin–1 system.

Review of the Spin–1/2 Case

For spin–1/2 systems we have from [12, 14, 18] that

$$E_F(\rho) = H(f(C)), \tag{3.3}$$

where H is the binary entropy function

$$H(x) = -x\log x - (1-x)\log(1-x),$$

f is given by

$$f(x) = \frac{1}{2} + \frac{1}{2}\sqrt{1-C^2},$$

and C is the generalized concurrence, or concurrence of formation,

$$C = \max(0,\ 2\lambda_{max} - \mathrm{Tr}(R)). \tag{3.4}$$

Here R is the product matrix $R = \sqrt{\rho\tilde{\rho}}$ of the density matrix, ρ, and the spin–flipped density matrix, $\tilde{\rho}$. This spin–flipped density matrix is obtaind by making a time reversal (TR) transformation. That is, we take

$$|\Psi\rangle \quad \stackrel{TR}{\longrightarrow} \quad U_{TR}|\Psi\rangle \equiv |\tilde{\Psi}\rangle = \sigma^y|\Psi^*\rangle$$

with the state vector, $|\Psi\rangle$, corresponding to the density matrix ρ. This is equivalent to the transformation

$$\rho \quad \stackrel{TR}{\longrightarrow} \quad \tilde{\rho} = \sigma^y\rho^*\sigma^y \tag{3.5}$$

of the density matrix. It should be stressed here that the σ^y denotes a spin–matrix in the y–direction for all of the reduced Hilbert space. That is

$$\sigma^y \equiv \otimes_{i=1}^N \sigma_i^y = \prod_{i=1}^N \sigma_i^y$$

where σ_i^y in the tensor product denote the spin matrix operating in the Hilbert space of particle i, while σ_i^y in the matrix product denotes $\mathbf{1} \otimes \sigma^y \otimes \mathbf{1}$. That is, the spin matrix extended to the whole Hilbert space, but with trivial acting in all but subspace i.

The statement (3.3) is by no means obvious and, as pointed out above, has evolved from a number of papers, where [12, 14, 18] are the main contributors. Despite of this, the generalization to spin–1 systems is not a very complicated matter. We will not derive equation (3.3) here, but rather refer to [12, 14, 18] for the proof of the spin–1/2 case. Instead we will state what has to be changed for the more general case of higher spin systems, in particular spin–1.

Generalization to Other Spin Systems

The form of equation (3.5) follows from the special relation

$$U_{TR} = UK$$

for the time reversal operator for angular momentum [3]. The operator U_{TR} is antilinear and consists of the unitary operator U and the complex conjugations operator K. Here

$$K|\Psi\rangle = |\Psi^*\rangle,$$

while U can be expressed by the formula [3]

$$U = e^{-i\pi/2\sigma^y}. \tag{3.6}$$

For a spin–1/2 system U in (3.6) (*and* its inverse U^{-1}!) happen to equal σ^y, thus the equation (3.5). However this is not the case for a spin–1 system where the y–component of the spin operator, call it σ_1^y, has the matrix representation

$$\sigma_1^y \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

This gives the expression

$$U \equiv i \begin{pmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix},$$

for U. We first note that $U \neq U^{-1}$. This forces us to use the general spin–flip operation

$$\rho \quad \stackrel{S.F.}{\longrightarrow} \quad \tilde{\rho} = U\rho^*U^{-1}.$$

In the literature one often see the formula

$$C = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4),$$

for the concurrence, where λ_1 is the largest eigenvalue of R. This expression is not valid in the spin–1 case any more since ρ is larger and R will now have nine eigenvalues. Thus the more general formula (3.4) has to be used. With this, the prescription above is valid for any spin system.

One more thing to note is that entanglement is basis dependent. The prescription stated here is also basis dependent. To be valid, the state of the system (and thus the density matrix) has to be expressed in the standard local spin basis.

This is all there is to it. All other relations remain valid for the spin–1 case. Thus we now have a prescription to calculate the entanglement of formation for a spin–1 system (or any higher spin system, with U modified accordingly).

3.4 Degenerate Ground States

According to the quantum mechanical postulates a system at zero temperature chooses the lowest lying energy state (the *ground state*). This is the eigenstate belonging to the smallest eigenvalue. Now it might be that this lowest eigenvalue is degenerate – that is two or more eigenvectors have the same eigenvalue. If this is the case the choice of eigenvectors is not unique. To see this, assume that $|E_1\rangle$ and $|E_2\rangle$ are eigenvectors to the operator H with the same eigenvalue E. Then the vector $\alpha|E_1\rangle + \beta|E_2\rangle$ is also an eigenvector. This is easily shown:

$$H(\alpha|E_1\rangle + \beta|E_2\rangle) = \alpha H|E_1\rangle + \beta H|E_2\rangle = E\alpha|E_1\rangle + E\beta|E_2\rangle = E(\alpha|E_1\rangle + \beta|E_2\rangle).$$

Note that to be able to perform this calculation the two eigenvectors to have the same eigenvalue. Since α and β are arbitrary and $|E_1\rangle$ and $|E_2\rangle$ are linear independent we can choose any pair of eigenvectors in the E_1, E_2–plane as the two eigenvectors.

For some models, like the Ising model, the ground state is degenerate. This can easily be seen for a two–particle system by an explicit calculation. The degeneration never exists in "reality" for macroscopic systems since small defects on the lattice or small external perturbations always force the system to choose one of its ground states (thus we have a *spontaneous symmetry breaking*). In analytical calculations this is not a problem since one can pick by hand one of the states as the ground state. In numerical calculations though, it is not as easy. To force the system to choose a particular ground state we add a term on line 7 in algorithm 1. This term is the small field ε mentioned in section 1.1 in connection with equations (1.1) and (1.2). Obviously this term will distort our results and we have to be careful in choosing it so that it does not corrupt them to much. A more careful discussion of this subject is carried out in section 4.1.

3.5 Finite Temperatures

A QPT occurs at zero temperature by the very definition of a QPT. Entanglement on the other hand can exist also at finite temperatures. But as soon as we have a finite temperature we get some distribution of our states. This is due to the fact that temperature is equivalent to excitations, thus distributions.

If we want to examine how entanglement behaves in systems at finite temperature we therefore need a way to find the distribution of the system. This is not a very simple thing. The problem is that none of the canonical distributions are valid for our system. The microcanonical distribution is not the way to go since temperature is not even defined there. (Also, most of our models include some terms representing a coupling to the environment.) The canonical ensemble is also not appropriate as the approximations done when deriving this ensemble are not valid for small systems (for example, Stirlings formula is not valid). However, we shall not pursue this problem further in this thesis, but rather leave it as an open question that would need some attention.

3.6 A Note on Complexity

The reason for us not being able to carry out exact diagonalisation on spin systems larger than ~ 10 spins is due to two facts. First the Hilbert space grows exponentially with system size. This is due to the tensor product, and makes the Hilbert space for a system consisting of 10 spins having dimension $2^{10} = 1024$, which is quite demanding in terms of memory storage. The second part is the problem of calculating the density matrix. When doing this we have to diagonalize the Hamiltonian and evaluate matrix functions. Algorithms for doing this are slow.

The other algorithms, like 4, are logarithmic in complexity, and no problem arises.

4 Results from Exact Diagonalisation

In this section we will present the results obtained from the exact diagonalisation described in section 3.

4.1 The Ising Model in a Transverse Filed

The ferromagnetic Ising model is obtained by setting $\gamma = 1/2$ in equation (1.3). We have carried out exact diagonalisations for Ising systems with 3 to 11 spins. In figure 4.1 the entropy of entanglement is shown for different system sizes.

Also the first and second derivative of the entanglement is of interest. The first derivatives corresponding to the entanglement in figure 4.1 are shown in figure 4.2 and the second derivatives in figure 4.3. The reason for this being interesting is that there have been conjectures in the literature [22] that it might be one of the derivatives of the entanglement that diverges at a QPT rather than the entanglement it self having a maximum. The derivations are done numerically.

