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# Solutions to the one-dimensional Heisenberg model

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## Abstract

In this thesis we take a look at the one-dimensional Heisenberg model. The Heisenberg model is the most used model to study the magnetic properties of materials and is of paramount importance for understanding magnets. First we sketch a brief derivation of the model and discuss its strengths and weaknesses. Afterwards we develop a transformation of the Heisenberg model to a model of spinless fermions, which allows for an easy solution of the  $J_z = 0$  model. After solving the model for  $J_z = 0$ , we solve the model for general  $J_z$ . The results we find are very complicated and it is hard to calculate anything explicitly. So we move to the thermodynamic limit to calculate the ground state energy for  $J_z = 1$ . After that we have found a solution for big system sizes, we use exact diagonalisation to solve the Heisenberg model. We do this for system sizes up to 12 particles. With our results we check how accurate some expansions for smaller system sizes are. We find some accurate expansions for small  $\Delta$  and  $\Delta = 1$ . We also look at an energy gap of the system for  $\Delta > 1$ . We find how this gap behaves as a function of  $\Delta$ .

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## 1 Introduction

One might logically assume that magnetic ordering is caused by interacting magnetic moments via the magnetic fields caused by these magnetic moments. But if we calculate the energy of this interaction we would find that the energy associated with aligning magnetic moments would correspond to a transition temperatures of 1 Kelvin. This is way off target, iron for example has a transition temperature of around 1000 K. The fact that our results using classical electrodynamics are so far off seems to suggest that the magnetic ordering of materials are regulated by non classical concepts. So in order to study the magnetic properties we need to use quantum physics.

The first question we seek to answer in this thesis is why do spins interact? As stated before, magnetic ordering is not caused by magnetic fields. We will follow a calculation first done by Heitler and London in 1927 to explain what causes magnetic ordering instead. We will find that the Coulomb interaction combined with fermi statistics causes magnetic ordering in a 2 electron system.

After we have found the reason for magnetic ordering for 2 electron system we generalise this to a system of  $N$  electrons on a lattice. We make some approximations to find a well known model for studying magnetic ordering: the Heisenberg model. The Heisenberg model was first proposed by Werner Heisenberg in 1928 and has ever since formed the basis of the study of the dynamics of spins.

After we have sketched a brief derivation of the Heisenberg model we arrive at the main question we seek to answer in this thesis: "what are the solutions to the 1-dimensional Heisenberg model?". We will answer this question with 2 different methods. We will solve the one-dimensional Heisenberg model using analytical and numerical methods. First we will use the coordinate Bethe Ansatz to solve the one-dimensional Heisenberg model analytically. In 1 dimension the Heisenberg model was first solved by Hans Bethe in 1931. In more than 1 dimension analytical solutions have not been found. The solutions we will find will be very complicated and it would be very difficult to calculate any properties of interest. Because of this we will look to the thermodynamic limit. In the thermodynamic limit we find the ground state energy of the XXX Heisenberg model.

Lastly we solve the system using numerical methods. With exact diagonalization we find the ground state energy and the energy of the excited states for system sizes up to 12 particles. We will do this for the isotropic and the anisotropic Heisenberg model. We will look at expansion for the ground state energy for finite system sizes. We will compare this with our numerical data to see how accurate this expansion is.

## 2 Origin of the spin interactions

In this section we take a look at interaction between spins. In this section we want to explain the physical reason why spins interact the way they do. One might logically assume magnetic field and magnetic moments cause the interaction between the spins. But magnetic fields are very weak and therefore can not explain an interaction with the strength which we see in spin interactions. In this section we will do a calculation which shows that the reason for the spins interaction has nothing to do with magnetic fields, but instead is a combination of the electrostatic potential and fermi statistics.

### 2.1 Heitler London calculation

In this section and the next section we will follow chapter 26 of Condensed matter physics by Marder[1]. We will first follow a calculation done by Heitler and London in 1927. This calculation will show us the origin of the interaction between spins.

We consider 2 atoms at positions  $\vec{R}_1$  and  $\vec{R}_2$  respectively. In our calculation the only electrons we will focus on will be the outermost electrons of the atoms. We will denote the spatial wave functions of the outermost electrons centered on atom 1 and 2 when the atoms are infinitely far apart by  $\phi_1(\vec{r})$  and  $\phi_2(\vec{r})$  respectively. Since these are wave functions centered around different positions the overlap integral is nonzero. We define the overlap integral as:

$$l = \left\| \int \phi_1^*(\vec{r}) \phi_2(\vec{r}) d\vec{r} \right\| \quad (2.1)$$

In the following calculations we will assume that the excited states of the electrons do not play a role. Furthermore, we will take the Coulomb interaction between the electrons and atoms to be a perturbation. The total wave function will be a product of the spatial and the spin part:

$$\Psi_{\text{total}} = \Phi_{\text{spatial}} \chi_{\text{spin}}, \quad (2.2)$$

where  $\Phi$  is the spatial wave function and  $\chi$  is the spin part of the wave function. The spatial wave function is either a symmetric or antisymmetric product of  $\phi_1(\vec{r})$  and  $\phi_2(\vec{r})$ :

$$\Phi_- = \frac{1}{\sqrt{2 - 2l^2}} (\phi_1(\vec{r}_1) \phi_2(\vec{r}_2) - \phi_1(\vec{r}_2) \phi_2(\vec{r}_1)), \quad (2.3)$$

$$\Phi_+ = \frac{1}{\sqrt{2 + 2l^2}} (\phi_1(\vec{r}_1) \phi_2(\vec{r}_2) + \phi_1(\vec{r}_2) \phi_2(\vec{r}_1)). \quad (2.4)$$

The spin part of the wave function is either in the singlet configuration:

$$\frac{1}{\sqrt{2}} (\chi_{\uparrow} \chi_{\downarrow} - \chi_{\downarrow} \chi_{\uparrow}).$$

Or the spin part could be either of the three triplet configurations:

$$\frac{1}{\sqrt{2}} (\chi_{\uparrow} \chi_{\downarrow} + \chi_{\downarrow} \chi_{\uparrow}),$$

$$\chi_{\uparrow} \chi_{\uparrow},$$

$$\chi_{\downarrow} \chi_{\downarrow}.$$

Since electrons are fermions the total wave function has to be antisymmetric under exchange of particles. So that means that you have to combine a symmetric and a antisymmetric part to find an antisymmetric total wave function. So 2.3 will be paired with the singlet configuration and 2.4 will be paired with a triplet configuration.

We will now calculate the energy expectation value of the antisymmetric and the symmetric wave function. We will ignore the spin wave function because the Hamiltonian does not depend on the spin of the electrons.

The Hamiltonian of this system is:

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{e^2}{|\vec{R}_2 - \vec{R}_1|} + \frac{e^2}{|\vec{r}_2 - \vec{r}_1|} - \frac{e^2}{|\vec{R}_1 - \vec{r}_1|} - \frac{e^2}{|\vec{R}_2 - \vec{r}_2|} - \frac{e^2}{|\vec{R}_1 - \vec{r}_2|} - \frac{e^2}{|\vec{R}_2 - \vec{r}_1|}, \quad (2.5)$$

where  $\vec{p}_1$  and  $\vec{p}_2$  are the momentum operators of electrons 1 and 2 respectively. The first 2 terms are kinetic terms, the other terms are the interactions between the electrons and the atoms. We now calculate the energy expectation value. Since the Hamiltonian does not depend on spin, we do this using only the spatial part of the wave function. This gives us:

$$\begin{aligned} E_{\pm} &= \int \Phi_{\pm}^*(\vec{r}_1, \vec{r}_2) H \Phi_{\pm}(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2 \\ &= \frac{1}{2 \pm 2l^2} \int [\phi_1^*(\vec{r}_1) \phi_2^*(\vec{r}_2) \pm \phi_1^*(\vec{r}_2) \phi_2^*(\vec{r}_1)] H [\phi_1(\vec{r}_1) \phi_2(\vec{r}_2) \pm \phi_1(\vec{r}_2) \phi_2(\vec{r}_1)] d\vec{r}_1 d\vec{r}_2. \end{aligned} \quad (2.6)$$

Here  $E_+$  is the energy of the (singlet) wave function of 2.4 and  $E_-$  is the energy of the (triplet) wave function of 2.3.

Let us now split 2.6 into multiple different integrals. To ease our notation we define the following integrals:

$$\begin{aligned} U &= \int |\phi_1(\vec{r}_1)|^2 |\phi_2(\vec{r}_2)|^2 \left[ \frac{e^2}{|\vec{R}_2 - \vec{r}_2|} - \frac{e^2}{|\vec{r}_2 - \vec{r}_1|} + \frac{e^2}{|\vec{r}_2 - \vec{R}_2|} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \right] d\vec{r}_1 d\vec{r}_2, \\ V &= \int \phi_1(\vec{r}_1)^* \phi_2(\vec{r}_1)^* \phi_2(\vec{r}_1) \phi_1(\vec{r}_2) \left[ \frac{e^2}{|\vec{R}_2 - \vec{r}_2|} - \frac{e^2}{|\vec{r}_2 - \vec{r}_1|} + \frac{e^2}{|\vec{r}_2 - \vec{R}_2|} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \right] d\vec{r}_1 d\vec{r}_2, \\ E_0 &= \int \phi_1(\vec{r}_1)^* \left[ \frac{p_1^2}{2m} - \frac{e^2}{|\vec{R}_1 - \vec{r}_1|} \right] \phi_1(\vec{r}_1) d\vec{r}_1 = \int \phi_2(\vec{r}_2)^* \left[ \frac{p_2^2}{2m} - \frac{e^2}{|\vec{R}_2 - \vec{r}_2|} \right] \phi_2(\vec{r}_2) d\vec{r}_2. \end{aligned}$$

Using this notation 2.6 become:

$$\begin{aligned} E_+ &= E_s = 2 \frac{2E_0 + U + V + 2l^2 E_0}{2 + 2l^2} = 2E_0 + \frac{U + V}{1 + l^2}, \\ E_- &= E_t = 2 \frac{2E_0 + U - V - 2l^2 E_0}{2 - 2l^2} = 2E_0 + \frac{U - V}{1 - l^2}. \end{aligned} \quad (2.7)$$

Now that we have these expression for the energy's we can calculate the energy difference.

$$\Delta E = E_t - E_s = 2E_0 + \frac{U - V}{1 - l^2} - \left( 2E_0 + \frac{U + V}{1 + l^2} \right) = \frac{2l^2 U - 2V}{1 - l^4} \equiv -J \quad (2.8)$$

The value of  $J$  depends on the integrals  $U, V$  and  $l$ . These integrals have different values depending on what type of atom we have. So  $J$  can be positive or negative. If  $J > 0$  then the triplet configuration has a lower energy. This means that it is favourable to have aligned spins. This correspond too ferromagnetic materials. If  $J < 0$  then the singlet configuration has a lower energy. In this case it is favourable to have the spins point in different directions. This corresponds to antiferromagnetic materials.

## 2.2 Replacing the Hamiltonian by spin operators

We have seen in the previous subsection that the energy is correlated with the spin wave function. The singlet and triplet state have a different energy. This motivates us to replace the Hamiltonian from a spatial Hamiltonian to a spin Hamiltonian. If we choose to replace the Hamiltonian, we require  $\Psi^* H_{\text{spin}} \Psi = \Psi^* H_{\text{spatial}} \Psi$ . In the previous section we have found  $\Psi^* H_{\text{spatial}} \Psi$  (see 2.7). We need to find a spin Hamiltonian which gives the same results. We will try:

$$H_{\text{spin}} = a + b \vec{S}_1 \cdot \vec{S}_2 = a + b(S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z), \quad (2.9)$$

where  $\vec{S}_1$  acts on electron 1 and  $\vec{S}_2$  acts on electron 2. To check if this Hamiltonian complies with our requirement we apply  $H_{\text{spin}}$  to  $\Psi$ . We only have to focus on the spin part because the Hamiltonian does not act on the spatial part of the wave function. We find:

$$\begin{aligned}\frac{1}{2}(\chi_{\uparrow}\chi_{\downarrow} - \chi_{\downarrow}\chi_{\uparrow})H_{\text{spin}}(\chi_{\uparrow}\chi_{\downarrow} - \chi_{\downarrow}\chi_{\uparrow}) &= a + \frac{b}{4}, \\ \frac{1}{2}(\chi_{\uparrow}\chi_{\downarrow} + \chi_{\downarrow}\chi_{\uparrow})H_{\text{spin}}(\chi_{\uparrow}\chi_{\downarrow} + \chi_{\downarrow}\chi_{\uparrow}) &= a - \frac{3b}{4}, \\ \chi_{\downarrow}\chi_{\downarrow}H_{\text{spin}}\chi_{\downarrow}\chi_{\downarrow} &= a - \frac{3b}{4}, \\ \chi_{\uparrow}\chi_{\uparrow}H_{\text{spin}}\chi_{\uparrow}\chi_{\uparrow} &= a - \frac{3b}{4}.\end{aligned}$$

We see that the 3 triplet states have the same energy. If this was not the case our new spin Hamiltonian would be invalid. For this new Hamiltonian to be equivalent to the old Hamiltonian we need:

$$a - \frac{3b}{4} = 2E_0 \frac{U - V}{1 - t^2}, \quad (2.10)$$

$$a + \frac{b}{4} = 2E_0 \frac{U + V}{1 + t^2}. \quad (2.11)$$

These are 2 linearly coupled equations. They can be easily solved. The solution are:

$$\begin{aligned}a &= 2E_0 + \frac{U - V}{1 - t^2} + \frac{J}{4}, \\ b &= -J.\end{aligned} \quad (2.12)$$

So we have now found a new Hamiltonian in terms of spin matrices. Our final spin Hamiltonian then becomes:

$$H = 2E_0 + \frac{U - V}{1 - t^2} + \frac{J}{4} - J\vec{S}_1\vec{S}_2. \quad (2.13)$$

### 3 Heisenberg model

In the last section we studied the spin interaction of a 2 electron system. We found that the spin interactions between these 2 atoms was based on minimizing the Coulomb repulsion of the atoms when fermi statistics are taken into account. In the following section we wish to generalize the idea to a lattice of ions with an electron on each site. By making a few approximation we will find the famous Heisenberg Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j. \quad (3.1)$$

In our derivation of the Heisenberg model we look at a lattice with one ion per lattice site, but more importantly also one electron per lattice site. Realistically there are more electrons of course, but we will only focus on the outermost electron. We look at lattice with  $N$  lattice sites. We assume that there is no electron hopping between lattice sites. We assume that our Hamiltonian for our electrons has the following form:

$$H = \sum_{l=1}^N \frac{p_l^2}{2m} + U, \quad (3.2)$$

$\frac{p_l^2}{2m}$  gives the kinetic contribution, and all interactions terms are collected into  $U$ . We assume that  $U$  only contains pairwise interactions. Besides that  $U$  can take any form that it wants. It can be a Coulomb interaction, or a more complicated interaction like screened interactions. We will focus our attention on  $U$  since it contains all magnetic effects. We will first rewrite  $U$  to a form containing the creation and annihilation operators. For an introduction on the fermionic creation and annihilation operators see appendix C.

### 3.1 Rewriting the Hamiltonian

Since we assume  $U$  only contains pairwise interaction we rewrite it to:

$$U = \sum_{j \neq j'} f_{jj'}, \quad (3.3)$$

where  $f_{jj'}$  acts identically on all pairs of particles  $j$  and  $j'$ . We now wish to rewrite to a  $U$ , so that the only operators it contains are the creation and annihilation operators. In order to do this we first rewrite  $U$  to:

$$\begin{aligned} U = \sum_{j \neq j'} f_{jj'} &= \sum_{\substack{j \neq j' \\ \sigma \sigma' \sigma'' \sigma'''}} \left( |w(\vec{R}_{l\sigma})(j)\rangle \langle w(\vec{R}_{l\sigma})(j)| \right) \left( |w(\vec{R}_{l'\sigma'})(j')\rangle \langle w(\vec{R}_{l'\sigma'})(j')| \right) \\ &\times \left( |w(\vec{R}_{l''\sigma''})(j)\rangle \langle w(\vec{R}_{l''\sigma''})(j)| \right) \left( |w(\vec{R}_{l'''\sigma'''})(j')\rangle \langle w(\vec{R}_{l'''\sigma'''})(j')| \right) f_{jj'}, \end{aligned} \quad (3.4)$$

where  $|w(\vec{R}_{l\sigma})(j)\rangle$  is the Wannier function localized on lattice site  $l$  combined with the spin state  $\sigma$ . The  $(j)$  indicates that particle  $j$  occupies this state. Wannier functions are complete functions that describe electrons localized on an atomic lattice site. Since Wannier functions describe electrons localized on a lattice site, Wannier functions localized on different lattice site have very little overlap. Here we used that  $\sum_{l,\sigma} |w(\vec{R}_{l\sigma})(j)\rangle \langle w(\vec{R}_{l\sigma})(j)|$  is equal to the unitary operator because the functions  $w(\vec{R}_{l\sigma})$  are complete. Now reshuffling the terms we get:

$$\begin{aligned} \sum_{j \neq j'} f_{jj'} &= \sum_{\substack{j \neq j' \\ \sigma \sigma' \sigma'' \sigma'''}} |w(\vec{R}_{l\sigma})(j)\rangle |w(\vec{R}_{l'\sigma'})(j')\rangle \langle w(\vec{R}_{l\sigma})(j)w(\vec{R}_{l'\sigma'})(j')| f_{jj'} |w(\vec{R}_{l''\sigma''})(j)w(\vec{R}_{l'''\sigma'''})(j')\rangle \\ &\times \langle w(\vec{R}_{l''\sigma''})(j)| \langle w(\vec{R}_{l'''\sigma'''})(j')|. \end{aligned} \quad (3.5)$$

We are allowed to reshuffle the terms like this because function states occupied by different particles commute with each other. For the next step we will allow to run the summation over  $j = j'$ . The second term subtracts then the terms  $j = j'$ . This gives us:

$$\begin{aligned} &\sum_{\substack{jj' \\ \sigma \sigma' \sigma'' \sigma'''}} \left( |w(\vec{R}_{l\sigma})(j)\rangle \langle w(\vec{R}_{l''\sigma''})(j)| \right) \left( |w(\vec{R}_{l'\sigma'})(j')\rangle \langle w(\vec{R}_{l'''\sigma'''})(j')| \right) \\ &\times \langle w(\vec{R}_{l\sigma})(j)| \langle w(\vec{R}_{l'\sigma'})(j')| f_{jj'} |w(\vec{R}_{l''\sigma''})(j)| |w(\vec{R}_{l'''\sigma'''})(j')\rangle \\ - \sum_{\substack{jj' \\ \sigma \sigma' \sigma'' \sigma'''}} \delta_{l'l'} \left( |w(\vec{R}_{l\sigma})(j)\rangle \langle w(\vec{R}_{l''\sigma''})(j)| \right) \langle w(\vec{R}_{l\sigma})(j)| \langle w(\vec{R}_{l'\sigma'})(j')| f_{jj'} |w(\vec{R}_{l''\sigma''})(j)\rangle |w(\vec{R}_{l'''\sigma'''})(j')\rangle. \end{aligned} \quad (3.6)$$

