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Phase transitions in the transverse-field Ising model

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Abstract

Phase transitions in Ising models are a broadly studied subject within physics. In this thesis we will study the quantum mechanical transverse-field Ising model in order to determine analytical critical points for quantum phase transitions.

This will be done by introducing the concept of fermionic operators and the Jordan-Wigner transformation. Hereafter it is possible to Fourier transform the transverse Ising Hamiltonian and derive an exact eigenenergy spectrum. With these eigenenergies it is possible to derive the condition(s) for which a phase transition can occur. This is done by looking when the eigenenergy solutions are equal to zero. This causes the system to become unstable and thus indicates a point of phase transition.

Further in this thesis we will cover two different variations of the transverse-field Ising model which are the di-atomic transverse Ising chain and the frustrated Ising chain. The frustrated Ising chain will be a modification of the mono-atomic Ising chain where there is an extra interaction term introduced which will require an assumption of lowest order approximation of perturbation theory to solve analytically.

I would like to thank Lars Fritz for the great learning experience as a physicist within my bachelor thesis.

Contents

1 Introduction

In physics, phase transitions are a broadly studied field with relevant applications. The existence of these phase transitions reveals a lot of information about the physical properties of a system. It is important for systems like magnets, superconductors, etc.

Within this thesis we attempt to solve a variation of a well known statistical physics model called the Ising model, postulated in the early 20^{th} century. The model is a quantum mechanical version of the Ising model named the 'transverse-field Ising model' with the following Hamiltonian(1):

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

The main difference between the classical Ising model and this transverse-field Ising model lies in the fact that in the classical model the Hamiltonian depends on commuting terms while the transverse Hamiltonian introduces non-commuting Pauli spin matrices(2). This makes the problem quantum mechanical in nature. This difference thus requires a different approach to solve the transverse Hamiltonian which will be the aim of this thesis for different kinds of Ising chains in one dimension in combination with determining if quantum phase transitions occur in those chains.

The thesis is organized as follows: chapter 2 will introduce a way of expressing the transverse Ising Hamiltonian in terms of fermionic operators and cover the Jordan-Wigner transformation. This transformation will make certain transverse Ising chains in one dimension exactly solvable. In chapter 3 it will be shown how to solve the mono-atomic transverse 1D Ising chain (MTIC) Hamiltonian and how to derive the condition(s) for its quantum phase transitions. Chapter 4 and 5 cover a way of constructing and solving modifications of the MTIC. These two chapters also focus on the possible quantum phase transitions.

2 Fermionic language for the transverse Ising model

In order to solve the transverse Ising model in one dimension we start with reviewing a concept called second quantization. This concept is a formalism within quantum mechanics which allows to create and annihilate fermions locally thereby parameterizing a local Hilbert space of dimension two at each lattice site. This will be identified later with the local Hilbert space of a spin S=1/2 with the same dimensionality.

2.1 Fermionic operators

The set of fermionic operators $\{c_1, ..., c_n\}$ obeys the following commutation relations(1):

$$\{c_i, c_j\} = 0, \tag{2.1.1}$$

$$\{c_i^\dagger, c_j^\dagger\} = 0, \tag{2.1.2}$$

$$\{c_i, c_j^\dagger\} = \delta_{ij}. \tag{2.1.3}$$

Here the curly brackets indicate anti commutation relations meaning that $\{X, Y\} = XY + YX$ and the indices are the spatial labeling within the chain but could be any other quantum number.
These fermionic operators are the creation and annihilation operators mentioned earlier for the second quantization. The number states that these fermionic operators will work on are limited in the occupation of each state due to the Pauli exclusion principle. This principle states that there cannot be two fermions in the same quantum state. Because of this the number states will look like this:

$$|n_1, n_2, ..., n_j, ..., n_N\rangle, \tag{2.1.4}$$

where n_j is either 0 or 1 with $j \in \{1, .., N\}$ and the length of the chain is defined by N.
An example of the creation operator working on an arbitrary state looks the following(3):

$$\begin{aligned} c_i^\dagger|n_1, .., n_i, ...n_N\rangle &= (-1)^{\sum_{v=1}^{i-1} n_v}(1 - n_i)|n_1, .., 1_i, ..n_N\rangle \\ c_i|n_1, .., n_i, ...n_N\rangle &= (-1)^{\sum_{v=1}^{i-1} n_v} n_i|n_1, .., 0_i, ..n_N\rangle \end{aligned} \tag{2.1.5}$$

where we can see that if n_i = 0, $c_i^\dagger$ creates a fermion and when $n_i = 1$, $c_i^\dagger$ destroys the number state entirely. The annihilation operator does the inverse of the creation operator. From equation (2.1.5) we can immediately conclude that $c_i c_i = 0$ and $c_i^\dagger c_i^\dagger = 0$. The operator $c_i^\dagger c_i \in \{0, 1\}$ is the counting operator.

2.2 Jordan-Wigner transformation

The Hamiltonian of the transverse Ising chain contains Pauli matrices that are connected with raising and lowering operators according to(1):

$$\begin{aligned} \sigma_j^+ &= (\sigma_j^z + i\sigma_j^y)/2 \\ \sigma_j^- &= (\sigma_j^z - i\sigma_j^y)/2 \\ \sigma_j^x &= 2\sigma_j^+\sigma_j^- - 1. \end{aligned} \tag{2.2.1}$$

We see that the operators do satisfy (2.1.3), $\{\sigma_j^+, \sigma_j^-\} = 1$, but the Pauli matrices do commute on different sites, $[\sigma_j^+, \sigma_i^-] = 0$ with $i \neq j$. For fermionic operators they should anti commute like (2.1.1). So there is a slight modification needed to transform the Pauli operators into fermionic operators. This procedure is called the Jordan-Wigner transformation. We define therefore the following operators(1):

$$\begin{aligned} c_j^\dagger &\equiv \exp(i\pi \sum_{n=1}^{j-1} \sigma_n^+\sigma_n^-)\sigma_j^+ \\ c_j &\equiv \exp(-i\pi \sum_{n=1}^{j-1} \sigma_n^+\sigma_n^-)\sigma_j^-, \end{aligned} \tag{2.2.2}$$

with $c_j^\dagger c_j = \sigma_j^+\sigma_j^-$. These operators are the fermionic operators that will be used to solve the transverse Ising chain and satisfy the conditions given in equations (2.1.1)-(2.1.3).

The phase shift in front of the Pauli operators in (2.2.2) can be simplified a bit further by

$$\exp(\pm i\pi \sum_{n=1}^{j-1} \sigma_n^+\sigma_n^-) = \prod_{n=1}^{j-1} \exp(\pm i\pi\sigma_n^+\sigma_n^-) = \prod_{n=1}^{j-1} (1 - 2\sigma_n^+\sigma_n^-) \tag{2.2.3}$$

where in the last equality we made use of the fact that $\sigma_n^+\sigma_n^- \in \{0, 1\}$.

3 The mono-atomic transverse 1D Ising chain

In this chapter we solve the mono-atomic transverse one dimensional Ising chain. Figure (1) gives some intuition about the MTIC and the states that occur within it.

