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Opleiding Natuur- en Sterrenkunde

Next nearest neighbour interactions in the Heisenberg model

Bachelor Thesis

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Abstract

The Bethe ansatz is used to analytically solve the Heisenberg Model with nearest neighbour interactions for spin-$\frac{1}{2}$ particles in an one dimensional chain. Our goal is to find out if the Bethe ansatz can be extended to nearest and next nearest neighbour interactions and to gain insight into the system with exact diagonalization. We find that this cannot be done. Because of certain assumptions made in the Bethe ansatz, the method fails for next nearest neighbour interactions.

Contents

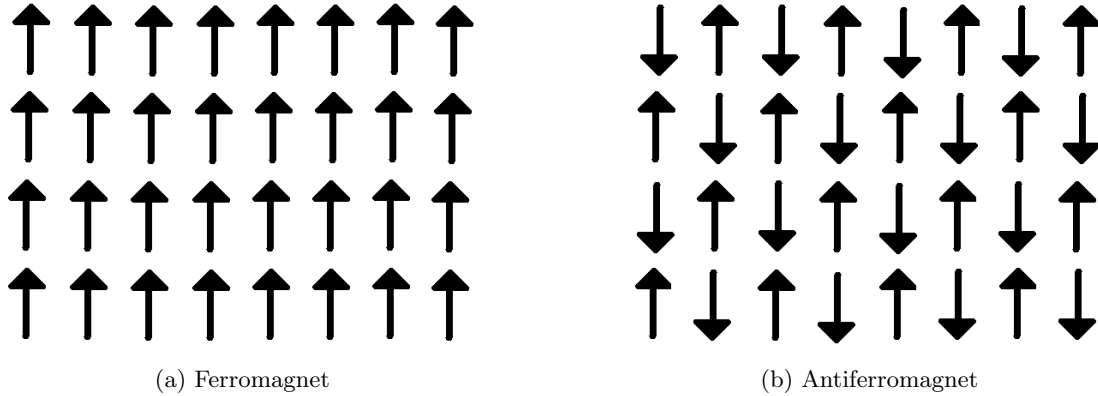(a) Ferromagnet   (b) Antiferromagnet

Figure 1: (1a) is a sketch of a ferromagnetic material, where the interactions favour a parallel alignment of neighbouring spins. Figure (1b) is a sketch of an antiferromagnetic material. Here the interactions favour anti parallel alignment of neighbouring spins.

1   Introduction

Classically, magnetism is described by the Maxwell equations[1]. To see how magnetism affects materials, we look at the magnetic moments in the material, which are either created by moving charges or by the intrinsic magnetic moment of the particles (the spin). We can classify a material by the respondence of its magnetic moments to the magnetic field. If the magnetic moments are attracted by the magnetic field, the material is called paramagnetic. If they are repelled by the magnetic field, the material is called diamagnetic.
When we take into account the interactions between the magnetic moments, we can make another classification: If the magnetic moments align with each other without an external magnetic field, the material is called ferromagnetic (figure 1a). If a material favours a configuration where neighbouring magnetic moments are in the opposite direction, the material is called antiferromagnetic (Figure 1b).

Ferromagnetic and antiferromagnetic systems can be described with an effective Hamiltonian called the Heisenberg model. This Hamiltonian describes the interaction between the spin of a particle and the spin of the neighbouring particle. In the first chapter of this thesis we will derive the Heisenberg model from the underlying electronic theory. WE also find out what the nature of the interaction between the particles is. In the remainder of this thesis we will look for solutions of the Heisenberg model of a one dimensional chain of spin-$\frac{1}{2}$ particles. We will do this numerically using exact diagonalization in Mathematica and analytically using the Bethe ansatz. This method was first used by Hans Bethe in 1931[2] to find the exact eigenvalues and eigenvectors of the Heisenberg Hamiltonian of a one dimensional chain with spin-$\frac{1}{2}$ particles. This approach by Bethe was done with only nearest neighbour interactions in the Heisenberg model. We will try to extend this approach for next nearest neighbour interactions. To get more insight into the problem we also do a numerical exact diagonalisation of the Heisenberg model in Mathematica. We then examine the behavior of the ground state for different ratios between the nearest neighbour and next nearest neighbour interaction. We will find that the ground is never degenerate except at $J_2 = \frac{1}{2}J_1$, where it is double degenerate. The model with this value for J_2 is known as the Majumdar-Ghosh model. We will shortly look into this model. When we extend the Bethe ansatz to next nearest neighbour interactions in the Heisenberg model we find that this does not work. The further reaching interactions cause the ansatz that is made to not be a valid eigenstate of the Hamiltonian when the particles are next to each other. Because of this we cannot analytically get the eigenvalues.

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[1]See for example Griffiths[1] chapter 7.3

(a) $\phi_s(\vec{r_1}, \vec{r_2})$
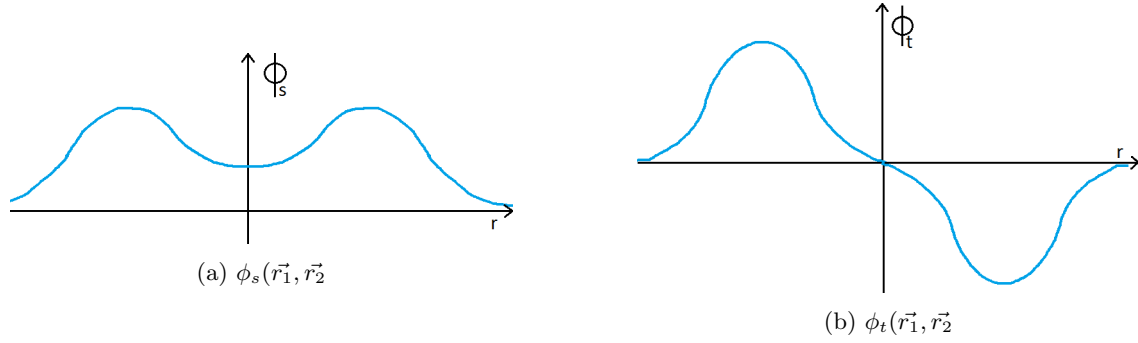
(b) $\phi_t(\vec{r_1}, \vec{r_2})$

Figure 2: Sketches of the spatial wave functions for the singlet and the triplet configuration of a system with two electrons.

