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Bachelor Thesis

Entanglement Entropy in a Finite Transverse Field Ising Chain

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Abstract

One of the exciting new phenomena that have risen from quantum mechanics is quantum entanglement. In this paper we study the basic mathematical properties of an entangled state as well as its entanglement entropy. These concepts together with the formalism of second quantization will be studied with respect to finite one-dimensional transverse field Ising models.

I would like to thank Lars Fritz and Sonja Fischer.

Contents

CHAPTER 1

Introduction

Entanglement is a very interesting phenomenon that appeals to the imagination. The paradoxical concept that two entities can be in a united state of being without physically being in touch is hard to grasp. It defies time and space and it makes the universe less detached than we thought it was.

The existence of entanglement has been confirmed experimentally[6], but it is still a relatively new field in physics. In this article I will try to give an overview of how entanglement manifests itself in a theoretical system: the Ising model.

We will look at chains of elementary particles with simple interactions. Each particle is affected equally by an external field and has an interaction with its nearest neighbors. States of such a system will naturally contain a certain amount of entanglement.

Chapter 2 will be an introduction to entanglement and entanglement entropy and contains some basic examples. In chapter 3, I will introduce second quantization, which is a method for efficiently describing many-particle systems. Chapter 4 contains the definition of the Schmidt decomposition and some basic implication this has for the entanglement in quantum mechanical systems. Chapter 5 and 6 finally deal with the transverse field Ising model, bringing into use everything from the previous chapters.

CHAPTER 2

Introduction to Entanglement

2.1 Entanglement

Entanglement is a quantum mechanical property which has met a lot of controversy in the past. It causes some counter intuitive and paradoxical phenomena which makes it very interesting to study.

When two quantum mechanical particles, that is, particles obeying quantum mechanical laws, are entangled, they are in a fundamentally joint state. The state of the first particle is always correlated with the state of the second particle. In that sense, it really is a joint state: the particles cannot be seen as independent but have to be described by their mutual wave function.

The controversy that this brings is that it seems like the two particles communicate with each other. This would not be a problem were it not that they seem to communicate *instantaneously*. Even if two entangled particles are both at another end of the universe, two observers would make correlated measurements. It seems like information has traveled across the universe to tell that because the first observer measured 'a', the second observer should measure 'b'. It seems also, that this means that the observers could exchange information instantaneously without being bothered by their distance. All this would contradict the principle that nothing can travel faster than light, not even information.

Unfortunately, or luckily, this is not the case. What has not been taken into account here is the unpredictable nature of quantum particles. When you measure a property of a quantum particle, it could always be 'a' or 'b' and you cannot know in advance. This also means it is impossible to force a particle in the exact state you want, making it impossible to exchange information; it is as if you write with a magic pen that writes down only random letters not taking into account its user.

The phenomenon of entanglement can be described mathematically. We want to express that the joint state of the two particles cannot be separated into two independent states. We start by considering the Hilbert space of the two particles. If particle 1 is in space $\mathcal{H}_1^N$ of dimension N and particle 2 is in space $\mathcal{H}_2^M$ of dimension M, the Hilbert space in which we can describe the two particles simultaneously is given by the tensor product space $\mathcal{H}_1^N \otimes \mathcal{H}_2^M$ of dimension $N \times M$.[4] If $\{|n\rangle\}$ is an orthonormal basis of $\mathcal{H}_1^N$ and $\{|m\rangle\}$ of $\mathcal{H}_2^M$, then the tensor product $\{|n\rangle\} \otimes \{|m\rangle\}$ forms an orthonormal basis for $\mathcal{H}_1^N \otimes \mathcal{H}_2^M$.

The most general state in this joint Hilbert space can be expressed as

$$|\Psi\rangle = \sum_{n,m} b_{nm} |n\rangle \otimes |m\rangle \,, \tag{2.1}$$

where b_{nm} are constants such that $\sum_{n,m} b_{nm}^2 = 1$. An *entangled* state is a state which cannot be written as a tensor product of two states from the different Hilbert spaces, i.e. a state $|\Psi\rangle$ which cannot be written in the form $|a\rangle \otimes |b\rangle$ where $|a\rangle \in \mathcal{H}_1^N, |b\rangle \in \mathcal{H}_2^M$. In our notation, this means we cannot factorize b_{nm} into the form $c_n d_m$; we cannot write equation 2.1 in the form

$$\sum_{n,m} c_n d_m |n\rangle \otimes |m\rangle = (\sum_n c_n |n\rangle) \otimes (\sum_m d_m |m\rangle) = |a\rangle \otimes |b\rangle . \tag{2.2}$$

An entangled state cannot be considered as the product of two independent states, in this sense.

2.2 Entanglement Entropy

Let us start by introducing a classic example of an entangled state. We consider two spin-$\frac{1}{2}$ particles and use the shorthand notation $|ij\rangle := |i\rangle_1 \otimes |j\rangle_2$: i represents the state of particle 1 and j the state of particle 2. We denote 0 for the state down and 1 for the state up.

We consider the state

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

Although not obvious, this state cannot be separated and is therefore entangled. One could try to prove this, but another way to check for entanglement is by determining the 'entanglement entropy'. Besides indicating whether your system is entangled, the entanglement entropy is also a measure of the *amount* of entanglement.

We first introduce the density matrix $\rho = |\Psi\rangle \langle\Psi|$. The reduced density matrix ρ_1 of particle 1 is defined by the partial trace of the density matrix over the Hilbert space of particle 2. In our example:

$$\begin{aligned}
\rho_1 &= \mathrm{tr}_2 \rho \\
&= \frac{1}{2} \langle 0|_2 (|01\rangle - |10\rangle)(\langle 01| - \langle 10|) |0\rangle_2 \\
&+ \frac{1}{2} \langle 1|_2 (|01\rangle - |10\rangle)(\langle 01| - \langle 10|) |1\rangle_2 \\
&= \frac{1}{2}(|0\rangle_1 \langle 0|_1 + |1\rangle_1 \langle 1|_1),
\end{aligned}$$

which is simply a diagonal matrix. The entanglement entropy S_1 of particle 1 is given by

$$S_1 = -\mathrm{tr}(\rho_1 \log \rho_1) = -\mathrm{tr}[\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \cdot \begin{pmatrix} \log 1/2 & 0 \\ 0 & \log 1/2 \end{pmatrix}] = \log 2.$$

In general, when we divide a system into two subsystems A and B, the entanglement entropy of system A is given by

$$S_A = -\mathrm{tr}(\rho_A \log \rho_A) \tag{2.3}$$

where $\rho_A = \mathrm{tr}_B \rho$ is the partial trace of the density matrix over the Hilbert space of system B.

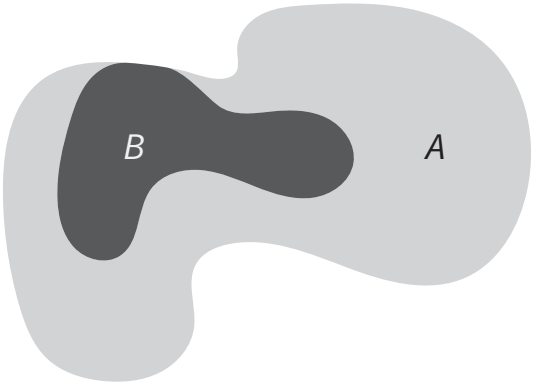

Figure 2.1: A representation of a system consisting of two subsystems A and B.

The expression $-\mathrm{tr}(\rho \log(\rho))$ is called the 'von Neumann entropy'. It is generally used to determine whether a state is a pure or a mixed state. When the Neumann entropy is zero, it is a pure state; when it is not zero, the state is mixed. In this context the entanglement entropy tells us whether subsystem A is in a pure, independent state, or whether it is mixed and entangled with its surroundings.

Let us look at what happens if we calculate the entanglement entropy of a non-entangled product state: $|\Psi\rangle = |a\rangle \otimes |b\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. We expect it to be zero. The reduced density matrix becomes:

$$\begin{aligned}\mathrm{tr}_B(|\Psi\rangle\langle\Psi|) &= \mathrm{tr}_B\left[(|a\rangle \otimes |b\rangle)(\langle a| \otimes \langle b|)\right] \\ &= |a\rangle\langle a|\,\mathrm{tr}_B(|b\rangle\langle b|) \\ &= |a\rangle\langle a|\end{aligned}$$

We can find a linear basis transformation U (using the Gram-Schmidt process [12]) such that $|a\rangle$ is one of the new basis vectors. In this basis, $|a\rangle\langle a|$ is a very simple matrix we call $\hat{m}_a$. Mathematically:

$$|a\rangle\langle a| = U^{-1}\begin{pmatrix}1 & 0 & \cdots & 0\\ 0 & 0 & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & 0\end{pmatrix}U = U^{-1}\hat{m}_a U.$$

For the entropy we get:

$$\begin{aligned}S_A &= -\mathrm{tr}\left[|a\rangle\langle a|\log(|a\rangle\langle a|)\right] = -\mathrm{tr}\left[U^{-1}\hat{m}_a U \ln(U^{-1}\hat{m}_a U)\right] \\ &= -\mathrm{tr}\left[U^{-1}\hat{m}_a U U^{-1}(\ln\hat{m}_a)U\right] = -\mathrm{tr}\left[\hat{m}_a(\ln\hat{m}_a)\right] \\ &= -\mathrm{tr}\left[\begin{pmatrix}1 & 0 & \cdots & 0\\ 0 & 0 & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & 0\end{pmatrix}\cdot\begin{pmatrix}0 & 0 & \cdots & 0\\ 0 & \infty & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \infty\end{pmatrix}\right] = 0,\end{aligned}$$

which is what we expected.