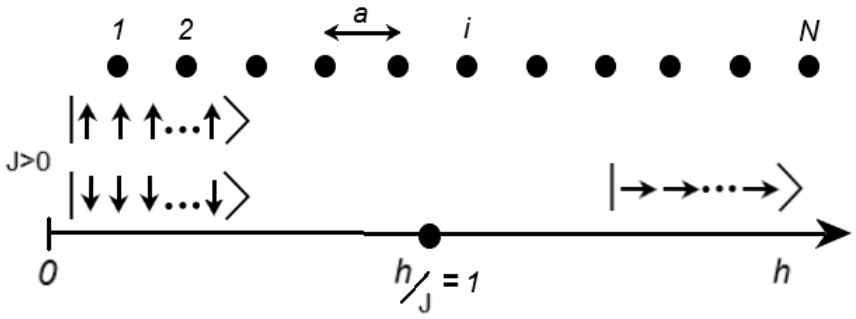

Figure 1: MTIC with ground states in different limits.

The upper chain in figure (1) indicates the N spin sites with lattice spacing a. The lower scale shows a phase diagram where at $h = 0$ we have the ferromagnetic ground state (anti-ferromagnetic is also valid for $J < 0$) and at some point for h we get the ground state aligned with the transverse field. The change in ground states with increasing h indicates that there is a critical point h for which a phase transition occurs.

3.1 Jordan-Wigner transform of MTIC

We start with our initial transverse Ising chain:

$$H = -J \sum_{j=1}^{N-1} \sigma_j^z \sigma_{j+1}^z - h \sum_{j=1}^{N} \sigma_j^x. \tag{3.1.1}$$

Now we are gonna apply the defined operators from (2.2.2) and the identities of (2.2.1). To begin we can write σ_j^z as $\sigma_j^z = \sigma_j^+ + \sigma_j^-$ which leads to:

$$\begin{aligned}
\sigma_j^z \sigma_{j+1}^z &= \prod_{n=1}^{j-1} (1 - 2c_n^\dagger c_n)(c_j^\dagger + c_j) \prod_{n=1}^{j} (1 - 2c_n^\dagger c_n)(c_{j+1}^\dagger + c_{j+1}) \\
&= \prod_{n=1}^{j-1} (1 - 2c_n^\dagger c_n)^2 (c_j^\dagger + c_j)(1 - 2c_j^\dagger c_j)(c_{j+1}^\dagger + c_{j+1}) \\
&= (c_j^\dagger + c_j)(1 - 2c_j^\dagger c_j)(c_{j+1}^\dagger + c_{j+1}) \\
&= (c_j^\dagger + c_j \cancel{- 2c_j^\dagger c_j^\dagger} c_j - 2c_j c_j^\dagger c_j)(c_{j+1}^\dagger + c_{j+1}) \\
&= (c_j^\dagger + (1 - 2c_j c_j^\dagger) c_j)(c_{j+1}^\dagger + c_{j+1}) \\
&= (c_j^\dagger + (1 - 2(1 - \cancel{c_j^\dagger c_j)) c_j})(c_{j+1}^\dagger + c_{j+1}) \\
&= (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})
\end{aligned} \tag{3.1.2}$$

Some comments on this derivation are that we made use of the fact that $c_j^\dagger c_j^\dagger = c_j c_j = 0$ in the fourth and sixth line respectively. In line six there was also made use of property (2.1.3) of the fermionic commutation relations.

For the last term in the Hamiltonian we can write σ_j^x as $\sigma_j^x = (\sigma_j^+ \sigma_j^- - \sigma_j^- \sigma_j^+)$ which transforms as follows:

$$\begin{aligned}
\sigma_j^x &= \prod_{n=1}^{j-1} (1 - 2c_j^\dagger c_j)^2 (c_j^\dagger c_j) - \prod_{n=1}^{j-1} (1 - 2c_j^\dagger c_j)^2 (c_j c_j^\dagger) \\
&= (c_j^\dagger c_j - c_j c_j^\dagger).
\end{aligned} \tag{3.1.3}$$

Combining both expression (3.1.2) and (3.1.3) leads to the new Hamiltonian in terms of fermionic operators:

$$H = -J \sum_{j=1}^{N-1} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) - h \sum_{j=1}^{N} (c_j^\dagger c_j - c_j c_j^\dagger). \tag{3.1.4}$$

3.2 Fourier transform of fermionic operators

We now want to transform the fermionic operators in (3.1.4) to Fourier space, but we need to make sure that the chain is periodic and that (2.1.1)-(2.1.3) are preserved by the Fourier transformation before we are allowed to do the transform.

To make the chain periodic we impose the following conditions:

$$\sigma^z_{N+1} = \sigma^z_1,\ \sigma^x_{N+1} = \sigma^x_1. \tag{3.2.1}$$

Because the elements of the chain are fermions it needs to be checked if there might arise a minus sign if we include the boundary term in the Hamiltonian in terms of fermionic operators.

$$\begin{aligned}
\sigma^z_N\sigma^z_{N+1} &= \sigma^z_N\sigma^z_1 \\
&= \prod_{k=1}^{N-1}(-1)^{c_k^\dagger c_k}(c_N^\dagger + c_N)(c_1^\dagger + c_1) \\
&= \prod_{k=1}^{N}(-1)^{c_k^\dagger c_k}((-1)^{c_N^\dagger c_N}c_N^\dagger + (-1)^{c_N^\dagger c_N}c_N)(c_1^\dagger + c_1) \\
&= (-1)^\beta((1-2c_N^\dagger c_N)c_N^\dagger + (1-\cancel{2c_N^\dagger c_N)c_N})(c_1^\dagger + c_1) \\
&= (-1)^\beta((1-2(1-\cancel{c_N c_N^\dagger)c_N^\dagger} + c_N)(c_1^\dagger + c_1) \\
&= (-1)^\beta(-c_N^\dagger + c_N)(c_1^\dagger + c_1) \\
&= (-1)^{\beta+1}(c_N^\dagger - c_N)(c_1^\dagger + c_1).
\end{aligned} \tag{3.2.2}$$

In this derivation $\beta = \sum_{k=1}^N c_k^\dagger c_k$ is the number of fermions in the chain. We see that depending on the amount of fermions the boundary conditions are periodic or anti periodic. If β is even we have anti periodic boundary conditions and if β is odd we have periodic boundary conditions. So the Hamiltonian for the (anti) periodic chain is:

$$H = -J\sum_{j=1}^{N-1}(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) \pm J(c_N^\dagger - c_N)(c_1^\dagger + c_1) - h\sum_{j=1}^{N}(c_j^\dagger c_j - c_j c_j^\dagger). \tag{3.2.3}$$

The last thing that needs to be shown before the Fourier transformation is whether or not the fermionic operators still obey the fermionic commutation relations after the Fourier transform. So we introduce the following inverse Fourier transform(1):

$$\tilde{c_k}^\dagger = \frac{1}{\sqrt{N}}\sum_j e^{-ikaj}c_j^\dagger. \tag{3.2.4}$$

From this we can apply (3.2.4) to (2.1.3) to get:

$$\begin{aligned}
\{\tilde{c_{j'}}, \tilde{c_k}^\dagger\} &= \tilde{c_{j'}}\tilde{c_k}^\dagger + \tilde{c_k}^\dagger\tilde{c_{j'}} \\
&= \frac{1}{N}\sum_n e^{ij'na}c_n \sum_j e^{-ikaj}c_j^\dagger + \frac{1}{N}\sum_j e^{-ikaj}c_j^\dagger \sum_n e^{ij'na}c_n \\
&= \frac{1}{N}\sum_{j,n} e^{ia(j'n-jk)}(c_n c_j^\dagger + c_j^\dagger c_n) \\
&= \frac{1}{N}\sum_{j,n} e^{ia(j'n-jk)}\delta_{j,n} \\
&= \frac{1}{N}\sum_j e^{iaj(j'-k)} \\
&= \delta_{j',k}.
\end{aligned} \tag{3.2.5}$$

We see that under Fourier transform (2.1.3) is still satisfied. The other two commutation relations are also satisfied by the fact that in line three of (3.2.5) instead of $c_n c_j^\dagger + c_j^\dagger c_n$ we have $c_n^\dagger c_j^\dagger + c_j^\dagger c_n^\dagger$ which is 0 by (2.1.2), which leads to $\{\tilde{c_{j'}}^\dagger, \tilde{c_k}^\dagger\}$= $\{\tilde{c_{j'}}, \tilde{c_k}\}$ = 0.