Now we note that  $\sum_j |w(\vec{R}_{l\sigma})(j)\rangle \langle w(\vec{R}_{l''\sigma''})(j)|$  is equal to  $c_{l\sigma}^\dagger c_{l''\sigma''}$ . This holds as well for other  $l$  and  $\sigma$ . Filling this in into 3.6 gives us:

$$\begin{aligned} &\sum_{\substack{jj' \\ \sigma \sigma' \sigma'' \sigma'''}} c_{l,\sigma}^\dagger c_{l',\sigma'} c_{l'',\sigma''}^\dagger c_{l''',\sigma'''} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | f_{jj'} |w(\vec{R}_{l''\sigma''})(1)w(\vec{R}_{l'''\sigma'''})(2)\rangle \\ - \sum_{\substack{jj' \\ \sigma \sigma' \sigma'' \sigma'''}} \delta_{l'l'} c_{l,\sigma}^\dagger c_{l',\sigma'} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | f_{jj'} |w(\vec{R}_{l''\sigma''})(1)w(\vec{R}_{l'''\sigma'''})(2)\rangle, \end{aligned} \quad (3.7)$$

at the same time we also replaced  $\langle w(\vec{R}_{l\sigma})(j)| \langle w(\vec{R}_{l'\sigma'})(j')| f_{jj'} |w(\vec{R}_{l''\sigma''})(j)| |w(\vec{R}_{l'''\sigma'''})(j')\rangle$  by  $\langle w(\vec{R}_{l\sigma})(1)| \langle w(\vec{R}_{l'\sigma'})(2) | f_{12} |w(\vec{R}_{l''\sigma''})(1)| |w(\vec{R}_{l'''\sigma'''})(2)\rangle$ . We are allowed to do this since  $f_{jj'}$  act the



same on all pairs of particles. We will now use the commutation relation of the creation and annihilation operators to switch around the terms  $c_{l'',\sigma''}c_{l',\sigma'}^\dagger$ . By doing this we will also cancel the second sum. This gives us:

$$\sum_{\substack{jj'l'l''l'''' \\ \sigma\sigma'\sigma''\sigma'''}} c_{l,\sigma}^\dagger c_{l',\sigma'}^\dagger c_{l'',\sigma''} c_{l''',\sigma'''} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | f_{jj'} | w(\vec{R}_{l''\sigma''})(1)w(\vec{R}_{l'''\sigma'''})(2) \rangle. \quad (3.8)$$

So to summarise we have now rewritten our interaction terms in terms of a scalar and the creation and annihilation operators.

$$U = \sum_{j \neq j'} f_{jj'} = \sum_{\substack{jj'l'l''l'''' \\ \sigma\sigma'\sigma''\sigma'''}} c_{l,\sigma}^\dagger c_{l',\sigma'}^\dagger c_{l'',\sigma''} c_{l''',\sigma'''} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | f_{jj'} | w(\vec{R}_{l''\sigma''})(1)w(\vec{R}_{l'''\sigma'''})(2) \rangle \quad (3.9)$$

Since  $U$  (and therefore also)  $f_{jj'}$  does not depend on spin, only the terms where  $\sigma = \sigma''$  and  $\sigma' = \sigma'''$  are nonzero. So we can restrict our sums to  $\sigma, \sigma'$ . This gives us:

$$U = \sum_{l,l',l'',l''',\sigma,\sigma'} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l''\sigma})(1)w(\vec{R}_{l'''\sigma'})(2) \rangle c_{l\sigma}^\dagger c_{l'\sigma'}^\dagger c_{l''\sigma} c_{l'''\sigma'} \quad (3.10)$$

### 3.2 Making approximations to find the Heisenberg model

In order to find the Heisenberg Hamiltonian we have to make multiple approximations. The first approximation we make is that only the terms where  $w(\vec{R}_{l'\sigma'}) = w(\vec{R}_{l''\sigma''})$  and  $w(\vec{R}_{l\sigma}) = w(\vec{R}_{l''\sigma''})$  or  $w(\vec{R}_{l\sigma}) = w(\vec{R}_{l'''\sigma'''})$  and  $w(\vec{R}_{l'\sigma'}) = w(\vec{R}_{l''\sigma''})$  are considered. The motivation for this approximation is that the Wannier functions are localized on a lattice site. So only the elements where  $\vec{R}_{l'\sigma'} = \vec{R}_{l''\sigma''}$  and  $\vec{R}_{l\sigma} = \vec{R}_{l''\sigma''}$  or  $\vec{R}_{l\sigma} = \vec{R}_{l'''\sigma'''} and  $\vec{R}_{l'\sigma'} = \vec{R}_{l''\sigma''}$  contribute significantly. We also assume that  $l$  and  $l'$  are neighbours. The motivation for this is again that the other terms in the sum contribute very little. These approximations transform 3.10 to:$

$$U = \sum_{\langle l,l',\rangle,\sigma,\sigma'} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle c_{l\sigma}^\dagger c_{l'\sigma'}^\dagger c_{l\sigma} c_{l'\sigma'} \\ + \sum_{\langle l,l',\rangle,\sigma,\sigma'} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle c_{l\sigma}^\dagger c_{l'\sigma'}^\dagger c_{l\sigma'} c_{l'\sigma}. \quad (3.11)$$

$\langle l,l',\rangle$  indicates that we only sum over neighbouring sites. We now rewrite this using the commutation relations for the creation and annihilation operators:

$$U = \sum_{\langle l,l',\rangle,\sigma,\sigma'} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle c_{l\sigma}^\dagger c_{l'\sigma'}^\dagger c_{l\sigma} c_{l'\sigma'} \\ + \sum_{\langle l,l',\rangle,\sigma,\sigma'} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle [n_{l\sigma} \delta_{ll'} - c_{l\sigma}^\dagger c_{l\sigma'} c_{l'\sigma'}^\dagger c_{l'\sigma}], \quad (3.12)$$

where  $n_{l\sigma} = c_{l\sigma}^\dagger c_{l\sigma}$ . We will now focus on the last term in 3.12. It can be put as an interaction between spins. First note the following identities:

$$S_l^z = \frac{1}{2} [n_{l\uparrow} - n_{l\downarrow}], \\ S_l^+ = c_{l\uparrow}^\dagger c_{l\downarrow}, \\ S_l^- = c_{l\downarrow}^\dagger c_{l\uparrow}, \\ n_{l\uparrow} n_{l'\uparrow} + n_{l\downarrow} n_{l'\downarrow} = \frac{1}{2} \left[ (n_{l\uparrow} + n_{l\downarrow})(n_{l'\uparrow} + n_{l'\downarrow}) + (n_{l\uparrow} - n_{l\downarrow})(n_{l'\downarrow} - n_{l'\uparrow}) \right] \\ = \frac{1}{2} [1 + 4S_l^z S_{l'}^z].$$

In the last step we use that at every site there is either an electron with spin up or an electron with spin down, so either  $n_{\downarrow}$  or  $n_{\uparrow}$  is 1 while the other is 0. We now explicitly evaluate the spin sum in the final term of 3.12. This gives us:

$$\begin{aligned}
& \sum_{\langle l, l' \rangle} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle [-c_{l\uparrow}^\dagger c_{l\downarrow} c_{l'\downarrow}^\dagger c_{l'\uparrow} - c_{l\downarrow}^\dagger c_{l\uparrow} c_{l'\uparrow}^\dagger c_{l'\downarrow} - n_{l\uparrow} n_{l'\uparrow} - n_{l\downarrow} n_{l'\downarrow}] \\
&= -2 \sum_{\langle l, l' \rangle} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle \left[ \frac{1}{4} + S_l^z S_{l'}^z + \frac{1}{2} (S_l^+ S_{l'}^- + S_l^- S_{l'}^+) \right] \\
&= -2 \sum_{\langle l, l' \rangle} \langle w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) | U | w(\vec{R}_{l\sigma})(1)w(\vec{R}_{l'\sigma'})(2) \rangle \left[ \frac{1}{4} + \vec{S}_l \vec{S}_{l'} \right]
\end{aligned} \tag{3.13}$$

We have now shown that the Hamiltonian contains the term  $\vec{S}_l \vec{S}_{l'}$ . In order to find our Heisenberg Hamiltonian we now disregard all other terms in the Hamiltonian. We do this because the other terms in the Hamiltonian do not depend on the spin of the electrons and is therefore not important when we only want to consider the magnetic properties of our material. This might seem like an preposterous approximation, but it turns out to be quite accurate if we only care about the magnetic properties of our material. Of course this approximation is only accurate if the kinetic energy of the electrons is small. If the kinetic energy of the electrons is big, the approximation is not accurate.

## 4 Transformation of the Heisenberg model

In this section we will look at 2 transformations of the Heisenberg model. We will work with a slightly more general Hamiltonian than the Hamiltonian we have found in our previous derivation. We will allow the coupling constant to be different in the z-direction. This gives us the following Hamiltonian:

$$\begin{aligned} H &= J_{xy} \sum_{j=1}^L [S_{j+1}^x S_j^x + S_{j+1}^y S_j^y] + J_z \sum_{j=1}^L S_{j+1}^z S_j^z \\ &= \frac{J_{xy}}{2} \sum_{j=1}^L [S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+] + J_z \sum_{j=1}^L S_{j+1}^z S_j^z. \end{aligned} \quad (4.1)$$

Here  $S^x$ ,  $S^y$  and  $S^z$  are the Pauli spin operators.  $S^+$  and  $S^-$  are the raising and lowering operators. This model is called the XXZ Heisenberg model since we allow for a different coupling constant in the z direction. If  $J_z = J_{xy}$  then we would have the XXX Heisenberg model.

We will look at 2 transformations in this section. We will do this following section 6.1 of Quantum Physics in One Dimension by Thierry Giamarchi[2]. The first transformation shows that we only have to take  $J_{xy} > 0$  into account. The second transformation will show that the one-dimensional Heisenberg model is equivalent to a model of interacting spinless fermions. The reason why we do this is because by doing this we get rid of the Pauli spin matrices in favor of the creation and annihilation operators. We like this because the Pauli spin matrices have unfavorable commutation relations. By getting rid of the Pauli spin matrices we can solve our model of interacting spinless fermions for  $J_z = 0$ .

For every transformation we make we have to make sure that the commutation relations of the spins operators are still satisfied. These commutation relations are given by:

$$[S_i^\alpha, S_j^\beta] = \delta_{ij} i \epsilon_{\alpha\beta\gamma} S_i^\gamma, \quad (4.2)$$

where  $\epsilon_{\alpha\beta\gamma}$  is the totally antisymmetric tensor.

For our first transformations we look at:

$$\begin{aligned} S_j^x &\rightarrow (-1)^j S_j^x \\ S_j^y &\rightarrow (-1)^j S_j^y \\ S_j^z &\rightarrow S_j^z \end{aligned} \quad (4.3)$$

This transformation does not change the commutation relation and is therefore allowed. This transformation is equivalent to changing  $J_{xy}$  to  $-J_{xy}$ . So because we can always change the sign of  $J_{xy}$ , we can always assume  $J_{xy}$  to be positive.

Next we want to transform the Heisenberg model from a model of interacting spins to a model of spinless fermions. To do this we would like to use the following transformation:

$$\begin{aligned} S_i^+ &\rightarrow c_i^\dagger, \\ S_i^- &\rightarrow c_i, \\ S_i^z &\rightarrow c_i^\dagger c_i - 1/2. \end{aligned} \quad (4.4)$$

This has the correct commutation relations for operators on the same site. Let us for example calculate  $[S_i^+, S_i^-]$ . Using our transformations this becomes:

$$[S_i^+, S_i^-] = [c_i^\dagger, c_i] = c_i^\dagger c_i - c_i c_i^\dagger = 2c_i^\dagger c_i - 1 = 2S_i^z. \quad (4.5)$$

Which is exactly what it should be. It is not that complicated to check that the other commutation relations for operators on the same site are also obeyed. But for  $[S_j^+, S_i^-]$  with  $i \neq j$ , we find:

$$[S_j^+, S_i^-] = [c_j^\dagger, c_i] = c_j^\dagger c_i - c_i c_j^\dagger = 2c_i^\dagger c_i \neq 0. \quad (4.6)$$

We can see that because fermionic operators on different sites anticommute this is not equal to 0, which it should be. In order to solve this problem we add a string of operators to  $c_i^\dagger$  and  $c_i$ :

$$\begin{aligned} c_j &\rightarrow c_j \exp \left[ -i\pi \sum_{k=-\infty}^{j-1} c_k^\dagger c_k \right] \\ c_j^\dagger &\rightarrow c_j^\dagger \exp \left[ i\pi \sum_{k=-\infty}^{j-1} c_k^\dagger c_k \right]. \end{aligned} \quad (4.7)$$

This gives us:

$$\begin{aligned} S_i^+ &\rightarrow c_i^\dagger e^{i\pi \sum_{k=-\infty}^{i-1} c_k^\dagger c_k} \\ S_i^- &\rightarrow c_i e^{-i\pi \sum_{k=-\infty}^{i-1} c_k^\dagger c_k} \\ S_i^z &\rightarrow c_i^\dagger c_i - 1/2 \end{aligned} \quad (4.8)$$

This transformation does not change the commutation relations which are already obeyed, but it does introduce the minus sign that is necessary for  $[S_j^+, S_i^-]$  to commute. Let us see how this works. In this calculation we will restrict ourselves to  $j > l$ , this is just for convenience's sake. The calculation would also work for  $l > j$ . With this restriction we get:

$$\begin{aligned} [S_j^+, S_l^-] &= c_j^\dagger \exp \left[ i\pi \sum_{k=-\infty}^{j-1} c_k^\dagger c_k \right] c_l \exp \left[ -i\pi \sum_{k=-\infty}^{l-1} c_k^\dagger c_k \right] - c_l \exp \left[ -i\pi \sum_{k=-\infty}^{l-1} c_k^\dagger c_k \right] c_j^\dagger \exp \left[ i\pi \sum_{k=-\infty}^{j-1} c_k^\dagger c_k \right] \\ &= c_j^\dagger \exp \left[ i\pi \sum_{k=l}^{j-1} c_k^\dagger c_k \right] c_l - c_l \exp \left[ i\pi \sum_{k=l}^{j-1} c_k^\dagger c_k \right] c_j^\dagger \\ &= c_j^\dagger c_l \exp \left[ i\pi \sum_{k=l+1}^{j-1} c_k^\dagger c_k \right] - c_l c_j^\dagger \exp \left[ i\pi \sum_{k=l}^{j-1} c_k^\dagger c_k \right] \\ &= \exp \left[ i\pi \sum_{k=l+1}^{j-1} c_k^\dagger c_k \right] \left( c_j^\dagger c_l - c_l c_j^\dagger \exp \left[ i\pi c_l^\dagger c_l \right] \right) = 0. \end{aligned} \quad (4.9)$$

Here we used that  $c_k^\dagger c_k$  and  $c_j$  commute as long as  $k \neq j$ . An easy way to see that the last expression is 0 is by dividing our problem in 2 cases: either  $l$  is occupied or  $l$  is unoccupied. If  $l$  is unoccupied the whole expression is 0, because we act on it with  $c_l$ . If  $l$  is occupied then  $\exp \left[ i\pi c_l^\dagger c_l \right]$  is  $-1$  and the last term is 0 using the commutation relations for the fermionic creation and annihilation operators. So we have now found that our transformation obeys the commutation relationships. Which means that the transformation:

$$\begin{aligned} S_i^+ &\rightarrow c_i^\dagger e^{i\pi \sum_{k=-\infty}^{i-1} c_k^\dagger c_k} \\ S_i^- &\rightarrow c_i e^{-i\pi \sum_{k=-\infty}^{i-1} c_k^\dagger c_k} \\ S_i^z &\rightarrow c_i^\dagger c_i - 1/2 \end{aligned} \quad (4.10)$$

is valid. Luckily these string of operators simplify in the case of a one-dimensional chain. For a one-dimensional chain we have:

$$\begin{aligned} S_{i+1}^+ S_i^- &= c_{i+1}^\dagger e^{i\pi c_i^\dagger c_i} c_i = c_{i+1}^\dagger c_i, \\ S_{i+1}^- S_i^+ &= c_{i+1} e^{i\pi c_i c_i^\dagger} c_i^\dagger = c_{i+1} c_i^\dagger. \end{aligned} \quad (4.11)$$

Filling this in into our Hamiltonian gives us:

$$H = -\frac{J_{xy}}{2} \sum_i c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} + J_z \sum_i (c_{i+1}^\dagger c_{i+1} - 1/2)(c_i^\dagger c_i - 1/2). \quad (4.12)$$

Note that in the case  $J_z = 0$ , this is equal to the free fermion problem. This problem can be solved without too much difficulty. This is done in the appendix A of [3]. This is a lot easier than the Bethe Ansatz we will use in the next section. Using perbutation theory it is also possible to find approximate solution for small  $J_z$ . This is a good alternative to the Bethe Ansatz since the solutions we will find with the Bethe Ansatz will be very complicated.

## 5 Bethe Ansatz

In this chapter we will solve the Heisenberg model, which we have derived in a previous chapter. We will work within an one-dimensional chain of length  $L$ . To simplify our notation we will set our lattice spacing to 1 in this entire chapter. We will work with the same Hamiltonian as in the previous section:

$$\begin{aligned}
 H &= J_{xy} \sum_{j=1}^L [S_{j+1}^x S_j^x + S_{j+1}^y S_j^y] + J_z \sum_{j=1}^L S_{j+1}^z S_j^z \\
 &= \frac{J_{xy}}{2} \sum_{j=1}^L [S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+] + J_z \sum_{j=1}^L S_{j+1}^z S_j^z.
 \end{aligned} \tag{5.1}$$

In this section we will use periodic boundary conditions. So we will use:

$$\begin{aligned}
 S_{L+1}^x &= S_1^x, \\
 S_{L+1}^y &= S_1^y, \\
 S_{L+1}^z &= S_1^z.
 \end{aligned}$$

Once we find the wave function, we will of course also require that the wave function will satisfy periodic boundary condition as well. We will in this chapter use the parametrisation  $J_{xy} = J$ ,  $J_z = J\Delta$ . With this parametrisation our Hamiltonian becomes:

$$H = \frac{J}{2} \sum_{j=1}^L [S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+ + \Delta S_{j+1}^z S_j^z]. \tag{5.2}$$

If we set  $\Delta = 1$  we get the Hamiltonian we derived in the previous chapter. This is equal to the isotropic system.

To solve the Heisenberg model we will a method called the coordinate Bethe Ansatz. We will do this following chapter 5 from the book Quantum Physics in One Dimension by Thierry Giamarchi [2].

As we can see, the Hamiltonian commutes with the total  $S^z$ . This means that the total spin is conserved. If the total spin is conserved then the number of spins down is also conserved. This motivates us to first look at the case of all but 1 spin up, or in other words 1 spin down. After that we will look at the case of 2 spins down. Only then will we take a look at  $N$  down spins. The reason we do this is because a lot phenomena which occur with 1 or 2 spins down also occur with more spins down. By first looking at the easier case of 1 or 2 spins down, it will be easier to solve the XXZ Heisenberg model for a general case of  $N$  spins down. We will find an expression for the wave function and energy's for  $N$  spins down. But since the energy's we find are in a system of non-linear coupled equations, it will be hard to find exact energy's. The wave functions we find will also be very complicated. So even though we will solve the system it will be hard to calculate a lot of properties of the system that we are interested in. What we can do however is calculate the ground state energy in the thermodynamic limit. So after we have found the solution to the XXZ Heisenberg model we will delve into the thermodynamic limit to find the ground state energy of the system.