In order to tackle the problems and complexities that arise when dealing with many particle systems, we first need to cover a few other concepts which we will do in the next chapters.

CHAPTER 3

Second Quantization and Fermionic Operators

3.1 First Quantization

3.1.1 Indistinguishability

When talking about more than one particle in quantum mechanics, one has to be careful. Different physical properties play a role which should always be taken into account in order to get the right results. At the quantum level, things do not work as we are used to and counter-intuitive rules dominate.

The first concept we have to introduce is the notion of indistinguishability. In our daily experience, when we see two similar objects, we can still always distinguish between them. When you have two green balls, you could place one in your left and one in your right hand. You could also paint one of the balls another colour to make distinguishing even more easy.

In quantum mechanics this is not possible. One can never distinguish between two identical particles.[1] When looking at electrons, for example, there is no way of tracking or labeling one single particle. This property relates to the fact that observing particles in quantum mechanics inevitably affects them: when we do not (want to) influence the system, we cannot observe it and thereby cannot distinguish between identical particles.

3.1.2 Multi-particle Wave Function

When you want to describe a quantum-mechanical system of two particles, for example, the statement 'particle one is in state a and particle two is in state b' wouldn't make sense. If it would, one could simply write for the total quantum state:

$$\Psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2),$$

where x_1, x_2 are the positions of particle one and two respectively. This statement doesn't take into account that one cannot distinguish between particle one and two, however. In practice, we can only say 'there are two particles in two different states'. Which particle is in which state is unknown. To express this mathematically, we write:[1]

$$\Psi_{\pm}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) \pm \psi_b(x_1)\psi_a(x_2)].$$

Finding particle one in state a and two in b is equally likely as finding one to be in state b and two in a. This requirement of symmetry can be written down more generally as:

$$\Psi(x_1, x_2) = \pm\Psi(x_2, x_1).$$

Whether there should be a plus or a minus depends on the type of particle. A minus sign implies that no two particles can be in the same place: if $x_1 = x_2$, we get

$$\Psi(x, x) = -\Psi(x, x),$$

which can only hold true when Ψ is zero. Particles with this property of not being able to be in the same place (or state in general) are called fermions. The other type of particles with a plus sign are called bosons. This thesis is focused on fermions, however.

If we want to describe a system with more than two fermions, this symmetry problem quickly becomes more complex. For example, for the three particle wave function to satisfy the symmetry conditions it is written down as:

$$\begin{aligned}\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}}[&\psi_a(x_1)\psi_b(x_2)\psi_c(x_3) - \psi_a(x_1)\psi_b(x_3)\psi_c(x_2) \\ &- \psi_a(x_2)\psi_b(x_1)\psi_c(x_3) + \psi_a(x_3)\psi_b(x_1)\psi_c(x_2) \\ &+ \psi_a(x_2)\psi_b(x_3)\psi_c(x_1) - \psi_a(x_3)\psi_b(x_2)\psi_c(x_1)].\end{aligned}$$

Swapping two coordinates in this equation results in the same equation with a minus sign, so as before, no two particles can be in the same place. In general, for many particles the wave function is given by (here, we label states by numbers instead of letters):

$$\Psi(x_1, x_2, ..., x_n) = \det \begin{pmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_n(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \cdots & \psi_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_1(x_n) & \psi_2(x_n) & \cdots & \psi_n(x_n) \end{pmatrix};$$

the so called Slater determinant.[9] When working with many-particle systems, this notation is very inefficient.

3.2 Second Quantization

3.2.1 Multi-particle Wave Function

Second quantization is a notation which makes it much more easy to work with wave functions involving more than one particle.

The idea is that states are built up from the so-called vacuum, or empty state $|0\rangle$. The empty state is the state where none of the possible states of the system is occupied by a particle.

Assume the system we are looking at has different states that we label by numbering them. A state with one particle in state 1 can be 'created' by working with a so-called creation operator on the empty state:

$$|1_1\rangle := c_1^\dagger |0\rangle$$

here, $c_1^\dagger$ is the creation operator that creates a particle in state one. We can also create a state with two particles in state 1 (bosons):

$$|2_1\rangle := c_1^\dagger c_1^\dagger |0\rangle = (c_1^\dagger)^2 |0\rangle ,$$

or a state with two particles in different states:

$$|1_1, 1_2\rangle := c_1^\dagger c_2^\dagger |0\rangle .$$

Besides the creation operators, there are also annihilation operators which are in fact the daggered version of the creation operators: $c_1 = (c_1^\dagger)^\dagger$. They remove a particle from the wave function:

$$c_1 |1_1\rangle = |0\rangle .$$

If there is no particle in that state to begin with, the state is destroyed; it is impossible to remove a particle from the empty state. Note that 0 is in this sense different from the empty state. For example:

$$c_2 |1_1\rangle = 0 \neq |0\rangle .$$

These types of creation and annihilation operators are called 'fermionic operators' when they regard fermions and 'bosonic operators' when they regard bosons.

One might wonder how the required symmetries of the fermions and bosons are represented in this notation. It is the commutation relations of the operators that take care of the symmetry: instead of worrying about how to write down a complicated state, one simply has to take into account the commutation relations to get the right symmetry. This will become clearer in the next subsection.

3.2.2 Fermionic Operators

I will now elaborate on the different relations of the fermionic operators. The bosonic operators are not relevant for this thesis.

First of all, we have, by the Pauli exclusion principle, that every state can be occupied by at most one particle. Adding another particle in the same state will destroy the wave function:

$$c_1^\dagger c_1^\dagger |0\rangle = c_1^\dagger |1_1\rangle = 0, \tag{3.1}$$

so $c_1^\dagger c_1^\dagger = 0$. Similarly, $c_1 c_1 = 0$.

Another feature is that when creating or destroying a particle, a minus sign might arise depending on the amount of particles in the preceding states. Mathematically:

$$c_j^\dagger |n_1, n_2, ..., n_{j-1}, 0, n_{j+1}, ...\rangle = (-1)^{\sum_{i<j} n_i} |n_1, n_2, ..., n_{j-1}, 1, n_{j+1}, ...\rangle , \tag{3.2}$$

where all n_i are 0 or 1. Here, we assume the j^{th} state is not occupied: if it were, the state would have been destroyed. We see that a minus sign arises precisely when the amount of occupied states *before* the j^{th} state is odd. E.g.:

$$c_2^\dagger c_1 |1,0\rangle = c_2^\dagger |0\rangle = |0,1\rangle$$
$$c_1 c_2^\dagger |1,0\rangle = -c_1 |1,1\rangle = -|0,1\rangle$$

The above example brings us to the following: the fermionic operators have anti-commutation relations. These are the same as commutation relations except that the minus is a plus: $\{a,b\} = a.b + b.a$. The anti-commutation relations can be checked on random states using properties 3.1 and 3.2 and are as follows:[2]

$$\{c_i, c_j\} = 0 \tag{3.3}$$
$$\{c_i^\dagger, c_j^\dagger\} = 0 \tag{3.4}$$
$$\{c_i, c_j^\dagger\} = \delta_{ij}. \tag{3.5}$$

These commutation relations are conserved under Fourier transformations. This can be seen by explicitly working out the anti-commutator of k-space operators a and $a^\dagger$ and using the inverse Fourier transformation:

$$\begin{aligned}
\{a_k, a_l^\dagger\} &= a_k a_l^\dagger + a_l^\dagger a_k \\
&= \frac{1}{N}\sum_j e^{-ikj} c_j \sum_{j'} e^{ilj'} c_{j'}^\dagger + \frac{1}{N}\sum_{j'} e^{ilj'} c_j^{\prime\dagger} \sum_j e^{-ikj} c_j \\
&= \frac{1}{N}\sum_{j,j'} e^{-i(kj-lj')}(c_j c_{j'}^\dagger + c_{j'}^\dagger c_j) \\
&= \frac{1}{N}\sum_j e^{-i(k-l)j} \text{ (because } (c_j c_{j'}^\dagger + c_{j'}^\dagger c_j) = \delta_{j,j'}) \\
&= \delta_{k,l}.
\end{aligned}$$

One can easily see that $\{a_k^\dagger, a_l^\dagger\} = \{a_k, a_l\} = 0$ by looking at the third line of the above equation and using $\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0$.