2   Physical origin of the Heisenberg model

In this chapter we will derive the Heisenberg model, which is used to calculate the Hamiltonian of an one dimensional chain with interacting spin-$\frac{1}{2}$ particles. We will first determine the interaction strength J and then show how it turns up in the Heisenberg model. In the remainder of this thesis we will try to solve the Heisenberg model with the Bethe ansatz.

Consider two atoms on an one dimensional chain. To describe the interaction between these two atoms we look only at the outermost electrons. An electron is a spin-$\frac{1}{2}$ particle and therefore it obeys the Pauli principle, e.g. its total wave function has to be anti symmetric: $\psi(x_1, x_2) = -\psi(x_2, x_1)$. The combination of two spin-$\frac{1}{2}$ wave functions gives a singlet and a triplet configuration. The singlet spin wave function is anti symmetric and therefore its spatial wave function has to be symmetric. The spatial wave function is given by

$$\phi_s(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2 + 2l^2}}[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)]. \tag{1}$$

Because the wave functions are not orthogonal, there is an overlap integral $l = \langle \phi_1 | \phi_2 \rangle$. $\phi_i(\vec{r}_j)$ denotes the spatial wave function of particle $\vec{r}_j$ in state i.
The triplet spin state is symmetric, so its spatial wave function has to be anti symmetric:

$$\phi_t(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2 - 2l^2}}[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)]. \tag{2}$$

Sketches for these wave functions are shown in figure (2).

The expected dominant forces in this system are the electric and the magnetic force. The magnetic moment of an electron is very small compared to its electric forces. Therefore, we neglect the contribution of the magnetic moment to the energy. The Hamiltonian, thus with only contributions of the Coulomb force, is given by

$$\hat{H} = \frac{\hat{p}_1^2}{2m} - \frac{e^2}{|\vec{r}_1 - \vec{R}_1|} + \frac{\hat{p}_2^2}{2m} - \frac{e^2}{|\vec{r}_2 - \vec{R}_2|} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} + \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} - \frac{e^2}{|\vec{r}_1 - \vec{R}_2|} - \frac{e^2}{|\vec{r}_2 - \vec{R}_1|}. \tag{3}$$

Here the upper case $\vec{R}$ the denotes the position of the atom and the lower case $\vec{r}$ denotes the position of the electron. We can now calculate the energy expectation value of respectively the singlet and the triplet state:

$$\epsilon_s = \langle \phi_s | \hat{H} | \phi_s \rangle = 2\epsilon_0 + \frac{U + V}{1 + l^2}, \tag{4}$$

$$\epsilon_t = \langle \phi_t | \hat{H} | \phi_t \rangle = 2\epsilon_0 + \frac{U - V}{1 - l^2}, \tag{5}$$

where ϵ_0 is the energy of one particle that is infinitely far away from the other particle. U and V are introduced to denote complicated integrals that arise because of all the different terms in (3).

$$
\begin{aligned}
U &= \int d\vec{r_1} d\vec{r_2} \phi_1^*(\vec{r_1}) \phi_2^* \left[\frac{e^2}{|\vec{r_1} - \vec{r_2}|} + \frac{e^2}{|\vec{R_1} - \vec{R_2}|} - \frac{e^2}{|\vec{r_1} - \vec{R_2}|} - \frac{e^2}{|\vec{r_2} - \vec{R_1}|} \right] \phi_1(\vec{r_1}) \phi_2(\vec{r_2}) \\
V &= \int d\vec{r_1} d\vec{r_2} \phi_1^*(\vec{r_1}) \phi_2^* \left[\frac{e^2}{|\vec{r_1} - \vec{r_2}|} + \frac{e^2}{|\vec{R_1} - \vec{R_2}|} - \frac{e^2}{|\vec{r_1} - \vec{R_1}|} - \frac{e^2}{|\vec{r_2} - \vec{R_2}|} \right] \phi_2(\vec{r_1}) \phi_1(\vec{r_2}).
\end{aligned}
\tag{6}
$$

The difference between the triplet and the singlet energy is called J and is given by

$$
J = \epsilon_t - \epsilon_s = -\frac{2V - 2l^2 U}{1 - l^4}.
\tag{7}
$$

We will show that this term describes the interaction between the electrons. As we have seen, it is a result of Pauli repulsion and electronic potentials between two electrons.[2]

We now want to obtain a Hamiltonian that describes the spin interactions in our system. At first, we start with two spin-$\frac{1}{2}$ particles. The total spin of this system is

$$
S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 = \frac{3}{2} + 2S_1 \cdot S_2,
\tag{8}
$$

which equals 2 if the spins are in a triplet state and 0 if they're in the singlet state. Thus we find $S_1 \cdot S_2 = \frac{1}{4}$ in the triplet states and $S_1 \cdot S_2 = -\frac{3}{4}$ in the singlet state.

Now we can construct a Hamiltonian:

$$
H = \frac{1}{4}(\epsilon_s + 3\epsilon_t) - (\epsilon_s - \epsilon_t) S_1 \cdot S_2.
\tag{9}
$$

This leaves the eigenvalue ϵ_s if the two particles are in the singlet state and ϵ_t if the two particles are in one of the triplet states. We can now omit the constant $\frac{1}{4}(\epsilon_s + 3\epsilon_t)$ and rewrite the Hamiltonian, using the definition of J (7), into

$$
H = J S_1 \cdot S_2.
\tag{10}
$$

If we generalize this to N particles, we find[3]

$$
H = \sum_{i,j}^{N} J_{ij} S_i \cdot S_j.
\tag{11}
$$

At large distances, the singlet and triplet energy splitting disappears and J_{ij} becomes zero. Thus for large separations of two particles, it is certainly not necessary (and way to complicated) to consider their interaction with each other in (11). We will thus only look at nearest and next nearest neighbour interactions. This model can be used for any dimension. It has only been analytically for nearest neighbour interactions in an one dimensional chain. This has been done using the Bethe ansatz. We will try to extend this to next nearest neighbour interactions. The Hamiltonian for these interactions, is given by

$$
\hat{H} = J_1 \sum_{i=1}^{N} \vec{S_i} \cdot \vec{S}_{i+1} + J_2 \sum_{i=1}^{N} \vec{S_i} \cdot \vec{S}_{i+2},
\tag{12}
$$

where J_1 is the interaction strength for nearest neighbour interactions and J_2 the interaction strength for next nearest neighbour interactions. In figure (3) is a sketch of a one dimensional of spin-$\frac{1}{2}$ particles. The interaction J_1 and J_2 are indicated.