### 5.1 1 spin down

Before we start, let us introduce some notation. Let  $|N\rangle$  be a state where there is one spin down on site  $N$ . At all other site we then have a spin up.  $|N_1, N_2, N_3, \dots\rangle$  is a state with spins down located at lattice sites  $N_1, N_2, N_3, \dots$ , the other sites are occupied by a spin up. Note that  $|N_1, N_2, N_3, \dots\rangle = |N_2, N_1, N_3, \dots\rangle$ , it does not matter in which order we put the down spins.

In this section we will solve the Hamiltonian of 5.1 for 1 spin down and all other spins up. We expect the wave function to be a superposition of the down spin at every lattice site, since there is no reason the down

spin should prefer one lattice site of another. The amplitude of our wave function should be the same on every site. We expect our total wave function for 1 spin down to have this form:

$$\Phi = \sum_x \phi(x) | x \rangle. \quad (5.3)$$

Let us see how the Hamiltonian acts on a wave function of this form:

$$H\Phi = \sum_x \left[ -J\Delta\phi(x) | x \rangle + \frac{J}{2}\phi(x) | x-1 \rangle + \frac{J}{2}\phi(x) | x+1 \rangle + E_0\phi(x) | x \rangle \right]. \quad (5.4)$$

Where  $E_0 = LJ/4$ , is the energy of the state where all spins are up. We see that there are 2 hopping terms. One to the right and one to the left. There is also one stationary term  $E_0 - \Delta$ . As an Ansatz for  $\phi(x)$  we try  $\Phi = \sum_x \phi(x) | x \rangle$ . We want to check if this wave function can be an eigenstate for correct choice of  $\phi(x)$ . To do this we try rewriting 5.4 to the form  $E\Phi$ . We will now look for all terms at position  $| x \rangle$ . There is one term which hopped there from the left with amplitude  $J\phi(x-1)/2$ , one term which hopped there from the right with amplitude  $J\phi(x+1)/2$  and one term with amplitude  $J(E_0 - \Delta)\phi(x)$ . Using this we can rewrite the sum to:

$$H\Phi = \sum_x \left[ (E_0 - J\Delta)\phi(x) | x \rangle + \frac{J}{2}\phi(x+1) | x \rangle + \frac{J}{2}\phi(x-1) | x \rangle \right]. \quad (5.5)$$

With the right choice of  $\phi(x)$  this  $\Phi$  could be an eigenstate. We try as an Ansatz for the wave function a plane wave with momentum  $k$ . So we have:

$$\phi(x) = \frac{e^{ikx}}{\sqrt{L}}. \quad (5.6)$$

If we fill this in into 5.5, we get:

$$\begin{aligned} H\Phi &= \left( J[-\Delta + \frac{1}{2}e^{-ik} + \frac{1}{2}e^{ik}] + E_0 \right) \sum_x e^{ikx} | x \rangle \\ &= (J \cos(k) - J\Delta + E_0) \sum_x e^{ikx} | x \rangle. \end{aligned} \quad (5.7)$$

So we have found that  $\Phi$  is an eigenstate of the Hamiltonian with an eigenenergy of:

$$E = J \cos(k) - J\Delta + E_0. \quad (5.8)$$

We still have to demand periodic boundary conditions on the wave function. Doing this will determine the allowed values of  $k$ . We demand:

$$\Phi(x) = \Phi(x+L). \quad (5.9)$$

This condition gives us the following allowed values for  $k$ :

$$k = \frac{2\pi n}{L}, \quad (5.10)$$

where  $n$  can be any integer. So we have now found a wave function for 1 down spin. Finding a solution for 1 spin down was quite easy. In the next section we will try finding the solution for 2 spins down. This will be a little bit more complicated since the 2 spins down will interfere with each other if they are close.

## 5.2 2 spins down

Just as for one spin down we expect the wave function to be a superposition of all possible ways to distribute the down spins:

$$\Phi = \sum_{x_1 \neq x_2} \phi(x_1, x_2) | x_1, x_2 \rangle. \quad (5.11)$$

Let us start again with calculating  $H\Phi$ . In the case of 2 spins the problem is slightly more complicated. The part of  $\Phi$  where  $x_1$  and  $x_2$  are next to each other give a different result from the part of  $\Phi$  where  $x_1$  and  $x_2$  are far apart. Let us first calculate  $H \sum_{x_1, x_2} \phi(x_1, x_2) |x_1, x_2\rangle$  seperately for  $x_1$  and  $x_2$  close together and far apart. If  $x_1$  and  $x_2$  are far apart we get:

$$H \sum_{x_1 \neq x_2 \pm 1} \phi(x_1, x_2) |x_1, x_2\rangle = \sum_{x_1 \neq x_2 \pm 1} \left[ \frac{J}{2} \phi(x_1, x_2) |x_1 - 1, x_2\rangle + \frac{J}{2} \phi(x_1, x_2) |x_1, x_2 - 1\rangle + \frac{J}{2} \phi(x_1, x_2) |x_1, x_2 + 1\rangle + \frac{J}{2} \phi(x_1, x_2) |x_1 + 1, x_2\rangle + (E_0 - 2J\Delta) \phi(x_1, x_2) |x_1, x_2\rangle \right]. \quad (5.12)$$

If  $x_1$  and  $x_2$  are close, we get:

$$H \sum_{x_1 = x_2 \pm 1} \phi(x_1, x_2) |x_1, x_2\rangle = \sum_{x_1 = x_2 \pm 1} \left[ \frac{J}{2} \phi(x_1, x_2) |x_1 - 1, x_2\rangle + \frac{J}{2} \phi(x_1, x_2) |x_1, x_2 + 1\rangle + (E_0 - J\Delta) \phi(x_1, x_2) |x_1, x_2\rangle \right]. \quad (5.13)$$

If we put both of these sums together, then we have  $H\Phi$ . We now again look for all terms containing  $|x_1, x_2\rangle$ . Here again we find different results depending on whether the spins are far apart or not. For the down spins far apart there are 4 hopping terms, one from the left and one from the right for both particles, and one term which remained stationary. Putting all the terms together we find for the down spins far apart:

$$\sum_{x_1 \neq x_2 \pm 1} \left[ \frac{J}{2} \phi(x_1 + 1, x_2) + \frac{J}{2} \phi(x_1 - 1, x_2) + \frac{J}{2} \phi(x_1, x_2 + 1) + \frac{J}{2} \phi(x_1, x_2 - 1) + \frac{J}{2} (E_0 - 4\Delta) \phi(x_1, x_2) \right] |x_1, x_2\rangle. \quad (5.14)$$

If we now try to find all terms with  $|x_1, x_2\rangle$  for the down spins close together we find a different result. There are 2 less hopping terms, also the stationary term has a different amplitude. For the spins down close together we find:

$$\sum_{x_1 = x_2 \pm 1} \left[ \frac{J}{2} \phi(x_1 - 1, x_2) + \frac{J}{2} \phi(x_1, x_2 + 1) + \frac{J}{2} (E_0 - 2\Delta) \phi(x_1, x_2) \right] |x_1, x_2\rangle. \quad (5.15)$$

We will deal with this complication by requiring that the difference in terms between 5.14 and 5.15 has to be 0. This way we can just solve the Schrödinger equation only with the terms we found in 3.12. The equation we then obtain is:

$$E\Phi = \sum_{x_1 \neq x_2} \left[ \frac{J}{2} \phi(x_1 + 1, x_2) + \frac{J}{2} \phi(x_1 - 1, x_2) + \frac{J}{2} \phi(x_1, x_2 + 1) + \frac{J}{2} \phi(x_1, x_2 - 1) + (E_0 - 2J\Delta) \phi(x_1, x_2) \right] |x_1, x_2\rangle. \quad (5.16)$$

The additional condition we will get from requiring that the difference in terms between 3.12 and 5.15 is 0 is:

$$\frac{J}{2} [-2\Delta \phi(x, x + 1) + \phi(x, x) + \phi(x + 1, x + 1)] = 0. \quad (5.17)$$

If 5.16 and 5.17 are both satisfied then we have found a solution to the Schrödinger equation. We will now first try solving 5.16. Later we will make sure that 5.17 is also satisfied.

In order to solve 5.16 we need an Ansatz for the wave function. Inspired by the wave function for 1 down spin we try as an Ansatz for 2 down spins:

$$\phi(x_1, x_2) = A e^{i(k_1 x_1 + k_2 x_2)} + B e^{i(k_2 x_1 + k_1 x_2)}, \quad (5.18)$$

where A and B are constants which will later be fixed to satisfy 5.17 and the normalisation of the wave function.  $k_1$  and  $k_2$  will be fixed by periodic boundary conditions and the symmetry requirement of the wave function.

We now check if the Ansatz solves 5.16. If we fill the Ansatz in into 5.16 we find:



$$\begin{aligned} & \sum_{x_1 \neq x_2} \left[ A e^{i(k_1 x_1 + k_2 x_2)} + B e^{i(k_2 x_1 + k_1 x_2)} \right] |x_1, x_2\rangle \left( \frac{J}{2} e^{ik_1} + \frac{J}{2} e^{-ik_1} + \frac{J}{2} e^{ik_2} + \frac{J}{2} e^{-ik_2} + E_0 - 2J\Delta \right) \\ &= (J \cos(k_1) + J \cos(k_2) + E_0 - 2J\Delta) \sum_{x_1 \neq x_2} \left( A e^{i(k_1 x_1 + k_2 x_2)} + B e^{i(k_2 x_1 + k_1 x_2)} \right) |x_1, x_2\rangle. \end{aligned}$$

So we find that our Ansatz is an eigenstate with an eigenenergy of:

$$J \cos(k_1) + J \cos(k_2) + E_0 - 2J\Delta. \quad (5.19)$$

Now that we have found that our Ansatz is a solution, we still have to satisfy requirement 5.17:

$$\frac{J}{2} [-2\Delta\phi(x, x+1) + \phi(x+1, x+1) + \phi(x, x)] = 0. \quad (5.20)$$

Filling in  $\phi$  we find:

$$\begin{aligned} & -2\Delta \left[ A e^{i(k_1 x + k_2(x+1))} + B e^{i(k_2 x + k_1(x+1))} \right] + A e^{i(k_1(x+1) + k_2(x+1))} + B e^{i(k_2(x+1) + k_1(x+1))} \\ & + A e^{i(k_1 x + k_2 x)} + B e^{i(k_2 x + k_1 x)} = 0. \end{aligned} \quad (5.21)$$

Now we bring everything but the  $\Delta$  term to the right, and then divide by  $e^{i(k_1 x + k_2 x)}$ , This gives us:

$$2\Delta (A e^{ik_2} + B e^{ik_1}) = A + B + A e^{i(k_1 + k_2)} + B e^{i(k_1 + k_2)}. \quad (5.22)$$

Now we collect all term with  $A$  on the left side and all term with  $B$  on the right side:

$$2\Delta A e^{ik_2} - A - A e^{i(k_1 + k_2)} = -2\Delta B e^{ik_1} + B + B e^{i(k_1 + k_2)} \quad (5.23)$$

Rewriting this gives:

$$\begin{aligned} \frac{A}{B} &= -\frac{2\Delta e^{ik_1} - 1 - e^{i(k_1 + k_2)}}{2\Delta e^{ik_2} - 1 - e^{i(k_1 + k_2)}} \\ &= -\frac{2\Delta e^{i\frac{k_1 - k_2}{2}} - e^{-i\frac{k_1 + k_2}{2}} - e^{i\frac{k_1 + k_2}{2}}}{2\Delta e^{-i\frac{k_1 - k_2}{2}} - e^{-i\frac{k_1 + k_2}{2}} - e^{i\frac{k_1 + k_2}{2}}} \\ &= -\frac{\Delta e^{i\frac{k_1 - k_2}{2}} - \cos\left(\frac{k_1 + k_2}{2}\right)}{\Delta e^{-i\frac{k_1 - k_2}{2}} - \cos\left(\frac{k_1 + k_2}{2}\right)}. \end{aligned} \quad (5.24)$$

Where in the first step we multiplied the denominator and the numerator with  $e^{-i\frac{k_1 + k_2}{2}}$ . So we have now found that our Ansatz wave function is an eigenstate as long as 5.24 is satisfied. 5.24 only fixes the ratio of  $\frac{A}{B}$ , normalisation will fix the amplitude of  $A$  and  $B$ .

In light of what will happen when there are more than 2 down spins it is useful to look at the result in 5.24 a little bit more closely.

It turns out that we can express  $\frac{A}{B}$  as a pure phase as long as  $k_1$  and  $k_2$  are real. To prove this note that the denominator and the numerator are complex conjugates. Because of this we can use the following parametrisations:

$$\begin{aligned} \Delta e^{i\frac{k_1 - k_2}{2}} - \cos\left(\frac{k_1 + k_2}{2}\right) &= r e^{i\Theta/2}, \\ \Delta e^{-i\frac{k_1 - k_2}{2}} - \cos\left(\frac{k_1 + k_2}{2}\right) &= r e^{-i\Theta/2}. \end{aligned}$$

If we fill in these equations, we find:

$$\frac{A}{B} = -\frac{re^{i\Theta/2}}{re^{-i\Theta/2}} = -e^{i\Theta}. \quad (5.25)$$

Since  $\Theta$  is the argument of a complex number we can calculate it by using simple geometry. The argument of a complex number is the arctangent of the imaginary part divided by its real part. So we find:

$$\Theta(k_1, k_2) = 2 \arctan \left( \frac{\Delta \sin(\frac{k_1-k_2}{2})}{\Delta \cos(\frac{k_1-k_2}{2}) - \cos(\frac{k_1+k_2}{2})} \right). \quad (5.26)$$

Note that  $\Theta(k_1, k_2) = -\Theta(k_2, k_1)$ . Also note that  $\Theta(k, k) = 0$ , this means that if  $k_1 = k_2$ ,  $A = -B$  and the whole wave function becomes 0. This is of course not allowed so we forbid  $k_1 = k_2$ .

So now that we have found that  $\Phi$  is an eigenstate of the Hamiltonian we still have to fix the periodic boundary condition and the symmetry requirement of the wave function. We combine these 2 requirements into one equation:

$$\phi(x_1, x_2) = \phi(x_2, x_1 + L). \quad (5.27)$$

This requirement will fix the allowed values of  $k_1$  and  $k_2$ . To find the allowed values of  $k_1$  and  $k_2$  we now fill in  $\phi$ :

$$Ae^{i(k_1x_1+k_2x_2)} + Be^{i(k_2x_1+k_1x_2)} = Ae^{i(k_1x_2+k_2(x_1+L))} + Be^{i(k_2x_2+k_1(x_1+L))}, \quad (5.28)$$

which gives:

$$A = B \left[ \frac{e^{i(k_2x_2+k_1(x_1+L))} - e^{i(k_2x_1+k_1x_2)}}{e^{i(k_1x_1+k_2x_2)} - e^{i(k_1x_2+k_2(x_1+L))}} \right]. \quad (5.29)$$

We can solve this equation by imposing  $\frac{A}{B} = e^{-ik_2L} = e^{ik_1L}$ . If we combine this with 5.25 we get the following equation for  $k_1$  and  $k_2$ :

$$\begin{aligned} k_1 + k_2 &= \frac{2\pi n}{L}, \\ k_1L &= 2\pi I_1 + \Theta(k_1, k_2), \\ k_2L &= 2\pi I_2 + \Theta(k_2, k_1). \end{aligned}$$

Where  $n$  can be any integer and  $I_1$  and  $I_2$  can be any half-integer.

So to summarize the results we have found for 2 spins down are:

$$\begin{aligned} \Phi &= \sum_{x_1, x_2} (Ae^{i(k_1x_1+k_2x_2)} + Be^{i(k_2x_1+k_1x_2)}) |x_1, x_2\rangle, \\ \frac{A}{B} &= -e^{i\Theta}, \\ \Theta &= 2 \arctan \left( \frac{\Delta \sin(\frac{k_1-k_2}{2})}{\Delta \cos(\frac{k_1-k_2}{2}) - \cos(\frac{k_1+k_2}{2})} \right), \\ E &= \frac{J}{2}(2 \cos(k_1) + 2 \cos(k_2) + E_0 - 4\Delta), \\ k_1L &= 2\pi I_1 + \Theta(k_1, k_2), \\ k_2L &= 2\pi I_2 + \Theta(k_2, k_1). \end{aligned}$$

We have now found the solution of the Heisenberg model for 2 spins down. We started with a wave function which had 4 parameters which we could tweak to ensure the wave function was an eigenstate. We used  $A$  and  $B$  to ensure that the Hamiltonian gave the same results regardless of whether the down spins were close or far apart. We used  $k_1$  and  $k_2$  to demand the periodic boundary conditions and the symmetry requirement.

Now that we have found the eigenstate for 2 spins down we are ready to tackle the system for an arbitrary  $N$  spins down.

### 5.3 Many spins down

Now that we have found the solution for 2 spins down we would like to generalize this to an arbitrary number of down spins. In this section we will deal with  $N$  down spins. As an Ansatz we try a wavefunction similar to the wave function we found for 2 particles. The Ansatz we use for  $N$  spins down is:

$$\Phi = \sum_P \phi(x_1, x_2, x_3, \dots, x_N) | x_1, x_2, x_3, \dots, x_N \rangle = \sum_P A_P e^{i(\sum_l k_{P_l} x_l)} | x_1, x_2, x_3, \dots, x_N \rangle. \quad (5.30)$$

Where  $P$  are all the permutations of ways to order the numbers 1 to  $N$ .  $P_l$  is then the number which is at the  $l$ th position in permutation  $P$ . So for example in the permutation  $(n, m, l, k, \dots)$   $P_1 = n, P_2 = m, P_3 = l$  and so on. As in the case for 2 particles we will once again pick the constants  $A_P$  in such a way that the difference in terms caused by neighbouring down spins is 0. Since there are now more ways in which the down spins can be distributed this will take a little bit more effort. To make sure the difference in terms caused by neighbouring down spins is 0 we set the following requirement:

$$2\Delta\phi(\dots, x_k, x_k + 1) = \phi(\dots, x_k + 1, x_k + 1, \dots) + \phi(\dots, x_k, x_k, \dots). \quad (5.31)$$

Note that this is similar to 5.17. 5.31 has to be satisfied for every possible value of  $k$ . The way we solve this equation is to associate with each permutations  $P$  a permutation which only differs from it by swichting 2 adjacent elements. We denote these permutations by  $P$  and  $P'$  respectively. Written this out into formula's we then have:

$$\begin{aligned} P_k &= P'_{k+1}, \\ P_{k+1} &= P'_k. \end{aligned}$$

Then we can rewrite  $\phi(x_1, x_2, x_3, \dots, x_l + m, x_l + n, \dots, x_N)$  as:

$$\phi(x_1, x_2, x_3, \dots, x_l + m, x_l + n, \dots, x_N) = \sum_P A_P e^{i(\sum_{l \neq k, k+1} k_{P_l} x_l)} e^{i(k_{P_l} + k_{P'_l})} \left[ A_P e^{i(mk_{P_l} + nk_{P'_l})} + A_{P'} e^{i(nk_{P_l} + mk_{P'_l})} \right]. \quad (5.32)$$

Here we have restricted the sum over only half the permutations  $P$ . For example we can sum only over the permutations with  $P(k+1) > P(k)$ . For 5.31 only  $m, n = 0, 1$  are relevant. If we fill 5.32 in into 5.31 we get the following equation:

$$2\Delta \left( A_P e^{iP'_k} + A_{P'} e^{iP_k} \right) = (A_P + A_{P'}) \left( 1 + e^{i(P_{k_l} + P'_{k_l})} \right). \quad (5.33)$$

Note that this is equivalent to 5.22. So the solution is also the same! So we have:

$$\frac{A_P}{A_{P'}} = -e^{i\Theta(k_{P_l}, k_{P'_l})}. \quad (5.34)$$

Where  $\Theta(k_{P_l}, k_{P'_l})$  is the same function as we found in 5.26. Again note that if  $k_{P_l} = k_{P'_l}$ , we would have  $A_P = -A_{P'}$ . This would lead again lead to the wave function becoming 0. This is most easily seen by looking at 5.32.