Now we have some tools to deal with many particle systems. We will first look at some useful properties of large systems and in the last chapter combine everything to get some real results.

CHAPTER 4

Spin Chains, Schmidt and Entanglement

What does entanglement entropy say about systems that consist of more than two spins? Consider a chain of N spins with a subsystem A consisting of k spins. We define B as the complement of subsystem A.

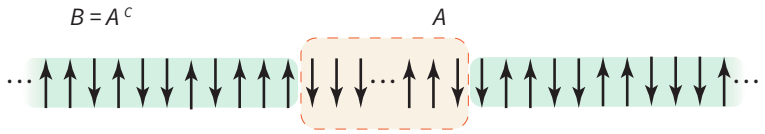

Figure 4.1: A schematic representation of a chain of spins divided into subsystems A and B.

The entanglement entropy of subsystem A tells us how many spins of A are entangled with B.[3] Remember that the most general state is written down as:

$$|\Psi\rangle = \sum_{\{s_i\}} c_{s_1 \dots s_N} |s_1\rangle |s_2\rangle \dots |s_N\rangle$$

where the s_i's are up or down and the c's are complex numbers such that $\sum_{\{s_i\}} c^2_{s_1 \dots s_N} = 1$. This sum contains 2^N elements, so for large N it is difficult to deal with this expression.

We are helped here by the 'Schmidt decomposition'. It comes from a theorem that can be formulated as follows:[10]

Assume we have a Hilbert space which we divide in two subsystems $\mathcal{H}_A$ and $\mathcal{H}_B$ such that the total space is $\mathcal{H}_A \otimes \mathcal{H}_B$. Assume subspace A has dimension m and subspace B dimension n, and $m \leq n$. Then for any vector $|\Psi\rangle$ from $\mathcal{H}_A \otimes \mathcal{H}_B$ there exist orthonormal bases $\{|1\rangle_A, ..., |m\rangle_A\}$ of $\mathcal{H}_A$ and $\{|1\rangle_B, ..., |n\rangle_B\}$ of $\mathcal{H}_B$ such that

$$|\Psi\rangle = \sum_{i}^{m} \lambda_i |i\rangle_A |i\rangle_B , \tag{4.1}$$

where λ_i are positive real numbers such that $\sum_i^m \lambda_i^2 = 1$. With this decomposition, we have reduced the amount of elements in the sum to the dimension of the smaller subspace.

Returning to the chain of length N with a small subsystem A of k spins, this means we can express any pure state from this system in the above form where the sum goes to 2^k.

A first result is that, in a pure state, the entanglement entropy of system A is equal to that of B; system A is entangled to B the same amount B is entangled to A. This is so because the reduced density matrices ρ_A and ρ_B have the same eigenvalues:[10]

$$\begin{aligned}\rho_A &= \sum_i \langle i|_B \Big(\sum_{i',i''} \lambda_{i'}\lambda_{i''} |i'\rangle_A |i'\rangle_B \langle i''|_A \langle i''|_B\Big) |i\rangle_B \\ &= \sum_i \lambda_i^2 |i\rangle_A \langle i|_A\end{aligned}$$

and similarly $\rho_B = \sum_i \lambda_i^2 |i\rangle_B \langle i|_B$. In both cases, the entropy becomes

$$S_A = S_B = -\sum_{i=1}^{2^k} \lambda_i^2 \log(\lambda_i^2).$$

We expect a random state, where the weights of all the product states are from a uniform distribution, to be almost maximally entangled. There is a theorem saying that for such a random state, in the Schmidt decomposition (in the limit $1 \ll k \ll N$) we have that $\lambda_i = \frac{1}{\sqrt{2^k}}$ for all i.[3] The Schmidt-decomposed state is thus a very simple state, contrary to the original state. We find the entanglement entropy to be

$$S_A = -\sum_{i=1}^{2^k} \frac{1}{2^k} \log(\frac{1}{2^k}) = 2^k * \frac{1}{2^k} * k \log(2) = k \log(2).$$

Here it becomes clear that the entropy scales linearly with the subsystem-size k. This is a result for random, maximally entangled states however, and we are also interested in more specific states. In the next chapter, we will look at the groundstates from the transverse field Ising model.

CHAPTER 5

The Ising Model for Small Systems

The model we are going to look at is called the 'transverse field Ising model'. Its Hamiltonian is given by

$$H = -J \sum_{i=1}^{N-1} S_i^x S_{i+1}^x - h \sum_{i=1}^{N} S_i^z, \tag{5.1}$$

where S^x, S^z are spin operators.[7] The coupling constant J expresses the interaction between neighboring spins: the energy gets lower if they have the same orientation in the x-direction and higher when they have different orientations. h expresses the interaction of the spins with a field pointing in the z-direction: for a spin, pointing along the positive z-direction is energetically more favorable then pointing in the negative direction. This model is more elaborate than the classical one: the fact that quantum spins can be in a superposition of two states plays a role in this model because spins have x- as well as z-interactions.

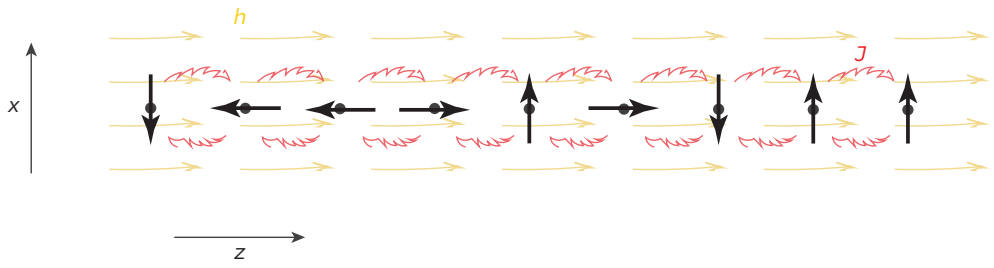

Figure 5.1: A schematic representation of the Ising model.

5.1 Solution for Two Spins

5.1.1 Finding the Eigenstates

The model is relatively easy to solve for two spins. To do so, we first simplify the Hamiltonian by including the factors $\frac{\hbar}{2}$ into the constants J and h. The Hamiltonian can now be expressed in terms of Pauli matrices:

$$\widetilde{H} = -J \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=1}^{N} \sigma_i^z. \tag{5.2}$$

For two spins:

$$\begin{aligned}\widetilde{H} &= -J\sigma_1^x \otimes \sigma_2^x - h(\sigma_1^z + \sigma_2^z) \\ &= -J\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \otimes \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} - h(\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}) \\ &= -\begin{pmatrix}2h & 0 & 0 & J\\ 0 & 0 & J & 0\\ 0 & J & 0 & 0\\ J & 0 & 0 & -2h\end{pmatrix},\end{aligned}$$

where the Hamiltonian is now expressed in the 2-spin z-basis: $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. This Hamiltonian can be diagonalized. Its eigenvectors and corresponding eigenvalues are given in the table below:

Eigenvector:	$\begin{pmatrix}0\\1\\1\\0\end{pmatrix}$	$\begin{pmatrix}0\\-1\\1\\0\end{pmatrix}$	$\begin{pmatrix}2h+\sqrt{4h^2+J^2}\\0\\0\\J\end{pmatrix}$	$\begin{pmatrix}-J\\0\\0\\2h+\sqrt{4h^2+J^2}\end{pmatrix}$
Eigenvalue:	$-J$	J	$-\sqrt{4h^2+J^2}$	$\sqrt{4h^2+J^2}$

Table 5.1: Eigenstates (not normalized) and corresponding eigenvalues of a two spin transverse field Ising model.

When plotting the eigenvalues as a function of J (setting h to 1), it becomes visible that in the limit of large J, states 1 and 3 as well as states 2 and 4 become degenerate.

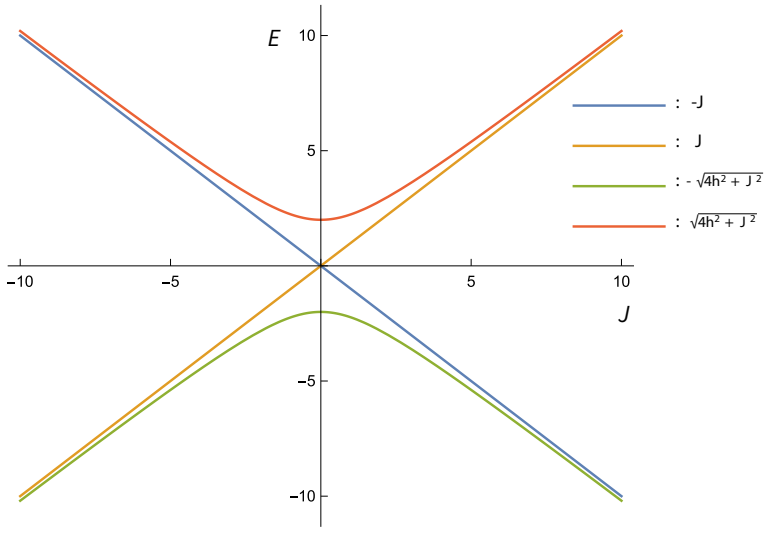

Figure 5.2: The eigenvalues of the two spin Ising model plotted as a function of J. Although no units are specified for the eigenvalues, physically they should correspond to energy.

