Excitation energies of the ordered long-range transverse field Ising chain

Bachelorarbeit

von

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Abstract

In this work, the low-energy behaviour of the ferromagnetic long-range transverse field Ising chain at zero temperature is investigated. Firstly, analytic expressions for the eigenenergies of the long-range Ising term are derived. They reveal a change of the nature of the elementary low-energy excitation from the topological single-domain wall excitation to the trivial spin-flip excitation if the long-range character of the Ising interaction is enhanced. This is different in the antiferromagnetic case. By applying a low-field expansion to the long-range Ising term it is shown that this crossover remains and is linked to a different character of the phase transition of the model from the ordered to the polarized phase. The critical values of the perturbation parameter at the phase transition stand in good agreement with the results obtained in the high-field limit of this model using linked cluster expansions. The comparison also suggests that the characteristic of the system in the crossover region lies in between the nearest-neighbour and the mean-field universality class. Additionally, a comparison with numerical data of the low-field approach is made showing as well a good accordance to the analytic expressions of the perturbative excitation energies.
Erklärung

Hiermit versichere ich, dass ich die vorliegende Bachelorarbeit mit dem Titel "Excitation energies of the ordered long-range Ising chain" ohne die Hilfe Dritter und nur unter Benutzung der angegebenen Quellen und Hilfsmittel angefertigt habe. Wörtliche und inhaltliche Übernahmen aus den Quellen sind als solche kenntlich gemacht. Diese Arbeit wurde in gleicher oder ähnlicher Form noch keiner anderen Prüfungsbehörde vorgelegt.

Erlangen, den 5. März 2019
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1 Introduction

Strongly interacting systems are a popular topic in the contemporary research on quantum matter. For example, they are used to model Coulomb interaction between charged particles as well as correlated spins in quantum magnets like so-called spin-ice materials [1]. Furthermore, in the enquiry towards reliable hardware for quantum computers, ensembles of several hundred trapped laser-cooled Be$^+$ ions that can be equipped with a tunable long-range interaction have been investigated [2]. The experimental work has proved to be able to induce an algebraically decaying interaction between the valence-electron spin states of each ion by the use of optical dipole-force laser beams. This setup enables basic scientific research in the field of low-temperature long-range interacting quantum systems.

In the theoretical field of study, the paradigmatic model is the long-range transverse field Ising model (lrTFIM). Proposed by E. Ising [3] in 1925, the Ising model is the simplest one to describe interacting spins on a lattice. The fundamental properties of the nearest-neighbour interacting Ising models are used to characterise an universality class of phase transitions in statistical physics. The simplest non-trivial phase transition at zero temperature arises in the one dimensional nearest-neighbour TFIM

$$H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x,$$

in which $J$ denotes the coupling constant and $h$ the strength of the transverse field. Due to the self-duality of this model (Sec. 2.1) the system undergoes a phase transition at $J = h$ from a $\mathbb{Z}_2$ symmetry-broken ‘ordered phase’ for $J > h$ to a ‘polarized phase’ for $J < h$ [4].

The aim of this work is to extend the one-dimensional nearest-neighbour Ising chain by an algebraically decaying long-range interaction and study its behaviour by considering the eigenenergies of the pure long-range Hamiltonian (Sec. 3) as well as the entire lrTFIM (Sec. 4). It will be seen that the value of $h/J$ at the phase transition will shift as the long-range interaction is turned on. The focus will lie on the ferromagnetic case where $J > 0$. However, the starting point for studying strongly frustrated antiferromagnetic systems will be made by also giving exact expressions for the antiferromagnetic Ising eigenenergies (Sec. 3.6).

Since the long-range interaction induces infinitely many different spin couplings, it is quite complicated to approach the model numerically. However, recent research has revealed suitable strategies to tackle long-range interactions with linked-cluster expansions (LCE) in the thermodynamic limit [5]. In this approach, the equidistant spectrum of the transverse field term is exploited to apply perturbative continuous transformations where the long-range Ising term is treated as the perturbation to the system. Figure 1.1 shows the results of the LCE for the ferromagnetic case.
Figure 1.1: Results for the critical parameter $\lambda_c = J_c/2h_c$ and the critical exponents $z\nu$ at the lrTFIM phase transition as a function of the coupling strength $\alpha$. The data corresponds to an extension of LCE with Makrow-chain Monte-Carlo methods (LCE/MCMC) in the high-field limit from Ref. [6] and data from exact diagonalization (ED) from Ref. [7].

Here, $\lambda := J/2h$ in the Hamiltonian

$$H = -\frac{1}{2} \sum_j \sigma_j^z - \lambda \sum_{i \neq j} \frac{1}{|i-j|^\alpha} \sigma_i^x \sigma_j^x. \tag{1.2}$$

It is seen that the values of the interaction exponent $\alpha$ changes the system’s behaviour from a mean-field criticality to a nearest-neighbour universality class, whereby passing an intermediate region, where the critical exponents $z\nu$ shift apparently continuously between the two universality classes. To get more insight into this transitional region of $5/3 < \alpha < 3$ [8] it seems reasonable to study the system directly in the $\mathbb{Z}_2$ symmetry-broken, ‘ordered’ phase and perturb it with a small transverse field.

Work in this direction has already been done by L. Vanderstraeten and M. van Damme in Ref. [9] using variational matrix product state techniques. In the framework of a quasiparticle ansatz the gaps of excitations of the long-range interacting spin chain have been calculated.
Fig. 1.2 shows the results within a region of $\alpha$ that corresponds to the transition region of Fig. 1.1. Here, the 'topological' excitation denotes an excited state with one domain wall between two symmetry-broken ground-state spin configurations. In comparison to the 'trivial' excitation corresponding to a single spin flip in the ground-state configuration, the topological excitation requires a large deformation of the ground state that changes the topological character of the chain. This topological state can only be reached in infinite order [10]. The data is gained from a perturbation of the Ising energies with a low transverse field where the perturbation parameter is defined as $\lambda := h/J$. A conversion to the $\lambda$ from the high-field limit can be made with $\lambda_{\text{high}} = 1/2\lambda_{\text{low}}$. The intersections of the gaps of the two lowest excitations for $\alpha \approx 2.3 - 2.4$ fundamentally change the nature of the low-energy excitation of the long-range Ising chain. This suggest a change in the characteristics of the phase transition in this $\alpha$-region which can be associated with the varying of the critical exponents $z\nu$ in the high-field limit.

The aim of this thesis is to gain further insight into the low-$\alpha$ region of the lrTFIM. As a first step, an iterative scheme for calculating the exact eigenenergies of the lrIM will be presented (Sec. 3). Furthermore, these expressions will be applied to conduct perturbation theory in $\lambda = h/J$ (Sec. 4). Finally, the results will be compared with the numerical data from the ordered phase [9] as well as with the data from the high-field limit LCE [6].
2 Transverse Field Ising Model

As already indicated in the previous section, the simplest model to describe ferromagnetism is the Ising model. It assumes that the ferromagnet can be subdivided into microscopic molecular magnets each of which carrying a magnetic moment that is able to interact with any other molecular magnet and can also be coupled to an external magnetic field. The magnetic moment itself arises from the intrinsic angular momentum (spin) of electrons in the inner unfilled shells of the atomic orbitals constituting the magnetic solid. For a ferromagnet the energy of the system is minimal if all spins are pointing in the same direction, whereas for an antiferromagnet the coupling between the spins works such that an antiparallel orientation between neighbouring spins is energetically favourable. The Ising model is a simple approximation of such a magnetic solid which fixes the position of each spin on a 1-, 2- or 3-dimensional lattice and restricts the orientation of each spin to one spatial axis [3].

For this work a 1D Ising spin chain with long-range interaction is considered. The spins sit on fixed sites and are coupled with the same strength with the neighbours to the left and right. In the following we focus on the thermodynamic limit of $N \to \infty$, $N$ denoting the number of spins. The interaction between pairs of spins is defined to decay algebraically $\propto 1/|\delta|^{\alpha}$, where $\delta = i - j$ denotes the distance between the two spins at site $i$ and site $j$. The parameter $\alpha$ denotes the long-range interaction constant. For $\alpha \to \infty$ the interaction energy of any two spins with distance $\delta > 1$ vanishes (nearest-neighbour model). The other limiting case is an ultra long-range interaction for $\alpha \to 1$ in the ferromagnetic case and an all-to-all coupling for $\alpha \to 0$ in the antiferromagnetic case.

Restricting the spins to the $z$-axis, hence representing them with $\sigma^z$-Pauli-matrices, the Hamiltonian of the system becomes

$$H = -J \sum_{i, \delta > 0} \frac{1}{\delta^{\alpha}} \sigma^z_i \sigma^z_{i+\delta},$$

(2.1)

where $J$ denotes the coupling constant. In order to prevent double counting of interaction distances $\delta$ in the sum over the chain, $\delta > 0$ is set. For $J > 0$ the system is ferromagnetic and its energy is lowered for parallel orientation of the spins at site $i$ and $i + \delta$ and increased for antiparallel orientation. $J < 0$ leads to opposite signs of the systems’ energy, increasing/decreasing it for parallel/antiparallel orientated spins, describing an antiferromagnetic system.