If the entropy of entanglement is a precursor for a QPT the location of its maximum should move towards $B = 1$ since this is where the Ising model has its QPT (or the derivative should diverge). We have identified the external magnetic field corresponding to the maximum entanglement for different system sizes. The result is shown as a solid line in figure 4.4(a). The data from the exact diagonalisation is then fitted to the curve $E(n) = 1 - c/n^{\lambda}$. The coefficient c and the exponent λ is found using MATLABs least square fit `lsqcurvefit`. The result of this fit is shown as the dotted line in the same figure. After optimization we get $c \simeq 2.167$ and $\lambda \simeq 0.9935$ for 3 to 10 spins and $c \simeq 2.2186$ and $\lambda \simeq 1.0114$ for 3 to 11 spins.

The Ising model undergoes a QPT for $B = 1$. This means that the spin expectation value along the x–direction, $\langle \sigma^x \rangle$ goes from

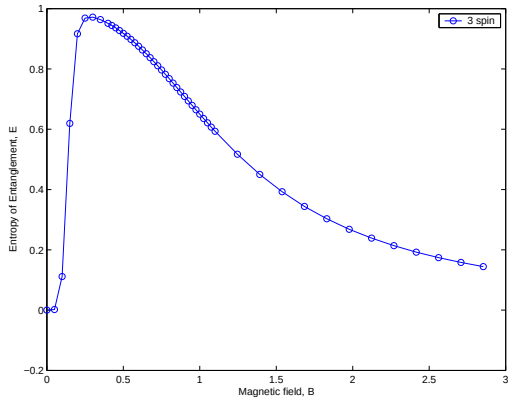
$$\langle \sigma_i^x \rangle \equiv 0, \ B \geq 1$$

to

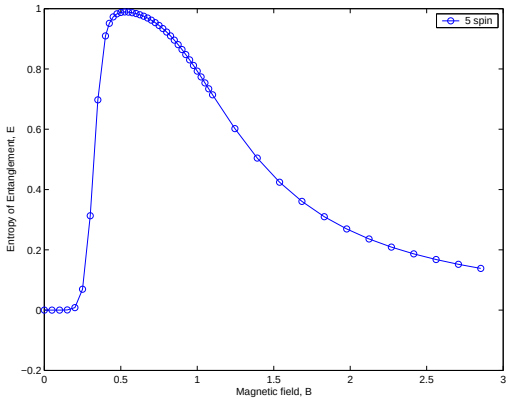
$$\langle \sigma^x \rangle = (1 - B^2)^{\frac{1}{8}}, \ B < 1.$$

That is, the Ising spin chain goes from being a ferromagnet for $B < 1$ to a paramagnet for $B > 1$; see [5, 23] and Ref. [38] in [23]. Since there is no analytic function connecting these two regimes one draws the conclusion that we have a phase transition [7]. Of course since this reasoning depends on the expectation value we are highly interested in how this looks for different system sizes. This is shown in figure 4.5. Here it can be seen that the transitions move towards $B = 1$ for increasing system size. The increase in expectation value on the left side of the transitions is due to the fact that we are calculating expectation value for the full system, and thus we get an increase by one when we increase our system size by one.

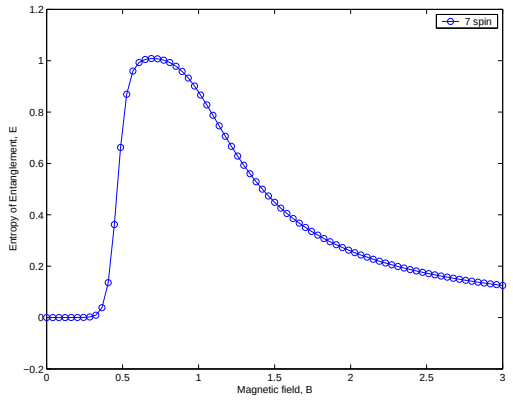
The Ising model has a degenerate ground state. Because of this the density matrix will look like a density matrix belonging to a mixed ensemble to E. But the Ising model in the thermodynamic limit has a spontaneous symmetry breaking in that it chooses one of its two possible ground states. To get a density matrix that better represents the Ising model with its broken symmetry we apply a very weak magnetic field ϵ in the positive coupling direction. Naturally this procedure will affect the result to some degree. See section 4.1 for a closer discussion of this problem. The entanglement of formation does not have this problem, as seen in figure 4.6. There are also two



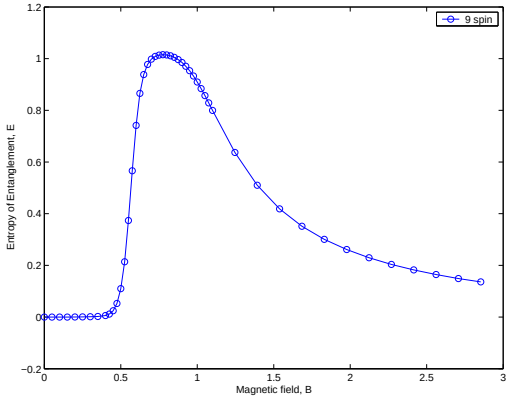
(a) 3 spins



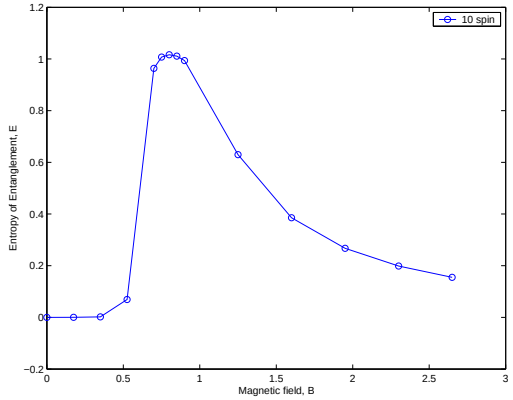
(b) 5 spins



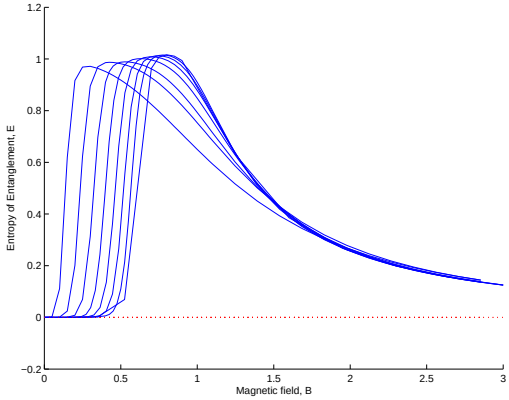
(c) 7 spins



(d) 9 spins

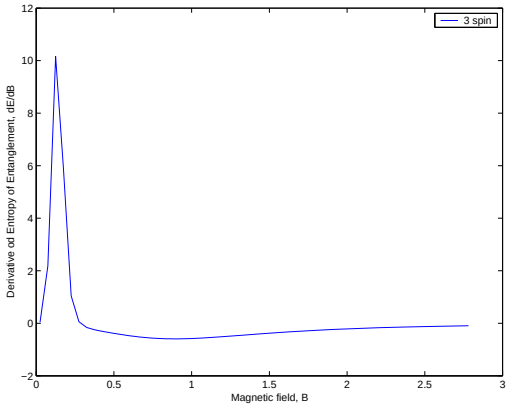


(e) 10 spins

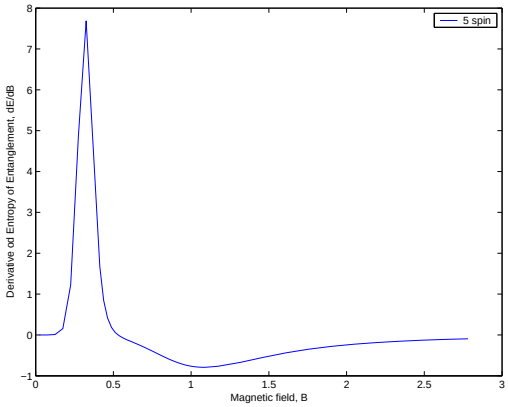


(f) 3 to 10 spins

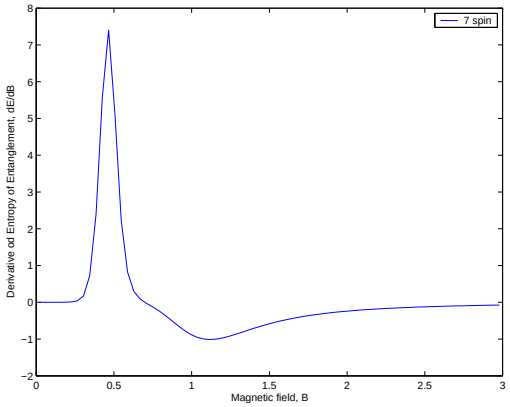
Figure 4.1: Entropy of entanglement for the Ising model for different system sizes. The de–degeneration field is set to $\epsilon = 1/(100 + 1000 \cdot B)$. In these curves all but the three last spins on the chain have been traced away when calculating the entropy of entanglement, except for the 3– and 4–spin chains where two spins have been kept.