Since the fermionic commutation relations are conserved under Fourier transformation we can transform the Hamiltonian of the (anti) periodic chain to Fourier space.

3.3 Solution of MTIC

We start with the Hamiltonian of the periodic chain which is:

$$\begin{aligned}
H &= -J\sum_{j=1}^{N}(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) - h\sum_{j=1}^{N}(c_j^\dagger c_j - c_j c_j^\dagger) \\
&= -J\sum_{j=1}^{N}(c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger - c_j c_{j+1}) - h\sum_{j=1}^{N}(c_j^\dagger c_j - c_j c_j^\dagger).
\end{aligned} \tag{3.3.1}$$

Now the individual operators can be Fourier transformed as follows:

$$c_j^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{ikaj}\tilde{c_k}^\dagger, \tag{3.3.2}$$

where $\tilde{c_k}^\dagger$ is the new fermionic Fourier operator and a the lattice spacing between individual fermions. Now applying (3.3.2) on (3.3.1) leads to:

$$H = -\frac{J}{N}\sum_{j=1}^{N}\sum_{k,k'}(e^{-ik'a}e^{-ija(k+k')}\tilde{c_k}^\dagger\tilde{c_{k'}}^\dagger + e^{ik'a}e^{-ija(k-k')}\tilde{c_k}^\dagger\tilde{c_{k'}}$$

$$- e^{-ik'a}e^{ija(k-k')}\tilde{c_k}\tilde{c_{k'}}^\dagger - e^{ik'a}e^{ija(k+k')}\tilde{c_k}\tilde{c_{k'}}) - \frac{h}{N}\sum_{j=1}^{N}\sum_{k}(\tilde{c_k}^\dagger\tilde{c_k} - \tilde{c_k}\tilde{c_k}^\dagger),$$

useful identities are: $\sum_{j=1}^{N} e^{-ija(k+k')} = N\delta_{k,-k'}$ and $\sum_{j=1}^{N} e^{-ija(k-k')} = N\delta_{k,k'}$.

$$= -J\sum_{k}(e^{ika}\tilde{c_k}^\dagger\tilde{c}^\dagger_{-k} + e^{ika}\tilde{c_k}^\dagger\tilde{c_k} - e^{-ika}\tilde{c_k}\tilde{c_k}^\dagger - e^{-ika}\tilde{c_k}\tilde{c}_{-k}) - h\sum_{k}(\tilde{c_k}^\dagger\tilde{c_k} - \tilde{c_k}\tilde{c_k}^\dagger).$$

Now we can make use of the commutation relations to get the following simplifications:

- $\sum_k e^{ika}\tilde{c_k}^\dagger\tilde{c}^\dagger_{-k} = \frac{1}{2}\sum_k e^{ika}\tilde{c_k}^\dagger\tilde{c}^\dagger_{-k} + e^{-ika}\tilde{c}^\dagger_{-k}\tilde{c_k}^\dagger = \sum_k i\sin(ka)\tilde{c_k}^\dagger\tilde{c}^\dagger_{-k},$
- $\sum_k e^{-ika}\tilde{c_k}\tilde{c}_{-k} = \sum_k i\sin(ka)\tilde{c}_{-k}\tilde{c_k},$
- $\sum_k e^{ika}\tilde{c_k}^\dagger\tilde{c_k} - e^{-ika}\tilde{c_k}\tilde{c_k}^\dagger = \sum_k \cos(ka)(\tilde{c_k}^\dagger\tilde{c_k} - \tilde{c}_{-k}\tilde{c}^\dagger_{-k}).$

  $= -J\sum_k \cos(ka)(\tilde{c_k}^\dagger\tilde{c_k} - \tilde{c}_{-k}\tilde{c}^\dagger_{-k}) + i\sin(ka)(\tilde{c_k}^\dagger\tilde{c}^\dagger_{-k} - \tilde{c}_{-k}\tilde{c_k}) - h\sum_k(\tilde{c_k}^\dagger\tilde{c_k} - \tilde{c}_{-k}\tilde{c}^\dagger_{-k}),$

$$H = \sum_k \begin{pmatrix}\tilde{c}^\dagger_k & \tilde{c}_{-k}\end{pmatrix}\begin{pmatrix}-J\cos(ka) - h & -iJ\sin(ka)\\ iJ\sin(ka) & J\cos(ka) + h\end{pmatrix}\begin{pmatrix}\tilde{c_k}\\ \tilde{c}^\dagger_{-k}\end{pmatrix}. \tag{3.3.3}$$

This is the final form of the periodic chain Hamiltonian which can be diagonalized to determine the energy spectrum of the one dimensional transverse Ising chain. The anti periodic chain results in the same final Hamiltonian as the periodic one which we initially started with.

We now can determine the eigenvalues/eigenenergies of the matrix in (3.3.3), which are the following: $\mu_k = \pm\sqrt{h^2 + J^2 + 2Jh\cos(ka)}$.
In figure (2) the positive eigenvalues are shown over the allowed k values.

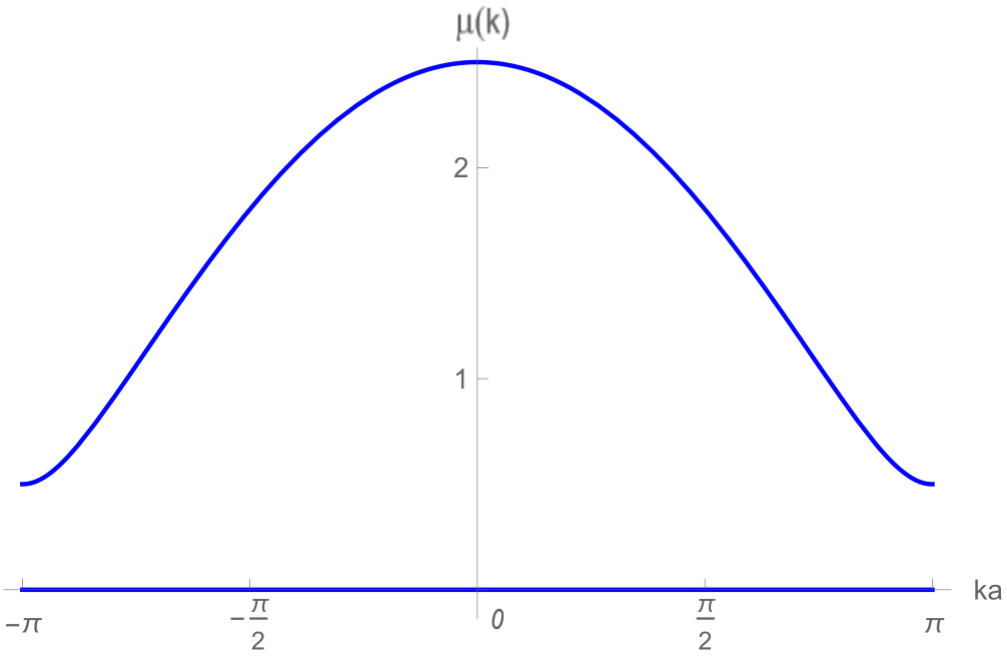

Figure 2: MTIC eigenenergies at J=1 and h=2.