5.1.2 Entanglement Entropy

The groundstate (the third state from table 5.1.1), when normalized, can be expressed as:

$$|\psi\rangle_{gs} = \frac{1}{\sqrt{2(4h^2 + J^2 + 2h\sqrt{4h^2 + J^2})}} \left[(2h + \sqrt{4h^2 + J^2}) \, |\uparrow\uparrow\rangle + J \, |\downarrow\downarrow\rangle \right].$$

The reduced density matrix of this state is given by

$$\rho_{red} = \frac{1}{2(4h^2 + J^2 + 2h\sqrt{4h^2 + J^2})} \left[(2h + \sqrt{4h^2 + J^2})^2 \, |\uparrow\rangle \langle\uparrow| + J^2 \, |\downarrow\rangle \langle\downarrow| \right].$$

This reduced matrix can be plugged into equation 2.3 directly, giving an analytical expression for the entanglement entropy. Setting h to 1, we can plot it as a function of J.

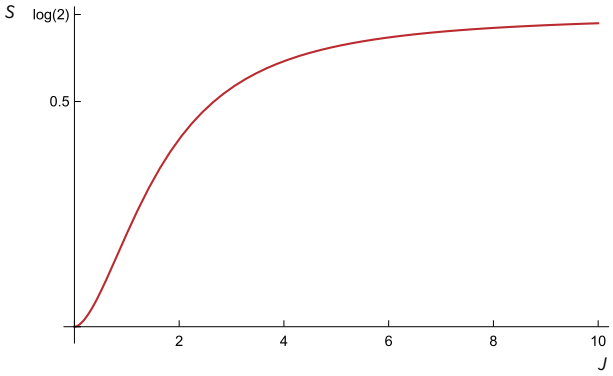

Figure 5.3: The entanglement entropy S in a two spin transverse field Ising model is plotted against the interaction factor J. The field h is set to 1.

We see that if J is zero, there is no entanglement. This is intuitive because zero J means there is no interaction. The groundstate will simply be all states aligning along the field h in the z-direction. For large J, meaning the interaction dominates, the state approaches maximum entanglement: $1 \log 2$.

The first two eigenstates, corresponding to the middle two values in the energy spectrum, are given by $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ and $\frac{1}{\sqrt{2}}(-|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ respectively. Both are independent of J and maximally entangled (they have entanglement entropy $\log 2$). They are very similar to the example given in section 2.2.

The fourth state exhibits the exact same entropy as the groundstate; their graphs overlap entirely. This is not very surprising because of the symmetry of the model. As can be seen in table 5.1.1, states with opposite energies are very symmetrical with respect to each other, in this case resulting in equal entanglement entropies.

5.2 Solution for 3 and 4 Spins

The 3- and 4-spin models are more complicated; their states have dimension 8 and 16 respectively. The matrix representation of the two models can be easily determined by

computing the tensor products (again setting $h = 1$):

$$H_3 = -J(\sigma_1^x \otimes \sigma_2^x + \sigma_2^x \otimes \sigma_3^x) - 1(\sigma_1^z + \sigma_2^z + \sigma_3^z)$$
$$= \begin{pmatrix} -3 & 0 & 0 & -J & 0 & 0 & -J & 0 \\ 0 & -1 & -J & 0 & 0 & 0 & 0 & -J \\ 0 & -J & -1 & 0 & -J & 0 & 0 & 0 \\ -J & 0 & 0 & 1 & 0 & -J & 0 & 0 \\ 0 & 0 & -J & 0 & -1 & 0 & 0 & -J \\ 0 & 0 & 0 & -J & 0 & 1 & -J & 0 \\ -J & 0 & 0 & 0 & 0 & -J & 1 & 0 \\ 0 & -J & 0 & 0 & -J & 0 & 0 & 3 \end{pmatrix}$$

and

$$H_4 = -J(\sigma_1^x \otimes \sigma_2^x + \sigma_2^x \otimes \sigma_3^x + \sigma_3^x \otimes \sigma_4^x) - 1(\sigma_1^z + \sigma_2^z + \sigma_3^z).$$

In the 3-spin model, the groundstate could be computed analytically. The 4-spin model was solved numerically, i.e. a value for J was entered first and then it was solved.

The reduced density matrices of the found eigenstates were computed using mathematica code.[11]

We can now compare the entropies of different subsystems of the groundstates.

When the system size is increased, the entanglement entropy of the leftmost spin increases as well. For larger systems, there are more spins this leftmost spin can entangle to. It still has a limit of $1 \log 2$, as could have been expected of a subsystem of size 1. Due to symmetry, the same result holds for the rightmost spin.

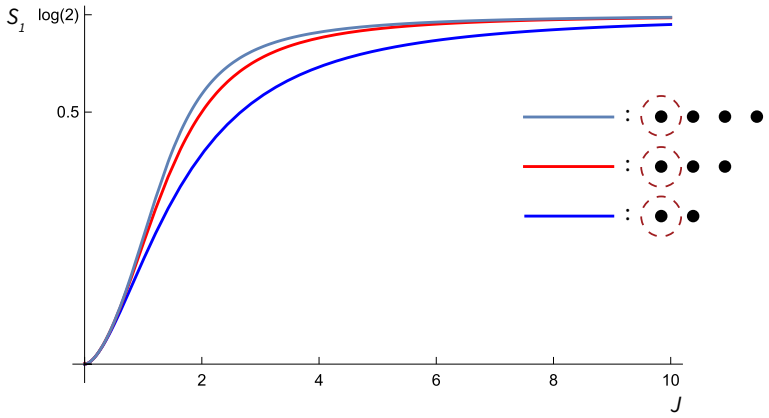

Figure 5.4: Entanglement entropies of the leftmost spins increase with the system size. Plotted here are the entropies of the leftmost spin in systems with 2,3 and 4 spins as a function of J.

In a system with 3 spins we can look at the entropy of the middle spin compared to a spin on the edge of the system. The middle spin has a larger entanglement entropy, which is in a way intuitive because this spin is more embedded in the system and can therefore mix more with its surroundings.

In a system with 3 spins, one could also take a subsystem of 2 spins, but the complement of this subsystem would then contain only 1 spin. As seen in chapter 4, the entanglement entropy of a subsystem and its complement are equal, so essentially we would again be dealing with a subsystem of size 1.

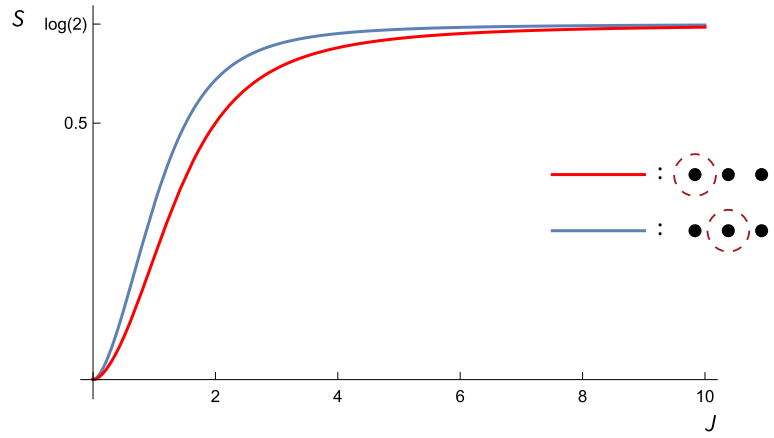

Figure 5.5: Comparison of the entanglement entropy of the middle and leftmost spin in a system of 3 spins.

Now when looking at a system with 4 spins, we can actually take subsystems larger than 1. There are 3 possible different subsystems we can take (taking into account that the entropy of a subsystem is equal to the entropy of its complement). Taking spin 1 and 3 gives the smallest entropy; spins 1 and 3 have no direct interaction so they do not form a coherent subsystem. Taking spins 2 and 3 gives a larger entropy, but their complement is very disconnected. The largest entropy is achieved by taking the subsystem containing spins 1 and 2. We see that the entropy actually exceeds our previous limit of $\log 2$, which is possible now the subsystem is larger than 1. It reaches a maximum value at a finite J but then returns to the limit of $\log 2$. This can be explained by the fact that in the limit of large J, the model becomes a simple fieldless ferromagnet where the groundstate is a superposition of all spins pointing left and all spins pointing right (along the x-axis). The entanglement of such a 'superposition of two states' is always $\log 2$.