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[2]The discussion above is based on chapter 26.2 of Marder[3]
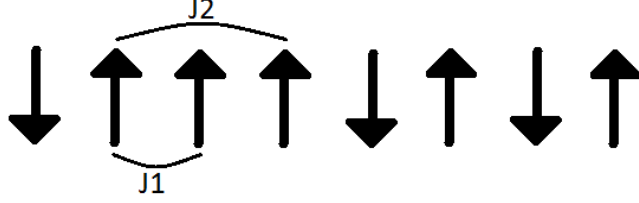[3]The derivation of the Heisenberg model is based on chapter 32 of Ashcroft and Mermin[4]

Figure 3: A sketch of a one dimensional chain of spin-$\frac{1}{2}$ particles the interactions J_1 and J_2 are between every particle with its nearest and next nearest neighbours.

3   Nearest neighbour interactions

In this chapter we follow Giarmarchi's[5] derivation of the Bethe equations for the Heisenberg model with nearest neighbour interactions. First, we do this for the trivial case of one flipped spin and secondly, we extend this approach to two flipped spins. Thereafter, we will extend this approach to many flipped spins. At final, we will look at the energy behavior in the continuum limit, which will give us an exact value for the ground state of this system.

To solve the Heisenberg model (12) analytically, we start with a system where there are only nearest neighbour interactions, e.g. $J_2 = 0$.
The Hamiltonian then becomes

$$
\begin{aligned}
H &= J \sum_{i=1}^{N} \vec{S}_i \vec{S}_{i+1} \\
&= J \sum_{i=1}^{N} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right) \\
&= J \sum_{i=1}^{N} \left[\frac{1}{2} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + S_i^z S_{i+1}^z \right].
\end{aligned}
\tag{13}
$$

Here $S_i^{\pm}$ are the standard spin ladder operators: $S_i^{\pm} = S_x \pm i S_y$.

3.1   One spin flipped

First we consider the fully polarized state $|F\rangle = |\uparrow ... \uparrow\rangle$, which has energy $H|F\rangle = \frac{L}{4}|F\rangle$ (to simplify notation we use $\hbar = 1$).
We now flip one spin at site N, $|\psi\rangle = S_n^- |F\rangle$. The Schrödinger equation then gives

$$
H S_n^- |F\rangle = J \left[\frac{1}{2} \left(S_{n+1}^- |F\rangle + S_{n-1}^- |F\rangle \right) + \left(\frac{L}{4} - 1 \right) |F\rangle \right],
\tag{14}
$$

where L is the length of the chain. Since adjacent up spins only contribute to an overall energy factor, but do not interact with each other, we can view this system as the down spin being a free particle. This we can describe with a plane wave ansatz:

$$
\psi(x) = \frac{1}{\sqrt{L}} e^{ikx}.
\tag{15}
$$

Combining this with the Schrödinger equation gives

$$
\begin{aligned}
H \psi(x) &= J \left[\frac{1}{2} \left(\psi(x+1) + \psi(x-1) \right) + \left(\frac{L}{4} - 1 \right) \psi(x) \right] \\
&= J \left[\cos(k) + \frac{L}{4} - 1 \right] \psi(x).
\end{aligned}
\tag{16}
$$

Because we can factor out the wave function (15), we see that the plane wave ansatz is an eigenstate of this system with energy

$$E(k) = J\left[\cos(k) + \frac{L}{4} - 1\right].\tag{17}$$

3.2   Two spins flipped

Because the Hamiltonian only has nearest neighbour interactions, two flipped spins that are not next to each other in an otherwise polarized chain $(S_n^- S_m^-|F\rangle)$, will behave like two separate free particles and can thus be described by

$$\psi(x_1, x_2) = \alpha e^{i(k_1 x_1 + k_2 x_2)} + \beta e^{i(k_1 x_2 + k_2 x_1)},\tag{18}$$

where we require the arguments of $\psi(x_1, x_2)$ to be ordered: $x_1 \leq x_2$. We now want this wave function to be valid at all distances. The two spins only interact with each other when they are next to each other. We want to find out whether the wave function (57) is still an eigenstate of the Hamiltonian if the two spins are adjacent. If this is the case, we want to find relations between α, β, k_1 and k_2. These relations will be the Bethe equations.

The Hamiltonian for a polarized chain with two flipped spins next to each other gives

$$HS_n^- S_{n+1}^-|F\rangle = J_1\left[\frac{1}{2}\left(S_n^- S_{n+2}^-|F\rangle + S_{n-1}^- S_{n+1}^-|F\rangle\right) + \frac{1}{4}(L-4)S_n^- S_{n+1}^-|F\rangle\right].\tag{19}$$

It is also possible to write these equations as wave functions, which are

$$H\psi(x, x+1) = J_1\left[\frac{1}{2}\left(\psi(x, x+2) + \psi(x-1, x+1)\right) + \frac{1}{4}(L-4)\psi(x, x+1)\right].\tag{20}$$

$\psi(x, x+1)$ can not be factored out here, which means the ansatz (57) we made, wouldn't be an eigenstate of the Hamiltonian. However, we can add a term which makes it possible to factor $\psi(x, x+1)$ out. This added term has to be zero everywhere, which leads to the following condition

$$\frac{1}{2}J_1\left[\psi(x+1, x+1) + \psi(x, x)\right] = J_1.\tag{21}$$

Using the wave function (57) and solving for α/β, gives

$$\begin{aligned}\frac{\alpha}{\beta} &= -\frac{e^{i\frac{k_1-k_2}{2}} - \cos\left(\frac{k_1+k_2}{2}\right)}{e^{i\frac{k_2-k_1}{2}} - \cos\left(\frac{k_1+k_2}{2}\right)} \\ &= -e^{i\Theta(k_1, k_2)},\end{aligned}\tag{22}$$

where $\Theta(k_1, k_2)$ is a phase shift, denoted by

$$\Theta(k_1, k_2) = 2\arctan\frac{\sin\left(\frac{k_1-k_2}{2}\right)}{\cos\left(\frac{k_1-k_2}{2}\right) - \cos\left(\frac{k_1+k_2}{2}\right)}.\tag{23}$$