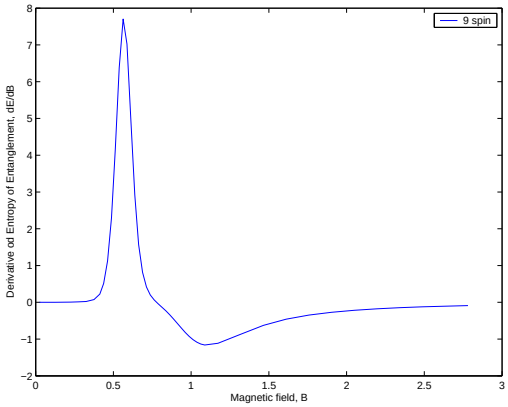
(a) 3 spins



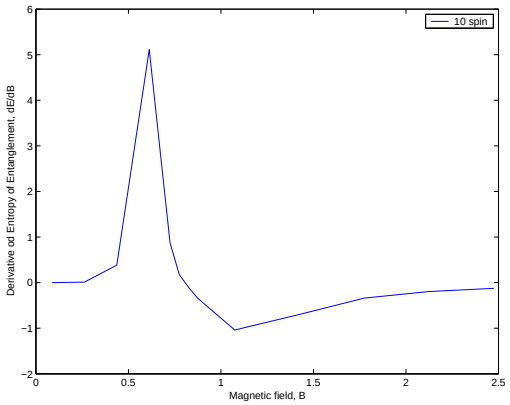
(b) 5 spins



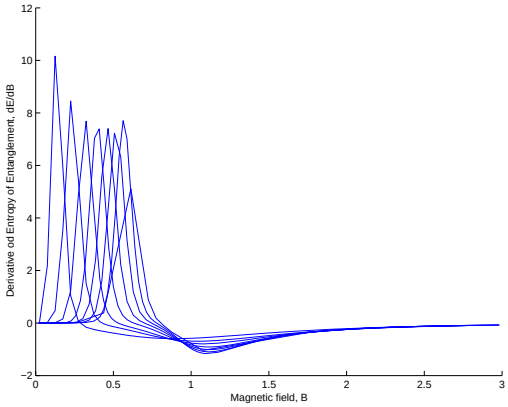
(c) 7 spins



(d) 9 spins

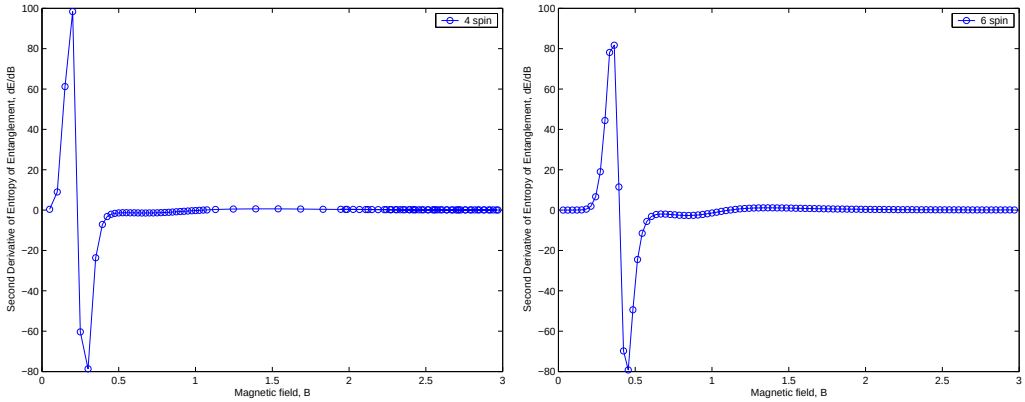


(e) 10 spins



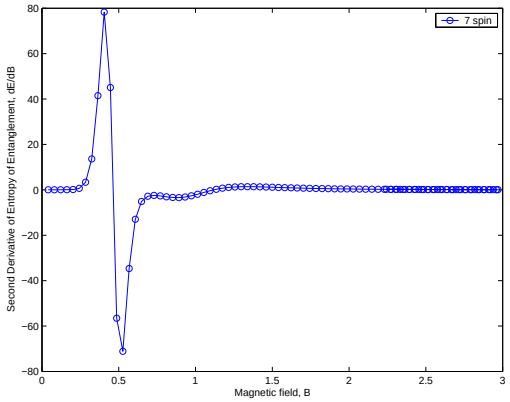
(f) 3 to 10 spins

Figure 4.2: Derivative of the entropy of entanglement for the Ising model for different system sizes. The de–degeneration field is set to $\epsilon = 1/(100 + 1000 \cdot B)$. In these curves all but the three last spins on the chain have been traced away when calculating the entropy of entanglement, except for the 3– and 4–spin chains where two spins have been kept.

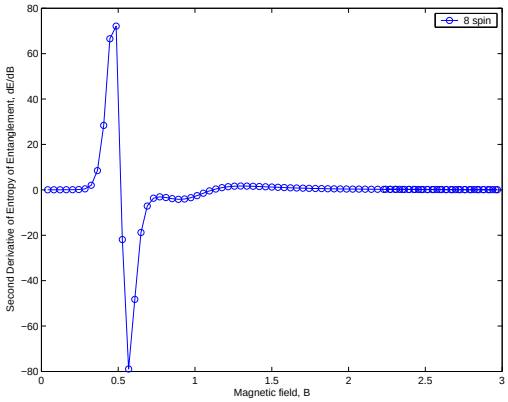


(a) 4 spins

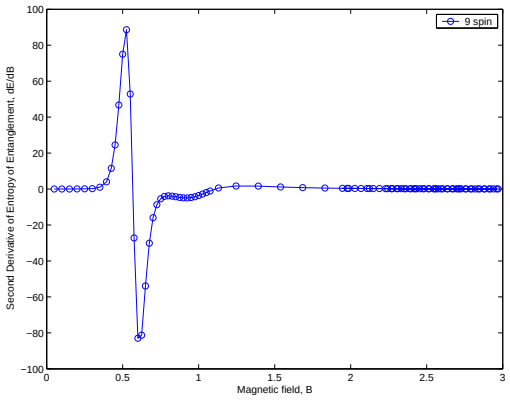
(b) 6 spins



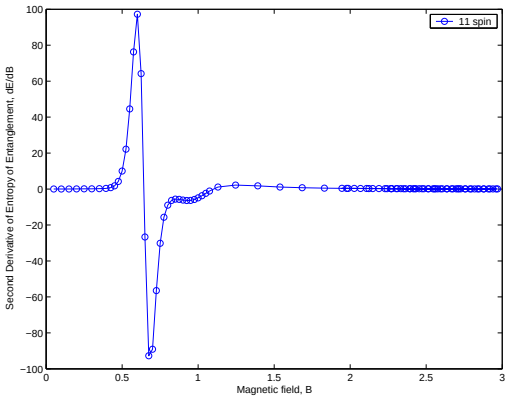
(c) 7 spins



(d) 8 spins

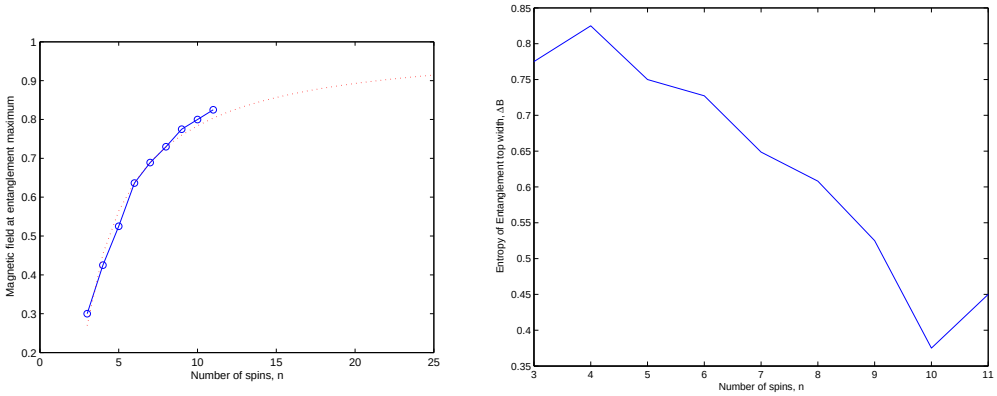


(e) 9 spins



(f) 11 spins

Figure 4.3: Second derivative of the entropy of entanglement for the Ising model for different system sizes. The de–degeneration field is set to $\epsilon = 1/(100 + 1000 \cdot B)$. In these curves all but the three last spins on the chain have been traced away when calculating the entropy of entanglement, except for the 3– and 4–spin chains where two spins have been kept.