The formula above is valid for all permutations which differ only by switching neighbouring elements. It is possible to compute the ratio's of every pair of permutations since we can compute every permutation by switching neighbouring elements. If we do this for  $A_{1,2,3,\dots,N}$  we find:

$$\frac{A_P}{A_{1,2,3,\dots,N}} = (-1)^\eta e^{\sum \Theta(k_i, k_j)}, \quad (5.35)$$

where  $\eta$  is the number of transpositions needed to compute  $A_P$  out of  $A_{1,2,3,\dots,N}$ . The sums is over all pairs of  $k_i, k_j$  which have been exchanged to create  $A_P$ . This in principle together with the normalisation defines all  $A_P$ . We can build every permutation by just switching adjacent elements. So we have now found all the factors  $A_P$  so that 5.22 is a solution.

At last we still have to fix the boundary conditions and require that the wave function is symmetric under exchange of particles. For this we require:

$$\phi(1, x_2, \dots, x_N) = \phi(x_2, \dots, x_N, L + 1). \quad (5.36)$$

We require 5.36 to be valid for all possible positions of  $\{x_2, \dots, x_N\}$ . In order to solve 5.36, we will first rewrite  $\phi(1, x_2, \dots, x_N)$  and  $\phi(x_2, \dots, x_N, L + 1)$ . To do this we define a permutation  $\tilde{P}$  which differs from  $P$  by a right shift of all elements. So  $(\tilde{P}_1, \tilde{P}_2, \dots, \tilde{P}_N) = (P_N, P_1, P_2, \dots, P_{N-1})$ . Using this we can rewrite  $\phi(1, x_2, \dots, x_N)$  and  $\phi(x_2, \dots, x_N, L + 1)$  in the following way:

$$\phi(1, x_2, \dots, x_N) = \sum_P A_P \exp\left(i \sum_{l=2}^N k_{P_l} x_l\right) e^{ik_{P_1}} = \sum_{\tilde{P}} A_{\tilde{P}} \exp\left(i \sum_{l=2}^N k_{\tilde{P}_l} x_l\right) e^{ik_{\tilde{P}_1}}, \quad (5.37)$$

$$\phi(x_2, \dots, x_N, L + 1) = \sum_P A_P \exp\left(i \sum_{l=1}^{N-1} k_{P_l} x_{l+1}\right) e^{ik_{P_N}(L+1)} = \sum_P A_P \exp\left(i \sum_{l=2}^N k_{\tilde{P}_l} x_l\right) e^{ik_{\tilde{P}_1}(L+1)}. \quad (5.38)$$

If we now fill this in into 5.36, we find:

$$\sum_{\tilde{P}} A_{\tilde{P}} \exp\left(i \sum_{l=2}^N k_{\tilde{P}_l} x_l\right) e^{ik_{\tilde{P}_1}} = \sum_P A_P \exp\left(i \sum_{l=2}^N k_{\tilde{P}_l} x_l\right) e^{ik_{\tilde{P}_1}(L+1)}. \quad (5.39)$$

This is solved by:

$$A_{\tilde{P}} e^{ik_{\tilde{P}_1}} = A_P e^{ik_{\tilde{P}_1}(L+1)}. \quad (5.40)$$

Which translates into:

$$\frac{A_P}{A_{\tilde{P}}} e^{ik_{\tilde{P}_1} L} = 1. \quad (5.41)$$

We can calculate  $A_P/A_{P'}$  explicitly by using 5.35 N-1 times. We then find:

$$(-1)^{N-1} \exp\left(i \sum_l \Theta(k_l, k_j)\right) e^{ik_j L} = 1. \quad (5.42)$$

So we find as the allowed values for  $k_i$ :

$$Lk_i = 2\pi I_i + \sum_l \Theta(k_i, k_l), \quad (5.43)$$

where  $I_i$  is a half integer if N is even, and  $I_i$  is an integer if N is odd.

We have now found the full solution for N spins down. To summarize the general solution for the one-dimensional XXZ Heisenberg model is:

$$\Phi = \sum_P A_P e^{i \sum_l k_{P_l} x_l} |x_1, x_2\rangle \quad (5.44)$$

With the following conditions on  $A_P$  and  $k_i$

$$\begin{aligned} \frac{A_P}{A_{1,2,3,\dots,N}} &= -1^\eta e^{i \sum \Theta(k_i, k_j)}, \\ \Theta(k_i, k_j) &= 2 \arctan\left(\frac{\Delta \sin(\frac{k_i - k_j}{2})}{\Delta \cos(\frac{k_i - k_j}{2}) - \cos(\frac{k_i + k_j}{2})}\right), \\ Lk_i &= 2\pi I_i + \sum_j \Theta(k_i, k_j). \end{aligned}$$

The state has an energy of:

$$E = E_0 + J \sum_j [\cos(k_i) - \Delta]. \quad (5.45)$$

Although we have found the wave function and the energy of the system the wave function is so complicated that it is hard to calculate any properties of interest. For example correlation functions will be very hard to explicitly calculate. And the energies are given in terms of  $N$  coupled non-linear equations. So even though we have found the solution to the Heisenberg model there is still very little we can calculate. This is why we look to the thermodynamic limit to calculate the ground state energy. We will do this in the next section.

## 5.4 Thermodynamic limit

In this section we will calculate the ground state energy of the Heisenberg model in the thermodynamic limit. We will do this for the 1 dimensional antiferromagnetic XXX Heisenberg model, so  $\Delta = 1$  and  $J > 0$ . The reason why we are interested in the thermodynamic limit is twofold. Firstly most materials we are interested in contain a lot of particles. So the hermodynamic limit is a good description of these system. The second reason we look to the thermodynamic limit is out of neccesity. Even though we found the an expression for the exact energy in the previous section, explicitly calculating the energy is a close to impossble task. The energy is given in terms of  $N$  coupled non-linear equations, which makes it hard to find the energy. But in the thermodynamic limit it is possible to find the exact ground state energy(It is also possible to find expresion for excited states but we will not do that here) of the system. This is why we use the thermodynamic limit.

In this section we will use the following parametrization:

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

With these parametrization we get the following equation for the energy and momentum:

$$\begin{aligned} E &= \frac{L|J|}{4} + |J| \sum_j [\cos(k_j) - 1] = \frac{L|J|}{4} - |J| \sum_j [1 + \cos(\bar{k}_j)] = \frac{L|J|}{4} - |J| \sum_j [2 \cos^2(\bar{k}_j/2)] \\ &= \frac{L|J|}{4} - |J| \sum_j \left[ \frac{2}{1 + \frac{\sin^2(\bar{k}_j/2)}{\cos^2(\bar{k}_j/2)}} \right] = \frac{L|J|}{4} - |J| \sum_j \frac{2}{1 + 4\lambda_j^2}, \\ 2\pi I_i &= 2L \arctan(2\lambda_i) - \sum_j 2 \arctan(\lambda_i - \lambda_j). \end{aligned} \quad (5.46)$$

To move to the thermodynamic limit we want to replace the sums with integrals. To do this we first have to find the density of states. In order to find the density of states we first introduce the counting function:

$$\Phi(\lambda) = 2L \arctan(2\lambda) - \sum_j 2 \arctan(\lambda - \lambda_j). \quad (5.47)$$

The function  $\Phi(\lambda)$  is parametrised by a set  $\{\lambda_j\}$ . If we then solve the equation  $\Phi(\lambda) = 2\pi I$ , for all possible values of  $I$ , the solution is a set of  $\{\lambda_\alpha\}$ . Every  $\lambda_\alpha$  then corresponds to a state which can be occupied. In order to satisfy 5.46 the set  $\{\lambda_j\}$  then needs to be a subset of  $\{\lambda_\alpha\}$ . Of course it is a very hard to find an original set  $\{\lambda_j\}$  which obeys this condition. Note that in principle the set  $\{\lambda_\alpha\}$  is bigger than  $\{\lambda_j\}$  Since the set  $\{\lambda_\alpha\}$  is bigger then the set  $\{\lambda_j\}$ , we find more allowed momenta than our original set  $\{\lambda_j\}$ . These extra momenta are called holes. The holes are chosen in such a way that the energy is minimalized.

We now introduce our density of states:  $\rho(\lambda)$ . The number of states in an interval  $d\lambda$  is then given by  $\rho(\lambda)d\lambda$ . Since every solution to  $\Phi(\lambda) = 2\pi I$  is a state, the number of states in the interval  $d\lambda$  is also given by  $\frac{d\Phi}{2\pi}$ . Combining these 2 expression for the number of states, one finds:

$$\rho(\lambda) = \frac{1}{2\pi} \frac{\partial \Phi}{\partial \lambda}. \quad (5.48)$$

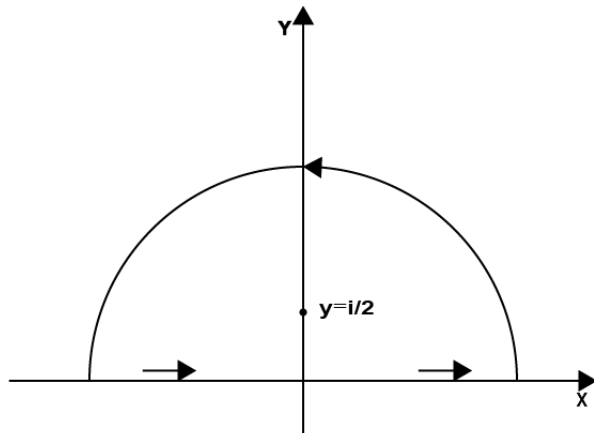


Figure 1: Our contour of integration for the Fourier transform of  $\frac{4L}{1+4\lambda^2}$  with a pole at  $y = i/2$

Since  $\rho(\lambda)$  is a density,  $\frac{\partial\Phi}{\partial\lambda}$  is always positive. This means that  $\Phi$  is an increasing function of  $\lambda$ . Note that  $\Phi(\lambda)$  has a minimal value of  $-\pi(L - N)$  and a maximum value of  $\pi(L - N)$ . Combine this with the fact that  $\Phi(\lambda)$  is an increasing function of  $\lambda$  and we find that the equation  $\Phi(\lambda) = 2\pi I$  has  $L - N$  solutions. This means that in the ground state (where  $N = \frac{L}{2}$ ) there are no holes. Thus in the ground state we have that all states are occupied. Because of this we can now use our density of states to calculate the ground state energy. If we would want to calculate the energy of excited states we would have to use a different density of states  $\rho - \rho_h$ , where  $\rho_h$  is the density of holes.

We now differentiate the counting function to  $\lambda$  to get:

$$2\pi\rho(\lambda) = \frac{4L}{1+4\lambda^2} - 2 \sum_j \frac{1}{1+(\lambda-\lambda_j)^2}. \quad (5.49)$$

Now we use the density of states to convert our sum to an integral. If we do this we find:

$$2\pi\rho(\lambda) = \frac{4L}{1+4\lambda^2} - 2 \int_{-\infty}^{+\infty} \rho(\lambda') \frac{d\lambda'}{1+(\lambda-\lambda')^2}. \quad (5.50)$$

So we have now found an integral equation for  $\rho(\lambda)$ . In order to solve this equation we use Fourier transformation and the residue theorem. Note that the integral is a convolution. Because of this we can rewrite it like this:

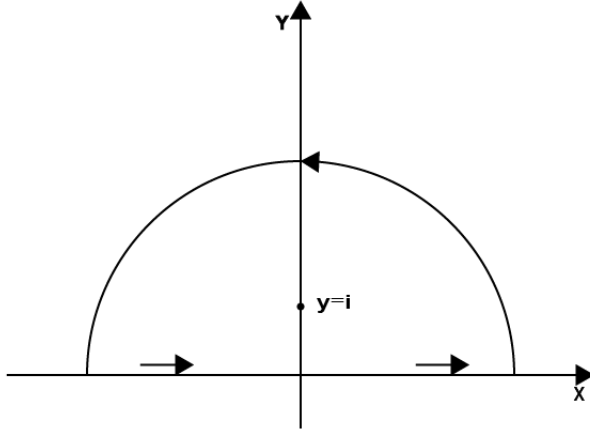
$$2\pi\rho(\lambda) = \frac{4L}{1+4\lambda^2} - 2 \int_{-\infty}^{+\infty} \tilde{\rho}(t) \tilde{F}(t) e^{-i\lambda t} dt, \quad (5.51)$$

where  $\tilde{F}(t)$  is the Fourier transform of  $\frac{1}{1+(\lambda-\lambda')^2}$  and  $\tilde{\rho}(t)$  is the Fourier transform of  $\rho(\lambda)$ . We now also rewrite all other terms to Fourier integrals. This gives us:

$$\sqrt{2\pi} \int_{-\infty}^{+\infty} \tilde{\rho}(t) e^{-i\lambda t} dt = \frac{4L}{2\pi} \int_{-\infty}^{+\infty} e^{-i\lambda t} dt \int_{-\infty}^{+\infty} \frac{1}{1+4\omega^2} e^{i\omega t} d\omega - 2 \int_{-\infty}^{+\infty} \tilde{\rho}(t) \tilde{F}(t) e^{-i\lambda t} dt. \quad (5.52)$$

We now explicitly evaluate the integral over  $\omega$  using the residue theorem. The function has 2 poles:  $\omega = \pm i/2$ . We will close the integration with an infinite semicircle in the positive imaginary plane (see figure 1). The only enclosed residue is at  $\omega = i/2$ . This pole is clearly of first order. This means that the residue is:

$$\lim_{\omega \rightarrow i/2} (\omega - i/2) \frac{e^{i\omega t}}{1+4\omega^2} = \lim_{\omega \rightarrow i/2} \frac{e^{i\omega t}}{4(\omega + i/2)} = \frac{e^{-t/2}}{4i}. \quad (5.53)$$

Figure 2: Our contour of integration for  $\tilde{F}$  with a pole at  $y = i$ 

With the residue, we now easily evaluate the integral:

$$\int_{-\infty}^{+\infty} \frac{1}{1+4\omega^2} e^{i\omega t} d\omega = 2\pi i \frac{e^{-t/2}}{4i} = \frac{\pi}{2} e^{-t/2}.$$

With the integral over  $\omega$  evaluated we get:

$$\begin{aligned} \sqrt{2\pi} \int_{-\infty}^{+\infty} \tilde{\rho}(t) e^{-i\lambda t} dt &= L \int_{-\infty}^{+\infty} e^{-t/2} e^{-i\lambda t} dt - 2 \int_{-\infty}^{+\infty} \tilde{\rho}(t) \tilde{F}(t) e^{-i\lambda t} dt \\ &= \int_{-\infty}^{+\infty} \left( L^2 e^{-t/2} e^{-i\lambda t} - 2\tilde{\rho}(t) \tilde{F}(t) e^{-i\lambda t} \right) dt. \end{aligned} \quad (5.54)$$

Since both sides are now an integral from  $-\infty$  to  $\infty$  we can now remove the integral sign. We then get:

$$\begin{aligned} \sqrt{2\pi} \tilde{\rho}(t) e^{-i\lambda t} &= L e^{-t/2} e^{-i\lambda t} - 2\tilde{\rho}(t) \tilde{F}(t) e^{-i\lambda t}, \\ \tilde{\rho}(t) &= \frac{L e^{-t/2}}{\sqrt{2\pi} + 2\tilde{F}(t)}. \end{aligned} \quad (5.55)$$

The Fourier transform of  $F$  is also calculated using the residue theorem.  $\frac{1}{1+(\lambda-\lambda')^2}$  has poles at  $\lambda - \lambda' = \pm i$ . These poles are of first order. We will close the integration with an infinite semicircle in the positive imaginary plane (see figure 2).