The ground state of this so-called Ising term (Eq. (2.1)) is a chain with all spins pointing in the same direction (ferromagnetic case), respectively an alternating spin orientation (antiferromagnetic case). Since the Ising term exhibits a $\mathbb{Z}_2$-symmetry with regard to the spin orientation either along ($\uparrow$) or in negative ($\downarrow$) $z$-direction, the ground state of Eq. (2.1) is 2-fold degenerate. Any excitation of the ground state leads to spin-flips increasing the energy of the system [10].
An exact expression for the eigenenergies of this Hamiltonian will be given in Sec. 3. In order to excite the system towards a higher energy a transversely orientated magnetic field with magnitude $h$ is applied in $x$-direction such that

$$H = -J \sum_{i,\delta \geq 0} \frac{1}{\delta} \sigma_i^z \sigma_{i+\delta}^z - h \sum_i \sigma_i^x.$$  \hspace{1cm} (2.2)

Rescaling Eq. (2.2) with the coupling constant gives

$$H = - \sum_{i,\delta \geq 0} \frac{1}{\delta} \sigma_i^z \sigma_{i+\delta}^z - \lambda \sum_i \sigma_i^x.$$  \hspace{1cm} (2.3)

with $H := H/J$, $\lambda := h/J$. As already seen in Sec. 1 this model is an extension of the nearest-neighbour TFIM at temperature $T = 0$ (Eq. (1.1)). The dynamics of the strongly correlated spin configuration comes solely from the application of the transverse field $h$ which induces non-local quantum fluctuations of the excitations along the chain. To study how the quantum fluctuations affect the behaviour of the system the transverse field term (which will be denoted with $V$) will be treated as a perturbation to the Ising term in Eq. (2.1) [4].

In the following, a useful transformation of the Hamiltonian in Eq. (2.3) will be performed to obtain a form that is feasible for perturbation theory.

2.1 Transformation to the dual lattice

With the Pauli matrices $\sigma_i^z$ and $\sigma_i^x$ the Hamilton operator in Eq. (2.3) is represented in terms of the fixed spin sites of the chain. However, it is suitable to exploit the $\mathbb{Z}_2$-symmetry of the system and transform it onto its dual lattice which can be represented by the interstitial sites $\nu := i - 1/2$ located between the actual spins at sites $i - 1$ and $i$. The advantage of this transformation is that each interstitial site can now be associated with the existence (indicated with 1) or absence (indicated with 0) of an excitation denoting a parallel or antiparallel orientation of the two spins edging the interstice. In the following, an antiparallel orientation of two neighbouring spins at sites $i - 1$ and $i$ will also be referred to as a domain wall at site $\nu$.

![Figure 2.1: Dual transformation of a state with two domain walls (in red): (Un)filled boxes indicate (in)existence of an excitation/domain wall at the respective site.](image)

Figure 2.1 shows the transition from the actual spin chain (labelled with $i$) towards the dual
lattice with domain walls at interstices labelled with \( \nu \). In bra-ket notation this corresponds to

\[
|... \uparrow\uparrow\uparrow\uparrow ... \rangle, |... \downarrow\downarrow\downarrow\downarrow ... \rangle \equiv |...00... \rangle \quad \text{(2.4)}
\]

\[
|... \uparrow\uparrow\downarrow\downarrow ... \rangle, |... \downarrow\downarrow\uparrow\uparrow ... \rangle \equiv |...010... \rangle \quad \text{(2.5)}
\]

\[
|... \uparrow\downarrow\uparrow\uparrow ... \rangle, |... \downarrow\uparrow\downarrow\downarrow ... \rangle \equiv |...0110... \rangle \quad \text{(2.6)}
\]

In the following these Fock states (i.e. the tensor product state of all sites in the chain) are labelled such that the excited sites entailing a domain wall (\( \equiv |1 \rangle \)) are indicated via their site number (e.g. \( |\nu, \nu + 1 \rangle \) resembles a state with an excitation at site \( \nu \) and \( \nu + 1 \) while any other site stays unexcited in state \( |0 \rangle \)).

Introducing Pauli-matrices \( \tau^z_\nu, \tau^x_\nu \) for the interstitial sites Eq. (2.4) - (2.6) suggest the transformation

\[
\tau^z_\nu = \tau^z_{i+1/2} = \sigma_i^z \sigma_{i+1}^z \quad \text{(2.7)}
\]

\[
\tau^x_\nu \tau^x_{\nu+1} = \tau^x_{i-1/2} \tau^x_{i+1/2} = \sigma_i^x \quad \text{(2.8)}
\]

Inserting Eq. (2.7) and Eq. (2.8) into Eq. (2.3) gives

\[
H = -\sum_{\nu, \delta > 0} \frac{1}{\delta^\alpha} \prod_{\kappa=0}^{\delta-1} \tau^z_{\nu+\kappa} - \lambda \sum_{\nu} \tau^x_\nu \tau^x_{\nu+1} \quad \text{(2.9)}
\]

Comparing Eq. (2.3) with Eq. (2.9) reveals a self-duality of the system. In particular in the nearest-neighbour (NN) case \( \alpha \to \infty \), the coupling term on the dual lattice exchanges roles with the field term on the original lattice and vice versa. This exact self-duality implies a phase transition for \( \lambda = 1 \) for the NN model [4].

The introduced domain walls (DW) may be interpreted as quasi-particles that can be created at any site of the \( \nu \)-chain. Hence, they are constituting a particle ensemble with indistinguishable and exchangeable quasi-particles. With these properties they describe a bosonic particle ensemble within which creation and annihilation operators can be defined for each site \( \nu \). However, it is only possible to create one quasi-particle on each site (if a domain wall is flipped twice the initial state is re-established). This can be described via an infinitely high potential well between adjacent quasi-particles and is equivalent to the fermionic property of an ensemble that in no case two quasi-particles can be in the exact same state at the exact same site (Pauli-exclusion principle). This mixture of bosonic and fermionic properties is called hardcore-bosonic [11]. By introducing creation (\( b^\dagger_\nu \)) and annihilation operators (\( b_\nu \)) for the domain walls at sites \( \nu \) such that

\[
\tau^z_\nu = 2b^\dagger_\nu b_\nu - 1 \quad \text{(2.10)}
\]

\[
\tau^x_\nu = b^\dagger_\nu + b_\nu \quad \text{(2.11)}
\]
the commutation relations of the hardcore-bosonic algebra

\[ [b_{\nu}, b_{\mu}] = 0 , \forall \ \nu \neq \mu \]  
\[ [b_{\nu}^\dagger, b_{\mu}^\dagger] = 0 , \forall \ \nu \neq \mu \]  
\[ [b_{\nu}, b_{\mu}^\dagger] = \delta_{\nu,\mu} (1 - 2 b_{\nu}^\dagger b_{\nu}) \]  

hold. Therewith, the Ising term of Eq. (2.3) can be rewritten to

\[
\begin{align*}
H_{\text{Ising}} &= E_0 + \sum_{\nu>0} \chi_1 \hat{b}_{\nu} \hat{b}_{\nu} + \sum_{\nu,d>0} \chi_2(d) \hat{b}_{\nu} \hat{b}_{\nu+d} b_{\nu+d}^\dagger + \\
&\quad \sum_{\nu,d_1,d_2>0} \chi_3(d_1,d_2) \hat{b}_{\nu} \hat{b}_{\nu+d_1} \hat{b}_{\nu+d_1}^\dagger \hat{b}_{\nu+d_2} b_{\nu+d_2}^\dagger + \ldots \\
&= E_0 + \sum_{\nu>0} \chi_1 \hat{n}_{\nu} + \sum_{\nu,d>0} \chi_2(d) \hat{n}_{\nu} \hat{n}_{\nu+d} + \\
&\quad \sum_{\nu,d_1,d_2>0} \chi_3(d_1,d_2) \hat{n}_{\nu} \hat{n}_{\nu+d_1} \hat{n}_{\nu+d_2} + \ldots .
\end{align*}
\]

\( \hat{n}_{\nu} := b_{\nu}^\dagger b_{\nu} \) counts the number of domain walls. The products \( \hat{n}_{\nu} \hat{n}_{\nu+d_1} \hat{n}_{\nu+d_1} \hat{n}_{\nu+d_2} \) describe many-body domain wall interactions counting the number of two domain walls with distance \( d \) respectively the number of three domain walls with distance \( d_1 \) and \( d_2 \). The coefficients \( \chi_i \) correspond to the energy difference of \( i \)-DW excitations to the ground-state energy \( E_0 \) under consideration of the overcount from lower excitations for \( i > 1 \). For example \( \chi_1 := E_1(\alpha) - E_0 \) and \( \chi_2(d) := E_2(d,\alpha) - E_0 - 2 \cdot \chi_1 \). The expressions for these prefactors get increasingly complicated, however it is in principle possible to determine all of them with the analytic expressions derived in Sec. 3.