(a) Location of the maximum of the entropy of entanglement and an extrapolated curve for the trend.

(b) Entropy of entanglement top width (the width is defined by the entropy of entanglement having decreased to $1/\sqrt{2}$ of its maximum value).

Figure 4.4: The behavior of the location of the maximum and the top of the entropy of entanglement for different system sizes.

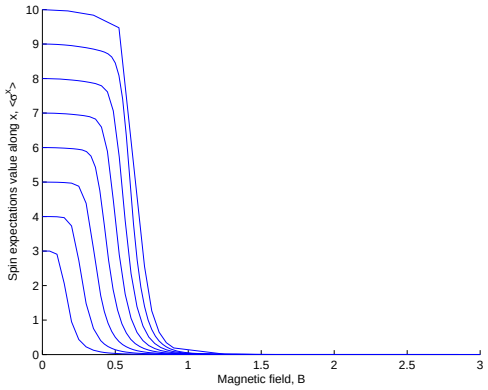


Figure 4.5: Spin expectation value $\langle \sigma^x \rangle$ for different Ising system sizes. The system size increases by one from 3 spins to 10 from left to right.

other very interesting things to note about figure 4.6. First the maximum – conjectured to occur at the phase transition moves away from $B = 1$. Thus the conjecture is obviously false for E_F and the Ising model. This actually agrees with the results in [22] where it is conjectured that it is the derivative, rather then the entanglement of formation itself, that should be at a maximum at the QPT. Secondly the maximum is much smaller than for the entropy of entanglement.

Dependence on the de–degeneration field ε

The dependence on the de–degeneration field for the Ising model with 6 spins is shown in figure 4.7. We want to preserve the expected sharp peak, and still not depress the maximum value. This makes $\varepsilon = 1/(100 + 1000 \cdot B)$ a good choice. In fact the actual handling of the de–degeneration field is a bit more delicate than just to stick to this value. It naturally depends on the system type – if we have no degeneracy in the ground state no field is needed – but also on the number of spins traced away. For example, if we have a 6-site spin Ising chain, and only trace away one spin the field

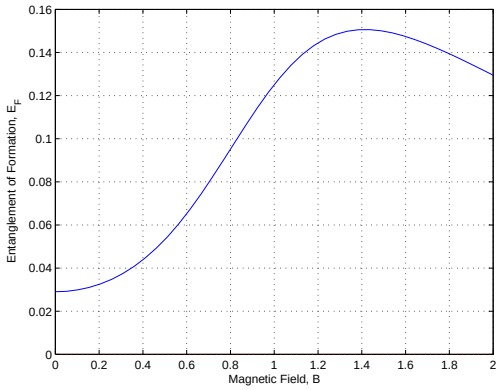


Figure 4.6: Entanglement of formation between two nearest neighbors for the Ising model.

above is too strong – it depresses the peak – and $\varepsilon = 1/(1000 + 10000 \cdot B)$ is a better choice. Why then can we in fact use the first value of the de–degenerations field? In the above calculations the de–degenerations field is always small enough that it will not depress the entanglement maximum. Thus it should be a safe choice.

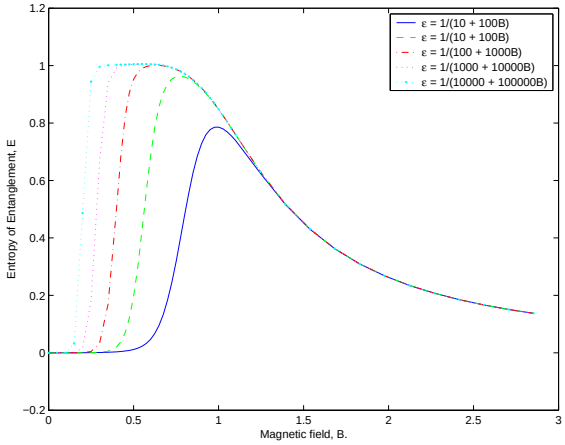


Figure 4.7: The entropy of entanglement for different de–degenerations fields. Here the system is an Ising type with 6 spins and the first three traced away.

For the full XX model the situation is different. Here the ground state of the system *is* unique *and* entangled (see the next section)! That is, this model will have a non-zero entanglement for the ground state. The result of a de–degeneration field here is only to destroy symmetry, as we shall see later.

Because of the rather unfortunate requirement, that an extra field have to be added "by hand", the results on the Ising model have to be questioned to some extent. However there are a number of factors suggesting the result to be plausible. To begin with, for the region $B > B_c$ we can skip the field since here we have no degeneration. If we do this the result for $B > B_c$ is the same as with the field ε. This can also be seen in figure 4.7 where the curve is essentially independent of ε when $B > B_c$. Secondly, similar investigations for the Ising model were carried out in [29]. The results there are very close to mine.

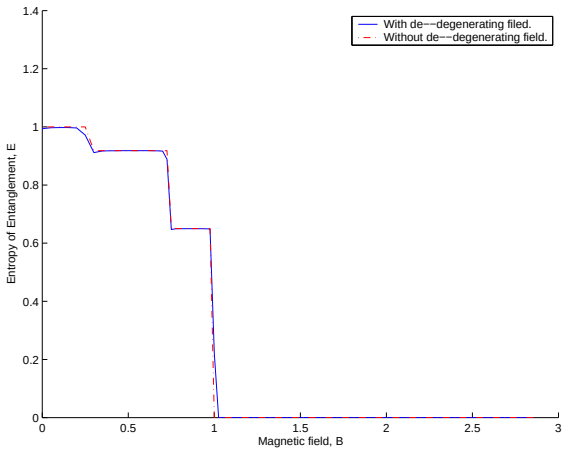


Figure 4.8: The entropy of entanglement for different de–degenerations fields. Here the system is an XX model with 6 spins and the first one traced away.

4.2 The XX Model in a Transverse Field

If we set $\gamma = 0$ in equation (1.3) we get the XX model. For $\gamma = 0$ we have a symmetry which we do not have for the other XY models. The Hamiltonian now commutes with σ^z, giving a $U(1)$–symmetry. This symmetry has implications which we shall discuss later. For the XX model the results are shown in figures 4.8 – 4.10.

The Ground State of the XX Model It is an easy matter to demonstrate that the Ising model has a product state ground state for $B = 0$. It is done in, for example, [5]. From this one would maybe think that also the XX model has a product ground state. This is however not the case. To verify this we do the calculations for a two particle XX Hamiltonian without any external field

$$H = -\sum_{i=1}^{2} \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y.$$

Now let $|0\rangle$ and $|1\rangle$ have the usual matrix representation. The Hamiltonian for two spins looks like

$$H = -(\sigma_1^x \sigma_2^x + \sigma_2^x \sigma_1^x + \sigma_1^y \sigma_2^y + \sigma_2^y \sigma_1^y).$$

In the matrix representation this is

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

which has eigenvalues

$$E_1 = -4, \; E_2 = E_3 = 0, \; E_4 = 4.$$

The ground state, is the eigenvector with the lowest eigenvalue E_1:

$$|E_1\rangle \equiv -\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ -1 \\ 0 \end{pmatrix} \equiv -\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

which is a singlet (that is, maximally entangled). This result is a bit deceptive since the ground state for a three–spin XX chain is not maximally entangled. My numerical calculations with exact

diagonalisation seem to imply that spins chains with an even number of spins are maximally entangled, whereas chains with an odd number of spins have entropy of entanglement of around 0.7 (see figure 4.10).