The only enclosed residue is at  $\lambda - \lambda' = i$ . This pole is clearly of first order, so the residue of this pole is:

$$\lim_{(\lambda'-\lambda) \rightarrow i} (\lambda' - \lambda - i) \frac{e^{i(\lambda'-\lambda)t}}{1 + (\lambda' - \lambda)^2} = \lim_{(\lambda'-\lambda) \rightarrow i} \frac{e^{i(\lambda'-\lambda)t}}{(\lambda' - \lambda + i)} = \frac{e^{-t}}{2i}. \quad (5.56)$$

So the Fourier transform of  $F$  is:

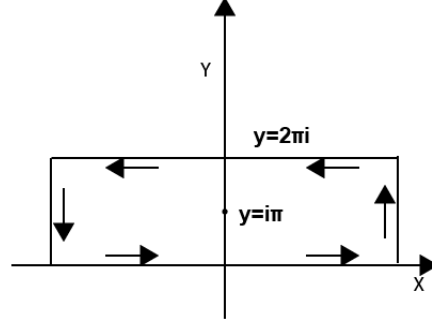
$$\tilde{F}(t) = \frac{1}{\sqrt{2\pi}} (2\pi i \frac{e^{-t}}{2i}) = \frac{\sqrt{2\pi}}{2} e^{-t}. \quad (5.57)$$

Filling this in, we find for  $\tilde{\rho}(t)$ :

$$\tilde{\rho}(t) = \frac{L e^{-t/2}}{\sqrt{2\pi} + \sqrt{2\pi} e^{-t}} = \frac{L}{\sqrt{2\pi} \cosh(t/2)}. \quad (5.58)$$

We now use the inverse Fourier transform to find  $\rho(\lambda)$ :

$$\rho(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{\rho}(t) e^{-i\lambda t} dt = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{L}{\cosh(t/2)} e^{-i\lambda t} dt. \quad (5.59)$$

Figure 3: Our contour of integration for  $\rho(\tilde{\lambda})$ 

To solve this integral we use our by now common tool, the residue theorem. But instead of closing the integration with an infinite semicircle we close the contour of integration with the line  $y = 2\pi i$  (see figure 3). By doing this we use the fact that  $\cosh(t) = -\cosh(t + \pi i)$ . There is only 1 pole included in this contour. The pole is at  $t = i\pi$ . To find the order of this pole we look at the Taylor expansion of  $\cosh(t/2)$ .  $\cosh(t/2)$  is analytical over its entire domain so we can Taylor expand it. If we Taylor expand  $\cosh(t/2)$  around its pole, we find:

$$\cosh(t/2) = \frac{1}{2}i(t - i\pi) + \frac{1}{48}i(t - i\pi)^3 + \mathcal{O}(t - i\pi)^5. \quad (5.60)$$

If we fill this in into  $\tilde{\rho}(t)$ , we find:

$$\tilde{\rho}(t) = \frac{L}{\sqrt{2\pi} \left[ \frac{1}{2}i(t - i\pi) + \frac{1}{48}i(t - i\pi)^3 + \mathcal{O}(t - i\pi)^5 \right]} \quad (5.61)$$

From this we can easily see that the pole is of first order. We now continue to calculate the residues. The residue of the pole is:

$$L \lim_{t \rightarrow i\pi} (t - i\pi) \frac{e^{-i\lambda t}}{\cosh(t/2)} = L \lim_{t \rightarrow i\pi} (t - i\pi) \frac{e^{-i\lambda t}}{\frac{1}{2}i(t - i\pi) + \frac{1}{48}i(t - i\pi)^3 + \mathcal{O}(t - i\pi)^5} = \frac{2Le^{-\pi\lambda}}{i}. \quad (5.62)$$

Now that we have found the residue we get the following equation:

$$\int_{-\infty}^{+\infty} \frac{L}{\cosh(t/2)} e^{-i\lambda t} e^{-2\pi\lambda} dt + \int_{-\infty}^{+\infty} \frac{L}{\cosh(t/2)} e^{-i\lambda t} dt = 4\pi L e^{-\pi\lambda}. \quad (5.63)$$

The integration around the sides vanish cause  $\tilde{\rho}(t) \rightarrow 0$  as  $|t| \rightarrow \infty$ . We can rewrite this to give:

$$\int_{-\infty}^{+\infty} \frac{L}{\cosh(t/2)} e^{-i\lambda t} dt = \frac{4\pi L e^{-\pi\lambda}}{1 + e^{-2\pi\lambda}} = \frac{2\pi L}{2 \cosh(\pi\lambda)}. \quad (5.64)$$

Filling in this integral gives us the following expression for  $\rho(\lambda)$ :

$$\rho(\lambda) = \frac{L}{2 \cosh(\pi\lambda)}. \quad (5.65)$$

Now that we have found the density of state, we can convert our sums to integrals. And these integrals can then be evaluated to give us the ground state energy.

$$\begin{aligned} E_0 &= \frac{L|J|}{4} - |J| \sum_j \frac{2}{1 + 4\lambda_j^2} \\ &= \frac{L|J|}{4} - |J| \int \rho(\lambda) \frac{2}{1 + 4\lambda^2} d\lambda \\ &= \frac{L|J|}{4} - L|J| \int \frac{1}{\cosh(\pi\lambda)} \frac{1}{1 + 4\lambda^2} d\lambda. \end{aligned} \quad (5.66)$$



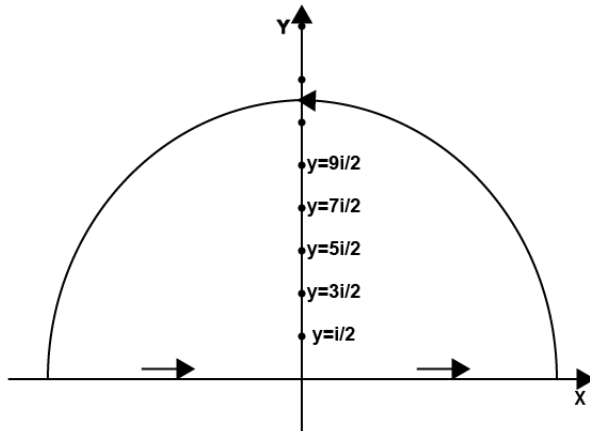


Figure 4: Our contour of integration for  $\frac{1}{\cosh(\pi\lambda)} \frac{1}{1+4\lambda^2}$

To solve this integral we use the residue theorem. To close the integration we use a semi-circle of infinite radius in the positive imaginary plane (see Figure 4). We first need to find all the poles of  $\frac{1}{\cosh(\pi\lambda)} \frac{1}{1+4\lambda^2}$ .  $\frac{1}{1+4\lambda^2}$  has poles at  $z = \pm \frac{i}{2}$ .  $\frac{1}{\cosh(\pi\lambda)}$  has poles at  $\lambda = i(\frac{1}{2} + n)$  for every integer  $n$ . Now that we have found the poles we need to find the residues of these poles. To find the residues we first need to find the order of these poles. As we have seen before the order of the poles due to the  $\cosh(\pi\lambda)$  are of order 1 (except the one at  $i = \frac{i}{2}$  since  $\frac{1}{1+4\lambda^2}$  also has a pole at that point). The pole at  $i = \frac{i}{2}$  is of second order because it is a combination of 2 first order poles.

Now that we know the order of the poles, we can calculate the residues associated with these poles. For a first order at  $\lambda_0 = i(\frac{1}{2} + n)$  the residue given by:

$$\begin{aligned} \lim_{\lambda \rightarrow \lambda_0} \frac{\lambda - \lambda_0}{\cosh(\pi\lambda)} \frac{1}{1+4\lambda^2} &= \lim_{\lambda \rightarrow \lambda_0} \frac{\lambda - \lambda_0}{(\lambda - \lambda_0)(-1)^n [i\pi + \frac{1}{6}i\pi^3(\lambda - \lambda_0)^2 + \mathcal{O}(\lambda - \lambda_0)^4]} \frac{1}{1+4\lambda^2} \\ &= \frac{(-1)^n}{i\pi} \frac{1}{1-4(\frac{1}{2} + n)^2}. \end{aligned}$$

The residue of the second order pole at  $\lambda = i/2$  is:

$$\begin{aligned} \frac{d}{d\lambda} [f(\lambda)(\lambda - \lambda_0)^2] \Big|_{\lambda=\lambda_0} &= \frac{d}{d\lambda} \frac{(\lambda - \lambda_0)^2}{\cosh(\pi\lambda)(1+4\lambda_j^2)} \Big|_{\lambda=\lambda_0} = \frac{d}{d\lambda} \frac{1}{(-1)^n [i\pi + \frac{1}{6}i\pi^3(\lambda - \lambda_0)^2 + \mathcal{O}(\lambda - \lambda_0)^4]} \frac{1}{\lambda + \lambda_0} \Big|_{\lambda=\lambda_0} \\ &= -\frac{1}{\lambda + \lambda_0^2} \frac{1}{i\pi} \Big|_{\lambda=\lambda_0} = \frac{1}{i\pi}. \end{aligned}$$

Now that we have found the residues, we can proceed to evaluate the integral:

$$\int \frac{1}{\cosh(\pi\lambda)} \frac{1}{1+4\lambda_j^2} = 2\pi i \left[ \frac{1}{4i\pi} + \sum_{n=1}^{n=\infty} \frac{(-1)^n}{i\pi(1-4(n+\frac{1}{2})^2)} \right] = 2 \left[ \frac{1}{4} + \sum_{n=1}^{n=\infty} \frac{(-1)^n}{(1-4(n+\frac{1}{2})^2)} \right]. \quad (5.67)$$

Now all that we have to do is evaluate the sum. We will do this by rewriting it to a known sum, the alternating harmonic series. We know that  $\sum_{n=1}^{n=\infty} \frac{(-1)^{n+1}}{n} = \ln 2$ . Using this we find:

$$\begin{aligned} &= 2 \left[ \frac{1}{4} + \sum_{n=1}^{n=\infty} \frac{(-1)^n}{(1-4(n+\frac{1}{2})^2)} \right] = \frac{1}{2} + \frac{1}{2} \sum_{n=1}^{n=\infty} \frac{(-1)^{n+1}}{n(n+1)} = \frac{1}{2} + \frac{1}{2} \sum_{n=1}^{n=\infty} \left[ \frac{(-1)^{n+2}}{n+1} + \frac{(-1)^{n+1}}{n} \right] \\ &= \frac{1}{2} + \frac{1}{2} \sum_{n=2}^{n=\infty} \frac{(-1)^{n+1}}{n} + \frac{1}{2} \sum_{n=1}^{n=\infty} \frac{(-1)^{n+1}}{n} = \frac{1}{2} + \frac{1}{2}(\ln 2 - 1) + \frac{1}{2} \ln 2 = \ln 2 \end{aligned} \quad (5.68)$$

So now we have finally found the ground state energy of anti-ferromagnetic chain is:

$$E_0 = L | J | \left[ \frac{1}{4} - \ln 2 \right] \approx -0.44L | J | . \quad (5.69)$$

It is interesting to compare this with the energy we found for a state which has alternating spins up and down. This state would have an energy of  $-L|J|/4$ , whereas the ground state we just found has an energy of  $-0.44L | J |$ . So we see that by taking quantum fluctuations into account we found a lower energy.

To summarize, in this chapter we found the solution to the 1 dimensional XXZ Heisenberg model. But since the wave functions we found were very complicated and the energy's were given in terms of N coupled non linear equations, it was not possible to explicitly calculate anything of interest. Luckily we could calculate the ground state energy of our system in the thermodynamic limit for the XXX model.

## 6 Numerical solution to the Heisenberg model

In the previous section we have found the ground state energy for the XXX Heisenberg model in the thermodynamic limit. The thermodynamic limit is a very useful approximation, but it is not suited for small systems. We would still like to find the energy eigenvalues of small systems. Since calculating the energy eigenvalues analytically is not possible we need another method for this. In this section we will use numerical methods to calculate the energy eigenvalues of small systems. Numerical methods work well for small systems where the amount of calculations to be done are not too big for a computer to handle. We will compare the results we found to expansions for the ground state energy. We will then see how accurate these expansions are if we only look at the first few terms. In this section we will first take a look at the case where  $\Delta = 1$ , afterwards we will also look at  $\Delta \neq 1$ .

Our numerical method consists of explicitly calculating the Hamiltonian for a system of size  $N$ . This Hamiltonian will be a  $2^N \times 2^N$  matrix. After we have computed the Hamiltonian we will use exact diagonalisation to find the eigenvalues of the system. The lowest eigenvalue then corresponds the ground state of the system. I did this using both Mathematica and Python. Since Mathematica could solve larger systems, I used Mathematica for my final results. For the exact code I used see appendix D.

### 6.1 XXX Heisenberg model

We first look at the XXX Heisenberg model for various system size. We look at system sizes up to 12 particles. This gave us the following results for the ground state energy:

$N$	$E_0/N/J$
6	-0.467129
8	-0.456387
10	-0.451545
12	-0.448949
$\infty$	-0.443147

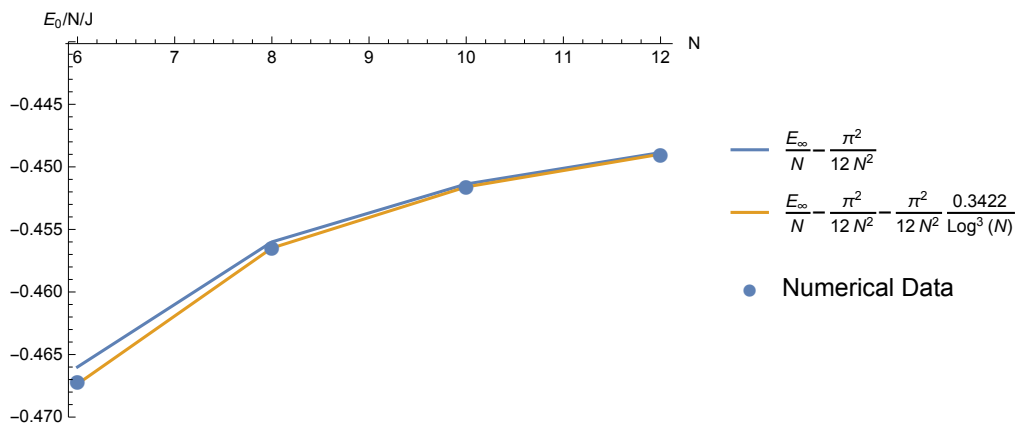


Figure 5: The ground state energy for various system sizes

As we expect, the bigger the system size, the closer the ground state energy gets to the energy in the thermodynamic limit.

Using exact diagonalisation we find more than only the ground state. We find the whole spectrum of eigenstates. This allows us to plot the spectrum of finite sized systems, see figure 6. Finding the whole spectrum can be useful when we want to calculate the thermodynamics of the system. We see that the middle of the spectrum of the most densely packed, while the edges are more sparsely packed.

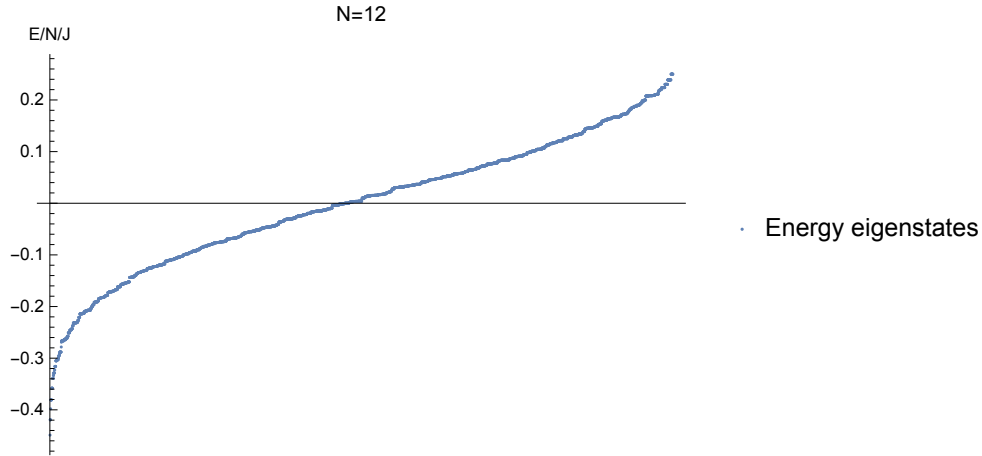


Figure 6: The spectrum of the XXX Heisenberg model

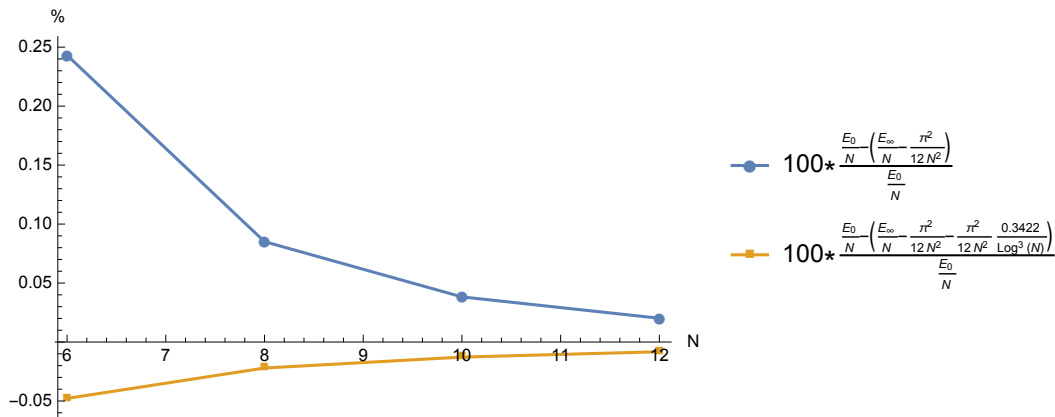


Figure 7: The percentual difference between the numerical data and the expansions

Our exact diagonalisation data also allows us to check the accuracy of various expansions for the ground state energy of finite system sizes. We will focus on the following expansion here[4]:

$$\frac{E_0}{N} = \frac{E_\infty}{N} - \frac{\pi^2}{12N^2} - \frac{\pi^2}{12N^2} \frac{0.3422}{\ln^3(N)} - \mathcal{O}\left(\frac{\ln(\ln(N))}{\ln^4(N)}, \frac{1}{\ln^4(N)}\right). \quad (6.1)$$

Here  $E_0$  is the ground state energy for system size  $N$ , and  $E_\infty$  is the ground state in the thermodynamic limit, which we have previously found with analytical methods. This expansion is plotted alongside our data in figure 5. We will check how accurate this expansion is with only the first 2/3 terms. We look at the percentual difference between the expansion and the exact diagonalisation data. This gives a better representation of the accuracy than absolute differences, since we do not know anything about the general energy scales.

We can see in figure 7 that both expansions are pretty accurate. With only the first 2 terms in the expansion, the error is 0.025% for  $N = 6$ . For  $N = 12$  the error is less than 0.05%.

If we take the first 3 terms of the expansion into consideration the error becomes smaller. For  $N = 6$  the error is less than 0.05%. For  $N = 12$  the error is less than 0.01%. We can see that the error becomes smaller the larger the system size for both expansions. This means that the bigger the system sizes the more accurate the expansions are. This is quite useful for systems which are too big to solve numerically but too small to use the thermodynamic limit. For these systems this expansion can be very useful.

## 6.2 XXZ Heisenberg model

Now we take a look at  $\Delta \neq 1$ . Using analytical methods solving the XXZ Heisenberg model is a lot more difficult than solving the XXX Heisenberg model, because one has to deal with trigonometric functions instead of rational functions. But using numerical methods the XXZ Heisenberg model can be solved using the same technique as  $\Delta = 1$ . All we have to do is change a factor in our Hamiltonian. This gave us the following results for the ground state energy:

$\Delta$	$E_0/N/J$
0	-0.321975
0.2	-0.343687
0.4	-0.367287
0.6	-0.392709
0.8	-0.419928
1.0	-0.448949
1.2	-0.4798
1.4	-0.512512
1.6	-0.547097
1.8	-0.583517
2.0	-0.621676

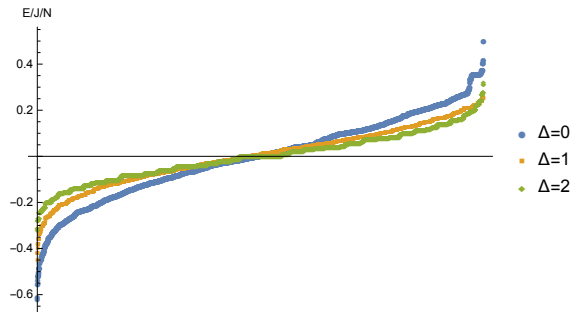


Figure 8: The spectrum for different  $\Delta$

All these results are for 12 particles. We can see that the higher the  $\Delta$  the lower the ground state energy. We plotted the spectrum for several values of  $\Delta$  in figure 8. We see that the shape of the spectrum looks a lot like the spectrum of  $\Delta = 1$ . Again we see that the middle of the spectrum is more densely packed and the edges are more sparsely packed. We can see that for higher  $\Delta$  the range becomes smaller.

