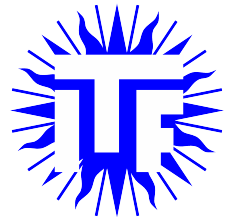




Utrecht University



Faculty of Science
Institute of Theoretical Physics
Condensed Matter

Study of the ground state of the one-dimensional Heisenberg spin- $\frac{1}{2}$ chain

BACHELOR THESIS

K.R. de Ruiter

Physics and astronomy

Supervisor:

Dr. D. Schuricht
Institute of Theoretical Physics

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Abstract

We discuss the ground state of the Heisenberg spin- $\frac{1}{2}$ chain in one dimension, considering nearest neighbor interactions. In the thermodynamic limit the energy is calculated analytically in several ways. We start by applying the Bethe ansatz to calculate the exact ground state energy of the XXX Heisenberg model. Next we study small perturbations of the system around $\Delta = 0$, the parameter for the interaction in the z -direction for the XXZ model, by applying time-independent perturbation theory. In addition we expand an exact integral expression of the energy of the XXZ model around $\Delta = 0$ in the thermodynamic limit. The results are compared to numerical solutions, which are obtained by means of exact diagonalization up to twelve lattice sites. We find that for ten or more lattice sites the numerics agree well with the expectation from the analytical calculations. Finally the concept of integrability is discussed in the context of the Heisenberg model.

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Notation

Symbol	Explanation
E_0	Ground state energy.
E_∞	Ground state energy in the thermodynamic limit.
L	Number of lattice sites.
N	Number down spins.
\hbar	In this entire thesis $\hbar = 1$.
a	Lattice spacing. Also $a = 1$ in this thesis.
x_{k+1}	Denotes site $k + 1$. This is equal to $x_k + 1$, as $a = 1$.
\uparrow	An up spin.
\downarrow	A down spin.

1 Introduction

Magnetism is caused by processes that take place on a microscopic level. To understand how magnetism arises we must therefore understand the structure of an atom [1]. An atom consists of a nucleus and electrons, which are in orbitals around the nucleus. Electrons have a characteristic called spin, which is a form of angular momentum. It is a property which has a magnitude and a direction. Because of the spin, electrons possess a magnetic moment, resulting in a magnetic field. The spin of an electron is pointed either upwards or downwards. It is therefore usually illustrated as an arrow, which points from the north pole to the south pole of the magnetic field induced by the magnetic moment. The orbitals of an atom are filled by electrons according to Hund's rules. In an atom each orbital can carry up to two electrons. This is because of the Pauli exclusion principle, which tells us that a specific state can never be occupied by more than one fermion. Therefore, if two electrons are in a single orbital, one of their spins must be pointed upwards and the other must be pointed downwards. This way they have different spin quantum numbers, and thus are in different states. Because of this their magnetic fields exactly cancel each other out. However, there are materials that have atoms with orbitals that are not completely filled, and thus contain unpaired electrons. If these electrons have spins in the same direction, then the magnetic fields of these electrons are not cancelled out, creating a net magnetization. These materials are magnets. More specifically, a material of which the spins of the unpaired electrons are aligned, is called a ferromagnet. Some objects are only magnetic when they are exposed to an external magnetic field. In the absence of an external magnetic field, the unpaired electrons of such an object are orientated in such a way that the total magnetic field is cancelled out. This is the case when there is no magnetic ordering, and thus the unpaired spins are all orientated in random directions. This is called a paramagnet. Another possibility is that neighboring spins have opposite directions, cancelling out the total field. In this case there is magnetic ordering, but no net magnetic field. These materials are called antiferromagnets. However, when either of these materials is exposed to an external magnetic field, the spins of the unpaired electrons are aligned due to the external field, resulting in a net magnetization. A few different types of magnets are shown in Figure 1, where the arrows represent the direction and magnitude of the spins of electrons.

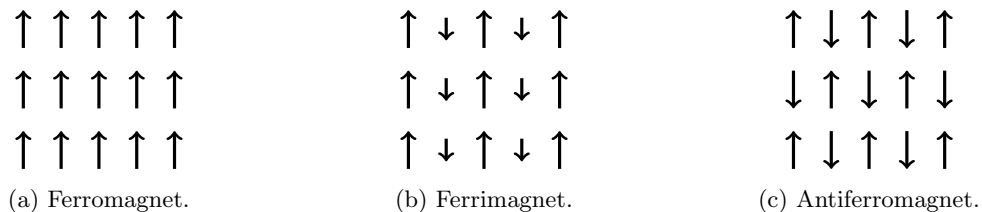


Figure 1: Different types of magnets.

In a ferrimagnet there are both up and down spins, but the magnitude of the moment in one direction is smaller than the other, resulting in a magnetization in the direction of the larger moment. This can for example happen when an object consists of different materials. We see that the ferromagnet and ferrimagnet both have a permanent magnetization, as opposed to the antiferromagnet, where the total magnetization is cancelled out. Most everyday magnets are either ferromagnets or ferrimagnets.

The Hamiltonian describing a magnetic material is of the following form

$$H = J_{xy} \sum_j [S_{j+1}^x S_j^x + S_{j+1}^y S_j^y] + J_z \sum_j S_{j+1}^z S_j^z.$$

This is known as the Heisenberg model. The \vec{S} are the spin- $\frac{1}{2}$ operators, and J is a coupling term related to the overlap of orbitals of neighboring atoms. More specifically, J is an exchange integral, which originates from quantum mechanics and Coulomb interaction. It describes both the antisymmetric quantum mechanical exchange interaction between electrons, and the electromagnetic Coulomb interaction between electrons.

In two and three dimensions the model can be studied using mean field theory. This theory approximates an interacting many-body system by averaging the interactions. A single particle is then considered in this average field, reducing it to a simple one-body system. Though this theory does not provide exact results, it

is used often to study phase transitions. For example, in two and three dimensions mean field theory can be used to study the behaviour of a material around its critical temperature, T_C . This is the temperature above which the magnetic ordering in a material is lost. In other words, above this temperature, a magnet becomes paramagnetic. In Figure 2 an ordered (ferromagnetic) and disordered (paramagnetic) phase are shown. The temperature dependence of magnetization is illustrated in Figure 3, together with the two phases.

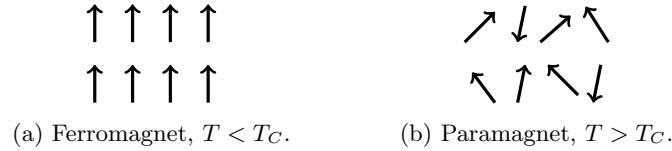


Figure 2: There is magnetic ordering below the critical temperature, T_C . Above the critical temperature there is no longer magnetic ordering.

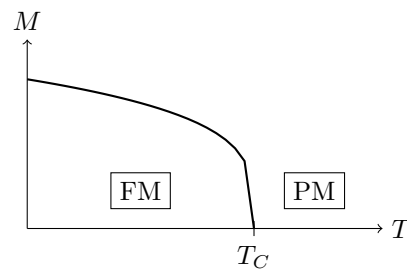


Figure 3: A sketch of magnetization as a function of temperature. At the critical temperature, T_C , magnetic ordering is lost. The ferromagnetic (FM) and paramagnetic (PM) phases are shown.

The critical temperature is called the Curie temperature for ferromagnets, and the Néel temperature for antiferromagnets. Magnetic ordering, the critical temperature, and mean field theory are discussed in more detail in Chapter 33 of Reference [2].

In this thesis we focus on one-dimensional spin chains. What makes the one-dimensional system interesting is that, in contrast with two and three dimensions, the one-dimensional system can be solved exactly. This will be discussed in Section 2 of this thesis. The method to exactly solve this system, the Bethe ansatz, was discovered by the German-American physicist Hans Bethe [3]. He is mostly known for his contribution in the field of nuclear physics. One of his biggest accomplishments is the discovery of the reactions which fuel a star. For this work he was awarded the Nobel Prize in 1967. However, before his work in nuclear physics, he also worked on solid-state physics. In 1931 Hans Bethe developed the Bethe ansatz. He used this method to find the exact solution to the one-dimensional antiferromagnetic Heisenberg model. See Reference [4] for his original paper. Bethe hoped to solve Heisenberg model in two and three dimensions as well by using this method. However, the Bethe ansatz failed in these cases. Later it was discovered that this is because the Heisenberg model is not an integrable system for dimensions higher than one. The concept of integrability is discussed in Section 6.

We will discuss the one-dimensional spin- $\frac{1}{2}$ Heisenberg model using different methods. First, in Section 2, the exact ground state energy in the thermodynamic limit of the XXX model is calculated analytically using the Bethe ansatz. Then in Sections 3 and 4 we do both a perturbation theory in Δ and an integral expansion to find the ground state energy of the XXZ model in the thermodynamic limit. Next we study the systems from a numerical perspective in Section 5. We solve the system numerically using exact diagonalization. The results are then compared to the expectations from the analytical calculations. Finally, the integrability of the one-dimensional Heisenberg model is discussed in Section 6.

2 The Bethe ansatz

This section closely follows the calculations from Chapter 5, pages 137–155, of the book *Quantum Physics in One Dimension* by Thierry Giamarchi [5]. The Bethe ansatz is a method used to analytically find exact solutions of one-dimensional quantum models. It can be used in so-called integrable systems, which are discussed in Section 6. Here it will be used to find the exact energy of the ground state of the one-dimensional antiferromagnetic spin- $\frac{1}{2}$ XXZ Heisenberg model. The Hamiltonian of such a model is of the form

$$\begin{aligned} H &= J_{xy} \sum_j [S_{j+1}^x S_j^x + S_{j+1}^y S_j^y] + J_z \sum_j S_{j+1}^z S_j^z, \\ &= \frac{J}{2} \sum_j [S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+] + \Delta J \sum_j S_{j+1}^z S_j^z, \end{aligned} \quad (1)$$

where J is the coupling constant, which is related to the overlap of the orbitals between neighboring sites. The parametrization $J_{xy} = J$, $J_z = \Delta J$ is used. Each lattice site contains a spin- $\frac{1}{2}$ particle. These particles can either have spin up (\uparrow), or spin down (\downarrow). This way each site creates a two-dimensional Hilbert space. The total Hilbert space for a spin- $\frac{1}{2}$ chain with L sites is then the tensor product of these Hilbert spaces, creating a 2^L -dimensional space, $\mathcal{H} = \mathbb{C}^{2^L}$. The spin- $\frac{1}{2}$ operators acting on lattice site j are notated by \vec{S}_j and are defined as

$$\vec{S}_j = \frac{\hbar}{2} \vec{\sigma}_j,$$

where $\vec{\sigma}_j$ are the Pauli matrices. Furthermore, $S^\pm = S^x \pm iS^y$. The operators S^\pm are the spin raising/lowering operators. These operators change the direction of the spin on the lattice site they act on. The spin raising operator S^+ changes the spin to an up spin, while the spin lowering operator S^- changes the spin to a down spin. For example, $S_{j+1}^+ S_j^-$ changes the spin on site j to a down spin, and the spin on site $j+1$ to an up spin. However, if the spin on a site is already in the direction of the spin operator acting on that site, it gives zero. In short:

$$\begin{aligned} S^+ |\uparrow\rangle &= 0, \\ S^+ |\downarrow\rangle &= |\uparrow\rangle, \\ S^- |\uparrow\rangle &= |\downarrow\rangle, \\ S^- |\downarrow\rangle &= 0. \end{aligned}$$

The goal is to find the exact energy of the ground state of a spin- $\frac{1}{2}$ chain with L lattice sites of which N are down spins at arbitrary locations. Let us first consider an easier problem to get an idea of what the system looks like.

2.1 Zero, one, and two down spins

The polarized state is defined as the state where all spins are up. This state is an exact eigenstate, since $S_{j+1}^+ S_j^- |\uparrow\uparrow\rangle = 0$. It is easy to see that in this case there are L pairs of two up spins. All of these spin pairs contribute an energy of $\Delta J/4$, adding up to a total energy of $E = L\Delta J/4$ for the polarized state.