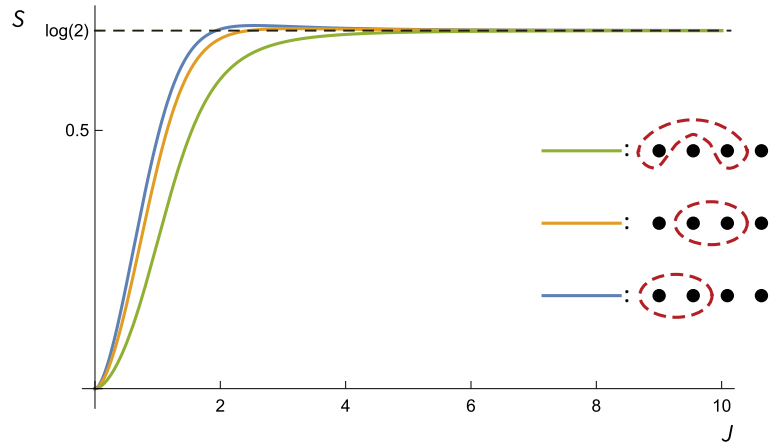

Figure 5.6: Comparison of the entanglement entropy of different subsystems in a system of 4 spins.

So far, we have looked at relatively small systems. Because the dimension of the system grows exponentially with $\sim 2^N$, the method used above quickly becomes too inefficient or even impossible. In the next chapter, methods are introduced which are used to solve larger systems.

CHAPTER 6

The Ising Model in Fermionic Language

6.1 Jordan Wigner Transformation

In order to deal with larger systems, it is convenient to express the Hamiltonian of the model in terms of fermionic operators. Somehow, there is a correspondence between the binary system of spins up or down and a system of fermions with occupied or unoccupied states.

The first thing we can note is that the correspondence between spins and fermions must lie in the creation and annihilation operators. In spin language, the dimensionless creation and annihilation operators are given by the Pauli matrices σ^+ and σ^-.[1] We cannot simply impose a 1-1 correspondence between spin and fermionic operators: spin operators have the wrong commutation relations. The spin operators commute ($\left[\sigma_i^+, \sigma_j^-\right] = 0$ if $i \neq j$) while fermionic operators anti-commute.

The following transformation remedies this:[5]

$$\sigma_i^+ = \Pi_{j<i}(1 - 2c_j^\dagger c_j)c_i^\dagger \qquad\qquad \sigma_i^- = \Pi_{j<i}(1 - 2c_j^\dagger c_j)c_i, \tag{6.1}$$

where $(1 - 2c_j^\dagger c_j)$ is equal to 1 if site j is empty and equal to -1 if it is full. In total, $\Pi_{j<i}(1 - 2c_j^\dagger c_j)$ will be +1 if the amount of filled sites before i is even and -1 if it is odd.

We have now expressed the spin creation and annihilation operators in terms of fermionic creation and annihilation operators such that the commutation relations are right. These transformed spin operators create and annihilate *fermions* instead of spins, but they behave in the exact same way, so this transformation gives us a 1-1 correspondence between fermions and spins. The benefit is that working with fermionic operators is easier than working with spin operators.

Now we are able to express $\sigma_i^x\sigma_{i+1}^x$ and σ_i^z in terms of fermionic operators. We use that $\sigma^x = (\sigma^+ + \sigma^-)$ and $\sigma^z = (\sigma^+\sigma^- - \sigma^-\sigma^+)$.

$$\begin{aligned}
\sigma_i^x\sigma_{i+1}^x &= (\sigma_i^+ + \sigma_i^-)(\sigma_{i+1}^+ + \sigma_{i+1}^-) \\
&= \Pi_{j<i}(1 - 2c_j^\dagger c_j)(c_i^\dagger + c_i)\Pi_{j<i+1}(1 - 2c_j^\dagger c_j)(c_{i+1}^\dagger + c_{i+1}) \\
&= \Pi_{j<i}(1 - 2c_j^\dagger c_j)^2(c_i^\dagger + c_i)(1 - 2c_i^\dagger c_i)(c_{i+1}^\dagger + c_{i+1}),
\end{aligned}$$

where in the last step, the commutation relations 3.3 were taken into account. We note that since $(1 - 2c_j^\dagger c_j)$ is either +1 or -1, its square is always 1. This means we can throw

away all the terms in the product:

$$\begin{aligned}\sigma_i^x\sigma_{i+1}^x &= (c_i^\dagger + c_i)(1-2c_i^\dagger c_i)(c_{i+1}^\dagger + c_{i+1}) \\ &= (c_i^\dagger - \cancel{2c_i^\dagger c_i^\dagger c_i} + c_i - 2c_i c_i^\dagger c_i)(c_{i+1}^\dagger + c_{i+1}) \\ &= (c_i^\dagger + c_i - 2(1-\cancel{c_i^\dagger c_i})c_i)(c_{i+1}^\dagger + c_{i+1}),\end{aligned}$$

so that finally

$$\sigma_i^x\sigma_{i+1}^x = (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}). \tag{6.2}$$

For σ_i^z we find

$$\begin{aligned}\sigma_i^z &= (\sigma_i^+\sigma_i^- - \sigma_i^-\sigma_i^+) \\ &= (\Pi_{j<i}(1-2c_j^\dagger c_j)c_i^\dagger\Pi_{j<i}(1-2c_j^\dagger c_j)c_i - \Pi_{j<i}(1-2c_j^\dagger c_j)c_i\Pi_{j<i}(1-2c_j^\dagger c_j)c_i^\dagger) \\ &= (c_i^\dagger c_i - c_i c_i^\dagger),\end{aligned} \tag{6.3}$$

where it was used again that $(1-2c_j^\dagger c_j)$ will always be 1 when squared. We now have everything to express the transverse field Ising model in terms of fermionic operators. Using equations 6.2 and 6.3 we find:

$$\begin{aligned}\widetilde{H} &= -J\sum_{i=1}^{N-1}\sigma_i^x\sigma_{i+1}^x - h\sum_{i=1}^{N}\sigma_i^z \\ &= -J\sum_{i=1}^{N-1}(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - h\sum_{i=1}^{N}(c_i^\dagger c_i - c_i c_i^\dagger).\end{aligned} \tag{6.4}$$

Having expressed the Hamiltonian in more familiar fermionic operators, we can move on to solving the model more efficiently for larger systems.

6.2 Reproducing the Result of 2 Spins

We want to compare results of the two-site fermionic Hamiltonian to the results we found directly for spins in section 5.1.1. For two sites, the Hamiltonian becomes (now in fermionic language):

$$\begin{aligned}H_2 &= -J(c_1^\dagger - c_1)(c_2^\dagger + c_2) - h(c_1^\dagger c_1 - c_1c_1^\dagger + c_2^\dagger c_2 - c_2c_2^\dagger) \\ &= -J(c_1^\dagger c_2 + c_1^\dagger c_2^\dagger + c_2c_1 + c_2^\dagger c_1) - h(c_1^\dagger c_1 - c_1c_1^\dagger + c_2^\dagger c_2 - c_2c_2^\dagger) \\ &= \begin{pmatrix} c_1^\dagger & c_2^\dagger & c_1 & c_2\end{pmatrix}\begin{pmatrix} -h & -J/2 & 0 & -J/2 \\ -J/2 & -h & J/2 & 0 \\ 0 & J/2 & h & J/2 \\ -J/2 & 0 & J/2 & h\end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger\end{pmatrix} \\ &= \vec{c^\dagger}\mathcal{H}\vec{c},\end{aligned} \tag{6.5}$$

where the matrix was made symmetrical by using the commutation relations 3.3, e.g. $c_1^\dagger c_2 = \frac{1}{2}(c_1^\dagger c_2 + c_1^\dagger c_2) = \frac{1}{2}(c_1^\dagger c_2 - c_2c_1^\dagger)$.

The eigenvectors and eigenvalues of the above matrix $\mathcal{H}$ (the above matrix inside the c-operator vectors) are as follows:

Eigenvectors:	$\begin{pmatrix} 2h+\sqrt{4h^2+J^2} \\ 2h+\sqrt{4h^2+J^2} \\ -J \\ J \end{pmatrix}$	$\begin{pmatrix} 2h+\sqrt{4h^2+J^2} \\ -2h-\sqrt{4h^2+J^2} \\ J \\ J \end{pmatrix}$	$\begin{pmatrix} J \\ J \\ 2h+\sqrt{4h^2+J^2} \\ -2h-\sqrt{4h^2+J^2} \end{pmatrix}$	$\begin{pmatrix} -J \\ J \\ 2h+\sqrt{4h^2+J^2} \\ 2h+\sqrt{4h^2+J^2} \end{pmatrix}$
	$\equiv \vec{u}_1$	$\equiv \vec{u}_2$	$\equiv \vec{u}_3$	$\equiv \vec{u}_4$
Eigenvalues:	$\frac{1}{2}(-J-\sqrt{4h^2+J^2})$	$\frac{1}{2}(J-\sqrt{4h^2+J^2})$	$\frac{1}{2}(-J+\sqrt{4h^2+J^2})$	$\frac{1}{2}(J+\sqrt{4h^2+J^2})$
	$\equiv -\epsilon_1$	$\equiv -\epsilon_2$	$= \epsilon_2$	$= \epsilon_1$

Table 6.1: The (not normalized) eigenvectors with corresponding eigenvalues of $\mathcal{H}$.