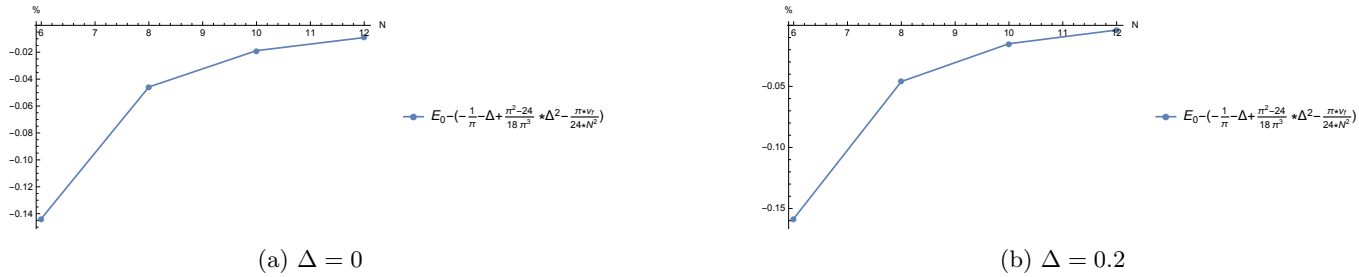
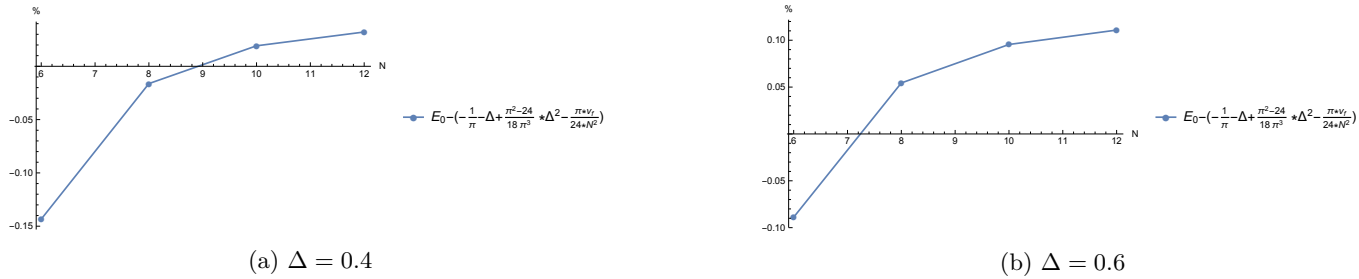
We will now again compare these results to an expansion of  $\frac{E_0}{N}$ . In order to do this we look at an expansion of  $E_0$  for small  $N$ . This expansion is given by [4]:

$$\frac{E_0}{N} = \frac{E_\infty}{N} - \frac{\pi v_f}{24N^2} - \mathcal{O}\left(\frac{1}{N^3}\right), \quad (6.2)$$

with  $v_f = \frac{2\pi \sin(\arccos(-\Delta))}{\pi - \arccos(-\Delta)}$ ,  $E_0$  and  $E_\infty$  are the ground state energy for finite system size and in the thermodynamic limit respectively. Since we do not know the ground state energy for  $\Delta \neq 1$ , we have to use an expansion for  $\frac{E_\infty}{N}$  as well. This expansion is only valid for small  $\Delta$  and is given by [4]:

$$\frac{E_\infty}{N} = -\frac{1}{\pi} - \frac{1}{\pi^2}\Delta - \frac{\pi^2 - 24}{18\pi^3}\Delta^2 + \mathcal{O}(\Delta^3). \quad (6.3)$$

We plotted the percentual error in figure 9 and 10. We can see that for  $\Delta = 0$  or  $\Delta = 0.2$  the error seems to converge to 0 for  $N \rightarrow \infty$ . We tried fitting our data for  $\Delta = 0$  and  $\Delta = 0.2$  to give an estimate for the error for large  $N$ . We used a fit of the form:  $a + \frac{b}{n^2}$ . We can use  $a$  as an estimation for the error for

Figure 9: The percentual error for various  $\Delta$ Figure 10: The percentual error for various  $\Delta$ 

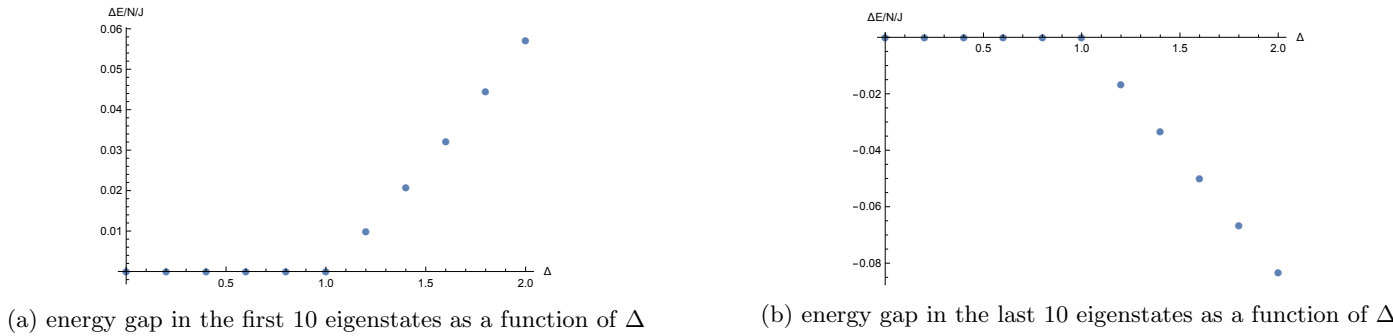
large  $N$ . The value we found for  $a$  is: 0.045534 and 0.0587903 for  $\Delta = 0$  or  $\Delta = 0.2$  respectively. So for  $\Delta \leq 0.2$  the combination of these expansions are very useful for larger system sizes. For  $\Delta = 0.4$  and  $\Delta = 0.6$  the percentual error are not very big. But since the error does not seem to converge too 0 the uses of this expansion seem to be small. Note that figure 9 and 10 do not prove the accuracy of the separate expansions 6.2 and 6.3. Figure 9 and 10 only looks at the accuracy of the combined expansions. It could be possible that the errors of both expansions cancel out and that the expansions are less accurate than figure 9 and 10 imply.

In the thermodynamic limit the system has an energy gap for  $\Delta > 1$ . We will look if we can find this energy gap for finite systems as well. For small  $\Delta - 1$  the energy gap behaves as:

$$\delta E \sim 11.7 \exp\left(-\frac{3.5}{\sqrt{\Delta - 1}}\right), \quad (6.4)$$

here  $\delta E$  is the size of the energy gap. This means that for small  $\Delta - 1$  this gap is hard to detect. So if we try to look for this energy gap, it is easiest to first look at  $\Delta = 2$ . As we can see in figure 8, there is no energy gap in the middle of the spectrum. To see if there are energy gaps we now zoom in on the edges of the spectrum, see figure 11. We see that between the first and second excited state there seems to be an energy gap. We see the same for the last 10 eigenstates but now between the third and second too last eigenstate.

To see if this is the energy gap we are looking for we plot the energy difference between the first and second excited state as a function of  $\Delta$ . We have done this in figure 12. We can see that the energy gap is absent for  $\Delta \leq 1$ , and the gap grows with  $\Delta$  for  $\Delta > 1$ . So we have found the energy gap we were looking for. We do not find the exponential behaviour. This is most likely because we take too large steps in  $\Delta$  to find the exponential behaviour off the gap. Another reason for not finding the exponential behaviour could be that we are looking at finite sized systems.

Figure 11: The edges of the spectrum for  $\Delta = 2$ Figure 12: The energy gap as a function of  $\Delta$ 

## A Calculus of complex functions

In this appendix we will follow chapter 6 and 7 of Mathematical methods for physicists by George B.Arffken and Hans J.Weber[6].

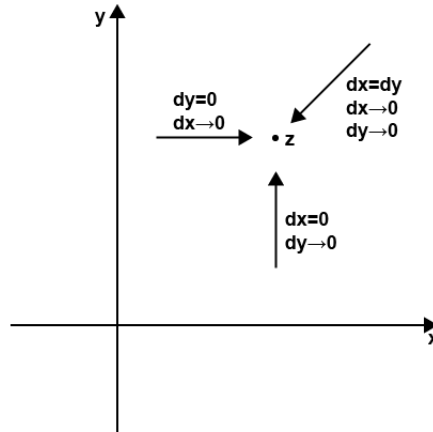
In this appendix we will develop some techniques involving the calculus of complex functions. We will first look at how to define functions of complex variables. After we have done that we will tackle how to differentiate and integrate complex functions. Once we have found how to integrate complex functions we will find some very powerful tools, such as the Cauchy integral theorem and the Cauchy integral theorem. This will help us develop a new type of function expansion, the Laurent expansion. After we have found the Laurent expansion, we will use this to find the residue theorem. The residue theorem is an extremely powerful tool in evaluating definite integrals.

### A.1 Permanence of algebraic form

Before we begin in working with complex functions, we must define how to interpret functions of complex variables. An easy way to define functions of complex variables is by a power series expansion. For example for the function  $e^z$ , we would get:

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!} = 1 + \frac{z}{1!} + \frac{z^2}{2!} + \dots \quad (\text{A.1})$$

This principle can be used for all our elementary functions. This is called the permanence of algebraic form.

Figure 13: A few of the possible ways to approach the point  $z_0$ 

## A.2 Cauchy Riemann conditions

Now that we have defined functions of a complex variable, we can start differentiating them. By the definition of the derivative we have:

$$f'(z) = \lim_{\delta z \rightarrow 0} \frac{f(z + \delta z) - f(z)}{\delta z}. \quad (\text{A.2})$$

For this derivative to exist it needs to be independent from the approach to the point  $z$ . As we will see this gives a restriction on which functions are differentiable. We now adopt the notation:

$$\begin{aligned} z &= x + iy, \\ f(z) &= u(x, y) + iv(x, y). \end{aligned} \quad (\text{A.3})$$

With this notation we can now write:

$$\begin{aligned} \delta z &= \delta x + i\delta y, \\ \delta f &= \delta u + i\delta v, \end{aligned} \quad (\text{A.4})$$

$$\frac{\delta f}{\delta z} = \frac{\delta u + i\delta v}{\delta x + i\delta y}.$$

There are multiple ways to approach the point  $z$  (see figure 13). If we approach horizontally, we have  $\delta y = 0$ . But we can also approach vertically, in which case  $\delta x = 0$ . By the definition of the derivative these must be equal. These two approaches give us the following expression for the derivative:

$$f'(z) = \lim_{\delta x \rightarrow 0} \frac{\delta u}{\delta x} + \frac{i\delta v}{\delta x} = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}, \quad (\text{A.5})$$

$$f'(z) = \lim_{\delta y \rightarrow 0} \frac{\delta u}{i\delta y} + \frac{i\delta v}{i\delta y} = \frac{\partial v}{\partial y} - i \frac{\partial u}{\partial y}. \quad (\text{A.6})$$

For the derivative to exist, these 2 expressions must be equal. Equating these expressions gives us:

$$\begin{aligned} \frac{\partial v}{\partial y} &= \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} &= -\frac{\partial v}{\partial x}. \end{aligned} \quad (\text{A.7})$$

These are the Cauchy-Riemann conditions. These conditions form the basis of the calculus of complex functions. If the derivative exists, these conditions are satisfied. It turns out that this also works the other way around. If the Cauchy-Riemann conditions are satisfied then the derivative exists. We will now prove that



if the Cauchy-Riemann conditions are satisfied, then the derivative is independent from direction of approach.

To show this, we write:

$$\delta f = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy. \quad (\text{A.8})$$

In A.5 and A.6 we have found  $\frac{\partial f}{\partial x}$  and  $\frac{\partial f}{\partial y}$ . If we fill this in we find:

$$\delta f = \left( \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} \right) \delta x + \left( \frac{\partial u}{\partial y} + i \frac{\partial v}{\partial y} \right) \delta y. \quad (\text{A.9})$$

With this expression we now calculate  $\frac{\delta f}{\delta z}$

$$\begin{aligned} \frac{\delta f}{\delta z} &= \frac{\left( \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} \right) \delta x + \left( \frac{\partial u}{\partial y} + i \frac{\partial v}{\partial y} \right) \delta y}{\delta x + i \delta y} \\ &= \frac{\left( \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} \right) + i \left( -i \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right) \delta y / \delta x}{1 + i(\delta y / \delta x)}. \end{aligned}$$

For this to be independent of the direction of approach we have to eliminate  $\delta y / \delta x$  from this expression. We do this by filling in the Cauchy-Riemann conditions:

$$\begin{aligned} \frac{\delta f}{\delta z} &= \frac{\left( \frac{\partial v}{\partial y} - i \frac{\partial u}{\partial y} \right) + i \left( \frac{\partial v}{\partial y} - i \frac{\partial u}{\partial y} \right) \delta y / \delta x}{1 + i(\delta y / \delta x)} \\ &= \frac{\partial v}{\partial y} - i \frac{\partial u}{\partial y}. \end{aligned} \quad (\text{A.10})$$

So we have now shown that if and only if the Cauchy-Riemann conditions are obeyed, the derivative of a complex function exists. Luckily for us, for almost all functions of interest the Cauchy-Riemann conditions are obeyed. For example all polynomials obey the Cauchy-Riemann conditions, and therefore all Taylor expansions as well. We will call a function  $f(z)$  analytic at  $z = z_0$  if it is differentiable at  $z_0$  and a small region surrounding  $z_0$ .

### A.3 Cauchy's integral theorem

In this subsection we turn our eyes towards integrating analytic complex functions. Analytic complex functions have to obey the Cauchy-Riemann conditions, because of this will find some useful and unexpected results which are not true for all real functions.

First we define how to treat an integral of a complex function. We define an integral over a complex function to be:

$$\int_{z_1}^{z_2} f(z) dz = \int_{x_1, y_1}^{x_2, y_2} (u(x, y) + iv(x, y)) (dx + idy) = \int_{x_1, y_1}^{x_2, y_2} u(x, y) dx - v(x, y) dy + i \int_{x_1, y_1}^{x_2, y_2} u(x, y) dy + v(x, y) dx. \quad (\text{A.11})$$

The nice part of this definition is that we do not have to change our way of integrating functions. We can just use the same techniques we also use for real functions.

Now that we have integration under control, we find some interesting results. Consider an function  $f(z)$  which is analytic in a simply connected region  $R$ . A simply connected region is simply put a region without a hole inside of it.

We consider the following integral:

$$\oint_C f(z) dz = \oint_C (u dx - v dy) + i \oint_C v dx + u dy = \oint_C V_x dx + V_y dy. \quad (\text{A.12})$$

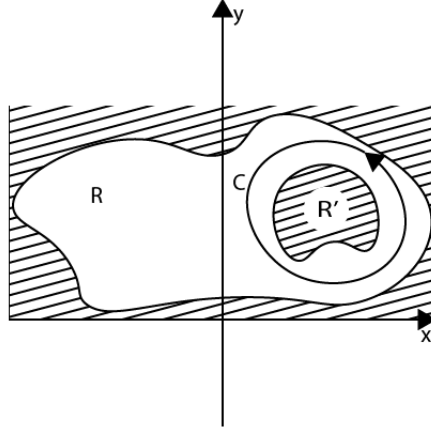


Figure 14

Here we used the following notation:  $V_x = u + iv$ ,  $V_y = iu - v$ .  $C$  is a arbitrary path through  $R$ . Now we use Stokes Theorem to rewrite this as:

$$\begin{aligned} \oint_C V_x dx + V_y dy &= \int \left( \frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y} \right) dx dy = \int \left( i \frac{\partial u}{\partial x} - \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} - i \frac{\partial v}{\partial y} \right) dx dy \\ &= i \int \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) dx dy - \int \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) dx dy. \end{aligned}$$

If the Cauchy-Riemann conditions are satisfied then both of these integrals vanish.

Notice that we did not assume much about the path  $C$ . All that we assumed is that  $f(z)$  is analytic on  $C$  and the area bounded by  $C$ . So we have found that:

$$\oint_C f(z) dz = 0, \tag{A.13}$$

as long as  $f(z)$  is analytic on and inside  $C$ . This result is also know as Cauchy's integral theorem. A disadvantage of Cauchy's integral theorem is that it is only valid for a function which is analytic on and inside our contour of integration. In the next subsection we will look at what happens when  $f(z)$  is analytic on our contour of integration but not everywhere inside of it.

### A.4 Multiply connected regions

Consider a function  $f(z)$  which is analytic in some region  $R$ . Inside this region  $R$  is a region  $R'$  where  $f(z)$  is not analytic. Say we want to integrate around a contour  $C$  which lies within  $R$  and encircles  $R'$ . For a picture of this, see figure 14. We want to use Cauchy's integral theorem on this integral. In order to this, we convert the region  $R$  into a simply connected region as in figure 15. By doing this we also need to change our contour of integration  $C$  so that it is completely within our simply connected region. Our new contour is now given by  $ABDEFGA$  Now that we have converted our multiply connected region  $R$  into a simply connected region, we can use Cauchy's integral theorem. Applying Cauchy's theorem gives us:

$$\oint_{ABDEFGA} f(z) dz = \int_{ABD} f(z) dz + \int_{EFG} f(z) dz = 0. \tag{A.14}$$

Note that  $\int_{DE} f(z) dz$  and  $\int_{AG} f(z) dz$  cancel out because the direction of integration is opposite to each other. We now reverse the direction of integration of  $EFG$  to find:

$$\int_{ABD} f(z) dz = \int_{GFE} f(z) dz. \tag{A.15}$$

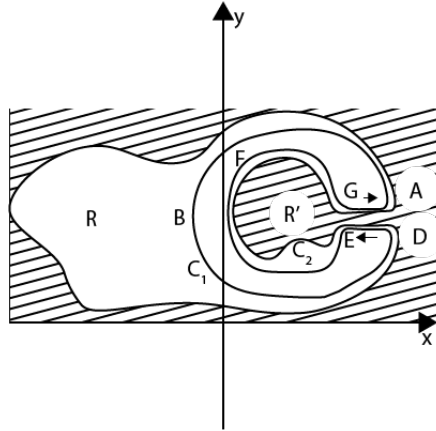


Figure 15

Since the distances AD and GE are infinitesimal, we can also write this as:

$$\oint_{C_1} f(z)dz = \oint_{C_2} f(z)dz. \tag{A.16}$$

Where  $C_1$  and  $C_2$  are the closed paths ABD and GFE respectively. We now have a formula for the integral over 2 closed paths within a multiply connected region. More specifically we now have found that every closed integral within a multiply connected region has the same value as long as both integrals are integrated in the counterclockwise direction(both integrated in the clockwise direction would work as well).