Using periodic boundary conditions, $\psi(x_1, x_2) = \psi(x_2, x_1 + L)$, it follows that

$$\alpha = \beta e^{-ik_2 L} = \beta e^{ik_1 L}.\tag{24}$$

This condition tells us that the total momentum should be quantized:

$$k_1 + k_2 = \frac{2\pi n}{L}.\tag{25}$$

We now have two equations for the ratio α/β (equations 22 and 24). If we combine these, we will find that

$$-e^{i\Theta(k_1, k_2)} = e^{ik_1 L} = e^{-ik_2 L},\tag{26}$$

which leads to the following equations:

$$
\begin{aligned}
Lk_1 &= 2\pi I_1 + \Theta(k_1, k_2), \\
Lk_2 &= 2\pi I_2 + \Theta(k_2, k_1),
\end{aligned}
\tag{27}
$$

where I_1 and I_2 are half integers. Now we can rewrite the wave function (57) as

$$
\psi(x_1, x_2) = e^{i\left(\frac{\Theta(k_1,k_2)}{2} + k_1 x_1 + k_2 x_2\right)} - e^{i\left(\frac{\Theta(k_2,k_1)}{2} + k_1 x_2 + k_2 x_1\right)}.
\tag{28}
$$

3.3   Many spin flips

We now take a polarized chain with L up spins. We flip N spins down at positions $x_1 < x_2 < ... < x_N$ and denote this by the list $\{x_j\}$. If none of the flipped spins are adjacent, the Schrödinger equation gives

$$
H\psi(\{x_j\}) = \frac{L}{4} - N + \frac{1}{2} \sum_{i=1}^{N} \left(S_{i-1}^- S_i^+ + S_i^+ S_{i+1}^-\right)\psi(\{x_j\}).
\tag{29}
$$

If two flipped spins are adjacent, we have seen in the two flipped spin case above, that there are two differences: The overall energy term is different and the movement of the spins is changed. When there is only one pair of adjacent down spins (say at x_k and x_{k+1}), we find that

$$
H\psi(\{x_j\}) = E_z^0\psi(\{x_j\}) + \frac{1}{2}\sum_{i \neq k, k+1}^{N}\left(S_{i-1}^- S_i^+ + S_i^+ S_{i+1}^-\right)\psi(\{x_j\}) + \frac{1}{2}\left(S_{k-1}^- S_k^+ + S_{k+1}^+ S_{k+2}^-\right)\psi(\{x_j\}) + \psi(\{x_j\}).
\tag{30}
$$

We want the equations (29) and (30) to be the same. To achieve this situation, we can add a term, just like we did in the two flipped spins case. Therefore we add

$$
\frac{1}{2}\psi(..., x_{k+1}, x_{k+1}, ...) + \frac{1}{2}\psi(..., x_k, x_k, ...) - \psi(..., x_k, x_{k+1}, ...).
\tag{31}
$$

We also want this term to be zero, which leads to the following equation

$$
2\psi(..., x_k, x_{k+1}, ...) = \psi(..., x_{k+1}, x_{k+1}, ...) + \psi(..., x_k, x_k, ...).
\tag{32}
$$

Just as before, we make an ansatz for the wave equation. The form is similar to the two flipped spins case. This leads to the following ansatz:

$$
\psi(x_1, ..., x_N) = \sum_P A_P \exp\left[i\sum_{j=1}^{N} k_{P_j} x_j\right].
\tag{33}
$$

In each exponent, every k is multiplied by the corresponding x. Thereafter, they are permuted (with permutation P) over all possible combinations, given a total of $N!$ terms. We can now insert this wave function into equation (32). Here fore, we first introduce a permutation P' which differs from P by the exchange of two adjacent elements $P'(j+1) = P(j)$, $P'(j) = P(j+1)$. We then have

$$
\psi(..., x_j + m, x_j + n, ...) = \sum_{\{P\}} e^{i\sum_{i \neq j, j+1} k_{P_i} x_i + i(k_{P_j} + k_{P_j'})x_j} \times \left(A_P e^{i(m k_{P_j} + n k_{P_j'})} + A_{P'}e^{i(m k_{P_j'} + n k_{P_j})}\right)
\tag{34}
$$

Here, the first sum is only over permutations that have $P(k) < P'(k)$.
It is now possible to solve (32) with this wave function. This gives

$$
2\left(A_P e^{i k_{P_k'}} + A_{P'}e^{i k_{P_k}}\right) = \left(A_P + A_{P'}\right)\left(1 + e^{i(k_{P_k} + k_{P_k'})}\right).
\tag{35}
$$

Just like we have done with equation (22), we can write this as

$$\frac{A_P}{A_{P'}} = -\frac{1 + e^{i(k_{P_k} + k_{P'_k})} - 2e^{ik_{P_k}}}{1 + e^{i(k_{P_k} + k_{P'_k})} - 2e^{ik_{P'_k}}} = -e^{-i\Theta(k_{P_k}, k_{P'_k})}. \tag{36}$$

Here, $\Theta(k_{P_k}, k_{P'_k})$ is the same phase shift as in (23).

This expression now fixes all coefficients A_P up to an overall normalization. Every permutation can be build up of a sequence of transpositions. To determine the normalization factor, we need to fix the identity permutation $A_{1,2,3,...,N}$. Using (36), we can write a permutation A_P as a product of transpositions and the identity permutation

$$\frac{A_P}{A_{1,2,3,...,N}} = (-1)^{\eta_P} \exp\left[\sum_T \Theta(k_i, k_j)\right], \tag{37}$$

where η_P is the number of transpositions required to get to P. The T in the sum denotes all transpositions required to get to P.