Now let us consider the state where there is one down spin. The energy of an $\uparrow\uparrow$ pair is $\Delta J/4$ as above. However, the energy of an $\uparrow\downarrow$ pair is $-\Delta J/4$ which is an energy difference of $-\Delta J/2$ compared to the $\uparrow\uparrow$ pair. Since for the state with one down spin there are two $\uparrow\downarrow$ pairs instead of two $\uparrow\uparrow$ pairs, there is a total energy difference of $\delta E = -\Delta J$ compared to the polarized state. This results in the following Schrödinger equation

$$H\psi(x) = \frac{J}{2} [\psi(x-1) + \psi(x+1)] + (E_0 - \Delta J)\psi(x), \quad (2)$$

where $\psi(x)$ has a down spin at lattice site x . The first term on the right hand side describes the hopping of the down spin to its neighboring sites. This term follows from the spin raising/lowering operators in expression (1). Furthermore, the $-\Delta J$ term describes the energy difference compared to the polarized state

due to the presence of a down spin, and E_0 is the energy of the polarized state. The Hamiltonian from (2) can be diagonalized via

$$\psi(x) = \frac{1}{\sqrt{L}} e^{ikx}. \quad (3)$$

Substituting the wavefunction of (3) into (2) we find

$$\begin{aligned} H\psi(x) &= \frac{J}{2}(e^{ik} + e^{-ik})\psi(x) + (E_0 - \Delta J)\psi(x), \\ &= J \left[\cos(k) + \frac{\Delta L}{4} - \Delta \right] \psi(x), \\ &= E\psi(x). \end{aligned}$$

The quantization of the momentum can be calculated from periodic boundary conditions ($\psi(x) = \psi(x + L)$) and is $k = 2\pi n/L$ with n an integer. The solution for the system with one down spin is

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{L}} e^{ikx}, \\ E &= J [\cos(k) - \Delta] + \frac{\Delta JL}{4}, \\ k &= \frac{2\pi n}{L}, \quad \text{where } n \in \mathbb{Z}. \end{aligned}$$

Next let us look at the state where there are two down spins. There are two ways the down spins can be distributed. This is shown in Figure 4. If the down spins are on adjacent lattice sites they will interact. However, if they are further away from each other they will not be able to interact, since only nearest neighbor interaction is taken into account.

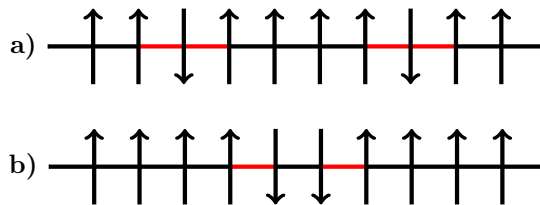


Figure 4: The two different cases in the presence of two down spins. a) the two down spins are far away from each other. b) the two down spins are adjacent and therefore there are two up-down pairs instead of four.

When the down spins are not adjacent it is possible to describe the situation as two particles with momenta k_1 and k_2 that scatter when they get close to each other. After scattering the particles are far away and have momenta k_3 and k_4 . From conservation of energy and momentum it follows that for two scattering particles the momenta should either be conserved ($k_1 = k_3$, $k_2 = k_4$) or exchanged ($k_1 = k_4$, $k_2 = k_3$). The wavefunction for two separated down spins is then

$$\psi(x_1, x_2) = \alpha e^{i(k_1 x_1 + k_2 x_2)} + \beta e^{i(k_1 x_2 + k_2 x_1)}. \quad (4)$$

The allowed momenta can be determined by imposing periodic boundary conditions on this wavefunction as follows

$$\begin{aligned} \psi(x_1, x_2) &= \psi(x_2, x_1 + L), \\ \alpha &= \beta e^{ik_1 L} = \beta e^{-ik_2 L}, \\ k_1 + k_2 &= \frac{2\pi n}{L}, \quad \text{where } n \in \mathbb{Z}. \end{aligned} \quad (5)$$

Furthermore, this implies the condition that $\alpha/\beta = e^{ik_1 L} = e^{-ik_2 L}$. This shows that the parameter α/β has an influence on how k_1 and k_2 are quantized. Since this is due to interactions between the two down spins,

it shows that the presence of more down spins affects the allowed values of the momentum k .

In the case of two separated down spins their individual wavefunctions (4) will be a solution to the Schrödinger equation in any case. This is true because we only take into account nearest neighbor interactions, so the Hamiltonian H can act on the wavefunctions of both down spins independently. However, for two adjacent down spins, as shown in Figure 4b, one must take into account the fact that the down spins cannot jump onto one another. Also, since the two down spins are adjacent, there are two $\uparrow\downarrow$ pairs and one $\downarrow\downarrow$ pair due to the presence of the down spins. The energy of a $\downarrow\downarrow$ pair is the same as that of an $\uparrow\uparrow$ pair, so the difference in energy to the polarized state is $\delta E = -\Delta J$, the same as when there is only one spin down. The Schrödinger equation is

$$H\psi(x, x+1) = \frac{J}{2}[\psi(x-1, x+1) + \psi(x, x+2)] + (E_0 - \Delta J)\psi(x, x+1). \quad (6)$$

The first term describes the hopping of the down spin at position x to the left, and at position $x+1$ to the right. The second is the energy difference to the polarized state. We want the Schrödinger equation to be equal to the one for an individual down spin (2) for any positions x_1 and x_2 of the down spins. This is not the case when the down spins are adjacent. Taking the difference between (6) and (2) gives the following term

$$-\frac{J}{2}[\psi(x, x) + \psi(x+1, x+1)] + \Delta J\psi(x, x+1), \quad (7)$$

where the term proportional to $J/2$ describes the hopping between two adjacent down spins. We want the wavefunction of (4) to satisfy the Schrödinger equation regardless of the positions x_1 and x_2 of the down spins. This can be accomplished by choosing α and β such that the difference term (7) is equal to zero. Plugging the wavefunction (4) into the difference term (7) and setting equal to zero gives

$$\begin{aligned} \frac{J}{2} \left[\alpha e^{i(k_1+k_2)x} + \beta e^{i(k_1+k_2)x} + \alpha e^{i(k_1+k_2)(x+1)} + \beta e^{i(k_1+k_2)(x+1)} \right] &= \Delta J \left[\alpha e^{i(k_1x+k_2(x+1))} + \beta e^{i(k_1(x+1)+k_2x)} \right], \\ J e^{i(k_1+k_2)x} \left[(\alpha + \beta) \left(1 + e^{i(k_1+k_2)} \right) \right] &= 2\Delta J e^{i(k_1+k_2)x} \left[\alpha e^{ik_2} + \beta e^{ik_1} \right], \\ (\alpha + \beta) \left(1 + e^{i(k_1+k_2)} \right) &= 2\Delta \left(\alpha e^{ik_2} + \beta e^{ik_1} \right), \\ \alpha \left(1 + e^{i(k_1+k_2)} - 2\Delta e^{ik_2} \right) &= \beta \left(2\Delta e^{ik_1} - e^{i(k_1+k_2)} - 1 \right), \\ \frac{\alpha}{\beta} &= -\frac{2\Delta e^{ik_1} - (1 + e^{i(k_1+k_2)})}{2\Delta e^{ik_2} - (1 + e^{i(k_1+k_2)})}. \end{aligned}$$

Using the relation $2 \cos(\theta) = e^{i\theta} + e^{-i\theta}$ this can be rewritten as

$$\frac{\alpha}{\beta} = -\frac{\Delta e^{i\left(\frac{k_1-k_2}{2}\right)} - \cos\left(\frac{k_1+k_2}{2}\right)}{\Delta e^{i\left(\frac{k_2-k_1}{2}\right)} - \cos\left(\frac{k_1+k_2}{2}\right)}. \quad (8)$$

Now we have found the value for α/β for which the wavefunction of (4) is the full wavefunction of the problem with two down spins. For real k_1 and k_2 this can be written as a phase

$$\frac{\alpha}{\beta} = -e^{i\Theta(k_1, k_2)},$$

with

$$\Theta(k_1, k_2) = 2 \arctan \left(\frac{\Delta \sin\left(\frac{k_1-k_2}{2}\right)}{\Delta \cos\left(\frac{k_1-k_2}{2}\right) - \cos\left(\frac{k_1+k_2}{2}\right)} \right). \quad (9)$$

By substituting α/β into the quantization of (5) we get

$$\begin{aligned} e^{i(k_2L + \Theta(k_1, k_2))} &= -1, \\ e^{i(k_1L - \Theta(k_1, k_2))} &= -1, \end{aligned}$$

which gives

$$\begin{aligned} Lk_1 &= 2\pi I_1 + \Theta(k_1, k_2), \\ Lk_2 &= 2\pi I_2 + \Theta(k_2, k_1), \end{aligned} \quad (10)$$

where we used $\Theta(k_1, k_2) = -\Theta(k_2, k_1)$. Both I_1 and I_2 are half-integers. These relations show that due to the presence of two down spins the allowed values for the momenta k_1 and k_2 are shifted. In particular we see that the shift in the momentum of one spin depends on the momentum of the other spin through $\Theta(k_1, k_2)$. By plugging the correct value for α/β into the wavefunction of (4) we can write the wavefunction as

$$\psi(x_1, x_2) = e^{i\left(\frac{\Theta(k_1, k_2)}{2} + k_1 x_1 + k_2 x_2\right)} - e^{i\left(-\frac{\Theta(k_1, k_2)}{2} + k_1 x_2 + k_2 x_1\right)}.$$

For $k_1 = k_2$ we find $\Theta(k_1, k_2) = 0$. This means that in this case the wavefunction $\psi(x_1, x_2) = 0$. Hence we need $k_1 \neq k_2$ to find a solution. From (9) it is easy to see that $\Theta(k_1, k_2) = 0$ when $\Delta = 0$. Thus in this case, if $k_1 \neq k_2$, the solution is simply a plane wave with independent momenta.

2.2 N down spins

Now that these simpler cases have been discussed we are ready to move on to the general case. Let us consider a system with N down spins at positions $x_1 < x_2 < \dots < x_N$. As shown in Figure 5 we again make a distinction between the case where there are no adjacent down spins, and the case where there are two down spins adjacent. If the down spins are not adjacent it can be treated analogous to the case of only one down spin, as there are only nearest neighbor interactions. Therefore, one can expect a Schrödinger equation similar to that of (2), but generalized for N down spins.

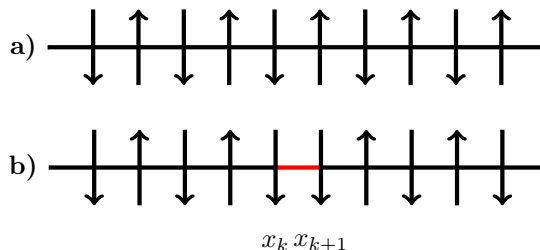


Figure 5: The loss of two up-down pairs due to the presence of a down-down pair. a) the system with N non-adjacent down spins (antiferromagnetic case). b) two out of N down spins are adjacent, creating a down-down pair while losing two up-down pairs.