### A.5 Cauchy's integral formula

In this section we will use Cauchy's integral theorem for a multiply connected region to derive the Cauchy integral formula. Cauchy's integral formula gives the value of  $f(z_0)$  at a point  $z_0$  in terms of a closed integral over  $\frac{f(z)}{z-z_0}$ . Here  $z_0$  has to be a point inside the contour of integration and  $f(z)$  has to be analytic inside and on the whole contour of integration. The Cauchy integral formula is:

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z-z_0} dz. \tag{A.17}$$

We will call the region bounded by  $C$ ,  $R$ . Note that while  $f(z)$  is analytic throughout  $R$ ,  $\frac{f(z)}{z-z_0}$  is not analytic at  $z = z_0$ . This means that  $\frac{f(z)}{z-z_0}$  is analytic in the multiply connected region  $R - z_0$ . This permits us to use A.16:

$$\oint_C \frac{f(z)}{z-z_0} dz = \oint_{C_2} \frac{f(z)}{z-z_0} dz. \tag{A.18}$$

We now take  $C_2$  to infinitesimal circle around  $z = z_0$  transversed in the counterclockwise direction(see figure 16). We will use the parametrisation  $z = z_0 + re^{i\theta}$ . Filling this in into the right side of A.18, we get:

$$\oint_{C_2} \frac{f(z_0 + re^{i\theta})}{re^{i\theta}} dz. \tag{A.19}$$

Since we are integrating over a circle the integration over  $z$  can be replaced by integration over  $\theta$ :

$$\oint_{C_2} \frac{f(z_0 + re^{i\theta})}{re^{i\theta}} rie^{i\theta} d\theta = \oint_{C_2} if(z_0 + re^{i\theta})d\theta. \tag{A.20}$$

We now take the limit  $r \rightarrow 0$ . This gives us:

$$\oint_{C_2} if(z_0 + re^{i\theta})d\theta = 2\pi if(z_0). \tag{A.21}$$

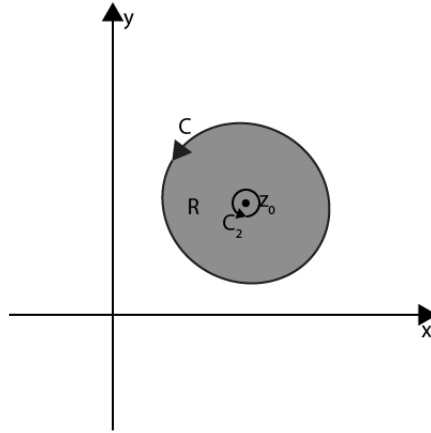


Figure 16

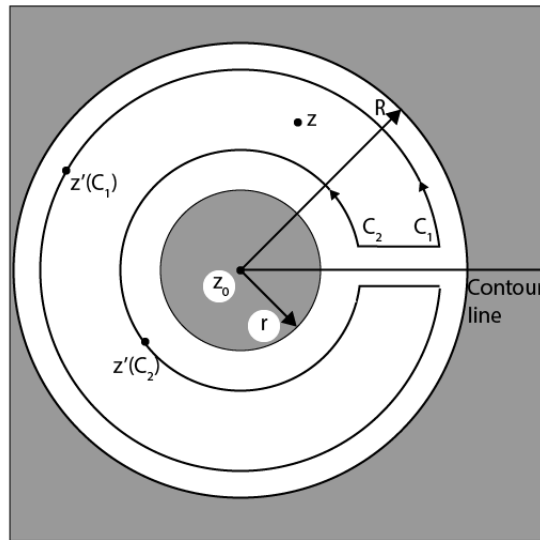


Figure 17

Remember that his integral was equal to  $\oint_C \frac{f(z)}{z-z_0} dz$ . So we find the formula:

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z-z_0} dz \quad (\text{A.22})$$

,which is equal to A.17. Note that  $C$  has to be transversered in the counter clockwise direction for this formula to be correct. This is because we transversered the infinitesimal circle  $C_2$  counter clockwise as well. The only 2 constraints on  $C$  are that it has encircle  $z_0$  and  $f(z)$  has to be analytic on and inside the contour  $C$ .

In the next subsection we will derive a new series expansion: the Laurent expansion. The special thing about the Laurent expansion is that with a Laurent expansion we can expand around a point where our function is not wel defined.

## A.6 Laurent expansion

Consider a function  $f(z)$  which is analytic in an annular region with inner radius  $r$  and outer radius  $R$ . We wish to use Cauchy's integral formula to calculate  $f(z)$ , where  $z$  is the in between the inner and outer circle.

We define the centre of the circles to be  $z_0$ . In order to transform the multiply connected are we draw a contour line as can be seen in figure 17. Now we use Cauchy's integral formula to calculate  $f(z)$ . This gives us:

$$f(z) = \frac{1}{2\pi i} \int_{C_1} \frac{f(z')dz'}{z' - z} - \frac{1}{2\pi i} \int_{C_2} \frac{f(z')dz'}{z' - z}. \quad (\text{A.23})$$

Here both  $C_1$  and  $C_2$  are transversed in the counterclockwise direction. We now rewrite the denominators in the integrals to:

$$f(z) = \frac{1}{2\pi i} \int_{C_1} \frac{f(z')dz'}{(z' - z_0)[1 - (z - z_0)/(z' - z_0)]} + \frac{1}{2\pi i} \int_{C_2} \frac{f(z')dz'}{(z' - z_0)[1 - (z' - z_0)/(z - z_0)]}. \quad (\text{A.24})$$

We will now rewrite both integrals further. To do this note the following identity:

$$\frac{1}{1 - t} = 1 + t + t^2 + t^3 + t^4 + \dots = \sum_{n=0}^{\infty} t^n. \quad (\text{A.25})$$

This is only valid for  $|t| < 1$  and can be verified by multiplying both sides by  $1 - t$ . We can use this identity to rewrite the denominators in both of the integrals. Note that for every point on  $C_1$ ,  $z' - z_0$  is always larger than  $z - z_0$ . For  $C_2$  the situation is the other way around,  $z - z_0$  is always larger than  $z' - z_0$ . So it turns out that for both denominators in the integrals we can use A.25. Filling in this identity, we find:

$$\begin{aligned} f(z) &= \frac{1}{2\pi i} \int_{C_1} \sum_{n=0}^{n=\infty} (z - z_0)^n \frac{f(z')dz'}{(z' - z_0)^{n+1}} + \frac{1}{2\pi i} \int_{C_2} \sum_{n=0}^{n=\infty} (z - z_0)^{-n-1} (z' - z_0)^n f(z')dz' \\ &= \frac{1}{2\pi i} \sum_{n=0}^{n=\infty} (z - z_0)^n \int_{C_1} \frac{f(z')dz'}{(z' - z_0)^{n+1}} + \frac{1}{2\pi i} \sum_{n=-1}^{n=-\infty} (z - z_0)^n \int_{C_2} (z' - z_0)^{-n-1} f(z')dz' \\ &= \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n. \end{aligned} \quad (\text{A.26})$$

Where in the last step we made the following substitution:

$$a_n = \frac{1}{2\pi i} \int_C \frac{f(z')dz'}{(z' - z_0)^{n+1}}. \quad (\text{A.27})$$

Here we changed the contour from  $C_1$  and  $C_2$  to  $C$ . We are allowed to do this since every closed integral in an multiply connected region has the same value.

For the series:

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \quad (\text{A.28})$$

to converge,  $z$  has to lie inbetween  $C_1$  and  $C_2$ . If  $z$  lies outside this region the series diverges.

We have now found a new power series expansion for a complex function. The special thing about this expansion is that we have expanded around a point  $z_0$  where  $f(z)$  does not have to be well defined.

We say that  $f(z)$  has a isolated singular point if  $f(z)$  is not analytic at  $z = z_0$  but at all neighbouring points. Since we will be dealing with isolated singular points a lot in the nex few subsections, I will now introduce some terms involving isolated singular points. If  $a_m = 0$  for all  $m < -n < 0$ , for negative  $-n$ , and  $a_n \neq 0$ , than we call  $z_0$  a pole of order  $n$ . If the summation continues to  $m = -\infty$ , then we call  $z_0$  an essential singularity.

A pole of order  $n$  can be erased by multiplying the Laurent expansion by  $(z - z_0)^n$ , but an essential singularity can not be erased.

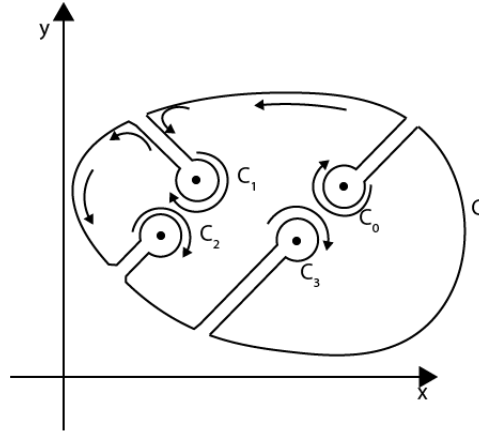


Figure 18

### A.7 Integrating around a singularity

In this subsection we will integrate around an isolated singularity. We will find that this gives an interesting result.

If we integrate around an isolated singularity at  $z = z_0$ , we find:

$$\oint_C f(z) dz = \sum_{n=-\infty}^{\infty} \oint_C a_n (z - z_0)^n dz. \quad (\text{A.29})$$

All the terms where  $n \neq -1$  vanish:

$$\oint_C a_n (z - z_0)^n dz = \frac{a_n}{n+1} (z - z_0)^{n+1} \Big|_{z_1 e^{2\pi i}}^{z_1} = 0. \quad (\text{A.30})$$

But the term  $n = -1$  gives us:

$$\oint_C \frac{a_{-1}}{(z - z_0)} dz = a_{-1} \ln(z - z_0) \Big|_{z_1 e^{2\pi i}}^{z_1} = 2\pi i a_{-1}. \quad (\text{A.31})$$

So in total we find:

$$\oint_C f(z) dz = 2\pi i a_{-1}. \quad (\text{A.32})$$

Note that since the only thing we assumed about the path is that the Laurent expansion exists on it, this result holds true for every closed integral around a singularity as long as the Laurent expansion converges on this path.

Since the coefficient  $a_{-1}$  will become very important, it has its own name. It is called the residue of a singularity.

### A.8 Residue theorem

In this subsection we will turn our interest to integrating around a contour which contains multiple singularities. Let us call this contour over which we integrate  $C$ . In order to integrate over  $C$  we once again draw contour lines to convert our region into a simply connected region. We do this as in figure 18. Note that in 18 there are only 4 singularities present but in principle there can be infinite singularities within the contour as long as they are isolated singular points. Since we converted our region into a simply connected region, we can use Cauchy's integral theorem. This gives us the following expression for our integral over  $C$ :

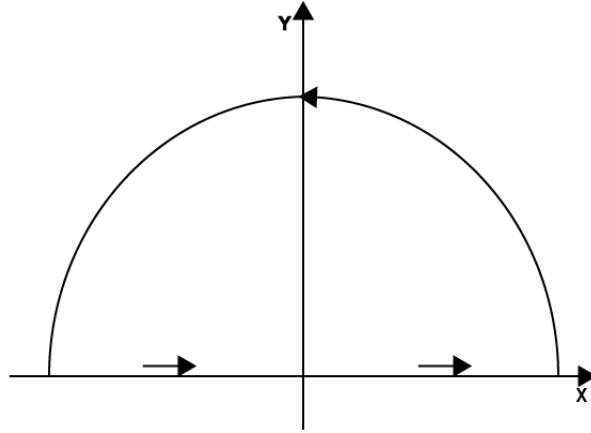


Figure 19

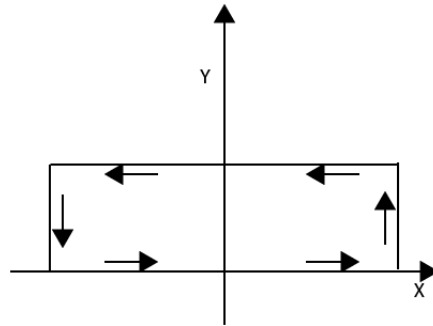


Figure 20

$$\oint_C f(z)dz = \oint_{C_0} f(z)dz + \oint_{C_1} f(z)dz + \oint_{C_2} f(z)dz + \oint_{C_3} f(z)dz. \tag{A.33}$$

Where  $C_0, C_1, C_2$  and  $C_3$  are small circles around the singularities. We have seen that integrating around a singularity is equal to  $2\pi i$  times the residue of that pole. So we find as an expression for our integral:

$$\oint_C f(z)dz = 2\pi i \sum_{\text{enclosed poles}} (\text{enclosed residues}). \tag{A.34}$$

Equation A.34 is called the residue theorem. It replaces the task of explicitly evaluating integrals by computing residues! It is an incredibly useful theorem. It provides a very powerful tool in evaluating definite integrals.

The residue theorem is also very useful in evaluating integrals over not closed paths. Say we have a non closed path  $C_1$ , we then look for a path  $C_2$  so that  $C_1 + C_2$  is a closed path. If we do this, we find:

$$\begin{aligned} \int_{C_1} f(z)dz &= \int_{C_1} f(z)dz + \int_{C_2} f(z)dz - \int_{C_2} f(z)dz = \oint_{C_1+C_2} f(z)dz - \int_{C_2} f(z)dz \\ &= 2\pi i \sum_{\text{enclosed poles}} (\text{enclosed residues}) - \int_{C_2} f(z)dz. \end{aligned} \tag{A.35}$$

The trick here is to choose the path  $C_2$  in such a manner that it is easily evaluated. This can be done by making sure that the integral over  $C_2$  is 0, or by using symmetries to evaluate the integral over  $C_2$ .

Two common examples of how to close our contour of integration are given in figures 19 and 20. In figure 19 we closed an integral from  $-\infty$  to  $\infty$  with an infinite semi-circle in the positive imaginary plane.

This can be useful if our integrand vanishes faster than  $1/|z|$ , then this extra integral vanishes.

Another example is given in figure 20. In this figure the contour is closed by the line  $y = ai$  and 2 vertical lines at  $x = \pm\infty$ . This may be useful if there are symmetries to be exploited and our integrands vanishes for  $z$  goes to  $\infty$ .

## A.9 Calculating residues

In the last section we found that with the residue theorem the task of evaluating definite integrals can be replaced by calculating residues. In this section we will look at how to calculate these residues. How to calculate residues depends on the order of the pole.

In order to find the residue of a first order pole, we look at the Laurent expansion of the function around a pole at  $z = z_0$ :

$$f(z) = \sum_{n=-1}^{\infty} a_n(z - z_0)^n \quad (\text{A.36})$$

By using the Laurent expansion we can check that the residue of a first order pole is given by:

$$a_{-1} = \lim_{z \rightarrow z_0} f(z)(z - z_0) \quad (\text{A.37})$$

For a higher order pole this method does not work. So for a higher order pole we need a different method. We consider a function  $f(z)$  with a pole of order  $m$  with a pole at  $z = z_0$ . The Laurent expansion of this function is given by:

$$f(z) = \sum_{n=-m}^{\infty} a_n(z - z_0)^n \quad (\text{A.38})$$

Using this Laurent expansion we find that the residue of a higher order pole is given by:

$$\frac{1}{(m-1)!} \left( \frac{d}{dz} \right)^{m-1} [f(z)(z-z_0)^m] \Big|_{z=z_0} = \frac{1}{(m-1)!} \left( \frac{d}{dz} \right)^{m-1} \sum_{n=-m}^{\infty} a_n(z-z_0)^{n+m} = \sum_{n=-1}^{\infty} a_n(z-z_0)^{n+1} \Big|_{z=z_0} = a_{-1} \quad (\text{A.39})$$



## B Fourier analysis

In this appendix we will develop some techniques involving Fourier analysis. Fourier analysis is incredibly rich and we will not even begin to scratch the surface of what is possible. We will start with a short derivation of the Fourier integral from the Fourier sums. From the Fourier integral we will define the Fourier transformation and the inverse Fourier transformation. We will also take a look at a short example to show the power of Fourier transformations. Finally we will also take a short look at the convolution product. We will do this following chapter 15 of Mathematical methods for physicists sixth edition by George B.Arffen and Hans J.Weber[6].

### B.1 From Fourier sums to Fourier integrals

In this subsection we will take the Fourier sum as a given. From it we will derive the Fourier integral. The Fourier sums is given by:

$$f(x) = \frac{1}{2L} \int_{-L}^{+L} f(t)dt + \frac{1}{L} \sum_{n=1}^{\infty} \int_{-L}^{+L} f(t) \cos\left(\frac{n\pi}{L}(t-x)\right) dt. \quad (\text{B.1})$$

The Fourier series is useful for describing functions on a finite interval  $[-L, L]$ . The Fourier series is valid as long as  $f(x)$  is piecewise continuous, piecewise differentiable and integrable on the interval  $[-L, L]$ .

In order to derive the Fourier integral from the Fourier series, we take the limit  $L \rightarrow \infty$ . By doing this we can represent our functions on the interval  $(-\infty, \infty)$ . We use the following parametrisation:

$$\begin{aligned} \omega &= \frac{n\pi}{L}, \\ \Delta\omega &= \frac{\pi}{L}. \end{aligned}$$

With these paramerisations we find:

$$f(x) = \frac{1}{\pi} \sum_{n=1}^{\infty} \Delta\omega \int_{-L}^{+L} f(t) \cos(\omega(t-x))dt. \quad (\text{B.2})$$

The first term of B.1 has been left out since it vanishes, assuming that  $\int_{-L}^{+L} f(t)dt$  exists. We can replace the sum over  $\omega$  with an integral to find:

$$f(x) = \frac{1}{\pi} \int_0^{\infty} d\omega \int_{-L}^{+L} f(t) \cos(\omega(t-x))dt \quad (\text{B.3})$$

We have now rewritten the Fourier series to an integral. This is only valid if  $\int_{-\infty}^{+\infty} f(t)dt$  exists,  $f(x)$  is piecewise continuous and piecewise differentiable. The Fourier integral is most often seen in an different form. In order to rewrite it to its more common form, note that  $\cos(\omega(t-x))$  is an even function and  $\sin(\omega(t-x))$  is an uneven function. So we have:

$$\begin{aligned} \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \int_0^{+\infty} f(t) \cos(\omega(t-x))dt &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) \cos(\omega(t-x))dt, \\ \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) \sin(\omega(t-x))dt &= 0. \end{aligned}$$

Because the integral over  $\sin(\omega(t-x))$  is 0. We can add  $\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) i \sin(\omega(t-x))dt$  to equation

B.3. If we do this we find:

$$\begin{aligned} f(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) \cos(\omega(t-x)) dt + \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) i \sin(\omega(t-x)) dt \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) [\cos(\omega(t-x)) + i \sin(\omega(t-x))] dt \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} f(t) e^{i\omega(t-x)} dt. \end{aligned}$$

We now reverse the order of integration to find:

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

We have now found the Fourier integral in its usual form. This will allow us to define the Fourier transform in the next subsection.

## B.2 Defining the Fourier transformation and the inverse transformation

Now that we have found the Fourier integral we can define our Fourier transform. We define the Fourier transform of a function as follows:

$$g(\omega) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt. \quad (\text{B.4})$$

Here  $g(\omega)$  is the Fourier transform of  $f(t)$ . From the Fourier integral we then find for the inverse transformation:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(\omega) e^{-i\omega x} d\omega. \quad (\text{B.5})$$

The prefactor  $\frac{1}{\sqrt{2\pi}}$  is a matter of choice. We could also put a factor of  $\frac{1}{2\pi}$  in front of one of the transformation.