In figure (2) we see the energy spectrum of the MTIC. The gap between the positive solution and zero energy indicate that there might be critical points where the spectrum is gapless and thus a phase transition occurs.

3.4 Phase transition in the mono-atomic transverse Ising chain

From the eigenvalues in the previous subsection we can compute whether or not the MTIC (mono-atomic transverse Ising chain) has a phase transition.
We can determine the condition(s) for a phase transition by taking the minimum energy of the eigenenergies and then looking at the point where the eigenenergy solutions are zero, i.e, the system becomes gapless.

So we start off with differentiating μ_k with respect to k to find the minimum energy:

$$\frac{d\mu_k}{dk}\Big|_{k_{ext}} = \frac{\pm Jh\sin(k_{ext}a)}{\sqrt{h^2+J^2+2Jh\cos(k_{ext}a)}} = 0,$$

which leads to $k_{ext} = \pm\frac{\pi j}{a}$ with j $\in \{0,1\}$ ('ext' means extrema) so:

$$\mu_{k,min} = \pm\sqrt{h^2+J^2-2Jh}.$$

Setting $\mu_{k,min}$ to zero for the positive eigenenergy gives $\mu_{k,min} = \sqrt{h^2 + J^2 - 2Jh} = 0$, which leads to:

$$\sqrt{(h-J)^2} = 0 \Rightarrow h = J.$$

The critical point $h = J$ is where the minimal energy in the system becomes zero.

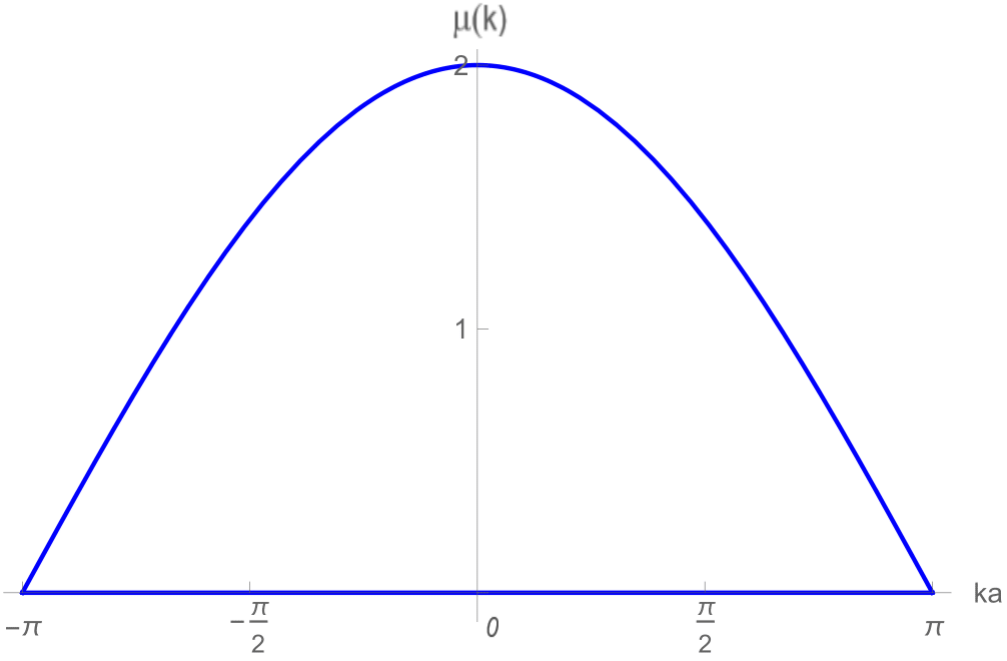

Figure 3: MTIC eigenenergies at the critical point J=1 and h=1.

In figure (3) it is visible that the energy spectrum has become gapless at the critical point in comparison to figure (2). We can therefore conclude that there is a phase transition for the one dimensional mono-atomic transverse Ising chain. This coincides with known literature(1).

4 The di-atomic transverse 1D Ising chain

In this chapter we can use the theory and methods explained in the previous chapters to solve a variation of the mono-atomic transverse Ising chain which will be the di-atomic transverse Ising chain (DTIC). This chain consists of two different fermionic operators that exist in a unit cell with internal and interconnected spin coupling. The following figure will give a schematic view of the chain.

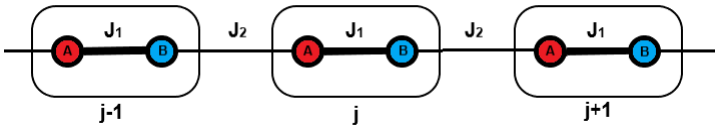

Figure 4: Di-atomic transverse Ising chain.

In figure (4) we can see the alterations in comparison to the MTIC. To begin with the chain is broken up into unit cells labelled with the index j. Within these unit cells we see the two different types of fermionic operators which couple via J_1. There is now also a coupling J_2 that couples the unit cells themselves. In the MTIC there was a lattice constant 'a' which indicated the spatial distance between the fermionic operator sites. For the di-atomic chain the lattice constant is defined as a'= 2a.

4.1 Change to the di-atomic Hamiltonian

In order to solve the Hamiltonian of the di-atomic chain we need to first know what that Hamiltonian is. In the mono-atomic chain we had the following Hamiltonian:

$$H_{mono} = -J\sum_{j=1}^{N}(c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j - c_{j+1}c_j) - h\sum_{j=1}^{N}(c_j^\dagger c_j - c_j c_j^\dagger). \quad (4.1.1)$$

Now in (4.1.1) we only have the coupling between neighbouring same species fermions. In the di-atomic chain however we have two different kinds of fermions which live in a unit cell. The di-atomic Hamiltonian will thus have a coupling energy between the fermions in the unit cell and between the unit cells themselves.