In the N non-adjacent down spins case there are $2N$ $\uparrow\downarrow$ pairs. This is an energy difference of $\delta E = -\Delta N J$ compared to the polarized state. The kinetic term, describing the hopping of down spins, can be extended to the general case by introducing the finite difference operator δ_i as

$$\delta_i \psi(\dots, x_i, \dots) = \psi(\dots, x_i - 1, \dots) + \psi(\dots, x_i + 1, \dots),$$

and using the notation $\{x_i\} = x_1, x_2, \dots, x_N$ for the locations of the down spins. The term describing the hopping of the spins then becomes

$$\frac{J}{2} \sum_{i=1}^N \delta_i \psi(\{x_i\}).$$

The Schrödinger equation now is

$$H\psi(\{x_i\}) = J \left[\frac{1}{2} \sum_{i=1}^N \delta_i \psi(\{x_i\}) - \left(\Delta N - \frac{\Delta L}{4} \right) \psi(\{x_i\}) \right] = E\psi(\{x_i\}).$$

Setting $J = 1$ to lighten notation and swapping terms this becomes

$$\epsilon\psi(\{x_i\}) = \frac{1}{2} \sum_{i=1}^N \delta_i \psi(\{x_i\}), \quad (11)$$

where $\epsilon = E + \Delta(N - \frac{L}{4})$. The $\Delta L/4$ term is the energy of the polarized state and E is the eigenvalue for the energy.

We have now found an expression for the Schrödinger equation for N separated down spins. Our goal is now to tweak this expression so that it holds for arbitrary locations of the down spins. To do so, let us again first consider a simpler case. Namely where only 2 out of N spins are adjacent on positions x_k and x_{k+1} , as shown in Figure 5b. Similar to the case of two adjacent down spins, this will give rise to two differences compared to the state without any adjacent down spins. Firstly, the energy difference compared to the polarized state will be different due to the presence of a $\downarrow\downarrow$ pair. Secondly, the neighboring down spins impose a restriction in movement of the spins, as down spins can not move to one another.

We begin by discussing the change in energy. When two down spins are adjacent both of them have a $\downarrow\downarrow$ bond with one another, and thus both lose an $\uparrow\downarrow$ pair. This means that there is now one $\downarrow\downarrow$ pair and only $2N - 2$ $\uparrow\downarrow$ pairs instead of $2N$ $\uparrow\downarrow$ pairs, as shown in Figure 5. The energy of a $\downarrow\downarrow$ pair is the same as that of an $\uparrow\uparrow$ pair. So, relative to the polarized state where all spins are up, the $\downarrow\downarrow$ has no contribution to the energy difference. From before, the energy difference between an $\uparrow\downarrow$ pair and an $\uparrow\uparrow$ pair is $-\Delta J/2$. This means that the total energy difference compared to the polarized state is $\delta E = (-\Delta J/2)(2N - 2) = -\Delta N J + \Delta J$.

The restriction in movement of the spins is represented by an extra kinetic term describing the displacement of the adjacent down spins.

Similar to the case where there are only two down spins, we find

$$\begin{aligned} \epsilon\psi(\dots, x_k, x_k + 1, \dots) &= \frac{1}{2} \sum_{i \neq k, k+1}^N \delta_i \psi(\dots, x_i, x_i + 1, \dots) \\ &+ \frac{1}{2} [\psi(\dots, x_k - 1, x_k + 1, \dots) + \psi(\dots, x_k, x_k + 2, \dots)] + \Delta\psi(\dots, x_k, x_k + 1, \dots). \end{aligned} \quad (12)$$

Recall that the $-\Delta N$ part of the energy difference term is already included in ϵ . From this we learn that whenever a spin down has a neighbor which is a spin down, the term describing the displacement to that site disappears, and an interaction term is gained. This gives an understanding of what the Schrödinger equation looks like when there are more adjacent down spins.

We will now generalize the wavefunction of (4) for two down spins to the case of N down spins by looking for a wavefunction of the form

$$\psi(x_1, \dots, x_N) = \sum_P A_P \exp \left[i \sum_{j=1}^N k_{P_j} x_j \right], \quad (13)$$

where P are all permutations of the index N of the down spins and A_P are coefficients (similar to α and β). In the exponent the momenta are permuted amongst the down spins. Looking for such a wavefunction is the actual ansatz of the Bethe ansatz. Just like in the earlier case of two down spins, we have two Schrödinger equations. One for separated spins (11), and one where there are two adjacent down spins (12). And again we can determine the coefficients (now A_P) such that the two Schrödinger equations become identical. Namely by setting the difference between the two equations to zero. This gives

$$2\Delta\psi(\dots, x_k, x_k + 1, \dots) = \psi(\dots, x_k + 1, x_k + 1, \dots) + \psi(\dots, x_k, x_k, \dots), \quad (14)$$

where the terms on the right hand side describe the hopping between two adjacent down spins. To solve this it is useful to define another permutation P' which only differs from P by exchanging two adjacent elements, meaning $P'(k) = P(k + 1)$.

Now we fill in $(x_1, \dots, x_l + m, x_l + n, \dots, x_N)$ in (13) as arbitrary positions of down spins, with m and n some integer. This gives

$$\psi(\dots, x_l + m, x_l + n, \dots) = \sum_P A_P \exp \left[i \sum_{j \neq l, l+1}^N k_{P_j} x_j + k_{P_l}(x_l + m) + k_{P_{l+1}}(x_l + n) \right],$$

which can be rewritten using $P'(k) = P(k+1)$ to

$$\psi(\dots, x_l + m, x_l + n, \dots) = \sum_P A_P \exp \left[i \sum_{j \neq l, l+1}^N k_{Pj} x_j \right] e^{i(k_{Pl} + k_{P'l})x_l} e^{i(mk_{Pl} + nk_{P'l})}.$$

Using the fact that P and P' differ only by one transposition this can be written as

$$\begin{aligned} \psi(\dots, x_l + m, x_l + n, \dots) &= \sum_P' \exp \left[i \sum_{j \neq l, l+1}^N k_{Pj} x_j \right] e^{i(k_{Pl} + k_{P'l})x_l} \\ &\times \left(A_P e^{i(mk_{Pl} + nk_{P'l})} + A_{P'} e^{i(mk_{P'l} + nk_{Pl})} \right), \end{aligned} \quad (15)$$

where \sum_P' is a summation over half of the permutations. The other half of the permutations is included in the extra term proportional to $A_{P'}$.

It is now possible to determine the coefficients A_P for which the difference term (14) is zero by plugging in our expression for the wavefunction (15). Note that the left hand side term of (14) requires $m = 0, n = 1$ while the terms on the right hand side require $m = n = 1$ and $m = n = 0$ respectively. This gives

$$2\Delta \left(A_P e^{ik_{P'k}} + A_{P'} e^{ik_{Pk}} \right) = (A_P + A_{P'}) \left(e^{i(k_{Pk} + k_{P'k})} + 1 \right).$$

By separating terms this is easily rewritten to

$$\frac{A_P}{A_{P'}} = - \frac{1 + e^{i(k_{Pk} + k_{P'k})} - 2\Delta e^{ik_{Pk}}}{1 + e^{i(k_{P'k} + k_{Pk})} - 2\Delta e^{ik_{P'k}}} = -e^{-i\Theta(k_{Pk}, k_{P'k})}, \quad (16)$$

with $\Theta(k_{Pk}, k_{P'k})$ as defined in (9). To determine the coefficients A_P from this we fix the permutation $P' = (12 \dots N)$. Next we use the fact that any permutation can be written as a product of adjacent transpositions (permutations of two adjacent elements). Each of the transpositions of which P consists contributes one factor of (16). We obtain

$$\frac{A_P}{A_{12 \dots N}} = (-1)^{\eta_P} e^{i \sum \Theta(k_j, k_l)},$$

where η_P is the number of transpositions of which permutation P is composed, and the summation is over these transpositions. Note that the minus sign in the exponent is gone. This is because the sequence of transpositions is not important due to the antisymmetry of $\Theta(k_j, k_l)$. Next we calculate the allowed values of the momenta k from the periodic boundary condition

$$\psi(x_1, x_2, \dots, x_N) = \psi(x_2, \dots, x_N, x_1 + L).$$

Plugging this into the wavefunction of (13) we obtain

$$\left(\frac{A_P}{A_{P'}} \right) e^{ik_{P'1}L} = 1. \quad (17)$$

Here P' is a permutation that follows from shifting all elements of permutation P one place to the right:

$$(P'1, P'2, \dots, P'N-1, P'N) = (PN, P1, P2, \dots, PN-1).$$

The ratio $A_P/A_{P'}$ can now be obtained by permuting PN to the right such that $(PN, P1, P2, \dots, PN-1) \mapsto (P1, P2, \dots, PN-1, PN)$. This corresponds to the permutation $(123 \dots N)$, which can be decomposed into $(12)(23) \dots (N-1 N)$. This consists of $N-1$ transpositions of adjacent elements. Using this together with (16) we find

$$\frac{A_P}{A_{P'}} = (-1)^{N-1} \exp \left(i \sum \Theta(k_{Pk}, k_{P'k}) \right).$$

Together with (17) this gives

$$(-1)^{N-1} \exp \left(i \sum_{j=1}^N \Theta(k_j, k_l) \right) \times \exp(ik_{Pl}L) = 1.$$

Note that there are two different cases for even and odd N . Solving this equation gives

$$Lk_l + \sum_{j=1}^N \Theta(k_j, k_l) = 2\pi I_l.$$

After renaming $l \mapsto i$ and using the antisymmetry condition $\Theta(k_i, k_j) = -\Theta(k_j, k_i)$ this results in

$$Lk_i = 2\pi I_i + \sum_{j=1}^N \Theta(k_i, k_j), \quad (18)$$

where I_i is integer when N is odd, and I_i is half-integer when N is even. Only solutions with $k_i \neq k_j$ are allowed, as the wavefunction of (15) is equal to zero when $k_i = k_j$. Looking back at the results for two down spins, it is clear that (18) is a generalization of the simpler case. Furthermore the energy is given by

$$E = \frac{\Delta JL}{4} + J \sum_j [\cos(k_j) - \Delta]. \quad (19)$$

We now have found the equations to describe the system of L lattice sites with N down spins on arbitrary locations.

2.3 Parametrization of the functions

To simplify the following calculation, we set $\Delta = 1$. Now we are going to calculate the exact energy of the ground state of the isotropic antiferromagnetic case, the XXX model. To do so we use the parametrization

$$\begin{aligned} k &= \bar{k} + \pi, \\ \lambda &= -\frac{1}{2} \tan(\bar{k}/2). \end{aligned}$$

The equations (18) and (19) now become

$$\begin{aligned} 2\pi \bar{I}_i &= 2L \arctan(2\lambda_i) - \sum_j 2 \arctan(\lambda - \lambda_j), \\ E_0 &= \frac{L|J|}{4} - |J| \sum_j [1 + \cos(\bar{k})], \end{aligned}$$

where \bar{I}_i is integer if L and N have opposite parities, and half-integer if L and N have the same parity. The parity of an integer is the property of being either even or odd. Furthermore, we use the absolute value of J . This is because this parametrization works not only for the isotropic antiferromagnet ($J > 0$), but also for the isotropic ferromagnet ($J < 0$). To solve the equation we define the function

$$\phi(\lambda) = 2L \arctan(2\lambda_i) - \sum_j 2 \arctan(\lambda - \lambda_j),$$

where $\phi(\lambda)$ is an increasing function of λ . Since the range of the arctangent is $[-\frac{\pi}{2}, \frac{\pi}{2}]$, we see that the function $\phi(\lambda)$ varies between $-\phi_0$ and ϕ_0 , where $\phi_0 = \pi[L - N]$. This means that the equation $\phi(\lambda_i) = 2\pi \bar{I}$ has $L - N$ solutions, as it goes through $2\pi[L - N]$ values (from $-\phi_0$ to ϕ_0) with steps of 2π times a (half-)integer. Of these solutions, only N are occupied. The rest are called holes. If there are any holes present, they are ordered in such a way that the total energy of the system is minimal. Let us now consider

a chain where there are no holes present. Also we assume zero net magnetization, hence $N_\uparrow = N_\downarrow = L/2$. Note that this requires L to be even. As the solutions of $\phi(\lambda_i) = 2\pi\bar{I}$ are regularly spaced, it is possible to define a density of states

$$\rho(\lambda) = \frac{1}{2\pi} \frac{d\phi}{d\lambda}. \quad (20)$$

One can now rewrite $\phi(\lambda)$ in the thermodynamic limit

$$\phi(\lambda) = 2L \arctan(2\lambda) - 2 \int_{-\infty}^{+\infty} \rho(\lambda') \arctan(\lambda - \lambda') d\lambda'.$$