## B.3 Fourier transforms of derivatives

In this subsection we will calculate the Fourier transforms for a function and its derivative. We will see that under the right condition these are very similar. Let us consider a function  $f(x)$  which goes to 0 for  $x \rightarrow \infty$ . Almost all functions which we Fourier transform obey this condition since the integral  $\int_{-\infty}^{\infty} f(x) dx$  has to exist. Its Fourier transform is given by:

$$g(\omega) = \int_{-\infty}^{+\infty} f(x) e^{i\omega x} dx. \quad (\text{B.6})$$

The Fourier transform of its derivative  $\frac{\partial f}{\partial x}$  is given by:

$$g_1(\omega) = \int_{-\infty}^{+\infty} \frac{\partial f}{\partial x} e^{i\omega x} dx. \quad (\text{B.7})$$

We now use partial integration to rewrite this Fourier transform. Note that the boundary terms vanish because  $f(x)$  goes to 0 for  $x \rightarrow \infty$ . This gives us:

$$g_1(\omega) = -i\omega \int_{-\infty}^{+\infty} f(x) e^{i\omega x} dx. \quad (\text{B.8})$$

We see that the Fourier transform of  $\frac{\partial f}{\partial x}$  is simply the Fourier transform of  $f(x)$  times  $-i\omega$ . This result is the reason why Fourier transforms are so often used in literature. Because of this result Fourier transform are incredibly useful in solving (partial) differential equations. The act of differentiating a function is a simply multiplication in Fourier space!

### B.4 Example of the uses of Fourier transformation

As an example of the power of Fourier transform we now solve the wave equation by using Fourier transforms. The wave equation has the following form:

$$\frac{\partial^2 y(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y(x, t)}{\partial t^2}, \quad (\text{B.9})$$

with  $y(x, 0) = f(x)$  as initial condition.  $f(x)$  goes to 0 for  $x \rightarrow \infty$ , this physically means that the wave has not reached  $\infty$  yet. We now Fourier transform both sides of this equation. This gives us:

$$\begin{aligned} \int_{-\infty}^{+\infty} \frac{\partial^2 y(x, t)}{\partial x^2} e^{i\omega x} dx &= \int_{-\infty}^{+\infty} \frac{1}{v^2} \frac{\partial^2 y(x, t)}{\partial t^2} e^{i\omega x} dx \\ (i\omega)^2 \int_{-\infty}^{+\infty} y(x, t) e^{i\omega x} dx &= \frac{\partial^2}{\partial t^2} \int_{-\infty}^{+\infty} \frac{1}{v^2} y(x, t) e^{i\omega x} dx \\ (-i\omega)^2 \tilde{y}(\omega, t) &= \frac{1}{v^2} \frac{\partial^2 \tilde{y}(\omega, t)}{\partial t^2}, \end{aligned} \quad (\text{B.10})$$

Here  $\tilde{y}(\omega, t)$  is the Fourier transform of  $y(x, t)$ . This is the power of Fourier transforms. We started with an partial differential equation. Using Fourier transformation we have rewritten this too a ordinary differential equation. What we are left with is an easy differential equation. Its solution is:

$$\tilde{y}(\omega, t) = \tilde{y}(\omega, 0) e^{\pm i\omega vt} = \tilde{f}(\omega) e^{\pm i\omega vt}, \quad (\text{B.11})$$

where  $\tilde{f}(\omega)$  is the Fourier transform of  $f(x)$ . Using the inverse transform to find  $y(x, t)$ , we find:

$$y(x, t) = \int_{-\infty}^{+\infty} \tilde{f}(\omega) e^{-i\omega(x \pm vt)} d\omega. \quad (\text{B.12})$$

Here we have shown that every solution of the wave function is a function of  $x \pm vt$ . Furthermore we have found an expression for the general solution of the wave equation. For appropriate initial conditions we can find the solution to the wave function.

### B.5 Convolution product

We define the convolution of 2 function to be:

$$f * g \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) f(x - y) dy. \quad (\text{B.13})$$

This product can be nicely rewritten in terms of a integral over Fourier transforms. We will denote the Fourier transform of  $f(x - y)$  by  $\tilde{f}(\omega)$  and the Fourier transform of  $g(y)$  by  $\tilde{g}(\omega)$

$$\begin{aligned} \int_{-\infty}^{\infty} f(y) g(x - y) dy &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) dy \left[ \int_{-\infty}^{\infty} \tilde{f}(\omega) e^{-i\omega(x-y)} d\omega \right] \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) e^{i\omega y} dy \left[ \int_{-\infty}^{\infty} \tilde{f}(\omega) e^{-i\omega x} d\omega \right] = \int_{-\infty}^{\infty} \tilde{g}(\omega) \tilde{f}(\omega) e^{-i\omega x} d\omega. \end{aligned} \quad (\text{B.14})$$

This turns out to be a nice way to rewrite an integral to Fourier space.

## C Introducing the annihilation and creation operators

In this appendix we will introduce 2 new operators: the fermionic annihilation and creation operators. In order to clearly we will first introduce some new notation.

Suppose we have a system with many identical fermions which can occupy multiple possible states. In such a case we want to write down our wave function in a short and tidy way. We do not want to write out antisymmetric products of states. For this we introduce the following notation:

$$|n, m, l, \dots\rangle.$$

This means there are  $n$  particles in the ground state,  $m$  in the first excited state,  $l$  in the second excited state and so on.

We define the fermionic creation operator as follows:

$$c_l^\dagger |n_1, n_2, \dots, n_l, \dots\rangle = \begin{cases} 0 & \text{if } n_l = 1 \\ |n_1, n_2, \dots, 0, \dots\rangle & \text{if } n_l = 0. \end{cases}$$

Similarly the fermionic annihilation operator is defined as:

$$c_l |n_1, n_2, \dots, n_l, \dots\rangle = \begin{cases} |n_1, n_2, \dots, 1, \dots\rangle, & \text{if } n_l = 1 \\ 0 & \text{if } n_l = 0. \end{cases}$$

The commutation relations of the operators are:

$$\begin{aligned} c_l^\dagger c_{l'}^\dagger + c_{l'}^\dagger c_l^\dagger &= 0, \\ c_l c_{l'} + c_{l'} c_l &= 0, \\ c_l c_{l'}^\dagger + c_{l'}^\dagger c_l &= \delta_{ll'}. \end{aligned}$$

The reason why these operators anticommute is due to the fact that the wave function has to be antisymmetric. If we add/remove a particle with the creation/annihilation operator we should always keep the wave function antisymmetric. Because of this it matters in which order we add/remove particles from the system. Adding/removing particles in a different order is equal to first exchanging the particles and thus gives a factor -1.

## D Mathematica code

### D.1 Mathematica code for the XXX Heisenberg model

$S_x = 0.5 * \{\{0, 1\}, \{1, 0\}\};$

$S_y = 0.5 * \{\{0, -i\}, \{i, 0\}\};$

$S_z = 0.5 * \{\{1, 0\}, \{0, -1\}\};$

$Id = \{\{1, 0\}, \{0, 1\}\};$

$L = 12;$

$SxN[N_, L_] := If [N == 1, KroneckerProduct [Sx, IdentityMatrix [2<sup>L-1</sup>]]$   
 $, If [N == L, KroneckerProduct [IdentityMatrix [2<sup>L-1</sup>], Sx], KroneckerProduct [IdentityMatrix [2<sup>N-1</sup>]$   
 $, Sx, IdentityMatrix [2<sup>L-N</sup>]]]]$

$SyN[N_, L_] := If [N == 1, KroneckerProduct [Sy, IdentityMatrix [2<sup>L-1</sup>]]$   
 $, If [N == L, KroneckerProduct [IdentityMatrix [2<sup>L-1</sup>], Sy], KroneckerProduct [IdentityMatrix [2<sup>N-1</sup>]$   
 $, Sy, IdentityMatrix [2<sup>L-N</sup>]]]]$

$SzN[N_, L_] := If [N == 1, KroneckerProduct [Sz, IdentityMatrix [2<sup>L-1</sup>]]$   
 $, If [N == L, KroneckerProduct [IdentityMatrix [2<sup>L-1</sup>], Sz], KroneckerProduct [IdentityMatrix [2<sup>N-1</sup>]$   
 $, Sz, IdentityMatrix [2<sup>L-N</sup>]]]]$

$HamiltonianXXX[L_] := Sum[SxN[i, L].SxN[i + 1, L] + SyN[i, L].SyN[i + 1, L] + SzN[i, L].SzN[i + 1, L]$   
 $, \{i, L - 1\}] + SyN[L, L].SyN[1, L] + SzN[L, L].SzN[1, L] + SxN[L, L].SxN[1, L];$

$EigXXX = Table \left\{ \left\{ i, \frac{Eigenvalues[HamiltonianXXX[i]]}{i} \right\}, \{i, 6, L, 2\} \right\};$

$Groundstate = Table [EigXXX[[i, 2, 1]], \{i, \frac{L-6}{2} + 1\}]$

$groundstateallsizes = Transpose[\{Table[i, \{i, 6, L, 2\}], Groundstate\}]$

$E_\infty = 1/4 - \text{Log}[2];$

$expansion1 = Table \left\{ \left\{ N, E_\infty - \frac{\pi^2}{12N^2} \right\}, \{N, 6, 12, 2\} \right\} // N;$

$expansion2 = Table \left\{ \left\{ N, E_\infty - \frac{\pi^2}{12N^2} - \frac{\pi^2}{12N^2} \frac{0.3422}{(\text{Log}[N])^3} \right\}, \{N, 6, 12, 2\} \right\};$

$accuracyexpansion1 = Table \left\{ \left\{ groundstateallsizes[[i, 1]], 100 * \frac{groundstateallsizes[[i, 2]] - expansion1[[i, 2]]}{groundstateallsizes[[i, 2]]} \right\} // N, \{i, 4\} \right\}$

$accuracyexpansion2 = Table \left\{ \left\{ groundstateallsizes[[i, 1]], 100 * \frac{groundstateallsizes[[i, 2]] - expansion2[[i, 2]]}{groundstateallsizes[[i, 2]]} \right\} // N, \{i, 4\} \right\}$

$groundstateplot = Show[ListPlot[\{expansion1, expansion2\}], PlotMarkers  $\rightarrow$  None$

$, PlotRange  $\rightarrow$   $\{-.47, -.44\}$ , AxesLabel  $\rightarrow$   $\{N, "E_0/N/J"\}$ , Joined  $\rightarrow$   $\{\text{True}, \text{True}\}$$

$, PlotLegends  $\rightarrow$   $\left\{ " \frac{E_\infty}{N} - \frac{\pi^2}{12N^2} ", " \frac{E_\infty}{N} - \frac{\pi^2}{12N^2} - \frac{\pi^2}{12N^2} \frac{0.3422}{\text{Log}^3(N)} " \right\}$ , ListPlot[\{groundstateallsizes$

```
, PlotMarkers → {Automatic, Medium}, PlotRange → {-0.47, -0.44}, AxesLabel → {N, "E0/N/J"}
, PlotLegends → {"Numerical Data"}]]
differenceplot = ListPlot[{accuracyexpansion1, accuracyexpansion2}, Joined → {True, True}
, PlotLegends → {
"100* $\frac{E_0}{N} - \left(\frac{E_\infty}{N} - \frac{\pi^2}{12N^2}\right)$ ", "100* $\frac{E_0}{N} - \left(\frac{E_\infty}{N} - \frac{\pi^2}{12N^2} - \frac{\pi^2}{12N^2} \frac{0.3422}{\text{Log}^3(N)}\right)$ "
}
, AxesLabel → {N, "%"}, PlotMarkers → {Automatic, Small}]
Spectrumlist = Sort[EigXXX[[-1, 2]], Less];
SpectrumPlot = ListPlot[Spectrumlist, Ticks → {None, Automatic}, AxesLabel → {"", "E/N/J"}
, PlotLegends → {"Energy eigenstates"}, PlotLabel → "N=12"]
```

## D.2 Mathematica code for the XXZ Heisenberg model

```
HamiltonianXXZ[J-, L-]:=Sum[SxN[i, L].SxN[i + 1, L] + SyN[i, L].SyN[i + 1, L] + J * SzN[i, L].SzN[i + 1, L]
, {i, L - 1}] + SyN[L, L].SyN[1, L] + J * SzN[L, L].SzN[1, L] + SxN[L, L].SxN[1, L];
```

```
XXZeigen6 = Table[{i,  $\frac{\text{Sort}[\text{Eigenvalues}[\text{HamiltonianXXZ}[i, 6], \text{Less}]}{6}$ }, {i, 0, 0.6, 0.2}];
```

```
XXZeigen8 = Table[{i,  $\frac{\text{Sort}[\text{Eigenvalues}[\text{HamiltonianXXZ}[i, 8], \text{Less}]}{8}$ }, {i, 0, 0.6, 0.2}];
```

```
XXZeigen10 = Table[{i,  $\frac{\text{Sort}[\text{Eigenvalues}[\text{HamiltonianXXZ}[i, 10], \text{Less}]}{10}$ }, {i, 0, 0.6, 0.2}];
```

```
XXZeigen12 = Table[{i,  $\frac{\text{Sort}[\text{Eigenvalues}[\text{HamiltonianXXZ}[i, 12], \text{Less}]}{12}$ }, {i, 0, 2, 0.2}];
```

```
XXZspectrum = ListPlot[{XXZeigen12[[-1, 2]], XXZeigen12[[-6, 2]], XXZeigen12[[-11, 2]]}
```

```
, Ticks → {None, Automatic}, AxesLabel → {None, "E/J/N"}, PlotMarkers → {Automatic, Tiny}
```

```
, PlotLegends → {"Δ=0", "Δ=1", "Δ=2"}]
```

```
groundstate12 = Table[XXZeigen12[[i, 2, 1]], {i, 11}]
```

```
groundstate6 = Table[XXZeigen6[[i, 2, 1]], {i, 4};
```

```
groundstate8 = Table[XXZeigen8[[i, 2, 1]], {i, 4};
```

```
groundstate10 = Table[XXZeigen10[[i, 2, 1]], {i, 4};
```

```
groundstate12 = Table[XXZeigen12[[i, 2, 1]], {i, 11};
```

```
Table[{groundstate6[[i]], groundstate8[[i]], groundstate10[[i]], groundstate12[[i]]}, {i, 4};
```

```
expansionaccuracy = Table[{
```

$$\left\{ 6, 100 * \left( \frac{-\frac{1}{\pi} - \frac{1}{\pi^2} (i/5 - 0.2) + \frac{\pi^2 - 24}{18\pi^3} (i/5 - 0.2)^2 - \frac{\pi * 2\pi * \text{Sin}[\text{ArcCos}[-(i/5 - 0.2)]]}{\pi - \text{ArcCos}[-(i/5 - 0.2)]} - \text{groundstate6}[[i]]}{\text{groundstate6}[[i]]} \right) \right\}$$

$$\left\{ 8, 100 * \left( \frac{-\frac{1}{\pi} - \frac{1}{\pi^2} (i/5 - 0.2) + \frac{\pi^2 - 24}{18\pi^3} (i/5 - 0.2)^2 - \frac{\pi * 2\pi * \text{Sin}[\text{ArcCos}[-(i/5 - 0.2)]]}{\pi - \text{ArcCos}[-(i/5 - 0.2)]} - \text{groundstate8}[[i]]}{\text{groundstate8}[[i]]} \right) \right\}$$

$$, \left\{ \left\{ 10, 100 * \left( \frac{-\frac{1}{\pi} - \frac{1}{\pi^2} (i/5-0.2) + \frac{\pi^2-24}{18\pi^3} (i/5-0.2)^2 - \frac{\pi * 2\pi * \text{Sin}[\text{ArcCos}[-(i/5-0.2)]]}{\pi - \text{ArcCos}[-(i/5-0.2)]} - \text{groundstate10}[[i]]}{\text{groundstate10}[[i]]} \right) \right\} \right\}, \left\{ \left\{ 12, 100 * \left( \frac{-\frac{1}{\pi} - \frac{1}{\pi^2} (i/5-0.2) + \frac{\pi^2-24}{18\pi^3} (i/5-0.2)^2 - \frac{\pi * 2\pi * \text{Sin}[\text{ArcCos}[-(i/5-0.2)]]}{\pi - \text{ArcCos}[-(i/5-0.2)]} - \text{groundstate12}[[i]]}{\text{groundstate12}[[i]]} \right) \right\} \right\}, \{i, 4\} ;$$

converge1 = Fit [expansionaccuracy[[1]], {1, N<sup>-2</sup>}, N] [[1]]

converge2 = Fit [expansionaccuracy[[2]], {1, N<sup>-2</sup>}, N] [[1]]

expansionaccuracyplot1 = ListPlot[expansionaccuracy[[1]], AxesLabel → {"Δ", "%"}]

, PlotLegends → {"E<sub>0</sub> - (-1/π - Δ + π<sup>2</sup>-24 / 18π<sup>3</sup> \* Δ<sup>2</sup> - π\*vf / 24\*N<sup>2</sup>)"},

Joined → True, PlotMarkers → {Automatic, Small}]

expansionaccuracyplot2 = ListPlot[expansionaccuracy[[2]], AxesLabel → {"Δ", "%"}]

, PlotLegends → {"E<sub>0</sub> - (-1/π - Δ + π<sup>2</sup>-24 / 18π<sup>3</sup> \* Δ<sup>2</sup> - π\*vf / 24\*N<sup>2</sup>)"},

Joined → True, PlotMarkers → {Automatic, Small}]

expansionaccuracyplot3 = ListPlot[expansionaccuracy[[3]], AxesLabel → {"Δ", "%"}]

, PlotLegends → {"E<sub>0</sub> - (-1/π - Δ + π<sup>2</sup>-24 / 18π<sup>3</sup> \* Δ<sup>2</sup> - π\*vf / 24\*N<sup>2</sup>)"},

Joined → True, PlotMarkers → {Automatic, Small}]

expansionaccuracyplot4 = ListPlot[expansionaccuracy[[4]], AxesLabel → {"Δ", "%"}]

, PlotLegends → {"E<sub>0</sub> - (-1/π - Δ + π<sup>2</sup>-24 / 18π<sup>3</sup> \* Δ<sup>2</sup> - π\*vf / 24\*N<sup>2</sup>)"},

Joined → True, PlotMarkers → {Automatic, Small}]

excitedstate12 = Table[XXZeigen12[[i, 2, 2]], {i, 11}];

secondexcitedstate12 = Table[XXZeigen12[[i, 2, 3]], {i, 11}];

diff = secondexcitedstate12 - excitedstate12;

diff12 = Table[secondexcitedstate12[[i]] - excitedstate12[[i]], {i, 11}]

Δ2 = ListPlot[XXZeigen12[[-1, 2, 1;;10]], AxesLabel → {"", "E/N/J"}, Ticks → {None, Automatic}]

energygap = ListPlot[Transpose[{{0, 0.2, 0.4, 0.6, 0.8, 1, 1.2, 1.4, 1.6, 1.8, 2}, diff12}]

, AxesLabel → {"Δ", "ΔE/N/J"}, PlotMarkers → Automatic]

secondhighestenergystate = Table[XXZeigen12[[i, 2, -2]], {i, 11}];

thirdhighestenergystate = Table[XXZeigen12[[i, 2, -3]], {i, 11}];

diffhigh = thirdhighestenergystate - secondhighestenergystate;

diff12high = Table[thirdhighestenergystate[[i]] - secondhighestenergystate[[i]], {i, 11}]

Δ2high = ListPlot[XXZeigen12[[-1, 2, -10;; -1]], AxesLabel → {"", "E/N/J"}, Ticks → {None, Automatic}]

energygaphigh = ListPlot[Transpose[{{0, 0.2, 0.4, 0.6, 0.8, 1, 1.2, 1.4, 1.6, 1.8, 2}, diff12high}]

, AxesLabel → {"Δ", "ΔE/N/J"}, PlotMarkers → Automatic]

## References

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