Therefore the following Hamiltonian applies for the di-atomic transverse Ising chain:

$$\begin{aligned} H_{di} = &\sum_j \{-J_1(a_j^\dagger b_j + b_j^\dagger a_j + a_j^\dagger b_j^\dagger + b_j a_j) - J_2(b_j^\dagger a_{j+1} + a_{j+1}^\dagger b_j + b_j^\dagger a_{j+1}^\dagger + a_{j+1}b_j)\} \\ &- h\sum_j (a_j^\dagger a_j - a_j a_j^\dagger + b_j^\dagger b_j - b_j b_j^\dagger). \end{aligned} \quad (4.1.2)$$

4.2 Di-atomic Hamiltonian solution

We can now use the theory introduced in the previous chapters to solve the di-atomic Hamiltonian. To start solving (4.1.2) we assume periodic boundary conditions which will not change the solutions of the chain just like with the mono-atomic chain.

$$
\begin{aligned}
H_{di} &= \sum_j -J_1(a_j^\dagger b_j + b_j^\dagger a_j + a_j^\dagger b_j^\dagger + b_j a_j) - J_2(b_j^\dagger a_{j+1} + a_{j+1}^\dagger b_j + b_j^\dagger a_{j+1}^\dagger + a_{j+1} b_j) \\
&\quad - h\sum_j (a_j^\dagger a_j - a_j a_j^\dagger + b_j^\dagger b_j - b_j b_j^\dagger) \\
&= \sum_k -\frac{J_1}{2}(A_k^\dagger B_k - B_{-k} A_{-k}^\dagger + B_k^\dagger A_k - A_{-k} B_{-k}^\dagger + A_k^\dagger B_{-k}^\dagger - B_k^\dagger A_{-k}^\dagger \\
&\quad + B_{-k} A_k - A_{-k} B_k) - \frac{J_2}{2}(B_k^\dagger A_k e^{ika'} - A_{-k} B_{-k}^\dagger e^{-ika'} + A_k^\dagger B_k e^{-ika'} \\
&\quad - B_{-k} A_{-k}^\dagger e^{ika'} + B_k^\dagger A_{-k}^\dagger e^{ika'} - A_k^\dagger B_{-k}^\dagger e^{-ika'} + A_{-k} B_k e^{-ika'} - B_{-k} A_k e^{ika'}) \\
&\quad - h\sum_k (A_k^\dagger A_k - A_{-k} A_{-k}^\dagger + B_k^\dagger B_k - B_{-k} B_{-k}^\dagger) \\
&= -\frac{1}{2}\sum_k \begin{pmatrix} A_k^\dagger \\ A_{-k} \\ B_k^\dagger \\ B_{-k} \end{pmatrix}^T \begin{pmatrix} 2h & 0 & \beta & \gamma \\ 0 & -2h & -\gamma & -\beta \\ \beta^\star & -\gamma^\star & 2h & 0 \\ \gamma^\star & -\beta^\star & 0 & -2h \end{pmatrix} \begin{pmatrix} A_k \\ A_{-k}^\dagger \\ B_k \\ B_{-k}^\dagger \end{pmatrix}.
\end{aligned}
\tag{4.2.1}
$$

In the last line of equation (4.2.1) we have derived the matrix for H_{di}, with $\beta = J_1 + J_2 e^{-ika'}$ and $\gamma = J_1 - J_2 e^{-ika'}$, from which we can determine the eigenvalues of the DTIC.

The eigenvalues are the following:

$$
\varepsilon_k = \pm\frac{1}{\sqrt{2}}\sqrt{2h^2 + (J_1^2 + J_2^2)(\pm)\sqrt{4h^2(J_1^2 + J_2^2) + (J_1^2 - J_2^2)^2 + 8h^2 J_1 J_2 \cos(ka')}}. \tag{4.2.2}
$$

The positive eigenvalues are shown in the figure below.

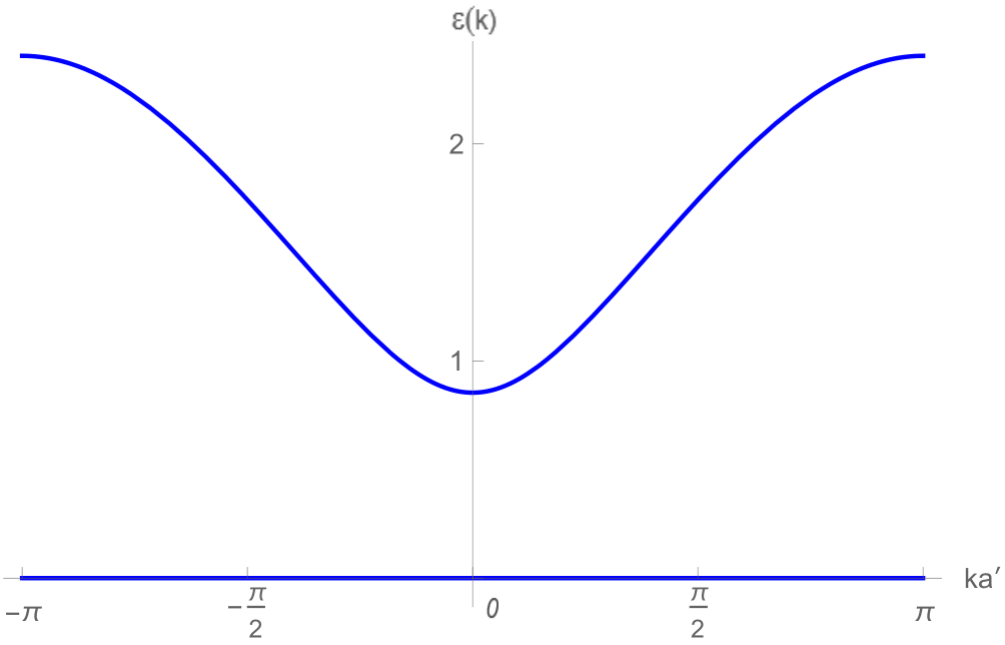

Figure 5: DTIC eigenenergies with J_1=1, J_2=4 and h=3.

In figure (5) we can see that there is a gap within the energy dispersion of the DTIC and zero energy. The existence of this gap indicates that there could be a critical point, just like with the MTIC, h where the energy spectrum is gapless so i.e. there is a phase transition in the system.

But first we need to check the validity of these eigenvalues. This can be checked by taking the limit $J_2 \to J_1$ to see if the eigenvalues of the mono-atomic chain come back from the di-atomic chain limit.

$$\lim_{J_2 \to J_1} \varepsilon_k = \pm \frac{1}{\sqrt{2}} \sqrt{2h^2 + 2J_1^2 + \sqrt{8h^2 J_1^2 + 8h^2 J_1^2 cos(ka')}}$$
$$= \pm \frac{1}{\sqrt{2}} \sqrt{2h^2 + 2J_1^2 + 4hJ_1 \sqrt{\frac{1 + \cos(ka')}{2}}}$$

We can use the trigonometric identity: $\sqrt{\frac{1 + \cos(ka')}{2}} = \cos(\frac{ka'}{2})$

$$= \pm \sqrt{h^2 + J_1^2 + 2hJ_1 \cos(\frac{ka'}{2})} = \pm \sqrt{h^2 + J_1^2 + 2hJ_1 \cos(ka)}. \tag{4.2.3}$$

In the last line we made use of the fact that a' = 2a. We see that in the limit $J_2 \to J_1$ it indeed holds that $\lim_{J_2 \to J_1} \varepsilon_k = \mu_k$. This gives a indication that the eigenvalues of (4.2.2) are valid for the di-atomic transverse Ising chain.