Taking the derivative with respect to λ gives

$$2\pi\rho(\lambda) = \frac{4L}{1+4\lambda^2} - 2 \int_{-\infty}^{+\infty} \rho(\lambda') \frac{d\lambda'}{1+(\lambda-\lambda')^2}. \quad (21)$$

This integral can be solved by using the Fourier transform. It is useful to notice that the integral is a convolution, so it is possible to apply the convolution theorem which is discussed in Appendix A. The integrals from the Fourier transforms can be done by using the Residue theorem. The derivation and application of the Residue theorem are discussed in more detail in Appendix B. Applying it here gives

$$\rho(\lambda) = \frac{L}{4\pi} \int_{-\infty}^{+\infty} \frac{e^{-i\omega\lambda}}{\cosh(\omega/2)} d\omega.$$

We again apply the Residue theorem to find the value for the density of states

$$\rho(\lambda) = \frac{L}{2 \cosh(\pi\lambda)}. \quad (22)$$

Now that we have an expression for the density of states, it is possible to calculate the total energy of the ground state. By using the parametrization $\bar{k} = -2 \arctan(2\lambda)$ we can rewrite our expression for the energy from before as

$$E_0 = \frac{L|J|}{4} - |J| \sum_j \frac{2}{1+4\lambda_j^2}.$$

In the thermodynamic limit this is

$$E_\infty = \frac{L|J|}{4} - |J| \int \rho(\lambda) \frac{2}{1+4\lambda^2} d\lambda,$$

where we use the notation E_∞ for the energy in the thermodynamic limit. Using the expression from (22) we can solve this integral using the Residue theorem to find

$$\frac{E_\infty}{L|J|} = \left[\frac{1}{4} - \ln(2) \right] \approx -0.44, \quad (23)$$

where the sum over infinite poles which appears is calculated using Reference [6]. Now we have found an expression for the exact energy per lattice site of the ground state of the XXX Heisenberg model. In Section 5 this result is compared to the numerical calculation of the system.

3 Perturbation to the ground state

In the previous section we have determined the exact energy of the ground state of the XXX Heisenberg model, so with $\Delta = 1$. Next we will discuss the XXZ model. Recall that the Hamiltonian of this system is

$$H = \frac{J}{2} \sum_j [S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+] + \Delta J \sum_j S_{j+1}^z S_j^z.$$

To avoid having to work with spin operators too much we will start by transforming the Hamiltonian.

3.1 Jordan-Wigner transformation

In order to discuss this model, we first map the spin operators in the Hamiltonian onto fermionic operators by applying the Jordan-Wigner transformation. This transformation is discussed in more detail in Appendix C. It is defined by

$$\begin{aligned} S_i^+ &\mapsto c_i^\dagger e^{i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j}, \\ S_i^- &\mapsto c_i e^{-i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j}, \\ S_i^z &= c_i^\dagger c_i - \frac{1}{2}. \end{aligned}$$

By applying this mapping the Hamiltonian becomes

$$H = \frac{J}{2} \sum_j [c_{j+1}^\dagger c_j + c_{j+1} c_j^\dagger] + \Delta J \sum_j \left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2} \right) \left(c_j^\dagger c_j - \frac{1}{2} \right), \quad (24)$$

where c^\dagger and c are the fermionic creation and annihilation operators, respectively. A spin down now corresponds to a lattice site occupied by a fermion, while a spin up corresponds to a free site. These fermionic operators create or annihilate a fermion on a specific site. For example, c_j^\dagger creates a fermion on site j , while c_j annihilates a fermion on site j . Following this logic we can understand the first term of the Hamiltonian of equation (24) effectively moves a fermion from site j to site $j + 1$. The fermionic operators obey the following algebra

$$\begin{aligned} \{c_i, c_j\} &= 0, \\ \{c_i^\dagger, c_j^\dagger\} &= 0, \\ \{c_i, c_j^\dagger\} &= \delta_{ij}, \end{aligned}$$

which implies that if the creation operator works on a site which is already occupied it gives zero, $c_j^\dagger c_j^\dagger = 0$. In other words, these anticommutation relations ensure that the Pauli exclusion principle is obeyed.

3.2 Perturbation theory

Now that we have expressed the Hamiltonian in terms of fermionic operators we are ready to discuss the system. We will again consider a chain of L lattice sites, and assume there to be no magnetic field. This effectively means that $\langle S_z \rangle = 0$. In other words, half of all spins will be up, and half will be down. Or, in terms of fermions, $L/2$ sites will be empty and $L/2$ sites will be occupied by fermions. Because of this L is required to be even. We will discuss the system by applying time-independent perturbation theory in Δ to the ground state. In perturbation theory one considers an unperturbed Hamiltonian H_0 , to which one adds a small perturbation, ΔH_1 . The whole Hamiltonian can then be expressed as

$$H = H_0 + \Delta H_1,$$

where Δ is a parameter. Note that for $\Delta = 0$ one has the unperturbed case, which corresponds to the XX Heisenberg model. In the case of the Hamiltonian from equation (24) it is easy to see that

$$H_0 = \frac{J}{2} \sum_j [c_{j+1}^\dagger c_j + c_{j+1} c_j^\dagger]$$

$$H_1 = J \sum_j \left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2} \right) \left(c_j^\dagger c_j - \frac{1}{2} \right).$$

We will start by calculating the ground state energy of the unperturbed Hamiltonian. To do so we first write H_0 in momentum representation by Fourier transforming it using the following identities

$$c_j = \frac{1}{\sqrt{L}} \sum_k a_k e^{ikx_j},$$

$$c_j^\dagger = \frac{1}{\sqrt{L}} \sum_k a_k^\dagger e^{-ikx_j},$$

where a_k^\dagger and a_k are the fermionic creation and annihilation operators for momentum k , respectively. Similar to the fermionic operators in real space, they obey the following algebra

$$\{a_k, a_{k'}\} = 0,$$

$$\{a_k^\dagger, a_{k'}^\dagger\} = 0,$$

$$\{a_k, a_k^\dagger\} = \delta_{kk'}.$$

Together with the identity for the Kronecker Delta,

$$\delta_{mn} = \frac{1}{L} \sum_{k=1}^L \exp\left(\frac{2\pi ik}{L}(m-n)\right),$$

the expression of H_0 simplifies to

$$H_0 = -J \sum_k \cos(k) a_k^\dagger a_k,$$

where the sum is over all allowed momenta k . Let us first define the ground state as follows

$$|\psi_0\rangle = \prod_q a_q^\dagger |0\rangle,$$

where $q = k_1, k_2, \dots, k_{L/2}$, and $|0\rangle$ is the vacuum. We take $|k_i| \leq \pi/2$. This creates exactly $L/2$ fermions with the allowed momenta in the lowest energy states. We assume the momenta to be ordered, meaning $k_1 < k_2 < \dots < k_{L/2}$. To calculate the ground state energy of the unperturbed Hamiltonian we let it act on the ground state

$$H_0 |\psi_0\rangle = -J \sum_k \cos(k) a_k^\dagger a_k \prod_q a_q^\dagger |0\rangle.$$

We calculate this by commuting the annihilation operator a_k through the string of $L/2$ creation operators from the ground state, making use of the fermionic anticommutation relation

$$a_k a_q^\dagger = \delta_{kq} - a_q^\dagger a_k.$$

As an annihilation operator acting on the vacuum gives zero, $a_k |0\rangle = 0$, one can see that what remains after $L/2$ commutations is a sum of $L/2$ Kronecker deltas. Due to the fact that fermions obey anticommutation

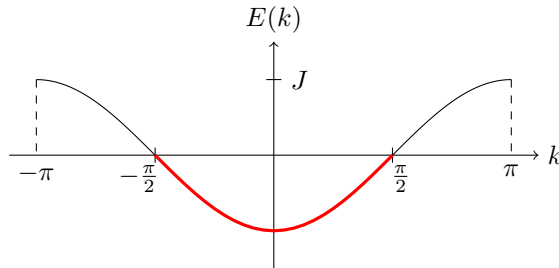


Figure 6: The dispersion of a single particle. In the ground state exactly the part from $-\pi/2$ to $\pi/2$ will be occupied by fermions.

relations, the deltas have alternating signs. It follows that

$$\begin{aligned} H_0 |\psi_0\rangle &= -J \sum_k \cos(k) a_k^\dagger \left(\sum_{p=1}^{L/2} \delta_{kp} (-1)^{p-1} \right) \prod_{q \neq p} a_q^\dagger |0\rangle, \\ &= -J \sum_{p=1}^{L/2} \cos(p) (-1)^{p-1} a_p^\dagger \prod_{q \neq p} a_q^\dagger |0\rangle. \end{aligned}$$

Note that the product of creation operators on the right is missing the a_p^\dagger operator, which is in front of the product. In order to rewrite the product of creation operators as the ground state we require the momenta to be ordered. From the relation $a_p^\dagger a_q^\dagger = -a_q^\dagger a_p^\dagger$ it is easy to see that placing a_p^\dagger back in the correct order, one gets an extra factor of $(-1)^{p-1}$. This exactly cancels the minus signs from the anticommutation relations, resulting in

$$\begin{aligned} H_0 |\psi_0\rangle &= -J \sum_{p=1}^{L/2} \cos(p) |\Psi_0\rangle, \\ E_0 &= -J \sum_{i=1}^{L/2} \cos(k_i). \end{aligned} \tag{25}$$

Changing the sum into an integral by taking the thermodynamic limit¹ yields

$$\begin{aligned} E_0 &= -\frac{JL}{2\pi} \int_{-\pi/2}^{\pi/2} \cos(k) dk, \\ &= -\frac{JL}{\pi}. \end{aligned}$$

We have found the ground state energy of the unperturbed Hamiltonian in the thermodynamic limit. In Figure 6 a single particle dispersion is plotted. In our case of the ground state, the $L/2$ fermions will occupy the states in the domain $[-\pi/2, \pi/2]$. The next step is to calculate the first order energy shift, which is $E_1 = \langle \psi_0 | H_1 | \psi_0 \rangle$. Similar to the unperturbed case, we first express H_1 , the Hamiltonian describing the perturbation, in momentum representation

$$H_1 = J \left[\frac{1}{L} \sum_{k_1} \sum_{k_2} \sum_{k_3} \sum_{k_4} e^{i(k_4 - k_3)} \delta_{k_2 + k_4 - k_1 - k_3} a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} - \frac{1}{2} \sum_{k_5} a_{k_5}^\dagger a_{k_5} - \frac{1}{2} \sum_{k_6} a_{k_6}^\dagger a_{k_6} + \sum_{i=1}^{L/2} \frac{1}{4} \right].$$

One can immediately recognize the second and third term as number operators with a prefactor. A number operator counts how many particles there are in each state. Since we are working with fermions, this can

¹In one dimension one can rewrite a sum into an integral in the thermodynamic limit as follows: $\sum_k \xrightarrow{L \rightarrow \infty} \frac{L}{2\pi} \int dk$

only be either 0 or 1 for each site. As we know there are a total of $L/2$ fermions in the ground state, these terms will both give $L/2$. Taking their prefactors into account they both are $-L/4$. Furthermore, the fourth term has no operators and thus will simply be $L/4$. The first term, however, is more interesting. Let us discuss this term separately by letting it act on the ground state. First we only take into account the four operators, as they are the only interacting parts.