Periodic boundary conditions give us

$$\left(A_P/A_{P'}\right)e^{ik_{P'_1}L} = 1. \tag{38}$$

This has to be satisfied for every permutation P. We can now calculate the ratio $A_P/A_{P'}$ by looking at the permutation P' as a 'right shift' of all elements:

$$(P'_1, P'_2, ..., P'_N) = (P_N, P_1, P_2, ..., P_{N-1}). \tag{39}$$

Combining this with (36), leads to

$$(-1)^{N-1} \exp\left(i\sum_{j=1}^N \Theta(k_j, k_l)\right)e^{ik_l L} = 1. \tag{40}$$

Therefore, it follows that

$$Lk_i = 2\pi I_i + \sum_j \Theta(k_i, k_j). \tag{41}$$

Here, I_i are half-integer, if N is even and I_i are integers, when N is odd. These are the Bethe equations, which couple the momenta of the spins.

Therefore, the energy of the system is just the eigenvalue of the Hamiltonian:

$$E = J\frac{L}{4} + J\sum_j^N \left[\cos(k_j) - 1\right]. \tag{42}$$

4   Continuum limit

Until now, we have looked at a finite system. In this section we look at the continuous limit, so we can come to an analytic expression for the ground state energy of our system. First, we introduce the shifted momentum $\overline{k}$ and the wavelength λ as

$$k = \overline{k} + \pi$$
$$\lambda = -\frac{1}{2}\tan\left(\overline{k}/2\right). \tag{43}$$

The energy (42) then becomes

$$E = \frac{1}{4}LJ - J\sum_i \left[1 + \cos(\overline{k})\right]. \tag{44}$$

From now on, we will drop the over-line to simplify notation. We can define a counting function

$$\Phi(\lambda) = 2L\arctan(2\lambda) - \sum_j 2\arctan(\lambda - \lambda_j), \tag{45}$$

which counts the number of flipped spins. In the thermodynamic limit, we can now define the density of states

$$\rho(\lambda) = \frac{1}{2\pi}\frac{d\Phi}{d\lambda}. \tag{46}$$

The second part of (45) can then be written as an integral:

$$\Phi(\lambda) = 2L\arctan(2\lambda) - 2\int_{-\infty}^{\infty} d\lambda' \rho(\lambda')\arctan(\lambda - \lambda'). \tag{47}$$

By differentiating this function, we can write the density of states as

$$2\pi\rho(\lambda) = \frac{4L}{1 + 4\lambda^2} - 2\int_{-\infty}^{\infty} d\lambda' \rho(\lambda')\frac{1}{1 + (\lambda - \lambda')^2}. \tag{48}$$

This is an integral equation and it can be solved by a Fourier transform (Appendix A). Thus we find

$$\rho(\lambda) = \frac{L}{2\cosh(\pi\lambda)}. \tag{49}$$

This density of state can be used to calculate the ground state energy, which is given by

$$\begin{aligned}
E_0 &= \frac{L|J|}{4} - |J|\sum_j \left[1 + \cos(k_j)\right] \\
&= \frac{L|J|}{4} - |J|\sum_j \frac{2}{1 + 4\lambda_j^2} \\
&= \frac{L|J|}{4} - |J|\int_{-\infty}^{\infty} d\lambda \rho(\lambda)\frac{2}{1 + 4\lambda^2} \\
&= L|J|\left[\frac{1}{4} - \log(2)\right].
\end{aligned} \tag{50}$$

The integral in the last equation is solved with Mathematica. This leads to a ground sate energy that is approximately $-0.44L|J|$. This is the exact ground state for an infinitely large system. We can compare this to the Néel state $|\uparrow\downarrow\uparrow\downarrow \dots \uparrow\downarrow\rangle$ which has energy $E_N = -0.25J$, we see that the true ground state of the system is much more complicated then the trivially thought of Néel state.

5   Next nearest neighbour interactions

We have just derived the exact ground state for a one dimensional chain with only nearest neighbour interaction, but is this enough? One can imagine that in real systems, the interactions reach further than just between nearest neighbours. The following step in the process of gaining a better model for a system, is adding next nearest neighbour interactions with an interaction J_2. We consider this interaction to be smaller than J_1 and of the same sign: $0 < J_2/J_1 < 1$. Looking at the problem through other methods can gain us some insight here. The Heisenberg Hamiltonian of a finite chain is just a matrix that can be solved for its eigenvalues using an exact diagonalization. For this I used Mathematica where I implemented a six site chain with spin-$\frac{1}{2}$ particles that interact through the spin matrices. This gives a $2^6 = 64$ by 64 matrix. The
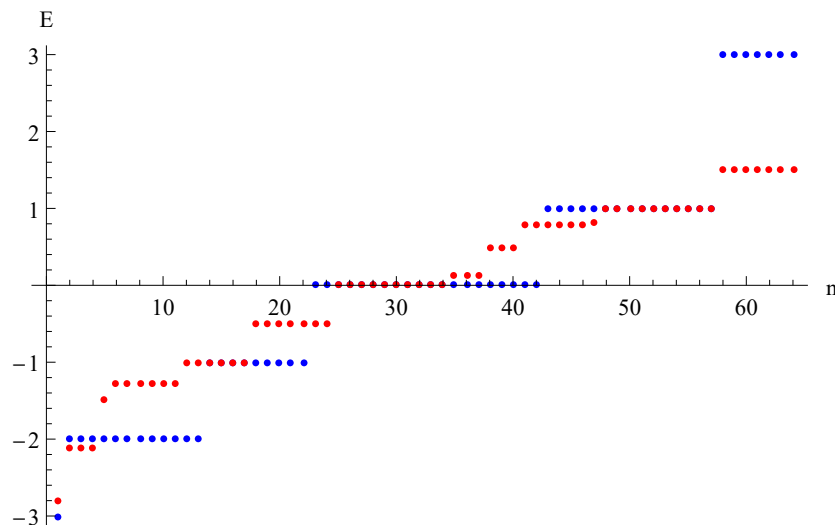
Figure 4: All of the energy eigenstates of a six site Heisenberg Hamiltonian (12), the red dots are the model with only nearest neighbour interactions $J_1 = 1, J_2 = 0$. The blue dots correspond to the energy states of the Heisenberg Hamiltonian (12) with J_1 and J_2 set to 1.

code used to get these results can be found in appendix (B). The numerical results for a chain interacting through the Heisenberg Hamiltonian (12) are shown in figure (4). A lot of degenerate energy states can be seen. This is because of spin multiplets arising from combining spins (as we have the singlet and the triplet configuration when there are just 2 spins). The figure shows that the ground state is not degenerate for these values of J_1 and J_2.