Applying Eq. (2.10) and Eq. (2.11) to the transverse field term in Eq. (2.9) gives

\[
V = -\lambda \sum_{\nu} \tau_{\nu} \tau_{\nu+1} = -\lambda \sum_{\nu} (b_{\nu}^\dagger + b_{\nu}) (b_{\nu+1}^\dagger + b_{\nu+1}) = -\lambda \sum_{\nu} (b_{\nu}^\dagger b_{\nu+1}^\dagger + b_{\nu}^\dagger b_{\nu+1} + b_{\nu} b_{\nu+1}^\dagger + b_{\nu} b_{\nu+1}) .
\]

This expression can be grouped into three processes of the transverse field onto the chain of quasi-particles: The term \( T_0 = \sum_{\nu} b_{\nu}^\dagger b_{\nu+1} + b_{\nu} b_{\nu+1}^\dagger \) causes a hopping from site \( \nu \) to \( \nu + 1 \) or vice versa conserving the total number of domain walls. The term \( T_2 = \sum_{\nu} b_{\nu}^\dagger b_{\nu+1}^\dagger \) creates two domain walls and its hermitic conjugate \( T_{-2} = \sum_{\nu} b_{\nu} b_{\nu+1} \) annihilates two adjacent domain walls. Hence

\[
V = T_0 + T_{-2} + T_2 .
\]

This notation will later be useful for the perturbation theory, since the effective Hamiltonian there needs to conserve the number of domain walls.
2.2 Sublattice rotation for the antiferromagnetic case

In the antiferromagnetic case the Ising term of the Hamiltonian of the 1D Ising chain (the coupling constant is already included in $\lambda$) becomes

$$H_{\text{Ising}}^{\text{AF}} = \sum_i \sum_{\delta > 0} \frac{1}{\delta \alpha} \sigma^z_i \sigma^z_{i+\delta}.$$  \hspace{1cm} (2.18)

Hence the ground state looks like:

$$... \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow ...$$

$$A \ B \ A \ B$$

Every second spin can be regarded as part of a sublattice A resp. B each of which containing spins of the same orientation. After rotating one sublattice (choose for example B) about the $x$-axis of the chain $\sigma^z_B \rightarrow -\sigma^z_B$ the ground state (2.19) looks like the ferromagnetic ground state with every spin pointing in the same direction.

$$... \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow ... \rightarrow ... \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow ...$$ \hspace{1cm} (2.20)

Applying this transformation to the Hamiltonian (Eq. (2.18)) gives

$$H_{\text{Ising}}^{\text{AF}} = \sum_i \sum_{\delta > 0} (-1)^\delta \frac{1}{\delta \alpha} \sigma^z_i \sigma^z_{i+\delta} + \delta.$$ \hspace{1cm} (2.21)

Rotating the system about the $x$-axis does not affect the $\sigma^x$ matrices, hence the transverse field term is the same as in the ferromagnetic case giving in total

$$H_{\text{AF}} = \sum_{i,\delta > 0} (-1)^\delta \frac{1}{\delta \alpha} \sigma^z_i \sigma^z_{i+\delta} - \lambda \sum_i \sigma^x_i.$$ \hspace{1cm} (2.22)

To perform perturbation theory onto the transformed lrTFIM it is necessary to evaluate the eigenenergies and eigenstates of the unperturbed Ising term. This will be done in the following chapter.
3 Eigenenergies of the Ising term

In the first place, the ferromagnetic Ising term

\[ H = -\sum_{i,\delta>0} \frac{1}{\delta^{\alpha}} \sigma_i^z \sigma_{i+\delta}^z \]  

(3.1)

will be considered. As will be seen later, the developed scheme can easily be transferred to the antiferromagnetic case.

3.1 Ground-state energy

Due to the \( \mathbb{Z}_2 \)-symmetry of the long-range Ising interaction, the ground state of the 1D chain is 2-fold degenerate with either all spins pointing upwards or downwards. We consider \( N \) spins, but have in mind, that \( N \to \infty \) for our system. In this arrangement each of the \( N \) spins interact ferromagnetically with any other spin running through all possible distances \( \delta \) in the sum. Therefore the ground-state energy is

\[ E_0 = -N \sum_{\delta>0} \frac{1}{\delta^{\alpha}}. \]  

(3.2)

As expected \( E_0 \) depends linearly on the size of the system i.e. is an extensive quantity.

3.2 Single-domain-wall excitation

As explained before the excitations of the system can be described using the concept of domain walls. The first excitation corresponds to one domain wall (vertical red line) that separates two sections of opposite spin orientation in the chain. This can also be viewed as two ground-state configurations with infinitely many spins that are separated by a domain wall. Because this deformation changes the topological nature of the state, the single-domain-wall (1DW) excitation will also be referred to as the ‘topological’ excitation.

\[ \ldots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow | \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \ldots \]  

(3.3)

Similar to the case of the ground-state energy \( E_0 \), the energy of this first excited state \( E_1 \) where any spin is flipped stays the same. For an infinitely long chain the domain wall can be moved
throughout the chain without loosing a binding partner of any distance, hence the degeneracy of $E_1$ is $N$ for $N \to \infty$.

In the NN case $\alpha \to \infty$, the only change in energy with respect to the ground-state results from the new antiferromagnetic (AF) bond between spin $i$ and $i+1$. All the other spins at sites left from $i$ and right from $i+1$ remain ferromagnetically bonded with their two nearest neighbours. Therefore only the first summand in the Ising Hamiltonian (Eq. (3.1), $\alpha \to \infty$) changes from $-1$ to $+1$ and the energy becomes $E_{1,NN} = E_{0,NN} + 2$.

For any finite $\alpha$ each spin on the left side of the domain wall interacts antiferromagnetically with each spin on the right side of the wall, hence is contributing to an increase in energy w.r.t. $E_0$. For an expression of $E_1$ the pairs of opposite spin for each distance $\delta$ are counted, each of which giving a contribution $\propto 1/\delta^\alpha$ to the energy. Sketch (3.3) shows one pair, namely $(i, i+1)$ with $\delta = 1$ in between, two pairs $(i-1, i+1), (i, i+2)$ with $\delta = 2$, three $(i-2, i+1), (i-1, i+2), (i, i+3)$ with $\delta = 3$ and so on. Because the chain is considered to be infinitely long in both directions, there is no lack of partners for a large distance to the left or right. As well as in the NN limit the summand in $H_0$ for each emerging AF bond changes sign from $-1/\delta^\alpha$ to $+1/\delta^\alpha$ w.r.t. $E_0$. Hence, the energy increases by $2 \cdot 1/\delta^\alpha$ for each AF bond. This gives

$$E_1(\alpha) = \lim_{N \to \infty} E_0 + 2 \cdot \frac{1}{\alpha} + 2 \cdot 2 \cdot \frac{1}{2^\alpha} + 2 \cdot 3 \cdot \frac{1}{3^\alpha} + \ldots + 2 \cdot N \cdot \frac{1}{N^\alpha}$$

$$= E_0 + 2 \cdot \sum_{\delta=1}^{\infty} \frac{\delta}{\delta^\alpha} = E_0 + 2 \cdot \zeta(\alpha - 1)$$

with the Zeta-function $\zeta(\alpha) = \sum_{m=1}^{\infty} \frac{1}{m^{\alpha}}$. Because $\zeta(\alpha)$ only converges for $\alpha > 1$, Eq. (3.4) is only a well-defined expression for $\alpha > 2$.

### 3.3 Two-domain-wall excitations

The second type of excitations corresponds to a spin arrangement with two domain walls as it is sketched in (3.5):

$$\ldots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \downarrow \ldots \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \ldots$$

$$= d$$

In contrast to the single-domain-wall excitation these states are reached by flipping a finite number of adjacent spins in the ground-state configuration. The corresponding energy depends on the thickness $d$ of the flipped spin block. Again considering the excitaion energy w.r.t. $E_0$ gives contributions from the AF bonds of the $d$ spins towards the spins left resp. right of the domain walls. The interaction energy of the spins within the $d$-block is already accounted for in the ground-state energy.

First of all, we assume that each of the $d$ spins has an opposite spin partner in both directions
leading to a factor of

\[ 2 \cdot d \sum_{\delta=1}^{\infty} \frac{1}{\delta^\alpha} = 2d \cdot \zeta(\alpha) . \]  

(3.6)

Because the spins within the \( d \)-block interact ferromagnetically, this expression needs to be corrected for each missing AF binding partner for bond lengths between \( \delta = 1 \) and \( \delta = d - 1 \). For a bond length of \( \delta = 1 \) only the outermost two spins of the \( d \)-block have an AF spin partner outside of the block. Therefore Eq. (3.6) gets reduced by \((2d - 2) \cdot 1/1^\alpha\). For \( \delta = 2 \) only the two \( \downarrow \) spins which are adjacent to each domain wall have an AF \( \uparrow \) spin partner. The sum in Eq. (3.6) gets reduced by \((2d - 2 \cdot 2) \cdot 2^{-\alpha}\). Subtracting all contributions up to \( \delta = d - 1 \) from Eq. (3.6) and considering again that each bond that switches from ferromagnetic to antiferromagnetic contributes a factor 2 to the energy increase w.r.t. the negative \( E_0 \), this leads to a total energy of

\[ E_2(d, \alpha) = E_0 + 2 \cdot 2 \left[ d \cdot \zeta(\alpha) - \sum_{i=1}^{d-1} \frac{1}{i^\alpha(d-i)} \right] . \]  

(3.7)

3.4 Comparison of the first two types of excitations

In the previous sections analytic formulae for the lowest-excitation energies of the long-range Ising chain corresponding to states with one and two domain walls have been deduced. Eq. (3.4) for \( E_1(\alpha) \) and Eq. (3.7) for \( E_2(d, \alpha) \) show a fundamental difference between these two excitations: Whereas for the energy of the single-domain-wall (1DW) state \( E_1 \) the number of AF bonds raising the ground-state energy increases with the bond length (for \( \delta = 1 \), 1 bond; \( \delta = 2 \), 2 bonds; \( \delta = 3 \), 3; ...), for the 2DW state this number is fixed by the distance between the domain walls \( d \). In Fig. 3.1 the excitation energies for different \( d \) are plotted as a function of the coupling strength \( \alpha \). It shows that the dependency of \( E_2 \) on \( d \) becomes infinitely small for large \( \alpha \). However, the degeneracy in \( d \) is never repealed for any finite \( \alpha \). For \( \alpha \to \infty \) the different 2DW excitation energies come arbitrarily close to another and approach an energy difference of +4 w.r.t. \( E_0 \) in accordance with the nearest-neighbour limit. For the plotted \( \alpha \)-region the degeneracy becomes more significant and the \( E_2 \)-energies get spread out as \( \alpha \) approaches the ultra-long-range regime. The 2DW energy \( E_{2;1} \) corresponding to a state with one flipped spin consistently remains the lowest among the 2DW excitations. As Eq. (3.7) indicates the \( E_2 \)-energies diverge at \( \alpha = 1 \) independent of the specific value of \( d \). However, more and more of the first summands of the zeta function get cut off as \( d \) becomes larger rising the respective curves already way before the actual divergence at \( \alpha = 1 \). For \( \alpha \leq 1 \) Eq. (3.1) indicates a super-extensivity of the ground-state energy \( \sum_{\delta>0} 1/\delta^\alpha \sim N \). There the system gets unstable and it is in the first instance no longer possible to give a systematic thermodynamically consistent description for it.