4.3 Phase transition in the di-atomic chain

Now we can do the same thing as for the mono-atomic chain to determine whether or not there is a phase transition. So we start by minimizing the eigenenergies from equation (4.2.2):

$$\frac{d\varepsilon_k}{dk}\Big|_{k_{ext}} = \frac{-a' h^2 J_1 J_2 \sin(k_{ext} a')}{\varepsilon_{k,ext} \sqrt{4h^2(J_1^2 + J_2^2) + (J_1^2 - J_2^2)^2 + 8h^2 J_1 J_2 \cos(k_{ext} a')}} = 0$$

This leads to $k_{ext} = \pm \frac{\pi j}{a'}$ with j $\in \{0, 1\}$. We can therefore express the minimum eigenenergies as follows:

$$\varepsilon_{k,min} = \pm \frac{1}{\sqrt{2}} \sqrt{2h^2 + (J_1^2 + J_2^2)(\pm) \sqrt{4h^2(J_1^2 + J_2^2) + (J_1^2 - J_2^2)^2 + 8h^2 J_1 J_2}}.$$
$$= \pm \frac{1}{\sqrt{2}} \sqrt{2h^2 + (J_1^2 + J_2^2)(\pm) \sqrt{4h^2(J_1 + J_2)^2 + (J_1^2 - J_2^2)^2}}$$

We can now equate $\varepsilon_{k,min}$ to zero to determine the condition(s) for phase transitions in the di-atomic chain if any exists.

$$\pm \frac{1}{\sqrt{2}}\sqrt{2h^2 + (J_1^2 + J_2^2)(\pm)\sqrt{4h^2(J_1 + J_2)^2 + (J_1^2 - J_2^2)^2}} = 0$$

$$\Rightarrow 2h^2 + (J_1^2 + J_2^2) = (\mp)\sqrt{4h^2(J_1 + J_2)^2 + (J_1^2 - J_2^2)^2}$$

$$\Rightarrow 4h^4 + (J_1^2 + J_2^2)^2 + 4h^2(J_1^2 + J_2^2) = 4h^2(J_1 + J_2)^2 + (J_1^2 - J_2^2)^2$$

$$\Rightarrow 4h^4 + 4h^2[(J_1^2 + J_2^2) - (J_1 + J_2)^2] + [(J_1^2 + J_2^2)^2 - (J_1^2 - J_2^2)^2] = 0$$

$$\Rightarrow 4h^4 - 8J_1J_2h^2 + 4J_1^2J_2^2 = 0.$$

Substituting x = h^2 leads to the following solution:

$$x = J_1J_2 \;\Rightarrow\; h = \pm\sqrt{J_1J_2}.$$

We see that there is indeed a phase transition occurring at $h = \pm\sqrt{J_1J_2}$.
However this solution holds true if both couplings are (anti-)ferromagnetic. If we take alternating coupling, i.e. $J_1 = -\alpha J_2$ with $\alpha \in \mathbb{R}$, then the derivation for $\varepsilon_{k,min}$ changes slightly. This alternating coupling results in $h = \pm\sqrt{-J_1J_2}$.

So for clarity we have the following conditions:

$$h = \begin{cases} \pm\sqrt{J_1J_2} & \text{for } J_1, J_2 > 0 \text{ or } J_1, J_2 < 0. \\ \pm\sqrt{-J_1J_2} & \text{for } J_1 > 0, J_2 < 0 \text{ or } J_1 < 0, J_2 > 0. \end{cases}$$

For different kinds of coupling we get a phase transition within the di-atomic transverse Ising chain. For the upper case we have that both the fermionic operators and the unit cells themselves couple (anti-)ferromagnetically and the lower case couples internally ferromagnetically and between unit cells anti-ferromagnetically or vice versa.

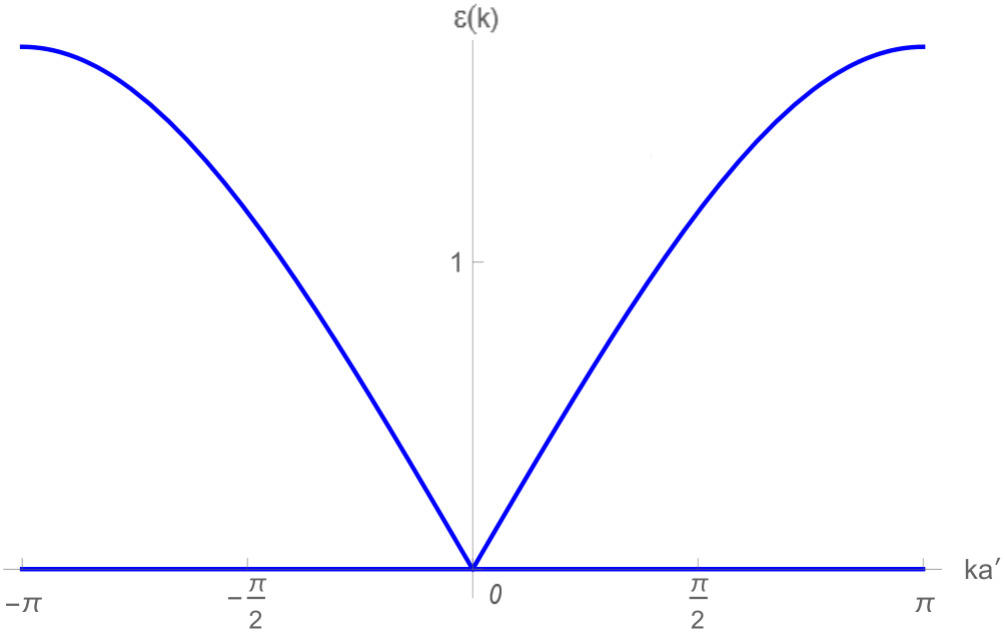

Figure 6: DTIC eigenvalues at J_1=1,$J_2 = 4$ and $h = 2$.

In figure (6) we see the DTIC eigenvalues at the critical point. The gap has vanished in comparison to figure (5).
Something else can be concluded by looking at the critical point h for the DTIC. In comparison with the critical point of the MTIC we can see that the difference between them is only up to a constant. So in essence we get that at the critical point $h_{MTIC} \propto h_{DTIC}$.

5 Frustrated Ising chain

In this chapter we will discuss the frustrated transverse Ising chain in one dimension. The frustrated chain is a modification of the mono-atomic chain where there is an extra interaction term added which is illustrated in the following figure.

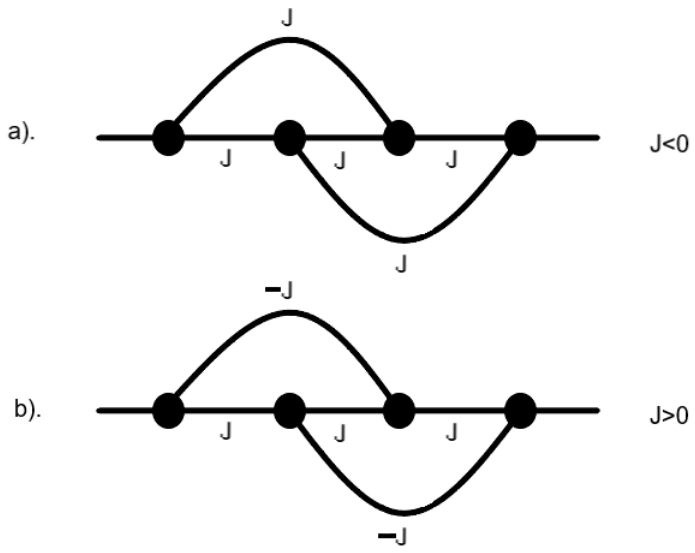

Figure 7: Frustrated chain a is with anti-ferromagnetic coupling and frustrated chain b is with ferromagnetic and anti-ferromagnetic coupling.

The reason it is called frustration can be best illustrated with an example from figure (7). In chain a there is anti-ferromagnetic coupling between the spin sites. In the case that the transverse field h is zero we should get the anti-ferromagnetic ground state back just like with the MTIC. We thus have that two neighbouring sites will anti-align with each other. However for the next neighbouring site it is impossible to anti-align with both of the neighbouring sites and is thus frustrated. This phenomenon is also referred to as geometrical frustration.
In figure (7) we see that there are multiple ways of creating frustration in the MTIC.