Note that these are not yet the eigenvectors and eigenvalues of the Hamiltonian.

Let U be the orthonormal matrix consisting of the normalized eigenvectors of $\mathcal{H}$: $U = \{\hat{\vec{u}}_1, \hat{\vec{u}}_2, \hat{\vec{u}}_3, \hat{\vec{u}}_4\}$ where $\hat{\vec{u}}_i = \frac{\vec{u}_i}{|\vec{u}_i|}$ are the normalized versions of the vectors above. We can rewrite equation 6.5 as follows:

$$
\begin{aligned}
H_2 &= \begin{pmatrix} c_1^\dagger & c_2^\dagger & c_1 & c_2 \end{pmatrix} UU^{-1} \begin{pmatrix} -h & -J/2 & 0 & -J/2 \\ -J/2 & -h & J/2 & 0 \\ 0 & J/2 & h & J/2 \\ -J/2 & 0 & J/2 & h \end{pmatrix} UU^{-1} \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix} \\
&= \begin{pmatrix} c_1^\dagger & c_2^\dagger & c_1 & c_2 \end{pmatrix} U \begin{pmatrix} -\epsilon_1 & 0 & 0 & 0 \\ 0 & -\epsilon_2 & 0 & 0 \\ 0 & 0 & \epsilon_2 & 0 \\ 0 & 0 & 0 & \epsilon_1 \end{pmatrix} U^{-1} \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix} \\
&= \begin{pmatrix} \hat{\vec{u}}_1 \cdot \vec{c}^\dagger & \hat{\vec{u}}_2 \cdot \vec{c}^\dagger & \hat{\vec{u}}_3 \cdot \vec{c}^\dagger & \hat{\vec{u}}_4 \cdot \vec{c}^\dagger \end{pmatrix} \begin{pmatrix} -\epsilon_1 & 0 & 0 & 0 \\ 0 & -\epsilon_2 & 0 & 0 \\ 0 & 0 & \epsilon_2 & 0 \\ 0 & 0 & 0 & \epsilon_1 \end{pmatrix} \begin{pmatrix} \hat{\vec{u}}_1 \cdot \vec{c} \\ \hat{\vec{u}}_2 \cdot \vec{c} \\ \hat{\vec{u}}_3 \cdot \vec{c} \\ \hat{\vec{u}}_4 \cdot \vec{c} \end{pmatrix} \\
&= \begin{pmatrix} \gamma_1 & \gamma_2 & \gamma_2^\dagger & \gamma_1^\dagger \end{pmatrix} \begin{pmatrix} -\epsilon_1 & 0 & 0 & 0 \\ 0 & -\epsilon_2 & 0 & 0 \\ 0 & 0 & \epsilon_2 & 0 \\ 0 & 0 & 0 & \epsilon_1 \end{pmatrix} \begin{pmatrix} \gamma_1^\dagger \\ \gamma_2^\dagger \\ \gamma_2 \\ \gamma_1 \end{pmatrix} \\
&= \epsilon_1(\gamma_1^\dagger\gamma_1 - \gamma_1\gamma_1^\dagger) + \epsilon_2(\gamma_2^\dagger\gamma_2 - \gamma_2\gamma_2^\dagger).
\end{aligned}
$$

One can easily check that $\gamma_1^\dagger := \hat{\vec{u}}_1 \cdot \vec{c}$ is indeed the daggered version of $\gamma_1 := \hat{\vec{u}}_4 \cdot \vec{c}$ by using the symmetry of the vectors $\vec{u}_1$ and $\vec{u}_4$. These gammas are new fermionic operators that create and destroy what are called 'Bogoliubons'. Expressed in the language of Bogoliubons, the Hamiltonian is easy to solve. The groundstate is simply given by the empty Bogoliubon state $|\text{VAC}\rangle$:

$$
H_2 |\text{VAC}\rangle = \epsilon_1(\cancel{\gamma_1^\dagger\gamma_1} - \gamma_1\gamma_1^\dagger) + \epsilon_2(\cancel{\gamma_2^\dagger\gamma_2} - \gamma_2\gamma_2^\dagger) |\text{VAC}\rangle = (-\epsilon_1 - \epsilon_2) |\text{VAC}\rangle ,
$$

where $-\epsilon_1 - \epsilon_2 = -\sqrt{4h^2+J^2}$. This energy is the same one we found in section 5.1.1.

We now also want to find the groundstate in terms of regular fermions, instead of Bogoliubov fermions. In other words: we want to express our Bogoliubov vacuum $|\text{VAC}\rangle$ in terms of fermions. To do so, we first write down $|\text{VAC}\rangle$ in the most general way possible:

$$
|\text{VAC}\rangle = \alpha c_1^\dagger c_2^\dagger |0\rangle + \beta c_1^\dagger |0\rangle + \gamma c_2^\dagger |0\rangle + \delta |0\rangle ,
$$

with $|0\rangle$ the fermion-vacuum and $\alpha, \beta, \gamma, \delta$ constants that we have to determine. We impose two requirements on the vacuum:

$$\gamma_1 |\text{VAC}\rangle = 0$$
$$\gamma_2 |\text{VAC}\rangle = 0;$$

in other words: the Bogoliubov annihilation operators should destroy it. These requirements give a series of relations from which finally follows:

$$\begin{aligned} |\text{VAC}\rangle &= \frac{1}{\sqrt{2(4h^2 + J^2 + 2h\sqrt{4h^2 + J^2}}} \left((2h + \sqrt{4h^2 + J^2}) c_1^\dagger c_2^\dagger + J \right) |0\rangle \\ &= \frac{1}{\sqrt{2(4h^2 + J^2 + 2h\sqrt{4h^2 + J^2}}} \left((2h + \sqrt{4h^2 + J^2}) |11\rangle + J |0\rangle \right), \end{aligned}$$

which is indeed what we found to be the groundstate in section 5.1.1, only now in language of fermions instead of spins. Because of the 1-1 correspondence we established, they can be regarded as equal. This Bogoliubov vacuum is known from the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity and it is often referred to as the BCS state.[8]

6.3 Solution for a Periodic Chain of N Sites

We are now going to look at periodic 1-dimensional Ising chains. The reason for the periodicity is that it will allow us to perform a Fourier transformation. Periodicity simply means here that if we have N sites, the $(N+1)$th site will be again the first site. On every site, there can be 1 or 0 fermions corresponding to spin up or down.

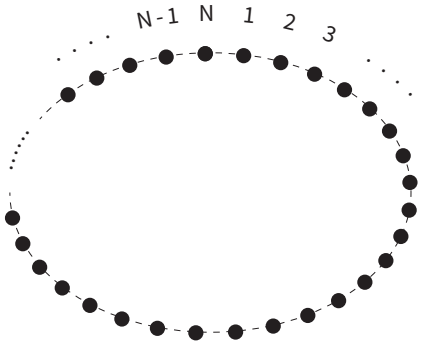

Figure 6.1: Schematic representation of a periodic chain of N different sites.

6.3.1 Periodic and Anti-periodic Boundary Conditions

Because of the periodicity, we have that for the spin matrices:

$$S^x_{N+1} = S^x_1, \qquad S^z_{N+1} = S^z_1.$$

This does not simply imply that $c_{N+1} = c_1$, however. We have to be careful and keep in mind that fermionic operators might give a minus sign depending on the amount of particles before them, as stated in equation 3.2.