The curve of \( E_1 \) corresponds to the 1DW excitation energy. For large \( \alpha \) it shows correctly the nearest-neighbour limit of +2 representing the appropriate low-energy excitation of the system. In the regime of small \( \alpha \) it already diverges as \( \alpha \to 2 \). This can be seen in Eq. (3.4) and comes from the fact that the number of energy contributions from one interaction length increases with
Figure 3.1: Lowest excitation energies of the ferromagnetic long-range Ising chain as a function of the coupling parameter $\alpha$. The parameter $d$ denotes the distance between the domain walls in Eq. (3.4).

This feature suggests a different behaviour at the ordered-polarized phase transition if the long-range system in Eq. (2.1) gets extended by an external source, in particular a transverse field. Detailed examination of the lrTFIM will be treated in Sec. 4 and will show indeed, that the 2DW gap (corresponding to $E_{2;1}$) drops below the 1DW gap at a critical value of $\alpha$ for a fixed field strength $\lambda$. 

A comparison of the two excitation modes in Fig. 3.1 shows, that due to the faster divergence of $E_1$ already for $\alpha \to 2$ the curves intersect and the lowest excitation mode changes from the 1DW (‘topological’) excitation to the 2DW with distance 1 (‘trivial’) excitation for $\alpha \approx 2.48$. This feature suggests a different behaviour at the ordered-polarized phase transition if the long-range system in Eq. (2.1) gets extended by an external source, in particular a transverse field. Detailed examination of the lrTFIM will be treated in Sec. 4 and will show indeed, that the 2DW gap (corresponding to $E_{2;1}$) drops below the 1DW gap at a critical value of $\alpha$ for a fixed field strength $\lambda$. 
3.5 Multi domain-wall excitations

For the second-order perturbation of the topological and the trivial excitation energies, expressions for the energies with a larger number of DWs are needed. It turns out, that an iterative formula for any excitation of the long-range Ising model can be found.

For a state with \( n \geq 3 \) domain walls, it is suitable to consider the energy difference w.r.t. the state with \((n - 2)\) domain walls. Hence, \( E_3 \) is stated w.r.t. \( E_1 \), \( E_4 \) w.r.t. \( E_2 \) and so on.

Let us consider the following state with three domain walls:

\[
\ldots \downarrow \downarrow | \uparrow \uparrow ... \uparrow \uparrow | \downarrow \downarrow ... \downarrow \downarrow | \uparrow \uparrow \ldots
\]

\[=(d_1) \quad = (d_2)\]  \hspace{1cm} (3.8)

Since the two outermost spin domains form an \( E_1 \)-state with one of the inner domains, only the contribution of the other inner domain is necessary to examine. This is shown in the following, where we imagine that the blue colored \( d_1 \uparrow \)-spins are inserted into the black 1DW-state. The considerations are equal to considering the \( d_2 \)-block inserted into its respective surrounding 1DW-state which would then be composed of the \( d_1 \)-block and the two outermost infinitely long domains:

\[
\ldots \downarrow \downarrow | \uparrow \uparrow ... \uparrow \uparrow | \downarrow \downarrow ... \downarrow \downarrow | \uparrow \uparrow \ldots
\]

\[=(d_1)\]  \hspace{1cm} (3.8)

The first contribution enhancing \( E_1 \) are the AF bonds with the \( \downarrow \)- spins leftwards. Since an infinite long spin chain is assumed, this contribution is the same which we have seen for the 2DW excitation but only in the left direction (Sketch 3.5). Again, the sum over all possible AF bond lengths of each \( d_1 \)-spin leftwards gets reduced by the missing AF binding partners for bond lengths that stay within the blue \( d_1 \)-block of spins with indentical orientation. Hence, the first \( E_3 \)-contribution becomes (Eq. (3.7)):

\[
d_1 \cdot \zeta(\alpha) - \sum_{i=1}^{d_1-1} \frac{1}{\delta^\alpha} (d_1 - i) . \]

\[= (3.9)\]

Secondly, the AF interaction of the blue domain with the \( d_2 \)-spins to the right needs to be considered: Each of these spins form an AF bond with each of the \( d_1 \) spins to the left, so in total \( d_1 \) AF bonds for each \( d_2 \)-spin. The bond lengths become longer by the distance to the domain wall with the \( d_1 \)-block. Summing up the contribution for all \( d_2 \)-spins gives

\[
\sum_{\delta=1}^{d_1} \frac{1}{\delta^\alpha} + \sum_{\delta=2}^{d_1+1} \frac{1}{\delta^\alpha} + \ldots + \sum_{\delta=d_2}^{d_1+d_2-1} \frac{1}{\delta^\alpha} = \sum_{c=1}^{d_2} \sum_{\delta=c}^{d_1+c-1} \frac{1}{\delta^\alpha} . \]

\[= (3.10)\]

As a third correction to the black \( E_1 \) state, the ferromagnetic interaction of the blue \( d_1 \)-block with the spins with same directions right of the third domain wall needs to be quantified. Similar to the latter case, each of the \( d_1 \)-spins form infinitely many ferromagnetic (F) bonds with this outermost spin block, starting from bond lengths of \( d_2 + 1 \) for the blue spin on the very right
and from $\delta = d_2 + d_1$ for the leftest blue spin. Due to the ferromagnetic character of the bonds this sums up with a minus sign to

$$- \sum_{b=d_2+1}^{d_1+d_2} \sum_{\delta=b}^{\infty} \frac{1}{\delta^\alpha}.$$ (3.11)

Adding Eq. (3.10) and Eq. (3.11) to Eq. (3.9) the expression for $E_3$ becomes

$$E_3(d_1, d_2, \alpha) = E_1 + 2 \cdot \left[ d_1 \cdot \zeta(\alpha) - \sum_{i=1}^{d_1-1} \frac{1}{\delta^\alpha} (d_1 - i) + \sum_{c=1}^{d_2} \sum_{\delta=c}^{d_1+c-1} \frac{1}{\delta^\alpha} \right] .$$ (3.12)

Again, any addend to $E_1$ describing a change from an AF to a F bond w.r.t. the reference state or vice versa gets multiplied by 2.

Introducing the Hurwitz-Zeta function $\zeta(\alpha, b) = \sum_{m=0}^{\infty} \frac{1}{(m+b)^\alpha}$, Eq. (3.12) becomes

$$E_3(d_1, d_2, \alpha) = E_1 + 2 \cdot \left[ - \zeta(\alpha - 1, d_1) + d_1 \cdot \zeta(\alpha, d_1) + \zeta(\alpha - 1) + \sum_{b=1}^{d_2} \zeta(\alpha, b) - \zeta(\alpha, b + d_1) - \sum_{c=d_2+1}^{d_1+d_2} \zeta(\alpha, c) \right] .$$ (3.13)

This scheme can now be transferred to higher (nth) excitations by using the second last (n-2)th state as the reference state and summing up all antiferromagnetic (with a plus sign) and ferromagnetic (with a minus sign) contributions of the inserted, ’new’ spin block w.r.t. the remaining n blocks into which the reference state can be divided. Explicitly for n= 4:

$$\ldots \downarrow \downarrow \uparrow \uparrow \ldots \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \ldots \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \ldots \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \ldots \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \ldots$$

$$= d_1 \quad = d_2 \quad = d_3$$

$$E_4(d_1, d_2, d_3, \alpha) = E_2(d_3, \alpha) + 2 \cdot \left[ - \zeta(\alpha - 1, d_1) + d_1 \cdot \zeta(\alpha, d_1) + \zeta(\alpha - 1) + \sum_{b=1}^{d_2} \zeta(\alpha, b) - \zeta(\alpha, b + d_1) + \sum_{b=d_2+d_1+1}^{d_1+d_2+d_3} \zeta(\alpha, b) \right] .$$ (3.14)
In principle, this can be carried on for any higher excitation. However, each higher excitation order extends the correction of the reference state by one summand.

From the preceding expressions it is seen, that the first term remains the same for all excitations (it treats the AF interactions to the infinitely many spins leftwards). Also, the argument in the sums summing the interactions of the inserted spins with the spins of the respective $d_i$-blocks stays the same, only the sign (according to AF or F binding) and the summation limits change (according to the distance to the inserted $d_1$-block). The same holds for the last term which represents the interaction with the infinite chain end.

It is useful to introduce the abbreviations

\[
\beta(\alpha, d_1) := \zeta(\alpha - 1, d_1) + d_1 \cdot \zeta(\alpha, d_1) + \zeta(\alpha - 1)
\]

\[
\gamma(\alpha, d_1, b) := \zeta(\alpha, b) - \zeta(\alpha, b + d_1)
\]

where $b$ denotes the summation index (Eq. (3.14)).