$$\begin{aligned} \langle \psi_0 | a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} | \psi_0 \rangle &= \langle 0 | \prod_{q'} a_{q'} \left(a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} \right) \prod_q a_q^\dagger | 0 \rangle, \\ &= - \langle 0 | \prod_{q'} a_{q'} \left(a_{k_1}^\dagger a_{k_3}^\dagger a_{k_2} a_{k_4} \right) \prod_q a_q^\dagger | 0 \rangle + \delta_{k_2 k_3} \langle 0 | \prod_{q'} a_{q'} \left(a_{k_1}^\dagger a_{k_4} \right) \prod_q a_q^\dagger | 0 \rangle. \end{aligned}$$

This expression can be treated similar to the case of the unperturbed Hamiltonian. It quickly follows that the second term is equal to zero. The main difference in the first term compared to the unperturbed case is that this time there are two creation and annihilation operators. Commuting both annihilation operators results in two summations of $L/2$ deltas, the second of which is restricted by the first. Important to note is that we must make a distinction between two cases. Namely the cases where $k_1 < k_3$ and where $k_1 > k_3$. The difference between them is that in the first case $a_{k_3}^\dagger$ commutes one time less when commuting it back into the string of creation operators, resulting in a minus sign. Taking this into account, one finds

$$\langle \psi_0 | a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} | \psi_0 \rangle = \delta_{k_1 k_2} \delta_{k_3 k_4} - \delta_{k_1 k_4} \delta_{k_2 k_3}.$$

Combining this result with the rest of the term gives

$$\begin{aligned} &\frac{J}{L} \sum_{k_1} \sum_{k_2} \sum_{k_3} \sum_{k_4} e^{i(k_4 - k_3)} \delta_{k_2 + k_4 - k_1 - k_3} \langle \psi_0 | a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} | \psi_0 \rangle, \\ &= \frac{J}{L} \sum_{k_1} \sum_{k_2} \sum_{k_3} \sum_{k_4} e^{i(k_4 - k_3)} \delta_{k_2 + k_4 - k_1 - k_3} (\delta_{k_1 k_2} \delta_{k_3 k_4} - \delta_{k_1 k_4} \delta_{k_2 k_3}), \\ &= \frac{J}{L} \sum_{k_1} \sum_{k_3} - \frac{J}{L} \sum_{k_1} \sum_{k_2} e^{i(k_1 - k_2)}, \\ &= \frac{JL}{4\pi^2} \iint_{-\pi/2}^{\pi/2} dk_1 dk_3 - \frac{JL}{4\pi^2} \iint_{-\pi/2}^{\pi/2} e^{i(k_1 - k_2)} dk_1 dk_2, \\ &= \frac{JL}{4} - \frac{JL}{\pi^2}, \end{aligned}$$

where we changed the sums into integrals using the thermodynamic limit. Recall that we already concluded the second and third term of H_1 to contribute $-L/4$, and the fourth to contribute $L/4$. Adding all terms we can find the first order energy shift in the thermodynamic limit.

$$\begin{aligned} E_1 &= \langle \psi_0 | H_1 | \psi_0 \rangle, \\ &= J \left[\frac{L}{4} - \frac{L}{\pi^2} - \frac{L}{4} - \frac{L}{4} + \frac{L}{4} \right], \\ &= -\frac{JL}{\pi^2}. \end{aligned}$$

Combining this result with the one from the unperturbed case gives us the energy of the ground state per lattice site in the thermodynamic limit

$$\frac{E_\infty}{LJ} = \frac{E_0 + \Delta E_1}{LJ} = -\frac{1}{\pi} - \frac{\Delta}{\pi^2}.$$

Note that for $\Delta = 0$ we have $E_\infty/LJ = -1/\pi$ as expected.

4 Expansion around $\Delta = 0$

From [7] we have the following exact expression for the ground state energy of the XXZ Heisenberg model in the thermodynamic limit

$$\frac{E_\infty}{LJ} = \frac{\Delta}{4} - \frac{1}{4} \frac{\sin^2(2\eta)}{\pi - 2\eta} \int_{-\infty}^{\infty} \frac{d\lambda}{\cosh\left(\frac{\pi\lambda}{\pi-2\eta}\right) \cosh(\lambda + i\eta) \cosh(\lambda - i\eta)}, \quad (26)$$

where $\Delta = -\cos(2\eta)$. To get an initial feel for how the ground state energy per lattice site depends on the parameter Δ we will do a first order Taylor expansion around $\Delta = 0$. Expressing η in terms of Δ we find $\eta = \frac{1}{2} \arccos(-\Delta)$. Expanding this around $\Delta = 0$ gives $\eta = \pi/4 + \Delta/2 + \mathcal{O}(\Delta^2)$. This means that expanding to first order around $\Delta = 0$ is equivalent to expanding around $\eta = \pi/4 + \Delta/2$. In order to find the expansion of expression (26) we first expand the term in front of the integral around $\eta = \pi/4 + \Delta/2$. This gives $2/\pi + 4\Delta/\pi^2 + \mathcal{O}(\Delta^2)$. Next we take the expansion of the integrand, also around $\eta = \pi/4 + \Delta/2$, and integrate it from $-\infty$ to ∞ . This yields $2 - 2\Delta/\pi + \pi\Delta/2$. Combining the results and keeping only terms up to first order in Δ

$$\begin{aligned} \frac{E_\infty}{LJ} &= \frac{\Delta}{4} - \frac{1}{4} \left(\frac{2}{\pi} + \frac{4\Delta}{\pi^2} \right) \left(2 - \frac{2\Delta}{\pi} + \frac{\pi\Delta}{2} \right), \\ &= \frac{\Delta}{4} - \frac{1}{\pi} + \frac{\Delta}{\pi^2} - \frac{\Delta}{4} - \frac{2\Delta}{\pi^2}, \\ &= -\frac{1}{\pi} - \frac{\Delta}{\pi^2}. \end{aligned}$$

The intermediate steps of the expansion are mostly skipped as the expansion of the integrand is quite complicated and does not provide much insight in the calculation. Note that the result of the expansion is the same result as we obtained from the perturbation theory.

5 Numerical solutions

In Section 2 we analytically solved the XXX Heisenberg model. Then in Sections 3 and 4 we analytically made approximations for the XXZ model. Next, we will consider the Heisenberg model from a numerical perspective. To solve the system numerically we use exact diagonalization. The goal of exact diagonalization is to find the eigenvalues of the Hamiltonian by simply diagonalizing it. This method is straightforward and easy to use. A complication, however, is the fact that for a chain of spin- $\frac{1}{2}$ particles with L sites the Hilbert space is 2^L -dimensional, and thus the Hamiltonian is a matrix of size $2^L \times 2^L$. This means that diagonalizing the Hamiltonian grows more complicated very quickly with increasing number of sites. However, as we only consider nearest neighbor interactions, most of the terms in the matrix are equal to zero. This significantly reduces the amount of input, allowing us to diagonalize the Hamiltonian for a reasonable amount of sites.

5.1 Exact diagonalization

5.1.1 XXX model

In Figure 7 the ground state energies obtained from exact diagonalization of the XXX model are plotted as a function of L . Furthermore, the exact ground state energy from the analytics is shown twice. One only taking into account first order corrections, and one taking into account corrections up to second order to the thermodynamic limit [7]. We can see that for $L = 4$ the error is relatively big. However, for larger L the error decreases rapidly and for $L \geq 10$ the data from exact diagonalization is already in good agreement with the analytical results. Furthermore it clearly shows that the larger L , the more the values grow to our analytical result obtained from the Bethe ansatz in the thermodynamic limit (23).

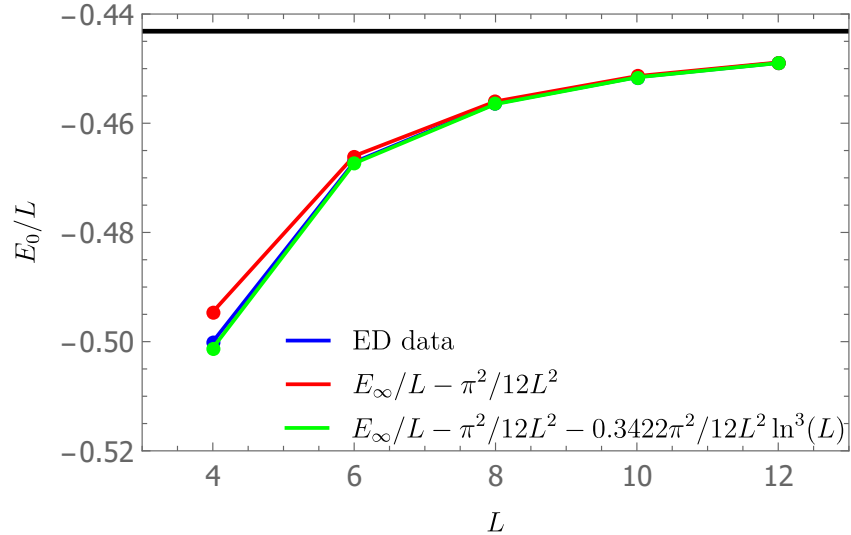


Figure 7: Ground state energies, E_0 , per lattice site in units of J for different number of lattice sites. The results of the exact diagonalization (blue) are plotted. In addition the exact results in the thermodynamic limit, E_∞ , are plotted with corrections up to first (red) and second (green) order taken from [7]. Note that the dots are the results, and they are connected with lines as a guide to the eye. Furthermore the exact energy of the ground state per lattice site in the thermodynamic limit is shown (black line).

Another representation of the data is shown in Figure 8. Plotted here is the difference between the result from the analytics and the exact diagonalization for the same values of L as in Figure 7. Note that it is plotted against $1/L^2$, meaning that L increases from right to left. One can see that as L increases, the results from the exact diagonalization grow closer to what is expected from the analytics. From the corrections to the thermodynamic limit of Reference [7] one would expect the slope of the fit to be $\pi^2/12 \approx 0.822467$. However, the slope we find is 0.897516. This is a difference of almost 8.4%. Most likely this difference is caused by the results for the lower numbers of L , as in Figure 7 we see that the results for $L = 4, 6, 8$ deviate a lot from the exact results, compared to the results for $L = 10$ or higher. Taking into account only the results for $L = 10, 12$ the slope of the fit is 0.838363. This is already much closer to the expected slope of $\pi^2/12$, confirming that the results for higher L are more accurate.

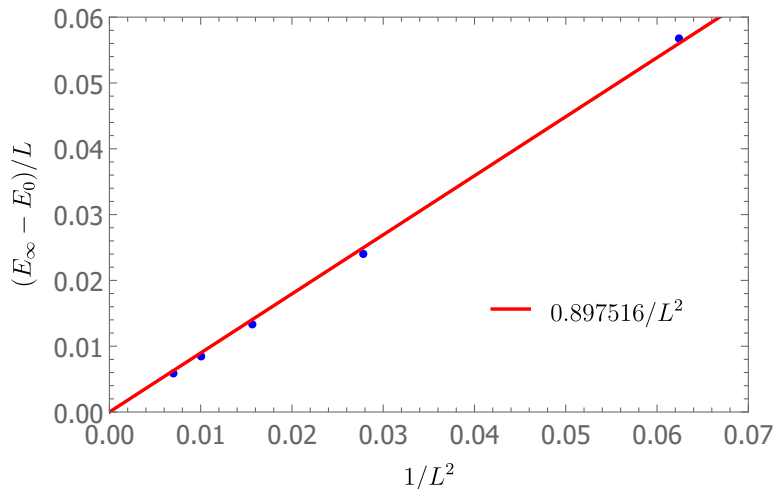


Figure 8: Difference between the exact result in the thermodynamic limit, E_∞ , from Bethe ansatz and the results from exact diagonalization, E_0 , with a fit through the points.

5.1.2 XXZ model

For this model we plot the ground state energy obtained from exact diagonalization against Δ . We do this for $L = 12$, which is the highest number of lattice sites our code can reach with reasonable computing time. The results are shown in Figure 9, together with the exact values from the integral expression of (26).