We will explicitly determine $S^x_N S^x_{N+1} = S^x_N S^x_1 = (\sigma^+_N + \sigma^-_N)(\sigma^+_1 + \sigma^-_1)$ in terms of fermions. Using the Jordan Wigner transformation:

$$\begin{aligned}\sigma^-_1 &= \Pi_{j<1}(1 - 2c^\dagger_j c_j)c_1 = c_1\\ \sigma^-_N &= \Pi_{j<N}(1 - 2c^\dagger_j c_j)c_N = (-1)^{\sum_{j=1}^{N-1} n_j} c_N,\end{aligned}$$

where n_j is 1 if site j is occupied and 0 if it is not. We get:

$$\begin{aligned}(\sigma^+_N + \sigma^-_N)(\sigma^+_1 + \sigma^-_1) &= \left((-1)^{\sum_{j=1}^{N-1} n_j} c^\dagger_N + (-1)^{\sum_{j=1}^{N-1} n_j} c_N\right)\left(c^\dagger_1 + c_1\right)\\ &= (-1)^{\sum_{j=1}^{N} n_j}\left((-1)^{n_N} c^\dagger_N + (-1)^{n_N} c_N\right)\left(c^\dagger_1 + c_1\right)\\ &= (-1)^{\mathcal{F}}\left((1 - 2c^\dagger_N c_N)c^\dagger_N + (1 - 2c^\dagger_N c_N)c_N\right)\left(c^\dagger_1 + c_1\right),\end{aligned}$$

where $\mathcal{F}$ is the amount of fermions in the system. $(-1)^{\mathcal{F}}$ is called the parity of the system. This expression can be simplified further using the commutation relations 3.3:

$$\begin{aligned}&= (-1)^{\mathcal{F}}\left((1 - 2(1 - \cancel{c_N c^\dagger_N}))c^\dagger_N + (1 - \cancel{2c^\dagger_N c_N})c_N\right)\left(c^\dagger_1 + c_1\right)\\ &= (-1)^{\mathcal{F}}\left(-c^\dagger_N + c_N\right)\left(c^\dagger_1 + c_1\right)\\ &= (-1)^{\mathcal{F}+1}\left(c^\dagger_N - c_N\right)\left(c^\dagger_1 + c_1\right).\end{aligned}$$

Comparing this with the term $\left(c^\dagger_N - c_N\right)\left(c^\dagger_{N+1} + c_{N+1}\right)$ we would naively get from the sum, we can conclude that

$$c_{N+1} = c_1 \qquad \text{if } \mathcal{F} \text{ is odd,} \tag{6.6}$$

$$c_{N+1} = -c_1 \qquad \text{if } \mathcal{F} \text{ is even.} \tag{6.7}$$

These conditions are called periodic and anti-periodic boundary conditions respectively.

6.3.2 Fourier Transformation

We write our Hamiltonian for an N-site periodic chain as

$$H = -J\sum_{i=1}^{N-1}(c^\dagger_i - c_i)(c^\dagger_{i+1} + c_{i+1}) \mp J(c^\dagger_N - c_N)(c^\dagger_1 + c_1) - h\sum_{i=1}^{N}(c^\dagger_i c_i - c_i c^\dagger_i)$$

where we have a minus at the second term if the amount of fermions in the system is odd and a plus if it is even. In other words: in the case of an odd number of fermions the Hamiltonian has periodic boundary conditions and in case of an even number anti-periodic.

We do not know in advance what the amount of states in the eigensystems will be. Furthermore, we do not know how an anti-periodic system will behave under a Fourier transformation.

Let us concentrate on anti-periodic boundary conditions. From the condition $c_{N+1} = -c_N$ we get a restriction on the possible momenta k of our momentum operators:

$$\begin{aligned}&c_{N+1} = -c_1\\ &\Rightarrow \sum_k e^{i(N+1)k} a_k = -\sum_k e^{ik} a_k\\ &\Rightarrow e^{iNk} = -1 \Rightarrow Nk = -\pi + 2\pi j\\ &\Rightarrow k = -\frac{\pi}{N} + \frac{2\pi j}{N}\end{aligned} \tag{6.8}$$

where k now has N different values for $j \in \{0, 1, 2, ..., N-1\}$.

We perform a Fourier transformation on the components of the anti-periodic Hamiltonian:

- $-J\sum_{j=1}^{N-1}(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})$ becomes:

$$\begin{aligned} -J\sum_{j=1}^{N-1}\sum_{k,k'}[&e^{-ik'}e^{-ij(k+k')}a_k^\dagger a_{k'}^\dagger + e^{ik'}e^{-ij(k-k')}a_k^\dagger a_{k'} + e^{-ik'}e^{ij(k-k')}a_{k'}^\dagger a_k \\ &- e^{ik'}e^{ij(k+k')}a_k a_{k'}]. \end{aligned} \tag{6.9}$$

- $J(c_N^\dagger - c_N)(c_1^\dagger + c_1)$ becomes:

$$\begin{aligned} &J\sum_{k,k'}[e^{-ikN}e^{-ik'}a_k^\dagger a_{k'}^\dagger + e^{-ikN}e^{ik'}a_k^\dagger a_{k'} + e^{ikN}e^{-ik'}a_{k'}^\dagger a_k - e^{ikN}e^{ik'}a_k a_{k'}] \\ &= -J\sum_{k,k'}[e^{-iN(k+k')}e^{-ik'}a_k^\dagger a_{k'}^\dagger + e^{-iN(k-k')}e^{ik'}a_k^\dagger a_{k'} + e^{iN(k-k')}e^{-ik'}a_{k'}^\dagger a_k \\ &\qquad - e^{iN(k+k')}e^{ik'}a_k a_{k'}] \end{aligned} \tag{6.10}$$

  where was used that $e^{ik'N} = e^{-ik'N} = -1$.

- $-h\sum_{i=1}^{N-1}(c_i^\dagger c_i - c_i c_i^\dagger)$ becomes:

$$-h\sum_k (c_k^\dagger c_k - c_k c_k^\dagger)$$

It becomes visible that expressions 6.9 and 6.10 match: expression 6.10 is simply the Nth term of the sum in 6.9. Combining everything, we get:

$$\begin{aligned} H = -J\sum_{j=1}^{N}\sum_{k,k'}[&e^{-ik'}e^{-ij(k+k')}a_k^\dagger a_{k'}^\dagger + e^{ik'}e^{-ij(k-k')}a_k^\dagger a_{k'} + e^{-ik'}e^{ij(k-k')}a_{k'}^\dagger a_k \\ &- e^{ik'}e^{ij(k+k')}a_k a_{k'}] - h\sum_k (c_k^\dagger c_k - c_k c_k^\dagger), \end{aligned}$$

so that finally, using $\sum_{j=1}^{N} e^{ij(k+k')} = \delta_{k,-k'}$, $\sum_{j=1}^{N} e^{ij(k-k')} = \delta_{k,k'}$:

$$H = -J\sum_k [e^{ik}c_k^\dagger c_{-k}^\dagger + e^{ik}c_k^\dagger c_k + e^{-ik}c_k^\dagger c_k - e^{-ik}c_k c_{-k}] - h\sum_k (c_k^\dagger c_k - c_k c_k^\dagger). \tag{6.11}$$

This expression for the Hamiltonian is actually not only right for the even (anti-periodic) case, but also for the odd (periodic) case. The difference between the two cases lies in the k-values. In equation 6.8 we saw the possible values for the even case. For the odd (periodic) case we have (again, $j \in \{0, 1, ..., N-1\}$):

$$e^{iNk} = 1 \Rightarrow k = \frac{2\pi j}{N}$$

6.3.3 Bogoliubov Transformation

We now want to find the eigenvalues and eigenvectors of the Fourier-transformed Hamiltonian 6.11. To do so, we first rewrite it in a more symmetrical way. We rewrite (using

commutation relations):

$$\sum_k e^{ik} c_k^\dagger c_{-k}^\dagger = \frac{1}{2}\sum_k (e^{ik} c_k^\dagger c_{-k}^\dagger - e^{-ik} c_k^\dagger c_{-k}^\dagger) = \sum_k i\sin(k) c_k^\dagger c_{-k}^\dagger,$$

$$\text{(and similarly)} \qquad -\sum_k e^{ik} c_k c_{-k} = -\sum_k i\sin(k) c_{-k} c_k,$$

and

$$\sum_k (e^{ik} c_k^\dagger c_k + e^{-ik} c_k^\dagger c_k) = \sum_k \cos(k)(c_k^\dagger c_k - c_{-k} c_{-k}^\dagger),$$

so that

$$H = -J\sum_k [i\sin(k)(c_k^\dagger c_{-k}^\dagger - c_{-k} c_k) + \cos(k)(c_k^\dagger c_k - c_{-k} c_{-k}^\dagger)] - h\sum_k (c_k^\dagger c_k - c_k c_k^\dagger).$$

This can be rewritten as

$$H = \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} -J\cos(k) - h & -iJ\sin(k) \\ iJ\sin(k) & J\cos(k) + h \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}. \tag{6.12}$$

This above matrix can be diagonalized: its eigenvalues are $\pm\lambda_k = \pm\sqrt{J^2 + h^2 + 2Jh\cos(k)}$ with corresponding eigenvectors

$$\vec{v_+} = \frac{1}{\sqrt{2\lambda_k(\lambda_k + J\cos(k) + h)}} \begin{pmatrix} -iJ\sin(k) \\ J\cos(k) + h + \lambda_k \end{pmatrix} \text{ for } +\lambda_k \tag{6.13}$$

$$\vec{v_-} = \frac{1}{\sqrt{2\lambda_k(\lambda_k + J\cos(k) + h)}} \begin{pmatrix} J\cos(k) + h + \lambda_k \\ -iJ\sin(k) \end{pmatrix} \text{ for } -\lambda_k. \tag{6.14}$$