For a state with $m$ domain walls ($m$th excitation) with $m$ an odd number we get

\[
E_{m, odd} = (d_1, \ldots, d_{m-1}, \alpha) = E_{m-2}(d_3, \ldots, d_{m-1}) + 2 \cdot \left[ \beta(\alpha, d_1) + \sum_{b=1}^{d_2} \gamma(\alpha, d_1, b) \right.
\]

\[
- \sum_{b=1+1+d_2}^{d_2+d_3} \gamma(\alpha, d_1, b) + \sum_{b=1+d_2+d_3}^{d_2+d_3+d_4} \gamma(\alpha, d_1, b)
\]

\[
- \sum_{b=1+d_2+d_3+d_4}^{d_2+d_3+d_4+d_5} \gamma(\alpha, d_1, b) + \ldots
\]

\[
+ \sum_{b=1+d_2+d_3+d_4}^{d_1+d_4+d_3+d_2+d_3+d_4+d_5+d_{m-2}+d_{m-1}} \gamma(\alpha, d_1, b)
\]

\[
- \sum_{c=1+d_2+d_3+d_4+d_5+d_{m-2}+d_{m-1}}^{c+d_2+d_3+d_4+d_5+d_{m-2}+d_{m-1}} \zeta(\alpha, c)
\].

For $m$ even, the signs of the last two terms change, because the interaction of the inserted $d_1$-block with the infinitely long chain end is antiferromagnetically. Respectively, the interaction with the last finite $d_{m-1}$-block changes from AF to F (Sketch 3.18)

\[
E_{m, even} = (d_1, \ldots, d_{m-1}, \alpha) = E_{m-2}(d_3, \ldots, d_{m-1}) + 2 \cdot \left[ \beta(\alpha, d_1) + \sum_{b=1}^{d_2} \gamma(\alpha, d_1, b) \right.
\]

\[
- \sum_{b=1+1+d_2}^{d_2+d_3} \gamma(\alpha, d_1, b) + \sum_{b=1+d_2+d_3}^{d_2+d_3+d_4} \gamma(\alpha, d_1, b)
\]

\[
- \sum_{b=1+d_2+d_3+d_4}^{d_2+d_3+d_4+d_5} \gamma(\alpha, d_1, b) + \ldots
\]

\[
+ \sum_{b=1+d_2+d_3+d_4}^{d_1+d_4+d_3+d_2+d_3+d_4+d_5+d_{m-2}+d_{m-1}} \gamma(\alpha, d_1, b)
\]

\[
- \sum_{c=1+d_2+d_3+d_4+d_5+d_{m-2}+d_{m-1}}^{c+d_2+d_3+d_4+d_5+d_{m-2}+d_{m-1}} \zeta(\alpha, c) - \sum_{b=1+1+d_2}^{d_2+d_3} \zeta(\alpha, d_1)
\].

For $m$ even, the signs of the last two terms change, because the interaction of the inserted $d_1$-block with the infinitely long chain end is antiferromagnetically. Respectively, the interaction with the last finite $d_{m-1}$-block changes from AF to F (Sketch 3.18)
\[ E_{m, \text{even}} = (d_1, \ldots, d_{m-1}, \alpha) = E_{m-2}(d_3, \ldots, d_{m-1}) + 2 \cdot \left[ \beta(\alpha, d_1) + \sum_{b=1}^{d_2} \gamma(\alpha, d_1, b) \right. \]
\[ - \sum_{b=1+d_2}^{d_2+d_3+d_4+d_5} \gamma(\alpha, d_1, b) + \ldots \]
\[ - \sum_{b=1+d_2+d_3+d_4}^{d_2+d_3+d_4+d_5} \gamma(\alpha, d_1, b) + \ldots \]
\[ - \sum_{b=1+d_2+d_3+d_4+\ldots+d_{m-2}+d_{m-1}}^{d_1+d_2+d_3+\ldots+d_{m-1}} \gamma(\alpha, d_1, b) \]
\[ + \sum_{c=1+d_2+d_3+\ldots+d_{m-1}}^{d_1+d_2+d_3+\ldots+d_{m-1}} \zeta(\alpha, c) \] . \hspace{1cm} (3.19)

### 3.6 Eigenenergies of the antiferromagnetic Ising chain

For the antiferromagnetic case, a sublattice rotation about the x-axis leads to an Ising Hamiltonian of

\[ H = \sum_{i, \delta > 0} (-1)^\delta \frac{1}{\delta^\alpha} \sigma^z_i \sigma^z_{i+\delta} . \hspace{1cm} (3.20) \]

Hence, the ground-state energy becomes

\[ E_0 = \sum_i \sum_{\delta=1}^{\delta > 0} (-1)^\delta \frac{1}{\delta^\alpha} = N \sum_{\delta=1} (-1)^\delta \frac{1}{\delta^\alpha} . \hspace{1cm} (3.21) \]

The first excited state of the system with one domain wall looks like

\[ \ldots \uparrow \downarrow \uparrow | \uparrow \downarrow \uparrow \uparrow \ldots \xrightarrow{\text{sublattice rotation}} \ldots \uparrow \uparrow \uparrow | \downarrow \downarrow \downarrow \ldots , \] \hspace{1cm} (3.22)

again after rotation of every second spin. Because the antiferromagnetic eigenstates transform into the ferromagnetic eigenstates through the sublattice rotation, the calculation for the unperturbed antiferro eigenenergies can be done similarly to the ferromagnetic case (with special care of the right signs).
In particular for the first excited state $E_1$:

$$E_1 = E_0 + 1 \cdot \frac{1}{1^\alpha} - 2 \cdot \frac{1}{2^\alpha} + 3 \cdot \frac{1}{3^\alpha} - 4 \cdot \frac{1}{4^\alpha} + \ldots$$

$$= E_0 + 2 \sum_{\delta=1}^{\infty} (-1)^{\delta+1} \frac{\delta}{\delta^\alpha}$$

$$= E_0 + 2 \sum_{\delta=1}^{\infty} (-1)^{\delta+1} \frac{1}{\delta^{\alpha-1}}.$$  \hspace{1cm} (3.23)

Rewriting this with $\zeta$-functions gives

$$E_1 = E_0 + 2 \cdot 2^{-\alpha} (2^\alpha - 4) \cdot \zeta(\alpha - 1).$$ \hspace{1cm} (3.24)

However, this formula is formally only valid for $\text{Re}(\alpha) > 1$. One interesting limit case is $\alpha = 0$ in which all spins interact with any other spin independent of their distances towards another. If one uses the analytic continuation of the $\zeta$-function (i.e. $\zeta(-1) = -1/12$) this gives for $\alpha = 0$

$$\Delta E_1(\alpha = 0) = 2 \cdot (1 - 4) \cdot \zeta(-1) = \frac{1}{2},$$ \hspace{1cm} (3.25)

where $\Delta E_1 := E_1 - E_0$. The energies for the second excitation with two domain walls (Sketch 3.26) can be computed similarly:

$$\ldots \uparrow \downarrow \uparrow \uparrow \downarrow \uparrow \downarrow \ldots \overset{\text{sublattice}}{\rightarrow} \ldots \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \downarrow \ldots \overset{\text{rot.}}{=} d$$ \hspace{1cm} (3.26)

Like in the ferromagnetic case, first the energy correction of each of the $d$ spins to the ground-state needs to be considered. This gets reduced by the overcount due to the bonds within the spins of the $d$-block which are arranged like in the ground state.

$$E_2(d, \alpha) = E_0 + 2 \cdot 2 \left[ d \cdot \sum_{\delta=1}^{d-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} - \sum_{i=1}^{d-1} (-1)^{i+1} \frac{1}{i^\alpha(d - i)} \right].$$ \hspace{1cm} (3.27)

Again, this can be rewritten to

$$E_2(d, \alpha) = E_0 + 4 \cdot \left[ d \cdot 2^{-\alpha} (2^\alpha - 2) \zeta(\alpha) - \sum_{i=1}^{d-1} (-1)^{i+1} \frac{1}{i^\alpha(d - i)} \right].$$ \hspace{1cm} (3.28)

for $\text{Re}(\alpha) > 1$. Using the analytic continuation $\zeta(0) = -1/2$ one can calculate the energy for $\alpha = 0$ for different $d$:

$$\Delta E_2(1, 0) = 4 \cdot (-1) \cdot (-1/2) = 2$$ \hspace{1cm} (3.29)

$$\Delta E_2(2, 0) = 4 \cdot (-2 \cdot (-1/2) - 1) = 0.$$ \hspace{1cm} (3.30)
It turns out that $\Delta E_2(d, 0) = 2$ for $d$ odd and $\Delta E_2(d, 0) = 0$ for even $d$. For the second-order perturbation also the 3DW and 4DW energies are needed. By replacing $1/i^\alpha$ with $(-1)^{i+1}/i^\alpha$ as the argument in the sums of any expression for the ferromagnetic energies this becomes for $E_3$

$$E_3(d_1, d_2, \alpha) = E_1(\alpha) + 2 \cdot \left[ d_1 \cdot \sum_{\delta=1}^{d_1-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} - \sum_{\delta=1}^{d_1-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} (d_1 - \delta) \right. \right.

+ \left. \sum_{b=1}^{d_2} \sum_{\delta=b}^{d_1+b-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} - \sum_{b=d_2+1}^{\infty} \sum_{\delta=b}^{\infty} (-1)^{\delta+1} \frac{1}{\delta^\alpha} \right] \tag{3.31}$$

and for $E_4$

$$E_4(d_1, d_2, d_3, \alpha) = E_2(d_3, \alpha) + 2 \cdot \left[ d_1 \cdot \sum_{\delta=1}^{d_1-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} - \sum_{\delta=1}^{d_1-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} (d_1 - \delta) \right. \right.

+ \left. \sum_{b=1}^{d_2} \sum_{\delta=b}^{d_1+b-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} - \sum_{b=d_2+1}^{d_2+d_3} \sum_{\delta=b}^{d_1+b-1} (-1)^{\delta+1} \frac{1}{\delta^\alpha} \right.

+ \left. \sum_{b=d_2+d_3+1}^{d_1+d_2+d_3} \sum_{\delta=b}^{\infty} (-1)^{\delta+1} \frac{1}{\delta^\alpha} \right] \tag{3.32}$$

In Fig. 3.2 these formulae are plotted.