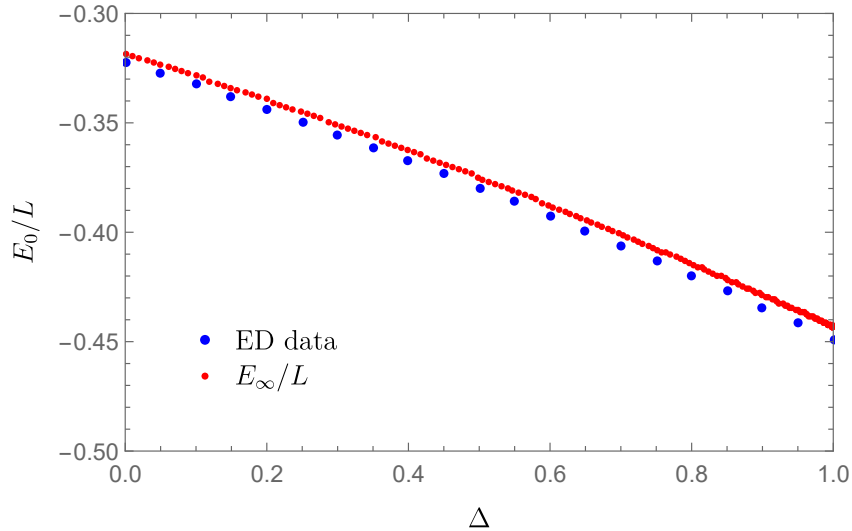


Figure 9: Ground state energy as a function of Δ obtained from exact diagonalization for $L = 12$ (blue dots), and the values from the integral expression (26) of the ground state energy in the thermodynamic limit [7] (red dots).

From the perturbation theory discussed before, we have an expectation of the ground state energy in the thermodynamic limit for the $\Delta = 0$ case. This is $E_\infty/LJ = -1/\pi$. Furthermore, from the Bethe ansatz, we have an analytically calculated expectation in the thermodynamic limit of the case where $\Delta = 1$. Recall from (23) that this is $E_\infty/LJ = 1/4 - \ln(2)$. In the following table we show for several values of Δ both the values of the exact diagonalization, E_0 , and the exact values from the integral expression from [7], E_∞ .

Δ	E_0/LJ	E_∞/LJ
0	-0.321975	-0.318310
0.25	-0.349413	-0.345180
0.50	-0.379773	-0.375000
0.75	-0.412955	-0.407659
1	-0.448949	-0.443147

One can see that already for $L = 12$ the results from exact diagonalization are close to the expectations obtained from analytics.

5.2 Approximations

In Sections 3 and 4 we made two different approximations of the system. First we studied perturbations in Δ in the thermodynamic limit. Then we did a first order expansion of the integral expression of the ground state energy in the thermodynamic limit. Both of these approximations yielded the same result, namely

$$\frac{E_\infty}{LJ} = -\frac{1}{\pi} - \frac{\Delta}{\pi^2}.$$

In Figure 10 the values of the integral expression from (26) are plotted against Δ , together with the result from the approximations. We immediately see that the error increases as Δ increases, and that the approximations are most accurate for Δ close to zero. The relative error between the perturbation theory and the exact result

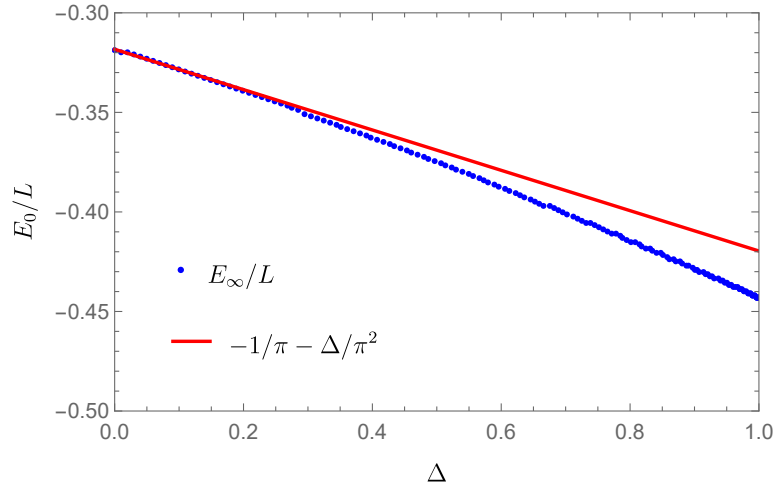


Figure 10: Values from the integral expression (26) of the ground state energy in the thermodynamic limit [7] (blue dots) plotted with the results from the first order expansion and perturbation theory (solid red line).

is plotted in Figure 11. One can see that the error roughly grows quadratically. This can be understood from the fact that we only took into account factors of Δ up to first order. Because of this the error is expected to be of second order, so quadratic. For small Δ (up to around $\Delta = 0.1$) the approximations are most accurate. For larger Δ , however, the accuracy quickly decreases significantly. This is no surprise, as perturbation theory is best applicable to systems with small perturbations only. However, even though the error increases, there error is still only a little over 5% for $\Delta = 1$.

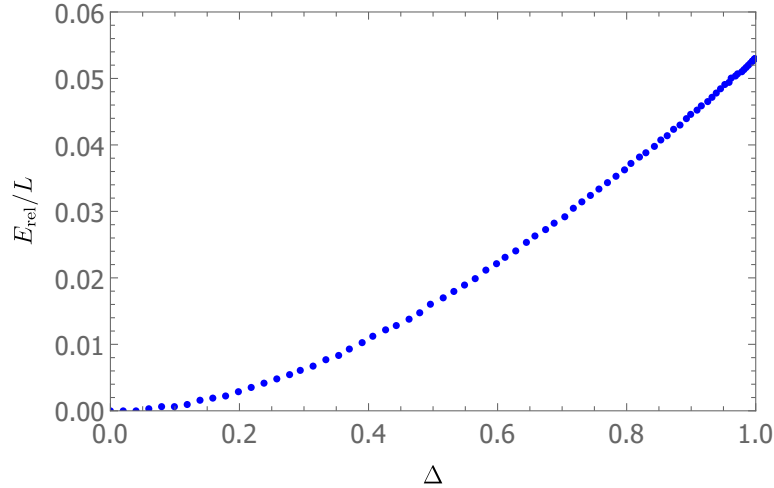


Figure 11: A plot of the relative error. Calculated by taking the difference between the exact result and the perturbation theory, and divide it by the exact result.

6 Integrability of the system

In Section 2 we analytically solved the Heisenberg model using the Bethe ansatz. As mentioned in Section 1, the reason this method works on this system is that the one-dimensional Heisenberg model is an integrable system. A quantum system is said to be integrable if it has infinitely many non-trivial, mutually commuting, conserved charges. This means that the one-dimensional Heisenberg model has infinitely many conserved charges. In this section we discuss a heuristic technique to construct some of these higher order conserved charges for the one-dimensional Heisenberg model, following the steps of Reference [8]. This method makes use of a Boost operator B , which acts on the conserved charges as

$$[B, H_n] = H_{n+1},$$

where H_2 is the Hamiltonian of the Heisenberg model. The Hamiltonian and Boost operator then take the form

$$\begin{aligned} H_2 &= \sum_j h_{j,j+1}, \\ B &= \sum_j j h_{j,j+1}. \end{aligned}$$

For example, in the case of the XXX Heisenberg model $h_{j,j+1} = S_j S_{j+1}$. However, for the moment we will use the general expression of $h_{j,j+1}$. We can now construct the first higher order conserved charge as follows

$$H_3 = [B, H_2] = \sum_{i,j} i [h_{i,i+1}, h_{j,j+1}].$$

As spins on different sites commute, one can see that this is only non-zero in the cases $i = j - 1$ and $i = j + 1$. This gives

$$H_3 = \sum_j \left((j-1) [h_{j-1,j}, h_{j,j+1}] + (j+1) [h_{j+1,j+2}, h_{j,j+1}] \right).$$

Next we rename j to $j+1$ in the first term. This is allowed because the system is translationally invariant, as we are discussing a lattice with periodic boundary conditions. Furthermore, we use the relation $[AB, CD] = -[CD, AB]$ in the second term.

$$\begin{aligned} H_3 &= \sum_j \left(j [h_{j,j+1}, h_{j+1,j+2}] - (j+1) [h_{j,j+1}, h_{j+1,j+2}] \right), \\ &= - \sum_j [h_{j,j+1}, h_{j+1,j+2}]. \end{aligned}$$

As H_3 is a conserved charge, it must commute with H_2 . This implies

$$[H_3, H_2] = - \sum_{i,j} \left[[h_{i,i+1}, h_{i+1,i+2}], h_{j,j+1} \right] = 0.$$

With a similar reasoning as before, one can see that this has non-zero terms for the cases $i = j - 2$, $i = j - 1$, $i = j$, $i = j + 1$. This gives the following four terms

$$\begin{aligned} &\sum_j \left(\left[[h_{j-2,j-1}, h_{j-1,j}], h_{j,j+1} \right] + \left[[h_{j-1,j}, h_{j,j+1}], h_{j,j+1} \right] \right. \\ &\quad \left. + \left[[h_{j,j+1}, h_{j+1,j+2}], h_{j,j+1} \right] + \left[[h_{j+1,j+2}, h_{j+2,j+3}], h_{j,j+1} \right] \right) = 0. \end{aligned} \tag{27}$$

We can use the Jacobi identity² to rewrite the first term as follows

$$\sum_j \left[[h_{j-2,j-1}, h_{j-1,j}], h_{j,j+1} \right] = - \sum_j \left(\left[[h_{j-1,j}, h_{j,j+1}], h_{j-2,j-1} \right] + \left[[h_{j,j+1}, h_{j-2,j-1}], h_{j-1,j} \right] \right),$$

where the last term is zero because spins on different sites commute. Shifting j to $j+1$ in the other term, we get

$$- \sum_j \left[[h_{j+1,j+2}, h_{j+2,j+3}], h_{j,j+1} \right].$$

This exactly cancels the last term in expression (27). Finally, replacing j by $j+1$ in the second term of (27), we get

$$\sum_j \left(\left[[h_{j,j+1}, h_{j+1,j+2}], h_{j+1,j+2} \right] + \left[[h_{j,j+1}, h_{j+1,j+2}], h_{j,j+1} \right] \right) = 0.$$

Adding them together we obtain the following condition of commutativity

$$[H_3, H_2] = \sum_j \left[[h_{j,j+1}, h_{j+1,j+2}], h_{j,j+1} + h_{j+1,j+2} \right] = 0.$$

If this condition is satisfied, it means that H_3 is a non-trivial conserved charge. Using $h_{j,j+1} = S_j S_{j+1}$ one can easily show that this condition is satisfied for the XXX Heisenberg model. And thus for the XXZ model as well, as the parameter Δ does not influence the commutations. Furthermore we can prove the existence of the next higher order conserved charge $H_4 = [B, H_3]$ as follows

$$[H_4, H_2] = \left[[B, H_3], H_2 \right].$$

Using the Jacobi identity again, we can write

$$[H_4, H_2] = - \left[[H_3, H_2], B \right] - \left[[H_2, B], H_3 \right] = 0,$$

where we used the commutativity of H_3 and H_2 , and the fact that $[H_2, B] = -H_3$. This shows that there exists another conserved charge H_4 which commutes with H_2 . Thus for the Heisenberg model we have found the first higher order conserved charge H_3 , and following from the commutativity of H_2 and H_3 we have proven the existence of the second higher order conserved charge H_4 . This already suggests that the one-dimensional Heisenberg model might be an integrable system, which is of course known to be true. Though we have not proven the existence of infinitely many conserved charges, this method does supply a quick and relatively easy way to suggest the possible integrability of a system. Thus for the one-dimensional Heisenberg model with nearest neighbor interactions we have shown that there are more conservation laws than just those of momentum and energy. We will illustrate the significance of this by discussing an example. Consider a two-particle scattering. Assuming both energy and momentum are conserved, one can solve this problem, as you have two conservation laws and two unknowns. However, if it is a three-particle scattering, and there are only two conservation laws, one cannot solve it. Thus to solve an N -particle scattering, one requires N conservation laws. This explains why the Bethe ansatz only works for integrable systems. To be able to solve an infinite spin- $\frac{1}{2}$ chain with N down spins one needs infinitely many conservation laws, requiring the system to be integrable. What one does by applying the Bethe ansatz, is taking these conservation laws, and combining them into the Bethe equations to solve the system.