With these orthonormal vectors we can construct a matrix U which diagonalizes the above matrix. Let $U = \begin{pmatrix} \vec{v_+} & \vec{v_-} \end{pmatrix}$, $U^{-1} = U^\dagger = \begin{pmatrix} \vec{v_+}^\dagger \\ \vec{v_-}^\dagger \end{pmatrix}$. Then equation 6.12 becomes:

$$\begin{aligned} H &= \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} UU^{-1} \begin{pmatrix} -J\cos(k) - h & -iJ\sin(k) \\ iJ\sin(k) & J\cos(k) + h \end{pmatrix} UU^{-1} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \\ &= \sum_k \begin{pmatrix} \gamma_k^\dagger & \gamma_{-k} \end{pmatrix} \begin{pmatrix} +\lambda_k & 0 \\ 0 & -\lambda_k \end{pmatrix} \begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix} \\ &= \sum_k \lambda_k(\gamma_k^\dagger \gamma_k - \gamma_k \gamma_k^\dagger), \end{aligned}$$

where

$$\begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix} = U^{-1} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} = \frac{1}{\sqrt{2\lambda_k(\lambda_k + J\cos(k) + h)}} \begin{pmatrix} iJ\sin(k) c_k + (J\cos(k) + h + \lambda_k) c_{-k}^\dagger \\ (J\cos(k) + h + \lambda_k) c_k + iJ\sin(k) c_{-k}^\dagger \end{pmatrix} \tag{6.15}$$

is now a vector consisting of two linear combinations of c_k and $c_{-k}^\dagger$. These two linear combinations define new fermionic operators, just like we saw in section 6.2. This 'transformation of fermionic operator basis' is called a Bogoliubov transformation.[8] The new operators γ and $\gamma^\dagger$ destroy and create 'Bogoliubov particles'.

With the Bogoliubov transformation, the Hamiltonian becomes a very simple expression. The groundstate is given by the empty Bogoliubov state with energy $E_{gs} = -\sum_k \lambda_k$.

6.3.4 Reproducing the Results of Two Spins

We can compare this energy with what was found in section 5.1.1. A two site model without periodicity is equivalent to a two site model *with* periodicity with half the interaction energy. In other words, if we replace J by $J/2$ we expect to get the same results. We now have to be careful and distinguish between the cases of an even and odd amount of particles.

Figure 6.2: Similarity between a 2-site periodic and non-periodic chain.

We start with the case of an even amount of particles (where we expect to find the groundstate, as can be seen in table 5.1.1). In this case, $k \in \{-\pi/2, \pi/2\}$. We find for the highest and lowest possible eigenenergies (corresponding to empty and full Bogoliubov states):

$$\begin{aligned} E_{gs}^{\text{even}} &= -\sum_k \lambda_k = -\sqrt{\frac{J^2}{4} + h^2 + Jh\cos(-\pi/2)} - \sqrt{\frac{J^2}{4} + h^2 + Jh\cos(\pi/2)} \\ &= -\sqrt{J^2 + 4h^2}, \\ E_{ex}^{\text{even}} &= \sum_k \lambda_k = \sqrt{J^2 + 4h^2}, \end{aligned}$$

which is what we had. For an odd amount of particles, we have $k \in \{0, \pi\}$, corresponding to energies

$$\begin{aligned} E_{gs}^{\text{odd}} &= -\sum_k \lambda_k = -\sqrt{\frac{J^2}{4} + h^2 + Jh\cos(0)} - \sqrt{\frac{J^2}{4} + h^2 + Jh\cos(\pi)} = -J, \\ E_{ex}^{\text{odd}} &= \sum_k \lambda_k = J. \end{aligned}$$

We have reproduced the correct energies as eigenenergies of the empty and full Bogoliubov states. States containing only one Bogoliubov particle are also eigenstates, but they do not give right energies. These 'extra results' are inconvenient. Usually, we are only interested in the groundstate, however, which is always the empty Bogoliubov state.

Finding the groundstate (now in k-space) is a matter of determining what exactly the empty Bogoliubov state, let's call it $|\text{VAC}\rangle$, is in terms of regular fermionic momentum operators. This is done by expressing $|\text{VAC}\rangle$ in the most general way possible as a superposition of all possible states and then imposing

$$\gamma_k |\text{VAC}\rangle = 0. \tag{6.16}$$

For two particles we can take the ansatz that the groundstate must be even, thus of the form $|\text{VAC}\rangle = (\alpha + \beta c_{-\pi/2}^\dagger c_{\pi/2}^\dagger)|0\rangle$. Using the γ_k from equation 6.15 (with $J/2$) we get the conditions (we neglect the cosine terms since they become zero):

$$\begin{aligned} \gamma_{-\pi/2}|\text{VAC}\rangle &= (-i\frac{J}{2}c_{-\pi/2} + (h + \sqrt{J^2/4 + h^2})c_{\pi/2}^\dagger)(\alpha + \beta c_{-\pi/2}^\dagger c_{\pi/2}^\dagger)|0\rangle \\ &= (-i\frac{J}{2}\beta + (h + \sqrt{J^2/4 + h^2})\alpha)c_{\pi/2}^\dagger|0\rangle = 0, \end{aligned}$$

and similarly

$$\gamma_{\pi/2}\left|\mathrm{VAC}\right\rangle = (-i\frac{J}{2}\beta + (h+\sqrt{J^2/4+h^2})\alpha)c^\dagger_{-\pi/2}\left|0\right\rangle = 0.$$

We see that $\alpha = \frac{iJ\beta}{2h+\sqrt{J^2+4h^2}}$. This together with the condition that $|\alpha|^2+|\beta|^2=1$ gives the following result for $|\mathrm{VAC}\rangle$:

$$\begin{aligned}\left|\mathrm{VAC}\right\rangle &= \frac{1}{\sqrt{2(4h^2+J^2+2h\sqrt{4h^2+J^2})}}(J - i(2h+\sqrt{J^2+4h^2})c^\dagger_{-\pi/2}c^\dagger_{\pi/2})\left|0\right\rangle \\ &= \frac{1}{\sqrt{2(4h^2+J^2+2h\sqrt{4h^2+J^2})}}(J + (2h+\sqrt{J^2+4h^2})c^\dagger_1 c^\dagger_2)\left|0\right\rangle,\end{aligned}$$

where in the last step a Fourier-transformation was taken. This is indeed the result we expected.

Condition 6.16 can also be solved in general, for any amount of particles. The general case is a quite well-known problem and it is solved in the Bardeen–Cooper–Schrieffer theory of superconductivity.[8] The result is that if

$$\gamma_k = u_k c_k + v_k c^\dagger_{-k},$$

with u_k, v_k momentum dependent variables, then

$$\left|\mathrm{VAC}\right\rangle = \prod_k (u_k - v_k c^\dagger_k c^\dagger_{-k})\left|0\right\rangle.$$

where $|0\rangle$ is the regular vacuum state. In our case:

$$\left|\mathrm{VAC}\right\rangle = \prod_k \frac{1}{\sqrt{2\lambda_k(\lambda_k + J\cos(k)+h)}}(iJ\sin(k) - (J\cos(k)+h+\lambda_k)c^\dagger_k c^\dagger_{-k})\left|0\right\rangle.$$

CHAPTER 7

Conclusion and Outlook

The concepts of entanglement and entanglement entropy have been introduced. They have been applied to the eigenstates of small sized transverse field Ising models.

In small models, we have seen that the groundstate naturally contains some entanglement provided the interaction constant is bigger than zero. The entanglement generally grows as a function of the interaction. For subsystems larger than one spin, we have seen that they can surpass the limit of $\log 2$ of one-spin subsystems. In the limit of large interaction, the model will behave as a fieldless ferromagnet and the groundstate will be a superposition of all spins left and all spins right. This means that in this limit, the entanglement again goes to $\log 2$, regardless of the size of the subsystem.

The formalism of second quantization has been introduced and applied to the transverse field Ising model in the form of a Jordan-Wigner transformation. Expressed in the more manageable fermionic operators, the Hamiltonian could be solved using a Fourier and then a Bogoliubov transformation.

The next step would be to try and find a way to determine the entanglement entropy efficiently from states in the fermionic language.

The groundstate that was determined at the end of chapter 6 is expressed in terms of fermionic *momentum* operators, instead of spacial fermionic operators. Transforming the groundstate from its momentum form back to its spatial form is not at all trivial so it is a question whether this process could be generalized.

For the entropy, the dimensions of the subsystems are very relevant. It remains a question whether the entropy can be determined efficiently without constructing enormous density matrices. The Schmidt decomposition has given a hopeful indication in that regard. In the Schmidt decomposition, the reduced density matrix still grows exponentially with the subsystem size, so there is still a limit.

If these difficulties are dealt with, the entanglement of different (small sized) subsystems of momentum states or spatial states could be studied and compared for any system size.

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