In section 2 we have the analytical solution to the ground state of the XY model in terms of free fermions. This solution, however is not very interesting to us when we want to calculate the entanglement since the fermion basis is not the spin basis.

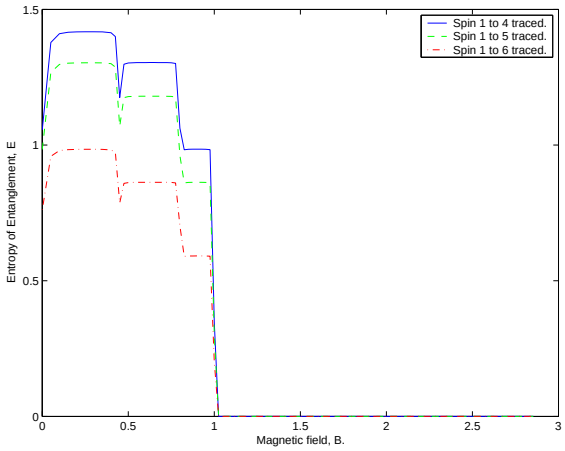


Figure 4.9: Entropy of entanglement for the XX model with 7 spins and different partitions.

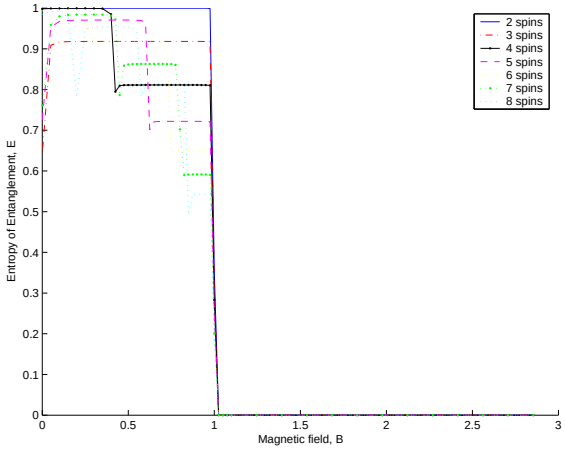


Figure 4.10: Entropy of entanglement for the XX model for different system sizes. One spin traced for all system sizes.

The discontinuities that appear in the entropy of entanglement in figures 4.9 and 4.10 might strike as very strange since we only deal with continuous functions. However they are easily explained. In one step of the calculations of the entanglement we are doing something discontinuous, namely when choosing the eigenvector. For $k_BT = 0$ the system resides in the eigenstate to the Hamiltonian corresponding to the lowest eigenvalue. When we start tuning the magnetic field these eigenvalues change continuously, with the system at all times staying in the eigenstate corresponding to the lowest eigenvalue. If we sketch how the two lowest–lying eigenvalues change we get the picture shown in figure 4.11. In other words, we have a level crossing. At the crossing point, B_d, the system changes from being in one eigenstate (corresponding to the solid line) to another (corresponding to the dashed line). At the point B_d these two eigenvalues are the same and the system is degenerate. The two eigenvectors belonging to these eigenvalues might (and do!)

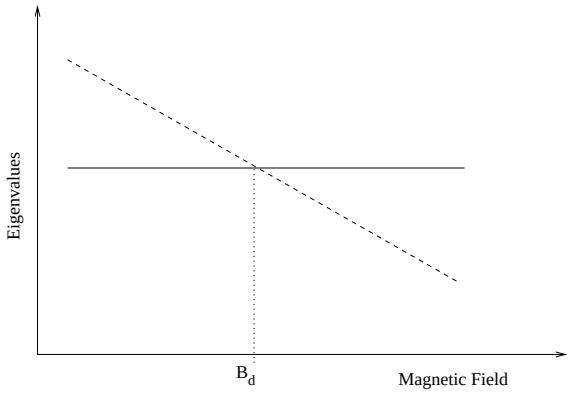


Figure 4.11: A sketch of how the two lowest eigenvalues for the XX model change as we tune the magnetic field.

look very different. This results in a discontinuity for our entanglement at B_d. Still there is one more thing that is very interesting to note about figure 4.9: The drop in entanglement at the level crossing. At the very crossing point the system is degenerate, which should result in an increase in the entropy of entanglement. This is however not the case, but instead we get a drop in the entanglement *around* the level crossing. In [29] Stegeby has found the same behavior.

Table 1 shows the number of steps in the entanglement for the XX and XXX[19] models for different systems sizes. These are the only two investigated systems showing this behavior. A

Size	XX	XXX
2	0	0
3	0	-
4	1	1
5	1	-
6	2	2
7	2	-
8	3	3
9	3	-

Table 1: Number of steps in the entropy of entanglement for the XX and the XXX models for different system sizes. The XX model is taken ferromagnetic, while the XXX is antiferromagnetic. Entries marked with "-" in the column for the antiferromagnetic XXX model comes from the fact that if we have an odd number of spins in an antiferromagnetic chain we will have some "frustration" in the system. This frustration creates a highly complex ground state, very sensitive to small numerical changes, and hence it is difficult to obtain reliable results for this case.

natural question to ask is how these discontinuities scale with system size. The assumption must be that they should approach the entanglement curve for an infinite system. In figure 4.10 it also looks as if this is the case. For the curves in figure 4.10 we can do an estimate of how they approach the infinite system size, $E_\infty(B)$, via the "distance function"

$$D(N) = \int_0^{B_c} |E_\infty(B) - E_N(B)| dB \tag{4.1}$$

where N is the system size and $E_\infty(B)$ is the entanglement in the infinite system from section 2. Since we only have a discrete set of data points for the finite models our integral in (4.1) changes

[19]The XXX model in a transverse field is quite similar to the XX model. The difference is that in the XXX model there are couplings in all directions, x, y, z. See later for a more extensive discussion of the XXX model.

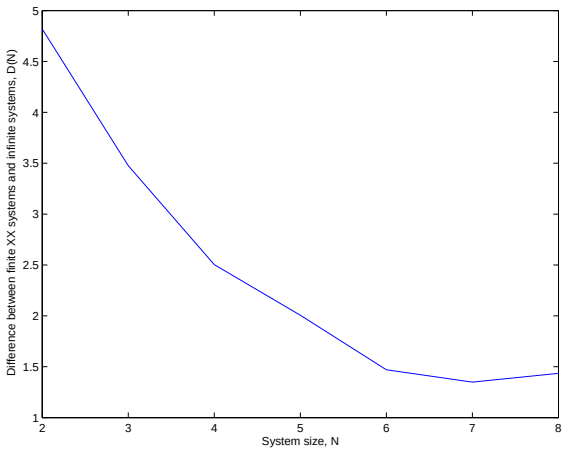


Figure 4.12: The scaling of the entropy of entanglement for different system sizes.

to a sum. If we do this calculation we get the result in figure 4.12 (note that the vertical axis is not to scale). I believe that the increase for a system of 8 spins is due to a numerical error from the finiteness of our data points. Apart from this, the behavior agrees with our expectation with the difference, $D(N)$, approaching zero. Later, in the section on the full XY model we will see why the Ising model does not have these discontinuities.

The next thing to note is the size of the entanglement. If we compare the XX model to the Ising model we see that the entanglement maximum is larger for XX. My interpretation of this is that for the Ising model we only have nearest neighbor entanglement (and this is only 1/2 ebit for each spin site) but for the full XX model we also have a small amount of next to nearest neighbor entanglement. It should be possible to do careful calculations, similar to those below for the antiferromagnetic XXX model, to see how fast the entropy of entanglement falls off, i.e. the entanglement length, l_E. Note: In the larger models (more than five spins, say) the entropy of the Ising model increases slightly above 1. This suggests that here might be a very small amount of next–to–nearest neighbor entanglement also in the Ising chain. This is also the result obtained in [23] when the concurrence is calculated for the infinite Ising model.