² $[A, B], C] + [B, C], A] + [C, A], B] = 0$

7 Summary

We have discussed several properties of the one-dimensional spin- $\frac{1}{2}$ Heisenberg model. First we analytically calculated the exact ground state energy in the thermodynamic limit by using the Bethe ansatz. Then we solved the XXZ model in the thermodynamic limit by studying small perturbations in Δ . In addition we did an expansion of the integral expression of the energy in the thermodynamic limit of the XXZ model. Both these methods yielded the same result. We solved the Heisenberg model numerically using exact diagonalization. The results are discussed and compared to the different analytical results. We found that for $L = 10$ and higher the numerical results agree well with the analytical results in the thermodynamic limit. The accuracy of the perturbation theory and the expansion is discussed in a relative error plot. This plot describes how well the perturbation theory and the expansion agree with the exact integral expression from [7], as a function of Δ . We found that the error roughly grows quadratically, as expected in first order perturbation theory. However, the error is still only slightly above 5% for $\Delta = 1$. Furthermore the integrability of the one-dimensional Heisenberg model is discussed. A heuristic method to construct some of the higher order conserved charges is discussed and applied, giving an initial feel of the integrability of the one-dimensional Heisenberg model.

8 Outlook

There are several directions a further study could follow. In this thesis only nearest neighbor interactions are discussed. In the future the interaction can be extended to next-nearest neighbor interactions. The Hamiltonian can be extended to include next-nearest neighbor interactions as follows

$$H = J_1 \sum_j \vec{S}_{j+1} \vec{S}_j + J_2 \sum_j \vec{S}_{j+2} \vec{S}_j,$$

where the term proportional to J_2 describes the next-nearest neighbor interactions. One can look into how a longer range interaction influences the interactions between spins. The entanglement of the spin- $\frac{1}{2}$ Heisenberg model with next-nearest neighbor interaction is discussed in Reference [9]. Furthermore one can look into the effect of next-nearest neighbor interactions on the integrability of the system. One will find that this system is not integrable.

One can generalize the system by studying the anisotropic XYZ model, where all directions have different interactions, $J_x \neq J_y \neq J_z$. In addition, one can introduce an external magnetic field. This adds an extra term to the Hamiltonian, proportional to the external field h .

The numerical calculations in Section 5 are done up to number of lattice sites $L = 12$. Even though these results were already close to the analytic results in the thermodynamic limit, the Mathematica code used for the exact diagonalization can definitely be improved so that higher numbers of lattice sites can be reached. This way the numerics will agree even more with the analytic results. One can also try a different numerical approach, such as DMRG. This is a numerical method mostly used to solve one-dimensional many-body quantum systems, and it can reach much higher numbers of lattice sites.

Furthermore, one can study the dynamics of the system. For example, what happens if you introduce a perturbation on a specific site. An example of a technique to describe such a perturbation is spin wave theory. This theory studies spin waves, which are disturbances that propagate through the lattice. More information on the dynamics of the Heisenberg antiferromagnetic chain can be found in Reference [10].

Another possibility is to look at the Heisenberg model at finite temperature. This is known as the thermodynamic Bethe ansatz. This way one introduces temperature dependence into the equations, making them more complicated. Then, for example, the temperature dependence of observables such as the heat capacity and the magnetic susceptibility can be studied.

One can also look further into the integrability. For example by constructing more higher order conserved charges. Or, as mentioned before, one could work out the condition of commutativity in the case of next-nearest neighbor interactions. In addition, one could study the proof of the existence of infinitely many conserved charges. However, this involves the algebraic Bethe ansatz, which is rather complicated.

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A Fourier theory

For this appendix Chapters 14 and 15 of Reference [11] are used.

In physics one often works with motions that are periodic in time, such as oscillating objects. Fourier series are a useful way to describe such motions. A Fourier series is the expansion of a function as a series of sines and cosines.

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx + \sum_{n=1}^{\infty} b_n \sin nx,$$

where a_n and b_n ($n = 0, 1, 2, \dots$) are coefficients defined by

$$a_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos(nx) dx,$$

$$b_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \sin(nx) dx.$$

There are many different ways to describe a function. An advantage of using a Fourier series is that it can also describe discontinuous functions.

As mentioned before, Fourier series are particularly useful in representing periodic functions. A function $f(x)$ with a period of 2π for example, can be expanded in series of functions with periods $2\pi/n$ with $n = 0, 1, 2, \dots$. Furthermore, Fourier series can be used to solve both ordinary and partial differential equations, such as motions induced by a periodic driving force. Using the Fourier series to expand the driving force gives a fundamental term plus a series of harmonics. This is useful because one can now solve the differential equation for each harmonic individually.

A disadvantage of Fourier series is that they require periodicity of the system to be useful. There is, however, an extension of the Fourier series which can describe non-periodic functions over an infinite interval. This is known as the Fourier transform and it is defined as

$$\hat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{i\omega x} dx,$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \hat{f}(\omega) e^{-i\omega x} d\omega,$$

where $\hat{f}(\omega)$ is the Fourier transform of $f(x)$, and ω is the variable in ω -space. The first expression is the Fourier transform and the second is its inverse transformation. Important to note is that this transformation works for a function of any variable. Position, x , is chosen as an example here. Just like the Fourier series, the Fourier transform is a very useful tool to solve both ordinary and partial differential equations. This can be demonstrated by considering the Fourier transform of the derivative

$$\hat{f}_1(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{df(x)}{dx} e^{i\omega x} dx, \quad (28)$$

where the subscript indicates the order of the derivative. Integrating by parts and assuming that $f(x)$ goes to zero as $x \rightarrow \pm\infty$ gives

$$\hat{f}_1(\omega) = (-i\omega) \hat{f}(\omega).$$

This result shows that the Fourier transform of the derivative of $f(x)$ is equal to $(-i\omega)$ times the Fourier transform of the original function $f(x)$. For higher order derivatives this generalizes to

$$\hat{f}_n(\omega) = (-i\omega)^n \hat{f}(\omega). \quad (29)$$

Exactly this is the reason why Fourier transformation is useful to solve differential equations. By taking the Fourier transform of an equation one can replace derivatives in the original space by a simple multiplication in the transformed ω -space. This way it is possible to reduce partial differential equations to ordinary differential

equations which are much easier to solve. The solution in the original space is then found by applying the inverse Fourier transformation to the solution in ω -space.

To illustrate how this works, let us study the wave equation in one dimension using Fourier transform. This is a partial differential equation describing the motion of waves. The equation is

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 f(x, t)}{\partial t^2},$$

where x and t are position and time, respectively. And $f(x, t)$ is a function of both of them. We Fourier transform both sides, transforming from x -space to ω -space. This gives

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{\partial^2 f(x, t)}{\partial x^2} e^{i\omega x} dx = \frac{1}{v^2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{\partial^2 f(x, t)}{\partial t^2} e^{i\omega x} dx.$$

The left hand side is of the form of equation (28), but with a second order derivative. This means we can simplify it using (29) for the second order. The right hand side is just the second order derivative with respect to time of the Fourier transform of $f(x, t)$. Together this simplifies to

$$(-i\omega)^2 \hat{f}(\omega, t) = \frac{1}{v^2} \frac{\partial^2 \hat{f}(\omega, t)}{\partial t^2},$$

where $\hat{f}(\omega, t)$ is the Fourier transform of $f(x, t)$. Note that we started with a partial differential equation in x -space. By Fourier transforming we have reduced the problem to an ordinary differential equation in ω -space. One can now solve the differential equation in ω -space using initial conditions, and then use the inverse Fourier transform to find the solution in x -space.

Next we will discuss the derivation of another useful result following from the Fourier transform, the convolution theorem. Consider two functions $f(x)$ and $g(x)$ and their Fourier transforms $\hat{f}(\omega)$ and $\hat{g}(\omega)$. The convolution of $f(x)$ and $g(x)$ is defined as

$$f * g \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(y) f(x - y) dy.$$

We substitute the definition of the inverse Fourier transform for $f(x - y)$ to find

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(y) \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \hat{f}(\omega) e^{-i\omega(x-y)} d\omega \right] dy.$$

Interchanging the order of integration yields

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \hat{f}(\omega) e^{-i\omega x} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(y) e^{i\omega y} dy \right] d\omega.$$

Note that the part between brackets is the definition of the Fourier transform. We can write

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \hat{f}(\omega) \hat{g}(\omega) e^{-i\omega x} d\omega.$$

This result is known as the convolution theorem. It tells us that the Fourier transform of a convolution of two functions is equal to the product of the Fourier transforms of the individual functions. This theorem is applied in Section 2 to solve equation (21).

B Complex analysis

The derivation of the Residue theorem is done following Chapters 6 and 7 of Reference [11].

The study of functions of complex numbers is called complex analysis. Though it has its roots in mathematics, there are many applications which are extremely useful in physics. One of these is the Residue theorem, which is a very effective method for solving difficult integrals. Not only in this thesis, but in physics in general it is commonly used and therefore a derivation of the theorem will be supplied in this appendix. It is a generalization of Cauchy's integral formula, so this will be proven first.

A function $f(z)$ is analytic at $z = z_0$ if the function is differentiable at $z = z_0$ and in a small region around z_0 , where z_0 is some point in the interior of the contour C . However, if the derivative of $f(z)$ at z_0 does not exist, we call z_0 a singularity or a singular point of $f(z)$.

Let us consider a function $f(z)$ which is analytic both in the interior and on the edge of a closed contour C in the complex plane. We will now prove Cauchy's integral formula, which is

$$\oint_C \frac{f(z)}{z - z_0} dz = 2\pi i f(z_0).$$

Note that the integrand is not analytic if $z = z_0$ unless $f(z_0) = 0$. To fix this we can deform the contour C in such a way that the singular point z_0 is excluded by a second circular contour C_2 . We can now apply Cauchy's integral theorem, which in this case states

$$\oint_C \frac{f(z)}{z - z_0} dz - \oint_{C_2} \frac{f(z)}{z - z_0} dz = 0.$$

Now we can express the integral over C_2 in polar coordinates since this contour is circular. Writing $z = z_0 + re^{i\theta}$ and $dz = ire^{i\theta} d\theta$ yields

$$\oint_C \frac{f(z)}{z - z_0} dz - \oint_{C_2} if(z_0 + re^{i\theta}) d\theta = 0.$$

Taking the limit $r \rightarrow 0$ gives

$$\oint_C \frac{f(z)}{z - z_0} dz = if(z_0) \oint_{C_2} d\theta = 2\pi i f(z_0).$$

This result is Cauchy's integral formula. It shows that the value of $f(z)$ at some point z_0 in the interior of C can be calculated if the boundaries of the contour are known.