![Figure 3.2: Eigenenergies of the Ising Hamiltonian with antiferromagnetic interaction (Eq. (3.20)).](image)

In contrast to the ferromagnetic energies, the sums also converge for $\alpha < 1$. For the concrete implementation, the analytic continuation of the $\zeta$-function has been used. To check its physical credibility the limiting case of $\alpha = 0$ can be considered: Here, the spin chain lacks any order.
since the spins may be exchanged within another without any energy cost (in this way it is an unphysical state for a spin chain). Hence, only the total number of spins pointing in up or down direction is important. Defining a macroscopic spin with \( \sigma^z_{\text{tot}} := \sum_i \sigma^z_i \), the Hamiltonian (Eq. 3.20) can be written as

\[
H_{\text{AF}, \alpha=0} = \sum_i \sum_{\delta > 0} \sigma^z_i \sigma^z_{i+\delta} = \frac{1}{2} (\sigma^z_{\text{tot}})^2 - \frac{N}{2}.
\]  

(3.33)

This formula gives the correct results for \( \Delta E_2 \), since for \( d = 1 \rightarrow \sigma^z_{\text{tot}} = 1; d = 2 \rightarrow \sigma^z_{\text{tot}} = 0 \) (compare with Eq. (3.29) and Eq. (3.30)). For \( E_1 \) however, one would expect to get \( \Delta E_1 = 0 \) for \( N \rightarrow \infty \), because then the contributions from the infinitely many spins left and right of the domain wall should cancel each other out. The circumstance that \( \Delta E_1 = 1/2 \) for \( \alpha = 0 \) seems unreasonable since it suggests a comparison of the \( E_1 \) state with an odd number of spins with a ground-state with an even number of spins, a finite size effect that is not expected for an infinitely large system.
4 Low-field approach to the IrTFIM

In order to examine the action of a transverse field on the long-range Ising model degenerate perturbation theory will be used. Therefore, the eigenenergies of the Ising Hamiltonian examined in Sec. 3 will be treated as the unperturbed energies and the transverse field will be regarded as the perturbation $V$. In the following, the second-order perturbation for the ferromagnetic ground state, the 1DW and 2DW with $d = 1$ state will be calculated.

4.1 Formalism of degenerate perturbation theory

The advantage of the degenerate perturbation theory is that with it each excitation can get decoupled from the complete many-body system and be treated separately with the perturbation term. Therefore an effective Hamiltonian containing an expansion in the perturbation term $V$ is derived for each $i$-quasi-particle state. Diagonalising it in the respective $i$-quasi-particle sub-Hilbertspace gives the corresponding corrections to the unperturbed energy in orders of the perturbation strength parameter (which is $\lambda$ in our case).

Up to second order in $V$ it looks like

$$H_{\text{eff},i} = P_i H_0 P_i + P_i V P_i + P_i V Q_i \left[ E^{(0)} - Q_i H_0 Q_i \right]^{-1} Q_i V P_i .$$  \hspace{1cm} \text{(4.1)}

$P_i$ denotes the projector on the Hilbert subspace spanned by the degenerate states with $i$-quasi-particles and $Q_i = 1 - P_i$ the projector on the Hilbert subspace spanned by all the other states. In our model, the quasi-particles are equivalent to domain walls. The formulae in the preceding section have showed that the 2DW energies with different $d$ are non-degenerate for $\alpha < \infty$. Hence, the respectively $N$-fold degenerate 1DW and 2DW with $d = 1$ states span their separate Hilbert subspace. $H_0$ denotes the unperturbed Hamiltonian (in our case the long-range Ising term in Eq. (3.1)) and $E^{(0)}$ the unperturbed energy of the degenerate Hilbert subspace that is considered. [12].
4.2 Ferromagnetic IrTFIM

As seen in Sec. 2.1 the transverse field perturbation term on the dual lattice $\nu$ is

$$V = -\lambda \sum_{\nu} (b_{\nu}^+ b_{\nu+1}^+ + b_{\nu}^+ b_{\nu+1} + b_{\nu} b_{\nu+1}^+ + b_{\nu} b_{\nu+1})$$

(4.2)

$$= T_0 + T_{-2} + T_{+2}.$$  

(4.3)

It therefore introduces different hopping processes to the excitations of the strongly correlated long-range Ising chain. Depending on the specific excitation and the order in $V$ different hopping patterns occur. These are evaluated in the following.

4.2.1 Ground-state energy

In order to examine the energy gap between the excited states and the ground-state (which will be represented by $|0\rangle$), it is first necessary to evaluate the perturbation of the ground state energy. The 0-th order becomes

$$E_0^{(0)} = \langle 0| P_0 H_0 P_0 |0 \rangle = E_0 = -N \cdot \zeta(\alpha) ,$$

(4.4)

according to Eq. (3.1). For the first-order in $V$, Eq. (4.2) is applied once to the ground state giving

$$E_0^{(1)} = \langle 0| P_0 V P_0 |0 \rangle = -\lambda \langle 0| P_0 \sum_{\nu} |\nu, \nu + 1 \rangle = 0 .$$

(4.5)

Here, $|\nu, \nu + 1 \rangle$ denotes a state with one domain wall at site $\nu$ and $\nu + 1$. Since the resulting 2DW states $|\nu, \nu + 1 \rangle$ are not in the ground-state Hilbert space the projection with $P_0$ gives 0.

For the second-order

$$E_0^{(2)} = \langle 0| P_0 V Q_0 \frac{1}{E_0^{(0)} - Q_0 H_0 Q_0} Q_0 V P_0 |0 \rangle ,$$

(4.6)

the only possible action of $V$ on the ground state is to create two domain walls $|\nu, \nu + 1 \rangle$ which corresponds to an energy of $E_2^{(0)}$ ($d = 1$). Hence,

$$E_0^{(2)} = \langle 0| P_0 V \sum_{\nu} |\nu, \nu + 1 \rangle \frac{-\lambda}{E_0^{(0)} - E_2^{(0)}(1)} .$$

(4.7)

Since the outcome of the second action of $V$ on the created 2DW states $|\nu, \nu + 1 \rangle$ gets projected onto the ground-state Hilbert space via $P_0$, the only non-zero possibility for the second $V$ is to annihilate the very same states $|\nu, \nu + 1 \rangle$. Hence,

$$E_0^{(2)} = \sum_{\nu} \frac{\lambda^2}{E_0^{(0)} - E_2^{(0)}(1)} = N \cdot \frac{\lambda^2}{4 \cdot \zeta(\alpha)} ,$$

(4.8)
with Eq. (3.7) and the assumption of the chain having \( N \) sites. In summary, the second order perturbation of the ground-state energy is

\[
E_0(\lambda) = -N \cdot \zeta(\alpha) - N \cdot \frac{\chi^2}{4 \cdot \zeta(\alpha)}.
\]  

(4.9)

Physically, Eq. (4.9) represents the fluctuations of the ground state to the higher energy level with \( E_2(d = 1) \) which is possible due to the application of a small transverse field. These fluctuations lower the ground-state energy.

### 4.2.2 Single-domain-wall state (topological excitation)

Similar to the calculation for the ground-state energy the 0-th order of the single-domain-wall state on the dual lattice \( |\nu\rangle \) gives according to Eq. (3.4)

\[
E_1^{(0)} = \langle \nu | P_1 H_0 P_1 | \nu \rangle = E_0^{(0)} + 2 \cdot \zeta(\alpha - 1).
\]  

(4.10)

For the first-order, the action of \( V \) on \( |\nu\rangle \) needs to be considered:

\[
P_1 V P_1 |\nu\rangle = -\lambda (|\nu - 1\rangle + |\nu + 1\rangle).
\]  

(4.11)

Since the outcome of \( V |\nu\rangle \) is projected onto the 1DW Hilbert subspace, only the quasi-particle conserving part \( T_0 \) takes action resulting in a hopping of the domain wall from site \( |\nu\rangle \) to \( |\nu - 1\rangle \), resp. \( |\nu + 1\rangle \) (Fig. 4.1).

![Figure 4.1](image)

Figure 4.1: Action of the perturbation term \( V \) for the first-order correction of the 1DW excitation with \( E_1 \).

The operator in Eq. (4.11) is not diagonal in \( \nu \)-space. However, the translational invariance of the systems’s Hamiltonian (and hence also the operator \( P_1 V P_1 \)) can be exploited via transforming it into the momentum space (\( k \)-space). For the change of basis \( |\nu\rangle \to |k\rangle \) the Fourier transform

\[
|k\rangle = \frac{1}{\sqrt{N}} \sum_\nu e^{-ik\nu} |\nu\rangle
\]  

(4.12)
is needed. Considering infinitely many sites and periodic boundary conditions Eq. (4.11) be-
comes

\[ P_1 V P_1 |k\rangle = \frac{1}{\sqrt{N}} \sum_{\nu} e^{-ik\nu} P_1 V P_1 |\nu\rangle \]

\[ = -\lambda \frac{1}{\sqrt{N}} (\sum_{\nu} e^{-ik\nu} |\nu - 1\rangle + \sum_{\nu} e^{-ik\nu} |\nu + 1\rangle) \]

\[ = -\lambda \frac{1}{\sqrt{N}} \sum_{\nu} (e^{-ik(\nu+1)} |\nu\rangle + e^{-ik(\nu-1)} |\nu\rangle) \]

\[ = -2\lambda \cos(k) |k\rangle. \quad (4.13) \]

Hence, the first-order correction of \( E_1 \) in k-space is

\[ E_1^{(1)} = -2\lambda \cos(k). \quad (4.14) \]