We can now vary the ratio between J_1 and J_2, figure (5) shows a numerical evaluation of the exact diagonalization for a spin-$\frac{1}{2}$ chain of six sites with nearest and next nearest neighbour interactions. The five lowest energies are plotted. This shows that the ground state is never degenerate, except at $J_2/J_1 = 0.5$. A model with this value for J_2, is known as the Majumdar-Ghosh model[6]. We will look into its special properties in the next section.

5.1 Majumdar-Ghosh model

A system with $J_2 = \frac{1}{2}J_1$ and an even number of spins, is known as the Majumdar-Ghosh chain[4]. A Hamiltonian of the form

$$H = \sum_i \left(S_i S_{i+1} + \frac{1}{2} S_i S_{i+2} + \frac{3}{8} \right), \tag{51}$$

can be rewritten as

$$H = \frac{1}{4} \sum_i \left[(S_i + S_{i+1} + S_{i+2})^2 - \frac{3}{4} \right]. \tag{52}$$

The total spin of three neighbouring sites can be constructed from $\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2} \oplus \frac{1}{2}$. Therefore, it can either be $\frac{1}{2}$ or $\frac{3}{2}$. For the ground state we want the total spin to be $\frac{1}{2}$, for the Hamiltonian above this value for the total spin gives exactly zero as energy. The total spin can only be $\frac{1}{2}$ when two of the spins form a singlet configuration together and the other spin does not interact with them. Since this has to be true for any position, the spins form singlet pairs. There are two configurations to form these singlet pairs:

$$\tag{53}$$

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[4]this derivation of the Majumdar-Ghosh chain is based on a paper Greiter[7]
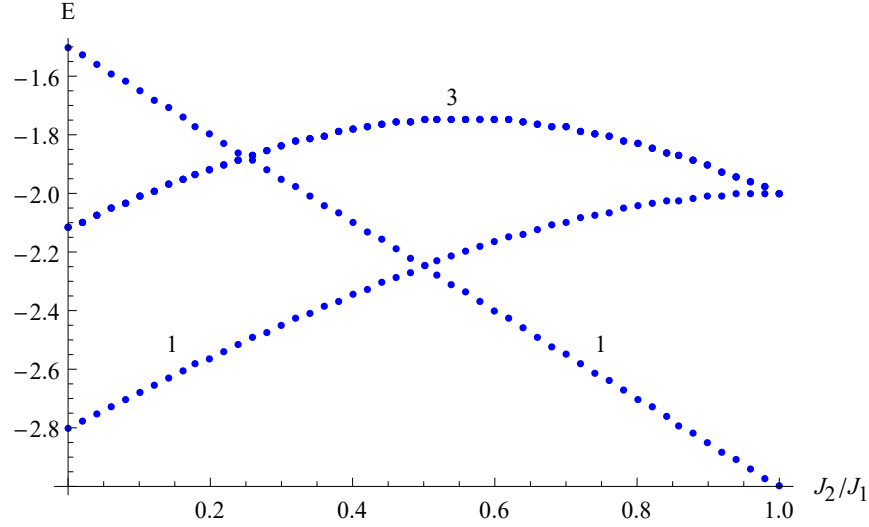
Figure 5: The five lowest energies of a six site spin-$\frac{1}{2}$ system with nearest and next nearest neighbour interactions J_1 and J_2. The ratio J_2/J_1 varies from 0 to 1. The numbers on the lines represent the number of degenerate states at that line. The ground state is only degenerate at $J_2/J_1 = 1/2$.

or

$$\tag{54}$$

where $\circ - \circ$ denotes a singlet pair. In the last state, the first and the last spin form a singlet configuration through periodic boundary conditions. As one can see, the condition that the number of spins should be even is vital for the way the ground state forms. If there is an odd number of spins, one spin at the end of chain would be left that cannot form a singlet pair with any of its neighbours, because all the other particles are already in pairs together. The states in (53) and (54) explain the twofold degeneracy of the ground state at $J_2/J_1 = 1/2$. Because of this special ground state configuration, we now have an exact ground state for the Heisenberg model with $J_2 = \frac{1}{2}J_1$. In the next subsection we will try to get a solution for general J_2 using the Bethe ansatz.

5.2   Bethe ansatz for next nearest neighbour interactions

We will now use the same approach as in the previous chapter to try to derive the Bethe equations in a system with a Hamiltonian that has also next nearest neighbour interactions (equation 12). We will first attempt this with a general next nearest neighbour interaction J_2.

The Hamiltonian can be written as

$$H = J_1 \sum_{i=1}^{N} \left[\frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + S_i^z S_{i+1}^z \right] + J_2 \sum_{i=1}^{N} \left[\frac{1}{2}\left(S_i^+ S_{i+2}^- + S_i^- S_{i+2}^+ \right) + S_i^z S_{i+2}^z \right]. \tag{55}$$

5.2.1   One spin flipped

As before, we start with the easiest case. We consider a spin chain with all spins up: $|F\rangle = |\uparrow ... \uparrow\rangle$. The same ansatz for the wave function as before (15) is used and the same periodic boundary conditions apply. The Schrödinger equation gives us

$$HS_n^-|F\rangle = J_1\left[\frac{1}{2}\big(S_{n+1}^-|F\rangle + S_{n-1}^-|F\rangle\big) + \frac{1}{4}(L-4)S_n^-|F\rangle\right] + J_2\left[\frac{1}{2}\big(S_{n+2}^-|F\rangle + S_{n-2}^-|F\rangle\big) + \frac{1}{4}(L-4)S_n^-|F\rangle\right],$$

$$H\psi(x) = J_1\left[\frac{1}{2}\big(\psi(x+1) + \psi(x-1)\big) + \frac{1}{4}(L-4)\psi(x)\right] + J_2\left[\frac{1}{2}\big(\psi(x+2) + \psi(x-2)\big) + \frac{1}{4}(L-4)\psi(x)\right],$$

$$H\psi(x) = J_1\left[\cos(k) + \frac{1}{4}(L-4)\right]\psi(x) + J_2\left[\cos(2k) + \frac{1}{4}(L-4)\right]\psi(x),$$

$$E = J_1\cos(k) + J_2\cos(2k) + (\frac{L}{4} - 1)(J_1 + J_2).$$

$$(56)$$

5.2.2 Two spins flipped

Now, the same wave function ansatz, as found in the previous chapter, (57) and the same periodic boundary conditions are used. Therefore