4.3 The Antiferromagnetic XXX Model in a Transverse Field

This model is obtained from equation (1.2) by setting

$$\begin{aligned} g_k^{ij} &= (\delta_k^x + \delta_k^y + \delta_k^z) \cdot \delta^{i+1,\,j} \\ d_l^k &= \delta_l^k \\ \varepsilon &= 0 \\ B_k &= 2B_z. \end{aligned}$$

In [20] Arnesen *et al.* have calculated the entanglement of formation in the Heisenberg chain using exact diagonalisation. They come to the conclusion that in the ferromagnetic, FM, case the entanglement is always absent. As expected this is also the that result I have come to. However this is not the case for the antiferromagnet, AFM. For a two spin system the entanglement is unity for a magnetic field below a threshold and rapidly vanishes above it. This is also the result that I obtained, see figure 4.13. For systems larger than two spins a more interesting behavior is displayed, see figure 4.14. Arnesen *et al.* has also done a calculation for how the entanglement of formation between nearest neighbors varies with the B-field.[20] We have done calculations to compare the entropy of entanglement with the entanglement of formation for the AFM XXX

[20]The method presented here for calculating the nearest neighbor entanglement are not based on [20] and thus might vary from the one used there.

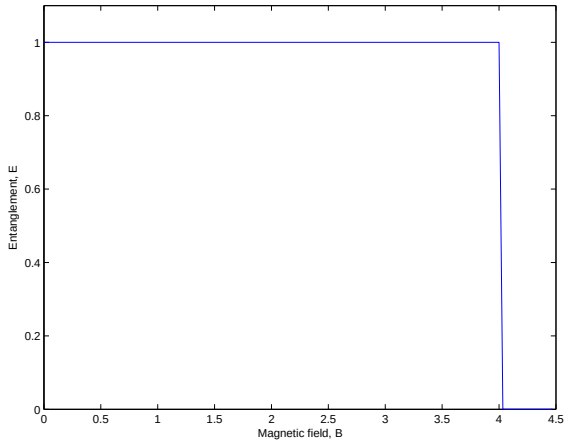


Figure 4.13: XXX result, no de-degeneration field, 2 spins In this plot the coupling constant is set so that we get a phase transition at $B = 4$.

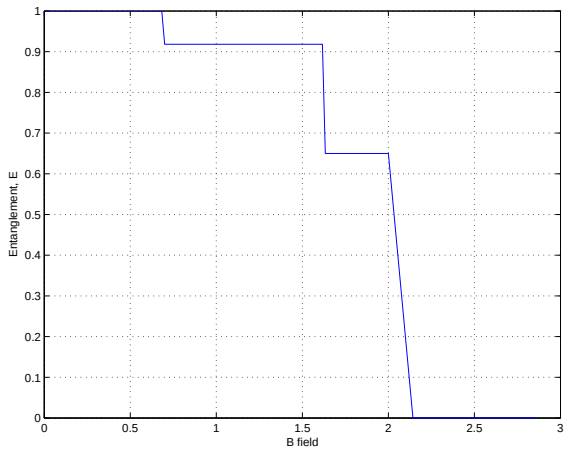


Figure 4.14: Entropy of entanglement in the XXX model with six spins and no de-degeneration field. All spins but one are traced out.

model. If we have a system with 6 spins and trace 4 of these, keeping say 1 and 2, we will get the entanglement between these two and the rest of the system. We call this entanglement E_{12}. If we trace all but one particle we will get the entanglement between this particle and the rest of the system, we call this entanglement $E_1 (= E_2 = ...)$. Now the entanglement between subsystem 12 and the rest of the system should be

$$E_{12} = E_1 + E_2 - 2 \cdot E^{12}, \tag{4.2}$$

where E^{12} $(= E^{21})$ denotes the entanglement between particle 1 and 2 (not to confuse with E_{12} denoting the entanglement of subsystem 12 with the rest of the system). Since E_{12} and $E_1 = E_2$ are known from exact diagonalisation, E^{12} can be calculated. In the same figure the result from Arnesen *et al.* [20] is shown. Note that their calculations are done for $k_B T = 0.1$ and with entanglement of formation as entanglement measure, while mine are done for $k_B T \equiv 0$.

We have also calculated the entanglement between two spins in a chain using the concurrence of formation and the entanglement of formation. When doing this, using the canonical ensemble to get the density matrix (in a similar way as done in [20]) for finite temperatures, we obtain the result shown in figure 4.16. If we compare figure 4.15 with figure 4.16 we see something interesting. The first discontinuity (corresponding to the level crossing where we switch from

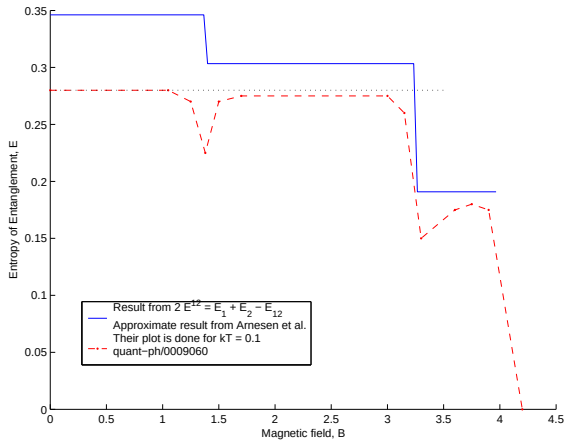


Figure 4.15: Nearest–neighbor entanglement for the XXX model with 6 spins.

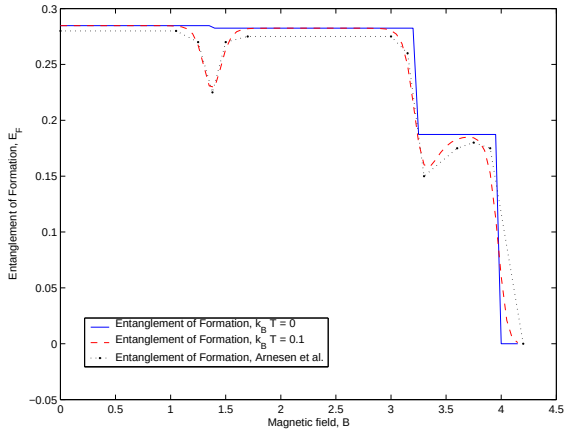


Figure 4.16: Nearest–neighbor entanglement of formation for the antiferromagnetic XXX Heisenberg model with six spins.

singlets to triplets [20]) for the $k_BT = 0$ case is much larger for the entropy of entanglement than it is for the entanglement of formation. This is surprising since for $k_BT = 0$ we are dealing with pure ensembles and one would expect the two measures to be equal. The mismatch might be due to some error in equation (4.2). A more plausible cause though, is that the two measures actually do not agree in the way expected. As was discussed in section 1.3.4 we are doing something rather strange when we optimize over actual ensembles corresponding to the density matrix. The result here obtained shows that there is a problem with the entanglement of formation.

4.4 The XY Model in a Transverse Field

The XY model is the more general model containing Ising and XX as special cases. It is displayed in equation (1.3) and its phase diagram is shown in figure 1.2. For $0 < \gamma \leq 1/2$ this model belongs to the Ising *universality class*. This means that all these models have the same set of Z_2 "spin flip" symmetries. For $N = \infty$ it undergoes a quantum phase transition at $B = 1$ [22]. For the XX model ($\gamma = 0$) we have a larger $U(1)$ symmetry, that is, the model is invariant under continuous rotations around the z–axis. In figures 4.17 and 4.18 we see the presence of a gap between the two lowest–lying eigenvalues (the degeneracy) and the rest for the Ising model. This gap is present, but gets smaller, for all γ down to 0 where it disappears. Of course we can not really talk of a true gap since this model is finite size, but we can easily imagine how the situation is for infinite

systems. Due to the difference in entanglement in the different ground states the level crossings are seen in the XXX case. These level crossings occur already for small (finite) systems. Thus we have a method to detect if a model is massless or not using entanglement on finite systems! If we have discontinuities in the entanglement this means level crossings and hence a massless phase. Of course a smooth curve does not guarantee a massive phase, but a discontinuous one does the opposite. Given this we can predict the spin systems considered here all but the Ising universality class to be massless.