For the second-order correction the term

\[ P_1 V Q_1 \frac{1}{E_1^{(0)} - Q_1 H_0 Q_1} Q_1 V P_1 |k\rangle \]

needs to be evaluated. Again, it is considered in k-space since the different hopping processes
of the domain walls are not diagonal in \( \nu \)-space. Because the operator \( Q_1 \) filters any 1DW state,
the only contribution of the first application of \( V \) is to create two domain walls with \( T_+2 \) and for
the second application of \( V \) to annihilate two domain walls with \( T_-2 \) giving

\[ E_1^{(2)} = \frac{1}{\sqrt{N}} \sum_{\nu} e^{-ik\nu} P_1 V Q_1 \frac{\lambda^2}{E_1^{(0)} - Q_1 H_0 Q_1} \sum_{\mu} \mu, \mu + 1) |\nu\rangle \]

\[ = \frac{1}{\sqrt{N}} \sum_{\nu} e^{-ik\nu} P_1 V Q_1 \left[ \sum_{\mu\neq\nu-1,\nu} \frac{\lambda^2}{E_1^{(0)} - E_3^{(0)}(1, d_2)} |\nu, \mu, \mu + 1) \right] \]

\[ + \frac{\lambda^2}{E_1^{(0)} - E_3^{(0)}(1, 1)} \left( |\nu, \nu + 1, \nu + 2) + |\nu - 2, \nu - 1, \nu) \right) \]

\[ = \frac{1}{\sqrt{N}} \sum_{\nu} e^{-ik\nu} \left[ \sum_{d_2 = 1}^{2} \frac{2 \cdot \lambda^2}{E_1^{(0)} - E_3^{(0)}(1, d_2)} |\nu\rangle + \frac{\lambda^2}{E_1^{(0)} - E_3^{(0)}(1, 1)} \left( |\nu + 2) + |\nu - 2) \right) \right]. \]

The first sum represents the contribution due to the creation of two arbitrary neighbouring do-
main walls and a subsequent annihilation of the very same domain walls with the second appli-
cation of \( V \) on the left hand side of Eq. (4.15) (Fig. 4.2). This contribution is already diagonal
in \( \nu \)-space.
The second term is due to the creation of two domain walls adjacent to the already existing one at site $\nu$, all together forming a 3DW state with $d_1 = 1$ and $d_2 = 1$ and the subsequent annihilation of the DW at $\nu$ and its respective direct neighbour $\nu - 1$ or $\nu + 1$ (Fig. 4.3).

Applying periodic boundary conditions with $N \to \infty$, this term can be rewritten as

$$E_1^{(2)} = -\frac{\lambda^2}{4} \frac{1}{\sqrt{N}} \sum_{\nu} (e^{-ik(\nu-2)} + e^{-ik(\nu+2)}) |\nu\rangle = -\frac{\lambda^2}{4} \cdot 2 \cos(2k) |k\rangle,$$

where we used Eq. (3.13) to evaluate $E_3^{(0)}(1, 1) = E_1^{(0)} + 4$.

Together, this gives the second-order correction of $E_1$

$$E_1^{(2)} = \lambda^2 \left[ 2 \cdot \sum_{d_2=1} \frac{1}{E_1^{(0)} - E_3^{(0)}(1, d_2)} - \frac{1}{2} \cos(2k) \right].$$

and in total

$$E_1(\lambda, k) = E_0 + 2\zeta(\alpha - 1) - 2\lambda \cos(k) + \lambda^2 \left[ 2 \sum_{d_2=1} \frac{1}{E_1^{(0)} - E_3^{(0)}(1, d_2)} - \frac{1}{2} \cos(2k) \right].$$
for the second-order corrected energy $E_1$.

To examine the phase transition of the system the gap between ground-state (Eq. (4.9)) and the 1DW state (Eq. (4.18)) is of interest. Eq. (4.18) is given in momentum space. To find its minimum the $\cos(k)$ needs to be evaluated at $k = 0$. Back in real space this corresponds to the excited state which is closest to the ground-state configuration having no phase difference between neighbouring spins [13]. Hence the gap $\Delta_{1\text{DW}}$ becomes

$$
\Delta_{1\text{DW}} = E_1(\lambda, 0) - E_0(\lambda) = E_0^{(0)} + 2\zeta(\alpha - 1) - 2\cdot \lambda + \lambda^2 \left[ 2 \cdot \sum_{d_2=1} \frac{1}{E_1^{(0)} - E_3^{(0)}(1, d_2)} - \frac{1}{2} \right] - E_0^{(0)} + N \cdot \frac{\lambda^2}{4\zeta(\alpha)} = 2\zeta(\alpha - 1) - 2\cdot \lambda - \frac{\lambda^2}{2} - 2\lambda^2 \sum_{d_2=1} \frac{1}{\Delta_1 E_3(d_2)} + \sum_\nu \frac{\lambda^2}{4 \cdot \zeta(\alpha)} = 2\zeta(\alpha - 1) - 2\zeta(\alpha - 1) - 2\lambda - \frac{\lambda^2}{2} + \lambda^2 \left[ \sum_{d_2=1} \frac{-2}{\Delta_1 E_3(d_2)} + \frac{2}{4 \cdot \zeta(\alpha)} \right] + \frac{2\lambda^2}{4\zeta(\alpha)},
$$

(4.19)

where $\Delta_1 E_3(d_2) := E_3^{(0)}(d_1 = 1, d_2) - E_1^{(0)}$ has been defined. The two sums in Eq. (4.19) have been condensed with the following consideration: The first sum running two times over $d_2$ contains $(N - 2)$ summands, since the second-order fluctuation of the 1DW state, which it describes, is possible at any site, except for the sites $\nu, \nu - 1$. The second sum running over $\nu$ describes the second-order fluctuation of the ground-state, hence containing $N$ summands. To condense this into an overall sum over $d_1$ (Eq. (4.20)), the two missing summands of the ground-state fluctuation need to be accounted for separately.

Eq. (4.20) can also be verified by considering the nearest-neighbour limit case: From the high-field-limit TFIM it is known that in the nearest-neighbour case a phase transition occurs at $h/J = 1$. Since no topological excitation may occur in the polarized phase established by a high field, the first excitation in this phase corresponds to a spin flip. The energy gap of this quasi-particle closes linearly at the critical point, because the NN interaction only allows local hopping to the directly neighbouring sites (first-order hopping). At the other side of the phase transition, described by the ordered phase, the low-field-limit TFIM deploys the aforementioned topological excitation as the first possible excitation (for large $\alpha$). Evaluating its respective gap (Eq. (4.20)) for $\alpha \to \infty$ gives

$$
\Delta_{1\text{NN}} = 2 - 2 \cdot \lambda ,
$$

(4.21)

where $\zeta(\alpha \to \infty) = 1$ and $\lim_{\alpha \to \infty} \Delta_1 E_3(d_2) = 4$ for any $d_2$ (Eq. (3.12)) have been used. This is exactly the expected mirrored linear gap closure known for the high-field limit and is a consequence of the self-duality of the system at $\alpha \to \infty$ (Sec. 4) [4], [10].

25
4.2.3 Two-domain-wall state with distance 1 (trivial excitation)

In the long-range interacting regime of $\alpha \ll \infty$ the lowest of the 2DW excitations is the one with one flipped spin between the domain walls. In order to compare the energies of the two lowest excitations of the system $E_1$ and $E_{2;1}$ the second-order perturbation of this state is needed. Again, the zeroth order gives according to Eq. (3.7)

$$E_{2;1}^{(0)} = E_0 + 4 \cdot \zeta(\alpha).$$

For the first-order the term $P_{2;1} V P_{2;1} |\nu, \nu + 1\rangle$ needs to be considered. Since there is no possible way for $V$ to act in such a way, that the resulting state remains in the Hilbert space of states with 2DW, $d = 1$ from each other, the first order perturbation $E_{2;1}^{(1)}$ vanishes.

In the second-order perturbation term

$$P_{2;1} V Q_{2;1} \frac{1}{E_{2;1}^{(0)} - Q_{2;1} H_0 Q_{2;1}} Q_{2;1} V P_{2;1} |\nu, \nu + 1\rangle$$

(4.23)

4 processes can occur via the dual action of $V$ on the chain.

1. **Firstly**, it is possible to create two domain walls $|\mu, \mu + 1\rangle$ in the first place and annihilate them through the second application of $V$ (Fig. 4.4)

![Diagram](image)

Figure 4.4: First local contribution to second-order perturbation of $E_{2;1}$.

2. **Secondly**, a hopping of the two initial DWs $|\nu, \nu + 1\rangle$ may occur through the creation of any two DWs along the chain and the subsequent annihilation of the initial DWs leading to the state $|\mu, \mu + 1\rangle$ (Fig. 4.5 for $\mu = \nu - 2$).

$$2 \cdot \sum_{d_{2;1}} \frac{\lambda^2}{E_{2;1}^{(0)} - E_4^{(0)}(1, d_{2;1})} |\nu, \nu + 1\rangle.$$ (4.24)
This gives

$$\sum_{d_2=1}^{2} \frac{\lambda^2}{E_{2;1}^{(0)} - E_{4}^{(0)}(1, d_2, 1)} \left( |\nu - (d_2 + 1), \nu - d_2\rangle + |\nu + d_2 + 1, \nu + 1 + d_2 + 1\rangle \right). \quad (4.25)$$

Similar to the case of the hopping term in the perturbation of $E_1$ (Eq. (4.16)) a Fourier transformation into momentum space is necessary to get the exact eigenvalues of the perturbed Hamiltonian.