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

$$(57)$$

If the two particles are far apart, this wave function is an eigenstate of the Hamiltonian. As in the previous chapter, the situation changes when they are adjacent. Therefore, it follows that

$$\begin{aligned}
HS_n^- S_{n+1}^-|F\rangle &= J_1\sum_i\left[\frac{1}{2}\big(S_i^- S_{i+1}^+ + S_i^+ S_{i+1}^-\big) + S_i^z S_{i+1}^z\right]S_n^- S_{n+1}^-|F\rangle \\
&+ J_2\sum_i\left[\frac{1}{2}\big(S_i^- S_{i+2}^+ + S_i^+ S_{i+2}^-\big) + S_i^z S_{i+2}^z\right]S_n^- S_{n+1}^-|F\rangle \\
&= J_1\left[\frac{1}{2}\big(S_n^- S_{n+2}^- + S_{n-1}^- S_{n+1}^-\big) + \frac{1}{4}(L-4)S_n^- S_{n+1}^-\right]|F\rangle \\
&+ J_2\left[\frac{1}{2}\big(S_{n-2}^- S_{n+1}^- + A + B + S_n^- S_{n+3}^-\big) + \frac{1}{4}(L-8)S_n^- S_{n+1}^-\right]|F\rangle.
\end{aligned}$$

$$(58)$$

The J_1 part is the same as we have seen before. Our wave function does not immediately follow, but we can add a term that makes it possible to factor the wave function out. This added term would again need to be zero, which gives us an extra condition. With this condition, the Bethe equations can be determined.

The J_2 part should equal the case where two free spins are far away from each other. However, something goes wrong in the terms A and B. We will examine those terms in more detail below. (The arguments for B are along the same lines as those for A, so only A will be treated here).

$$\begin{aligned}
A &= S_{n-1}^- S_{n+1}^+ S_n^- S_{n+1}^- \\
&= S_{n-1}^- S_n^-.
\end{aligned}$$

$$(59)$$

The spin at position $x+1$ is moved two spaces to the left, making its position lower than that of the spin at position x. When we made the ansatz for the wave function (15), we restricted the elements in $\psi(x_1, x_2)$ to be ordered. The term A thus becomes

$$A|F\rangle = \psi(x-1, x).$$

$$(60)$$

In the case where x_1 and x_2 are far apart, this part of the Hamiltonian gives a term $\psi(x_1, x_2 - 2)$. We see that in our case, x_1 and x_2 are switched in the wave function, because one overtakes the other. Therefore, it is no longer possible to factor out $\psi(x, x+1)$, which makes this state an invalid eigenstate of the Hamiltonian. We could try the same approach as we did before, in which we added a term to factor the wave function out. Thereafter, this added term should equal zero again. We need to add terms that form cosines with the terms $\psi(x-2, x+1)$ and $\psi(x, x+3)$ from (58). To do so, we have to add $\psi(x+2, x+1)$ and $\psi(x, x-1)$. However, these wave functions cannot exist, because there second argument is smaller than their first argument. Thus

we see that it is impossible to factor $\psi(x, x + 1)$ out, which means that the ansatz we have made is wrong; it is not an eigenstate of the Hamiltonian. When we look at (58), it follows that the problematic part is found in the part of the equation that is proportional to J_2. If we set J_2 to zero, it is possible to solve the system, but there are no other values for J_2 for which this holds. This means that even for the special case with $J_2 = \frac{1}{2}J_1$ there is no clear way to solve this using the Bethe ansatz. We do, however, have an exact eigenstate for that value of J_2 that we got by using the approach by Majumdar-Ghosh in section (5.1)

6   Discussion

In this thesis we have tried to solve the Heisenberg model for nearest and next nearest neighbour interactions analytically. In order to do this, we have used the Bethe ansatz to make an ansatz for the wave function. We then required this wave function to be true for all distances and the arguments in this wave function to be ordered. The restriction that the wave function should be valid everywhere, combined with periodic boundary conditions, led us to relations between the different parameters from our ansatz, which are called the Bethe equations. When we tried to extend this approach by including next nearest neighbour interactions, it became clear that the method fails when the two flipped particles are adjacent. The arguments of the wave function had to be flipped, because of the restriction which states that the arguments should be ordered. Therefore, we see that our ansatz does not fully describe the system.

There may still be some other ways to get solutions for this system. One might try perturbation theory or try to solve the model with numerical methods like we did for a very small system in section (5)

A   Fourier transforms

With a Fourier transform we map a function $f(x)$ in x-space to a function $g(\omega)$ in ω-space. The Fourier transform is given by

$$g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{i\omega x}. \tag{61}$$

If in physics an equation is translationally invariant in its x-space it can be usefull to Fourier transform it to its ω-space. The wave description that is produced with this transform fits the symmetries of the system, which can make it easier to solve the equation. After solving the equation in ω-space we can use the inverse Fourier transform to get a solution for the original function. The inverse Fourier transform is given by

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega g(\omega) e^{-i\omega x}. \tag{62}$$

We can show that this is indeed the inverse Fourier transform by inserting the normal Fourier transform (61) into the inverse Fourier transform (62), this gives

$$\begin{aligned}
f(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} dx' f(x') e^{i\omega x} e^{-i\omega x'} \\
&= \int_{-\infty}^{\infty} dx' f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(x-x')} \right] \\
&= \int_{-\infty}^{\infty} dx' f(x') \delta(x - x') = f(x).
\end{aligned} \tag{63}$$

Here I used the definition of the Dirac delta function.
Some of integral equations will become easier to solve by first Fourier transforming them. We will try this approach with the density of states in the following subsection.