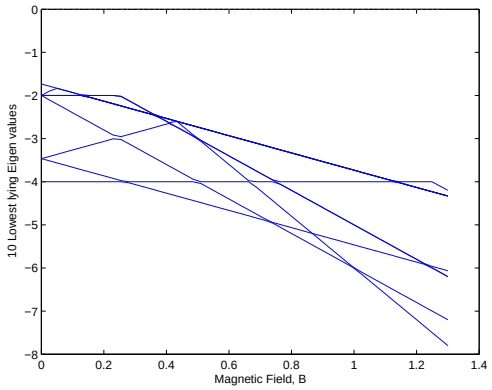


Figure 4.17: The 10 lowest–lying eigenvalues for the XX model.

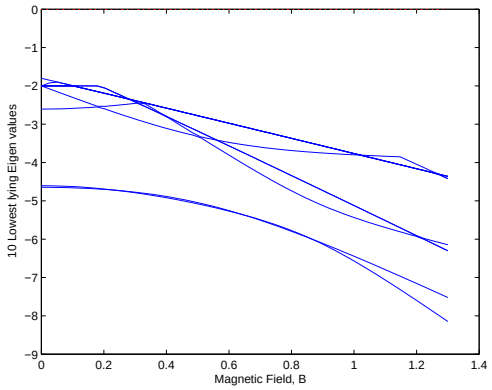


Figure 4.18: The 10 lowest–lying eigenvalues for the Ising model.

4.5 The XYZ Model

In this section we study the XYZ model. This is a model with the Hamiltonian

$$H = \pm \sum_{n=1}^{N} S_n^x S_{n+1}^x + \Gamma S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z.$$

The operators S_n^i are spin operators for spin 1/2 or spin 1 (or higher spin operators, which however will not be considered here). The signs $\pm$ define the AFM and FM model respectively. We have computed the entropy of entanglement in the usual way and the entanglement of formation using the equations derived in section 3.3 for this family of systems. The results are shown i figures

4.20–4.23. The size of the systems are the same and the partitioning is dome in the same way in this section, and in 4.6 and 4.7. It is shown in figure 4.19. Thus for the entropy of entanglement we calculate the entanglement between the spins 1 and 2 and the rest of the system, while for the entanglement of formations we calculate the entanglement between spin 1 and 2.

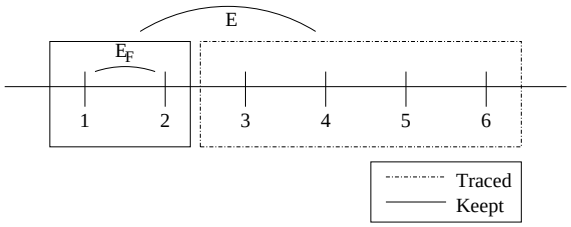
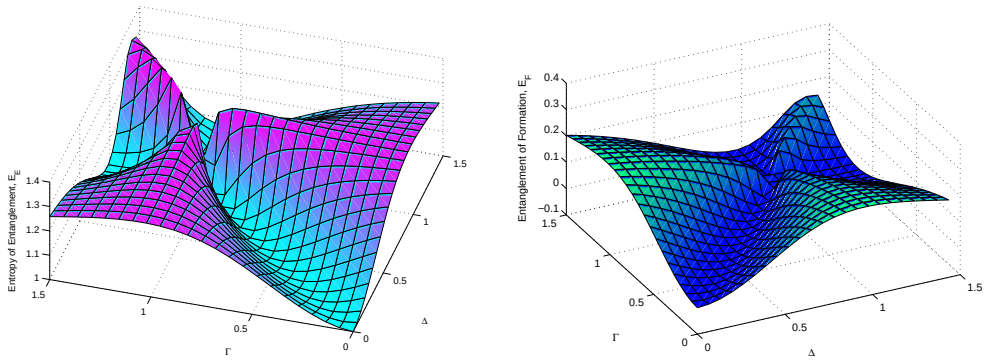


Figure 4.19: The partitioning used in this and the next two sections.



(a) Entropy of Entanglement

(b) Entanglement of Formation

Figure 4.20: Entanglement in the spin–1/2 FM XYZ model with 6 particles and 4 traced away. Note the different in scales on the z–axis, and also the different perspectives of the two graphs.

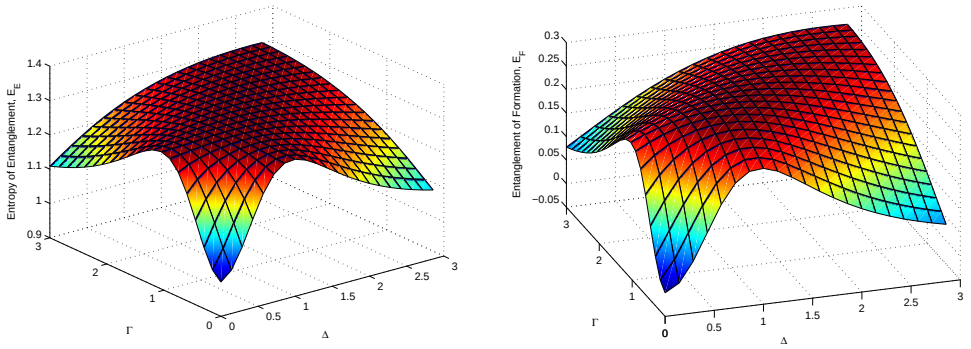
Several very interesting things can be seen from these results. We will point out some of them here. To begin with it looks as if the entanglement behaves very similar in the spin–half and spin–one cases. The entropy of entanglement has exactly the same qualitative behavior in the spin–1/2 and spin–1 FM model. Also the entanglement of formation looks very similar. However in the spin–1 model the entanglement of formation is not symmetric in the same way as in the spin–1/2 case. This is very surprising since the tuning of Γ and Δ should be symmetric in the way it appears in the other figures.

The same asymmetry also appears in the entanglement of formation for the AFM spin–1 case. Otherwise also the AFM case seems to behave quite similar in the two spin cases. It is however interesting to note that in the limit $\Gamma,\ \Delta \to 0$ the entanglement of formation increases in the spin–1 cases whereas it decreases in the spin–1/2 case.

4.6 The Spin–1 AFM XXX Model with Single–Ion Anisotropy

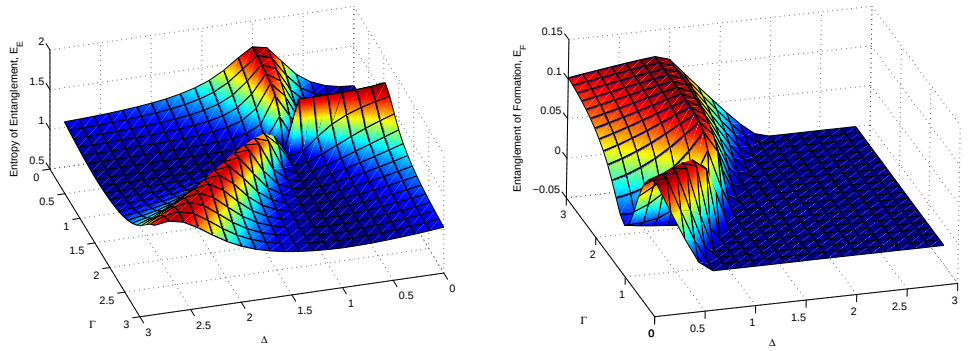
This model is described by

$$H = J \sum_{n=1}^{N} \bar{S}_n \cdot \bar{S}_{n+1} + B \sum_{n=1}^{N} (\bar{S}_n^z)^2,$$



(a) Entropy of Entanglement (b) Entanglement of Formation

Figure 4.21: Entanglement in the spin–1/2 AFM XYZ model with 6 particles and 4 traced away. Note the different scales on the z–axis, and also the different perspectives of the two graphs.



(a) Entropy of Entanglement (b) Entanglement of Formation

Figure 4.22: Entanglement in the spin–1 FM XYZ model with 4 particles and 2 traced away. Note the different scales on the z–axis.