Because the frustrated chain is an extension of the MTIC it is relatively easy to compose the Hamiltonian:

$$H_{frustrated} = -J \sum_{j=1}^{N-1} \{\sigma_j^z \sigma_{j+1}^z - \sigma_j^z \sigma_{j+2}^z\} - h \sum_{j=1}^{N} \sigma_j^x. \tag{5.0.1}$$

In the way we have constructed (5.0.1) the chain has two types of coupling namely ferromagnetic coupling between $\sigma_j^z \sigma_{j+1}^z$ and anti-ferromagnetic coupling between $\sigma_j^z \sigma_{j+2}^z$ for $J > 0$ (figure (7)b).

However we could have made the frustrated Hamiltonian differently by only taking anti-ferromagnetic coupling between the spin sites, which is shown in figure (7)a, as follows:

$$H^{\star}_{frustrated} = J \sum_{j=1}^{N-1} \{\sigma_j^z \sigma_{j+1}^z + \sigma_j^z \sigma_{j+2}^z\} - h \sum_{j=1}^{N} \sigma_j^x \tag{5.0.2}$$

where we also have $J > 0$. We can thus compare the solutions of both Hamiltonian's to see if they differ from each other in any way.
With these new Hamiltonian's we can proceed with the same procedure as with the previous two chains to see if there are analytical solutions.

5.1 Frustrated chain Hamiltonian

We will start with equation (5.0.1) and apply a Jordan-Wigner transformation to the Pauli spin matrices. We could do the same calculations for (5.0.2) but that would be to cumbersome so in the end of this chapter the solution of that Hamiltonian will just be given.
As a side note we already know what H_{mono} is gonna be (which is part of the frustrated Hamiltonian's) so we can focus on the next nearest neighbour interaction term in $H_{frustrated}$.
So the coupling term $\sigma_j^z \sigma_{j+2}^z$ in terms of fermionic operators is given by:

$$\begin{aligned}
\sigma_j^z \sigma_{j+2}^z &= \prod_{n=1}^{j-1} (1 - 2c_n^\dagger c_n)(c_j^\dagger + c_j) \prod_{n=1}^{j+1} (1 - 2c_n^\dagger c_n)(c_{j+2}^\dagger + c_{j+2}) \\
&= \prod_{n=1}^{j-1} (1 - 2c_n^\dagger c_n)^2 (c_j^\dagger + c_j)(1 - 2c_j^\dagger c_j)(1 - 2c_{j+1}^\dagger c_{j+1})(c_{j+2}^\dagger + c_{j+2}) \\
&= (c_j^\dagger + c_j)(1 - 2c_j^\dagger c_j)(1 - 2c_{j+1}^\dagger c_{j+1})(c_{j+2}^\dagger + c_{j+2}) \\
&= (c_j^\dagger - c_j)(c_{j+2}^\dagger + c_{j+2}) - 2(c_j^\dagger - c_j)(c_{j+1}^\dagger c_{j+1})(c_{j+2}^\dagger + c_{j+2}).
\end{aligned} \tag{5.1.1}$$

We see that there is an extra term in comparison to (3.1.2).
The way $\sigma_j^z\sigma_{j+2}^z$ is composed does not lead to an analytical solution for $H_{frustrated}$ because the last term includes fermionic operator products higher than two. This means that we need to make an assumption for (5.1.1) to continue.

The extra interaction term in (5.1.1) indicates a perturbation of a otherwise analytically solvable Hamiltonian. We approximate $\sigma_j^z\sigma_{j+2}^z$ to lowest order, i.e. assume that the extra interaction term equals zero. This will change (5.1.1) to:

$$\sigma_j^z\sigma_{j+2}^z = (c_j^\dagger - c_j)(c_{j+2}^\dagger + c_{j+2}).$$

So from this we can write $H_{frustrated}$ in fermionic operators as:

$$H_{frustrated} = -J\sum_{j=1}^{N}\{(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) - (c_j^\dagger - c_j)(c_{j+2}^\dagger + c_{j+2})\} - h\sum_{j=1}^{N}(c_j^\dagger c_j - c_j c_j^\dagger). \tag{5.1.2}$$

With this we can apply the Fourier transformation in the same way we did in the chapter about the MTIC. This will result in the the frustrated Hamiltonian in matrix form as follows:

$$H_{frus} = \sum_k \begin{pmatrix}\tilde{c_k}^\dagger & \tilde{c_{-k}}\end{pmatrix}\begin{pmatrix}-J(\cos(ka)-\cos(2ka))-h & -iJ(\sin(ka)-\sin(2ka)) \\ iJ(\sin(ka)-\sin(2ka)) & J(\cos(ka)-\cos(2ka))+h\end{pmatrix}\begin{pmatrix}\tilde{c_k} \\ \tilde{c_{-k}}^\dagger\end{pmatrix}. \tag{5.1.3}$$

We can now take a look at the eigenenergies that are associated with this matrix and the matrix that arises from (5.0.2) which are:

$$E_k = \pm\sqrt{h^2 + 2hJ(\cos(ka)-\cos(2ka)) + 2J^2(1-\cos(ka))}, \tag{5.1.4}$$

$$E_k^\star = \pm\sqrt{h^2 - 2hJ(\cos(ka)+\cos(2ka)) + 2J^2(1+\cos(ka))}. \tag{5.1.5}$$

Equation (5.1.4) belongs to (5.0.1) and equation (5.1.5) to (5.0.2).

Initially looking at the two energy spectra we can see that they are different from each other with respect to some $\pm$ signs. However we cannot conclude just yet that they will not produce the same phase transition(s), if they exist.

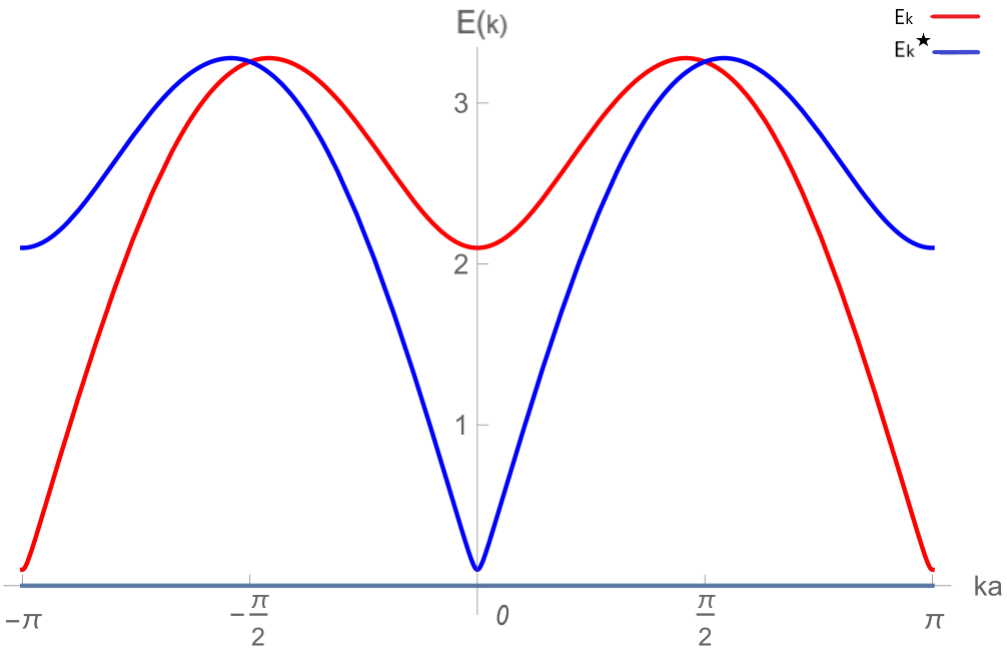

Figure 8: Frustrated eigenenergies at J=1 and h=2.1.