A.1   Density of states

We want to solve the following equation for $\rho(\lambda)$

$$2\pi\rho(\lambda) = \frac{4L}{1 + 4\lambda^2} - 2 \int_{-\infty}^{\infty} \frac{d\lambda'}{1 + (\lambda - \lambda')^2} \rho(\lambda'). \tag{64}$$

For notational convenience, we introduce two new functions

$$\begin{aligned}
f(\lambda) &= \frac{4L}{1 + 4\lambda^2}, \\
k(\lambda) &= \frac{1}{1 + \lambda^2}.
\end{aligned} \tag{65}$$

With these we can rewrite (64) as

$$\begin{aligned}
2\pi\rho(\lambda) &= f(\lambda) - 2 \int_{-\infty}^{\infty} k(\lambda - \lambda') \rho(\lambda') d\lambda' \\
&= f(\lambda) - 2g(\lambda),
\end{aligned} \tag{66}$$

where the integral is denoted by $g(\lambda)$:

$$g(\lambda) = \int_{-\infty}^{\infty} k(\lambda - \lambda') \rho(\lambda') d\lambda' \tag{67}$$

$g(\lambda)$ is a convolution integral, this means that its Fourier transform is a product of the Fourier transforms of the $k(\lambda)$ and $\rho(\lambda)$.

$$G(\omega) = \sqrt{2\pi}R(\omega)K(\omega), \tag{68}$$

where $G(\omega)$, $R(\omega)$ and $K(\omega)$ are the Fourier transforms of respectively $g(\lambda)$, $\rho(\lambda)$ and $k(\lambda)$

We now also use a Fourier transform on (66), which gives us

$$\begin{aligned} 2\pi R(\omega) &= F(\omega) - 2G(\omega) \\ &= F(\omega) - 2\sqrt{2\pi}R(\omega)K(\omega), \end{aligned} \tag{69}$$

where $F(\omega)$ is the Fourier transform of $f(\lambda)$. Solving for $R(\omega)$, gives

$$R(\omega) = \frac{F(\omega)}{2\pi + \sqrt{8\pi}K(\omega)}. \tag{70}$$

To find the density states, we first need to find the Fourier transforms for $f(\lambda)$ and $k(\lambda - \lambda')$ and then use an inverse Fourier transform on this equation for $R(\omega)$.

From this point on the problem is just solving integrals. I solved these integrals by using Mathematica. $F(\omega)$ and $K(\omega)$ can be computed by taking Fourier transforms, which are given by

$$\begin{aligned} F(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\lambda)e^{-i\lambda\omega} d\lambda \\ &= \frac{4L}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{1 + 4\lambda^2} e^{-i\lambda\omega} d\lambda \\ &= \sqrt{2\pi}Le^{-|\omega|/2}. \end{aligned} \tag{71}$$

$$\begin{aligned} K(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} k(\lambda)e^{-i\lambda\omega} d\lambda \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{1 + \lambda^2} e^{-i\lambda\omega} d\lambda \\ &= \sqrt{\frac{\pi}{2}}e^{-|\omega|}. \end{aligned} \tag{72}$$

Inserting these results into the equation for the Fourier transform of the density of states (70), gives

$$\begin{aligned} R(\omega) &= \frac{\sqrt{2\pi}Le^{-|\omega|/2}}{2\pi + 2\pi e^{-|\omega|}} \\ &= \frac{1}{\sqrt{2\pi}}L\frac{1}{e^{|\omega|/2} + e^{-|\omega|/2}} \\ &= \frac{L}{\sqrt{2\pi}}\frac{1}{2\cosh(|\omega|/2)}. \end{aligned} \tag{73}$$

Using the inverse Fourier transformation (which I again solved using Mathematica) gives us the density of states:

$$\begin{aligned} \rho(\lambda) &= \frac{L}{4\pi} \int_{-\infty}^{\infty} \frac{1}{\cosh(\omega/2)} e^{i\lambda\omega} d\omega \\ &= \frac{L}{2\cosh(\pi\lambda)}. \end{aligned} \tag{74}$$

B Mathematica code

```mathematica
spinx[i_, Nchain_] := 1/2 * Apply[KroneckerProduct, Table[If[n == i, PauliMatrix[1], IdentityMatrix[2]], {n, 1, Nchain}]];

spiny[i_, Nchain_] := 1/2 Apply[KroneckerProduct, Table[If[n == i, PauliMatrix[2], IdentityMatrix[2]], {n, 1, Nchain}]];

spinz[i_, Nchain_] := 1/2 Apply[KroneckerProduct, Table[If[n == i, PauliMatrix[3], IdentityMatrix[2]], {n, 1, Nchain}]];

XXZHamiltonian[Nc_, Δ_, J_, J2_] := J * Sum[spinx[i, Nc].spinx[Mod[i + 1, Nc, 1], Nc]
    + spiny[i, Nc].spiny[Mod[i + 1, Nc, 1], Nc] + Δ * spinz[i, Nc].spinz[Mod[i + 1, Nc, 1], Nc], {i, Nc}]
    + J2 * Sum[spinx[i, Nc].spinx[Mod[i + 2, Nc, 1], Nc] + spiny[i, Nc].spiny[Mod[i + 2, Nc, 1], Nc]
    + Δ * spinz[i, Nc].spinz[Mod[i + 2, Nc, 1], Nc], {i, Nc}];

XXZEnergies[Nc_, Δ_, J_, J2_] := Sort[N[Eigenvalues[XXZHamiltonian[Nc, Δ, J, J2]]]];

ListPlot[{XXZEnergies[6, 1, 1, 1], XXZEnergies[6, 1, 1, 0]}, AxesLabel → {"n", "E"},
 PlotLegends → {"Nearest and next nearest neighbour interactions", "Nearest neighbour interactions"},
 PlotStyle → {Blue, Red}]

ListPlot[Transpose[{xas, #}] & /@ {l[1], l[2], l[3], l[4], l[5]}, AxesLabel → {"J2/J1", "E"},
 PlotStyle → {Blue, Blue, Blue, Blue, Blue}]
```

References

[1] D. J. Griffiths, *Introduction to Electrodynamics* (Pearson, 2013), 4th ed.

[2] H. Bethe, *Zur theorie der metalle. i. eigenwerte und eigenfunktionen der linearen atomkette. (on the theory of metals k. eigenvalues and eigenfunctions of the linear atom chain).*

[3] M. P. Marder, *Condensed Matter Physics* (Wiley, 2010).

[4] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Harcourt, 1976).

[5] T. Giamarchi, *Quantum Physics in One Dimension* (Oxford science publications, 2003).

[6] C. K. Majumdar and D. Ghosh, *On next-nearest neighbour interaction in linear chain* (1969).

[7] M. Greiter, $s = 1$ *spin liquids: Broken discrete symmetries restored* (2002).