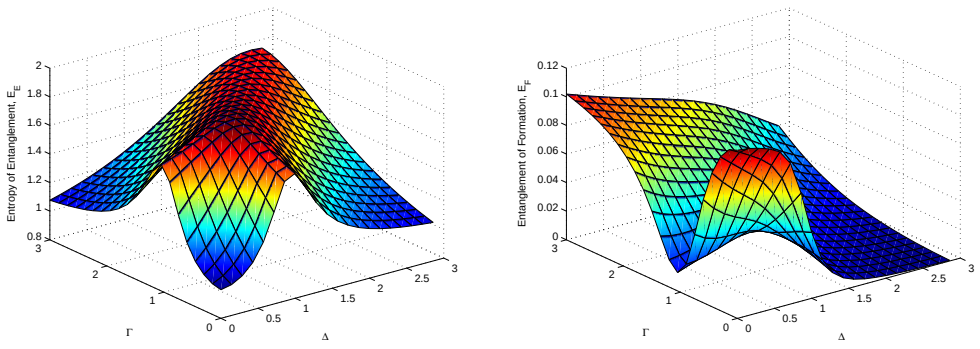
where $\bar{S}_n$ are spin–1 operators. The second term is the single–ion anisotropy. When $B > 0$ this term will favor states where the spin are aligned in the xy–plane ("easy–plane"). For $B < 0$ the term will favor spins in the z–direction ("easy–axis"). The entanglement is shown in figure 4.24.

4.7 The Spin–1 AFM XXZ Model with Single–Ion Anisotropy

The Hamiltonian is defined by

$$H = \sum_{n=1}^{N} (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) + B \sum_{n=1}^{N} (S_n^z)^2. \tag{4.3}$$

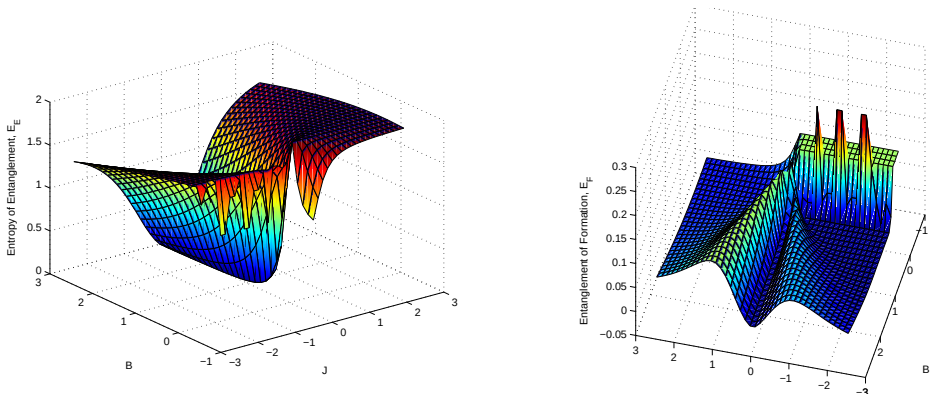
This model has a rich phase diagram. It can be found in for example [11]. A future project would be to study this model in more detail and compare the entanglement to the phase diagram found in [11] to see if we can discern any of its structure using entanglement. The entanglement is shown in figure 4.25.



(a) Entropy of Entanglement

(b) Entanglement of Formation

Figure 4.23: Entanglement in the spin–1 AFM XYZ model with 4 particles and 2 traced away. Note the different scales on the z–axis.



(a) Entropy of Entanglement

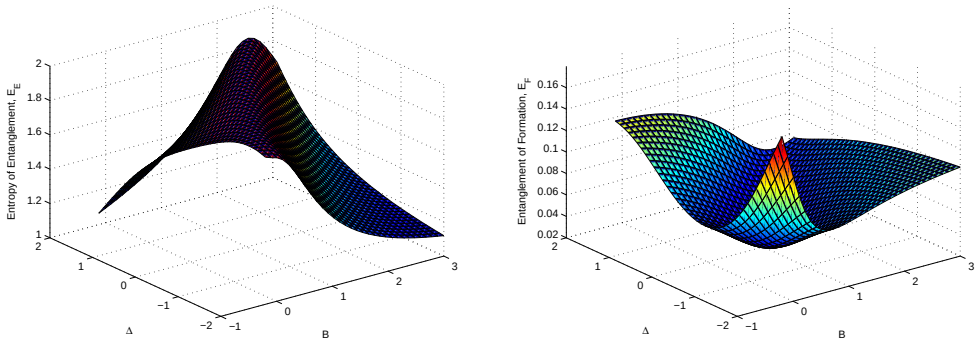
(b) Entanglement of Formation

Figure 4.24: Entanglement in the spin–1 XXX model with single–ion anisotropy with 4 particles and 2 traced away. Note the different scales on the z–axis, and also the different perspectives of the two graphs.

5 Discussion, Things to Do in the Future and Conclusion

In [23] it is conjectured that it is not the entanglement that is maximized at the phase transition but rather the *entanglement sharing*. That is, near the critical point the entanglement spread to include not only nearest neighbors but also qubits further apart. In using entanglement to characterize a quantum phase transition it is then important to find a suitable measure for this entanglement length. In [22] on the other hand the authors focus on the derivative of the entanglement of formation. The idea is that it is the derivative that should diverge, not the entanglement itself. If one compares to the classical theory of second order phase transitions, where the derivative of the order parameter (like the susceptibility) diverges at the critical point, this seems a natural suggestion.

If entanglement is a physical resource, similar to energy, it should be possible to transfer entanglement from one system to another. This has been done many times, and it is not anything



(a) Entropy of Entanglement

(b) Entanglement of Formation

Figure 4.25: Entanglement in the spin–1 XXZ model with single–ion anisotropy with 4 particles and 2 traced away. Note the different scales on the z–axis, and also the different perspectives of the two graphs.

strange [17]. But if entanglement is really a physical resource we should also be able to transfer entanglement between *different types* of systems. For instance, one would maybe like to use one ebit in the form of a spin singlet to create one ebit in the form of a maximally entangled superconductor circuit pair. This is analogous to transfer of kinetic energy to heat or potential energy. How to carry out this more general type of entanglement transfer is an open problem.

Another interesting problem would be to "de–kron" a state vector $|\psi\rangle$ to get the state vector on the regular form

$$|\psi\rangle = |A_1\rangle \otimes ... \otimes |A_n\rangle + ... + |N_1\rangle \otimes ... \otimes |N_n\rangle.$$

This is however quite a hard task to accomplish since N is in general unknown. Therefore we do not do this.

In the future it would be interesting to further explore the entanglement measure we introduced in section 1.4: vector entanglement. Since entanglement is basis dependent it is not sufficient to have a solution like the one obtained in section 2 for doing this. Since we need the ground state expressed in the standard basis we have no use of fermion solutions unless we can transform them back to our spin basis. Also it can be seen than additional work on choosing the correct ensemble for systems of the type considered here is needed. With the generalization from section 1.4 for entanglement of formation to higher spin–systems, more work should be done to see how these systems behave.

In conclusion it is hard to establish any firm quantitative connection between entanglement and QPT based of the results obtained here. That there *is* a connection seems undoubtable, but how this connection is to be characterized in detail is hard to tell. Also in many cases this "extreme" behavior is not located *at* the transition, but rather close to it. This most likely comes from the fact that we do not work with infinite system sizes.

In the thesis we have pointed out that the entanglement is basis dependent in the sense that, for example, the fermionic basis can not be used to calculate entanglement. We have required the basis to be "local". Perhaps this requirement can be relaxed. Every measurement operation specifies a basis (for example a position measurement or a localized spin measurement). Maybe one should use the basis defined by such a measurement to calculate entanglement. This has the drawback that there will be a doubt in how much entangled a system "really" is. But it will probably be a very useful tool when calculating entanglement in systems more complex than spin systems. Maybe it even is a *necessary* condition if one wants to be able to talk of entanglement in any meaningful way at all! To be specific one will have to talk about "entanglement in the basis

of O", where O represent some measurement.

In section 4.1 we investigated how entanglement behaves in the Ising model. To get rid of the degenerate ground state we applied a small field to remove the degeneration. This was motivated by the fact that for the infinite Isning model there is a spontaneous symmetry breaking in the system. Thus we can choose one of the two possible ground stats without hesitation.

Still the choice of one of the ground states in the Ising model may not be a very good idea. In fact if we do not make this choice, the Ising model seems to behave more like the other models in the XY–class. Then the entanglement maximum will not be located near the QPT, instead we will get an abrupt change in the entanglement near the QPT, like in the XX model case.

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