Next we will deduce the Laurent series. To do this we start by applying Cauchy's integral formula. This time we consider a circular contour, centered around z_0 , with radius R with a hole in it with a smaller radius r . To connect the boundary of the inner circle to that of the outer one we draw two more circular contours in the interior and connect these. We label these C_1 and C_2 with radii r_1 and r_2 respectively, where $r < r_2 < r_1 < R$. A sketch of the contours is given in Figure 12. By drawing these contours we have created one simply connected region and this allows us to apply Cauchy's integral formula

$$f(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(z')}{z' - z} dz' - \frac{1}{2\pi i} \oint_{C_2} \frac{f(z')}{z' - z} dz',$$

where z is some point in the interior of the contours, and z' are points on the contours C_1 and C_2 , and $f(z)$ is again an analytic function in and on the domain. Next we rewrite the denominators as follows

$$f(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(z')}{(z' - z_0) - (z - z_0)} dz' - \frac{1}{2\pi i} \oint_{C_2} \frac{f(z')}{(z' - z_0) - (z - z_0)} dz'.$$

Now we can use the geometric series $1/(1-x) = \sum_{n=0}^{\infty} x^n$ (for $|x| < 1$) to rewrite the integrals. To do so we take out a factor of $z' - z_0$ in the denominator in the integral over C_1 . However, for C_2 it holds that $z' < z$, so to be able to use the geometric series in this integral we take out a factor of $z - z_0$ in the denominator.

$$f(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(z')}{(z' - z_0) [1 - (z - z_0)/(z' - z_0)]} dz' - \frac{1}{2\pi i} \oint_{C_2} \frac{f(z')}{(z - z_0) [(z' - z_0)/(z - z_0) - 1]} dz'.$$

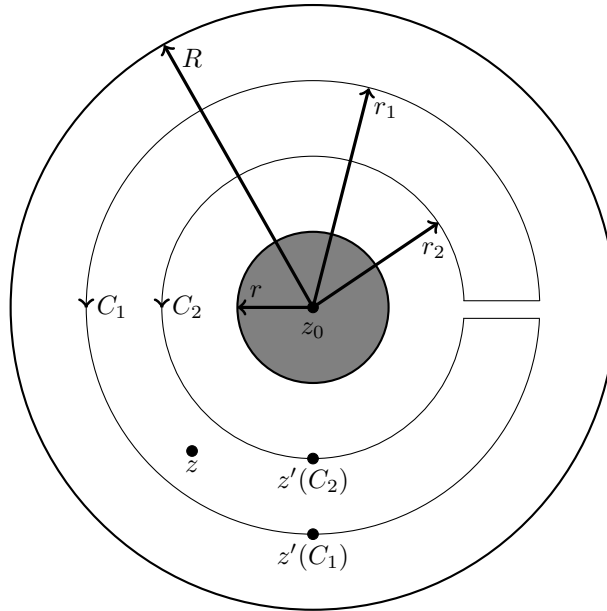


Figure 12: Sketch of the contours C_1 and C_2 , creating a simply connected region.

Applying the geometric series in both integrals we get

$$f(z) = \frac{1}{2\pi i} \sum_{n=0}^{\infty} (z - z_0)^n \oint_{C_1} (z' - z_0)^{-n-1} f(z') dz' + \frac{1}{2\pi i} \sum_{n=0}^{\infty} (z - z_0)^{-n-1} \oint_{C_2} (z' - z_0)^n f(z') dz'.$$

The next step is shifting the summation by replacing n with $n - 1$ in the second term, which results in

$$f(z) = \frac{1}{2\pi i} \sum_{n=0}^{\infty} (z - z_0)^n \oint_{C_1} (z' - z_0)^{-n-1} f(z') dz' + \frac{1}{2\pi i} \sum_{n=1}^{\infty} (z - z_0)^{-n} \oint_{C_2} (z' - z_0)^{n-1} f(z') dz'.$$

Finally we change n to $-n$ in the second series so we can add the two terms together to find

$$f(z) = \sum_{n=-\infty}^{+\infty} a_n (z - z_0)^n,$$

where z_0 are singular points and the coefficients a_n are

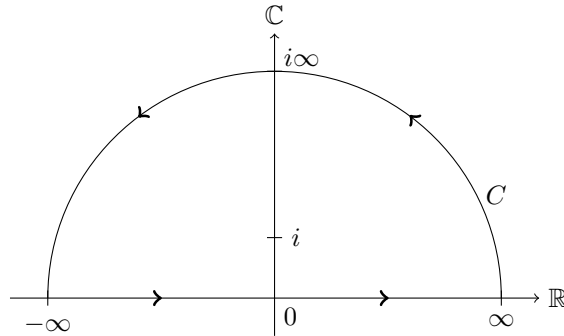
$$a_n = \frac{1}{2\pi i} \oint_C \frac{f(z')}{(z' - z_0)^{n+1}} dz'.$$

This is known as the Laurent expansion of $f(z)$. Laurent expansions are generalizations of Taylor expansions in the presence of singularities. The Residue theorem can be found by integrating over the terms of a Laurent expansion. Consider a Laurent expansion of some function $f(z) = \sum_{n=-\infty}^{+\infty} a_n (z - z_0)^n$. We integrate over a closed contour which contains a singular point z_0 of $f(z)$. For each term except for $n = -1$ this gives

$$a_n \oint (z' - z_0)^n dz' = a_n \left. \frac{(z' - z_0)^{n+1}}{n+1} \right|_z^z = 0.$$

However, if $n = -1$ the integral yields

$$a_{-1z_0} \oint (z' - z_0)^{-1} dz' = a_{-1z_0} \oint id\theta = 2\pi i a_{-1z_0},$$

Figure 13: Sketch of contour C .

where we again used the polar coordinates $z' = z_0 + re^{i\theta}$, $dz' = ire^{i\theta}d\theta$ to rewrite the integral. Combining the two gives the full expression for the integral of $f(z)$

$$\oint_C f(z)dz = 2\pi ia_{-1z_0}.$$

The coefficient a_{-1z_0} is called the residue of $f(z)$ at z_0 . This can be done for any singular point z_j enclosed by a contour C . Generalizing for any number of singular points enclosed by some contour C we get

$$\oint_C f(z)dz = 2\pi i (a_{-1z_0} + a_{-1z_1} + a_{-1z_2} + \dots) = 2\pi i \sum_j a_{-1z_j}. \quad (30)$$

This result is the Residue theorem. It tells us that the integral of $f(z)$ over some contour C is equal to $2\pi i$ times the sum of the residues enclosed by the contour. This is a remarkable expression as it simplifies performing contour integrals to calculating the value of the residues of the function at the isolated points. Even though it appears to be a theorem for complex functions, the theorem can also be used for real integrals. One then extends the real integral to the complex plane and chooses an appropriate contour in the complex plane. Sometimes one can choose the contour in such a way that the integral in the complex plane has no contribution, as we will do in the example below. After this it is just a matter of applying the theorem.

To show how the Residue theorem is applied, we will work out an example. In the Fourier transformation of equation (21) in Section 2 an integral of the following form is encountered

$$\int_{-\infty}^{\infty} \frac{1}{1+x^2} e^{i\omega x} dx.$$

To be able to apply the Residue theorem we extend the integral to the complex plane, creating a closed contour C . This contour goes from from $-\infty$ to ∞ along the real axis, and then back to $-\infty$ along a semicircle through $i\infty$ on the complex axis in a counterclockwise fashion. A sketch of C is shown in Figure 13. One could also take the negative semicircle, going through $-i\infty$. In this case the extra minus sign is cancelled as in this case the contour is of a clockwise fashion, giving the same result in the end. We can write the integral over contour C as the sum of two integrals, one along the real axis and one in the complex plane.

$$\int_C \frac{1}{1+z^2} e^{i\omega z} dz = \int_{\mathbb{R}} \frac{1}{1+x^2} e^{i\omega x} dx + \int_{\mathbb{C}} \frac{1}{1+z^2} e^{i\omega z} dz,$$

where z is a complex number. Note, however, that the complex integral has no contribution as the integrand is zero along the integral by our convenient choice of contour C . Applying the Residue theorem from (30) gives

$$\int_C \frac{1}{1+z^2} e^{i\omega z} dz = \int_{\mathbb{R}} \frac{1}{1+x^2} e^{i\omega x} dx = 2\pi i \sum_j a_{-1z_j}, \quad (31)$$

where the sum is over all residues enclosed by contour C . To solve the integral we have to calculate the residues enclosed by C . Note that $e^{i\omega z}$ is defined for all z , and thus has no singularities. However, $1/(1+z^2)$ has a singularity for $z = \pm i$. Of these points only $z = i$ is enclosed by our contour. The residue of a function $f(z)$ at a singularity z_0 is calculated as follows

$$\text{Res}(f(z), z_0) = \lim_{z \rightarrow z_0} (z - z_0)f(z).$$

Using this to calculate the residue at $z = i$ gives

$$\begin{aligned} \text{Res}\left(\frac{1}{1+z^2} e^{i\omega z}, i\right) &= \lim_{z \rightarrow i} (z - i) \frac{1}{1+z^2} e^{i\omega z}, \\ &= \lim_{z \rightarrow i} (z - i) \frac{1}{(z - i)(z + i)} e^{i\omega z}, \\ &= \lim_{z \rightarrow i} \frac{1}{z + i} e^{i\omega z}, \\ &= \frac{1}{2i} e^{-\omega} \end{aligned}$$

Filling this into equation (31) we find

$$\int_{\mathbb{R}} \frac{1}{1+x^2} e^{i\omega x} dx = \pi e^{-\omega}$$

Thus we successfully calculated the integral using the Residue theorem. This theorem is used several times to calculate integrals in Section 2. The most convenient choice of the contour depends on the integral one wants to calculate.

C Jordan-Wigner transformation

Chapter 6, pages 160–163, of Reference [5] is used for this appendix on the Jordan-Wigner transformation. In many quantum systems one deals with spin particles. However, in many-body systems for example, the spin operators are not very pleasant to work with. In the case of spin- $\frac{1}{2}$ particles one can avoid having to use the spin operators by using a mapping, which replaces the spin operators by fermionic creation and annihilation operators. It makes use of the analogy between spin- $\frac{1}{2}$ particles and fermions in the sense that the spin up state can be seen as an empty lattice site, whereas the spin down state can be seen as a site occupied by a single fermion. This gives rise to the following notation

$$\begin{aligned} S^x + iS^y &= S^+ \mapsto c^\dagger, \\ S^x - iS^y &= S^- \mapsto c, \\ S^z &= c^\dagger c - \frac{1}{2}, \end{aligned}$$

where c are the fermionic operators. With this notation, the commutation relations for the spin operators are obeyed. There is still a problem, however, as the fermionic operators obey the following algebra

$$\begin{aligned} \{c_i, c_j\} &= 0, \\ \{c_i^\dagger, c_j^\dagger\} &= 0, \\ \{c_i, c_j^\dagger\} &= \delta_{ij}. \end{aligned}$$

We see that the fermionic operators on different sites anticommute, whereas spin operators on different sites commute. This means the mapping must be altered in such a way that the spins also anticommute on different sites. This is known as the Jordan-Wigner transformation and it is as follows

$$\begin{aligned} S_i^+ &\mapsto c_i^\dagger e^{i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j}, \\ S_i^- &\mapsto c_i e^{-i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j}, \\ S_i^z &= c_i^\dagger c_i - \frac{1}{2}, \end{aligned}$$

where the exponents are phase factors. The term in the sum in the exponent, $c_j^\dagger c_j$, is the number operator, which in this case counts the number of fermions on the left of site i . Depending on whether this is even or odd, the exponent is ± 1 . To illustrate how this phase factor works, let us take a look at a term which arises in the Heisenberg Hamiltonian.

$$\begin{aligned} S_{i+1}^+ S_i^- &= c_{i+1}^\dagger e^{i\pi \sum_{j=-\infty}^i c_j^\dagger c_j} c_i e^{-i\pi \sum_{j=-\infty}^{i-1} c_j^\dagger c_j}, \\ &= c_{i+1}^\dagger e^{i\pi c_i^\dagger c_i} c_i, \\ &= c_{i+1}^\dagger c_i, \end{aligned}$$

where $e^{i\pi c_i^\dagger c_i} c_i = c_i$. This is because c_i annihilates a fermion on site i , and therefore the number operator $c_i^\dagger c_i = 0$ in the exponent. By using this transformation all commutation relations are obeyed, and one can successfully describe spin- $\frac{1}{2}$ particles in terms of fermionic operators.