In figure (8) it is shown how both versions of the frustrated chains disperse in relation to the eigenenergies of the system. This can be compared with figure (2) to see the difference in eigenenergies when an extra interaction term is introduced in the transverse Ising model. Just like with the MTIC and DTIC we have a gap between the positive eigenenergies and zero thus a phase transition can occur.

5.2 Phase transition in frustrated chain

With the eigenenergies for the frustrated transverse Ising chains we can see if there are phase transitions in these particular kind of chains. We minimize the positive eigenenergies with respect to k in E_k.

$$\begin{aligned}
\frac{dE_k}{dk}\Big|_{k_{ext}} &= \frac{1}{2E_{k,ext}}(2ahJ(-\sin(k_{ext}a) + 2\sin(2k_{ext}a)) + 2J^2a\sin(k_{ext}a)) = 0 \\
&\Rightarrow 2ahJ(-\sin(k_{ext}a) + 2\sin(2k_{ext}a)) + 2J^2a\sin(k_{ext}a)) = 0 \\
&\Rightarrow \sin(k_{ext}a)(J^2 - hJ + 4hJ\cos(k_{ext}a)) = 0 \\
&\Rightarrow \sin(k_{ext}a) = 0 \,\text{and}\, J^2 - hJ + 4hJ\cos(k_{ext}a) = 0.
\end{aligned}$$

From this we get $k_{ext} = \pm\frac{\pi j}{a}$ with $j \in \{0, 1\}$, which holds also true for $E_k^\star$. The other solution for k leads to non analytical results so the mentioned values for k will suffice for now.
If we plug k_{ext} into (5.1.4) and (5.1.5) we can get the global minimum in E_k and $E_k^\star$ from which we can derive the condition(s) for a phase transition to occur.

$$E_{k,min} = \pm\sqrt{h^2 - 4hJ + 4J^2}, \text{ at } k = \pm\pi.$$
$$E^\star_{k,min} = \pm\sqrt{h^2 - 4hJ + 4J^2}, \text{ at } k = 0.$$

From this it follows that a phase transition occurs at $h = 2J$ for both ways of designing the frustrated chain in the beginning of the chapter. We can thus conclude that the way we make the chain frustrated in this case doesn't influence the critical points of phase transition.

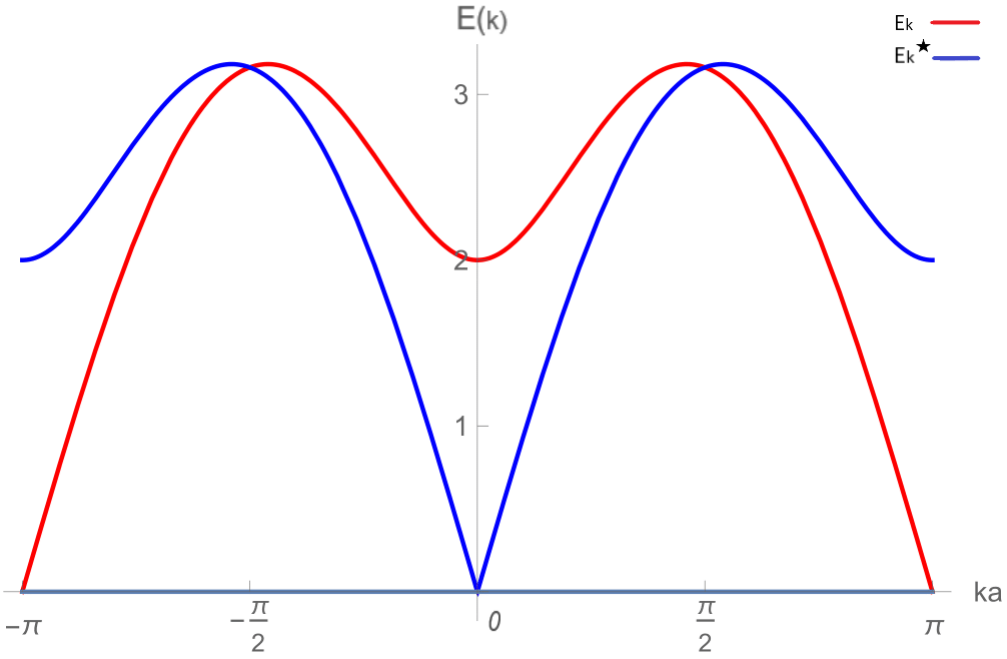

Figure 9: Frustrated chain at $J = 1$ and $h = 2$.

In figure (9) we see that the eigenenergies of both frustrated chains are gapless at the critical point and thus a phase transition occurs.

6 Conclusion

The main findings of this thesis are summarized as follows. The discussed Jordan-Wigner transformation applied to the MTIC resulted in a exact solution of the critical point $h = J$ for a quantum phase transition.

We found that the MTIC can be modified to a DTIC (and possibly more kinds of fermionic operators in a unit cell) or a frustrated Ising chain. The DTIC eigenenergies transform back to the MTIC eigenenergies in the limit $J_2 \Rightarrow J_1$ as shown in (4.2.3). From these modified chains we derived that both the di-atomic transverse Ising chain and the frustrated transverse Ising chain have quantum phase transitions at finite value's for the transverse field.

- $\mathrm{h}_{di} = \begin{cases} \pm\sqrt{J_1 J_2} & \text{for } J_1, J_2 > 0 \text{ or } J_1, J_2 < 0. \\ \pm\sqrt{-J_1 J_2} & \text{for } J_1 > 0, J_2 < 0 \text{ or } J_1 < 0, J_2 > 0. \end{cases}$
- $h_{frus} = 2J.$

7 Discussion and outlook

It is important within physics to analyze if we made any assumptions in our calculations to arrive at the final results and if these assumptions are reasonable to make. By doing this we can make sure that we are aware of the limitations of our results and where we can improve upon as it comes to making better assumptions.

For the mono/di-atomic transverse Ising chain there were no assumptions made in the derivations and thus the solutions are exact theoretical results. We saw already that the critical point for the MTIC agreed with existing theory which gives credence to the methodology used. To see if there is a quantum phase transition in the DTIC it could be verified by calculating the critical point of the DTIC with numerical calculations for a small number of sites and then compare it to our exact results.

For the frustrated Ising chain in chapter 5 it is already mentioned that an assumption was needed to get an analytical solution. This assumption was that we approximated the next nearest neighbour term in the frustrated Hamiltonian to lowest order. Since we do not posses theoretical/numerical values for the critical points of this frustrated Ising chain to compare to ours it is hard to judge the credibility of this assumption. We can imagine however that this approximation could be rather crude and improvements could be made. A different approach could be to apply mean field theory or higher order perturbation theory. This could lead to better approximations and solutions if it turns out that ours was not very accurate.

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