The momentum of the two domain walls $|\nu, \nu + 1\rangle$ can be characterised via a relative and a center of mass momentum. The resulting state after second-order perturbation remains in the $(2\text{DW}, d = 1)$-Hilbert space, hence the relative component of the momentum stays fixed. Only the center of mass momentum is hopping along the chain, hence the Fourier transform of the center of excitation $\nu' := (\nu + \nu + 1)/2$ is

$$|K\rangle = \frac{1}{\sqrt{N}} \sum_{\nu} e^{-iK\nu'} |\nu'\rangle \quad (4.26)$$

with $K$ denoting the center of mass momentum of the state $|K\rangle$. Eq. (4.25) contains a hopping of $|\nu\rangle$ to any place along the chain, hence the application of $|K\rangle$ on Eq. (4.25) gives

$$\begin{align*}
&= \left[ \frac{\lambda^2}{E_{2;1}^{(0)} - E_{4}^{(0)}(1, 1, 1)} - \frac{2 \cdot \cos(2K)}{2} + \frac{\lambda^2}{E_{2;1}^{(0)} - E_{4}^{(0)}(1, 2, 1)} - \frac{2 \cdot \cos(3K)}{2} + \ldots \right] |K\rangle \\
&= \lambda^2 \sum_{d_2=1}^{2} \frac{2}{E_{2;1}^{(0)} - E_{4}^{(0)}(1, d_2, 1)} \cos((d_2 + 1)K) |K\rangle. \quad (4.27)
\end{align*}$$
The third contribution is due to firstly annihilating $|\nu, \nu + 1\rangle$ arriving in the ground state and secondly creating two new domain walls $|\mu, \mu + 1\rangle$ somewhere on the chain (Fig. 4.6 and Fig. 4.7).

\[
\sum_{\mu} \lambda^2 E^{(0)}_{2;1} \left| \mu, \mu + 1 \right\rangle - E^{(0)}_0 \left| \nu, \nu + 1 \right\rangle + \sum_{\mu \neq \nu} \lambda^2 E^{(0)}_{2;1} \left| \mu, \mu + 1 \right\rangle - E^{(0)}_0 \left| \nu, \nu + 1 \right\rangle + \sum_{a=1} \left\{ \left| \nu, \nu + 1 \right\rangle + \sum_{a=1} \left| \nu + a, \nu + a + 1 \right\rangle + \left| \nu - a, \nu + 1 - a \right\rangle \right\}.
\]

Fourier transforming this expression in the same way as Eq. (4.27) gives

\[
\frac{\lambda^2}{E^{(0)}_{2;1} - E^{(0)}_0} \left[ 1 + 2 \cdot \sum_{a=1} \cos(aK) \right] |K\rangle . \quad (4.28)
\]

The last contribution to the second-order correction of $E_{2;1}$ is received through the application of the hopping term twice, arriving at an intermediate state $E_{2;2}$, the energy for which is different from $E_{2;1}$ in the long-range interacting system (Fig. 4.8):
The expression in the text is:

\[
T_0 T_0 |\nu, \nu + 1\rangle = T_0 (-\lambda) \sum_{\mu} b_{\mu}^\dagger b_{\mu+1} + b_{\mu} b_{\mu+1}^\dagger |\nu, \nu + 1\rangle
\]

\[
= T_0 (-\lambda) \left( |\nu - 1, \nu + 1\rangle + |\nu, \nu + 2\rangle \right)
\]

\[
= \lambda^2 \sum_{\mu} b_{\mu}^\dagger b_{\mu+1} + b_{\mu} b_{\mu+1}^\dagger (|\nu - 1, \nu + 1\rangle + |\nu, \nu + 2\rangle)
\]

\[
= \lambda^2 (|\nu - 1, \nu\rangle + |\nu + 1, \nu + 2\rangle + 2 \cdot |\nu, \nu + 1\rangle).
\]

Changing into $k$-space and evaluating the denominator of Eq. (4.23) gives

\[
\frac{\lambda^2}{\Delta E_{2;1} - \Delta E_{2;2}} \left( 2 \cdot \cos(K) + 2 \right) |K\rangle
\]

with $\Delta E_{2;i} = E_{2;i} - E_0$.

In total, Eq. (4.24), Eq. (4.27), Eq. (4.28) and Eq. (4.29) give the second-order correction of

\[
E_{2;1}^{(2)} = \sum_{d_2=1}^{\lambda^2} \frac{E_{2;1}^{(0)} - E_{2;2}^{(0)}}{E_{2;1}^{(0)} - E_{2;2}^{(0)}} \left[ 2 + 2 \cdot \cos((d_2 + 1)K) \right]
\]

\[
+ \frac{\lambda^2}{E_{2;1}^{(0)} - E_{0}^{(0)}} \left[ 1 + 2 \cdot \sum_{a=1}^{1} \cos(aK) \right]
\]

\[
+ \frac{\lambda^2}{\Delta E_{2;1} - \Delta E_{2;2}} [2 + 2 \cdot \cos(K)]
\]

This shows that the three $T-$operators $T_0, T_{+2}, T_{-2}$ in Eq. (4.3) respectively give a local and a hopping contribution to the second-order perturbation of a $(2;1)$ state.

One needs to be careful about the number of summands of the two sums in Eq. (4.30). The first
sum $2 \cdot \sum_{d_2=1} \text{contains} (N - 3) \text{summands since the process of adding two domain walls to already two existing ones is restricted by the hardcore nature of the domain walls allowing only one of such at any site. The second sum } 2 \cdot \sum_{a=1} \text{runs over } (N - 1) \text{summands because it covers the creation of two domain walls after having annihilated the initial ones. Hence, the sum runs over any site except the local term which is accounted for separately.}

Defining the total perturbed energy $E_{2;1}(\lambda, K) := E_{2;1}^{(0)} + E_{2;1}^{(2)}$ the gap between ground state and the $(2\text{DW}, d = 1)$ trivial state $\Delta^{2\text{DW}}$ evaluated at $K = 0$ becomes

$$
\Delta^{2\text{DW}} = E_{2;1}(\lambda, 0) - E_0(\lambda)
= 4 \cdot \zeta(\alpha) + \left( 2 \cdot \sum_{d_2=1} \frac{2 \cdot \lambda^2}{E_{2;1}^{(0)} - E_{1}^{(0)}(1, d_2, 1)} \right) + \frac{\lambda^2}{E_{2;1}^{(0)} - E_0^{(0)}} + (N - 1) \cdot \frac{\lambda^2}{E_{2;1}^{(0)} - E_0^{(0)}} + 4 \cdot \frac{\lambda^2}{\Delta E_{2;1} - \Delta E_{2;2}} + N \cdot \frac{\lambda^2}{4 \cdot \zeta(\alpha)}.
$$

Using $E_{2;1}^{(0)} - E_0^{(0)} = 4 \cdot \zeta(\alpha)$ (Eq. (3.7)) and $E_{2;1}^{(0)} - E_{4}^{(0)}(1, d_2, 1) := \Delta_{2;1} E_4(1, d_2, 1)$ this gives

$$
\Delta^{2\text{DW}} = 4 \cdot \zeta(\alpha) + \frac{\lambda^2}{4 \cdot \zeta(\alpha)} + \frac{4 \cdot \lambda^2}{\Delta E_{2;1} - \Delta E_{2;2}} + 2 \cdot \sum_{d_2=1} \left( - \frac{2 \cdot \lambda^2}{\Delta_{2;1} E_4(1, d_2, 1)} \right) + 2 \cdot N \cdot \frac{\lambda^2}{4 \cdot \zeta(\alpha)} - \frac{\lambda^2}{4 \cdot \zeta(\alpha)}.
$$

Condensing the extensive summand $2N \cdot \frac{\lambda^2}{4 \cdot \zeta(\alpha)} = (N - 3) \cdot \frac{2\lambda^2}{4 \cdot \zeta(\alpha)} + 3 \cdot \frac{2\lambda^2}{4 \cdot \zeta(\alpha)}$ with the sum over $d_2$ the final expression becomes

$$
\Delta^{2\text{DW}} = 4 \cdot \zeta(\alpha) + \frac{6\lambda^2}{4 \cdot \zeta(\alpha)} + \frac{4 \cdot \lambda^2}{\Delta_0 E_{2;1} - \Delta E_{2;2}} + 2 \cdot \sum_{d_2=1} \left( - \frac{2 \cdot \lambda^2}{\Delta_{2;1} E_4(1, d_2, 1)} + \frac{2\lambda^2}{4 \cdot \zeta(\alpha)} \right).
$$

(4.31)
5 Conclusions

In this section, the results of this work will be placed in the context of the current state of research regarding one-dimensional long-range interacting quantum Ising models. In particular, the publication of Laurens Vanderstraeten and his group [9] entails comparable numerical results for the topological and trivial excitations of the long-range TFIM at which a closer look will be taken in Sec. 5.2. Also, it is possible to bring the findings of this work in accordance with the high-field approach to the lrTFIM done by Sebastian Fey and Kai Schmidt [5] [6].

5.1 Evaluation of the results from second-order perturbation theory

In the first place, the outcomes for the ferromagnetic long-range TFIM will be considered.

![Figure 5.1: Energy gap of the 1DW (topological) and 2DW (trivial) excitation as a function of $\alpha$ for different field strengths $\lambda$.](image)

Fig. 5.1 shows the energy gaps of the two lowest excited states with 1DW (topological state) and 2DW with distance 1 (trivial state) as a function of $\alpha$ for fixed $\lambda$. As already seen in Sec. 3.4, the lowest excitation of the pure long-range Ising term ($\lambda = 0$) changes at $\alpha_c \approx 2.47875$ from the topological for $\alpha > \alpha_c$ to the trivial state for $\alpha < \alpha_c$. As Fig. 5.1 shows, the intersection value shifts to lower $\alpha$ as the transverse field is turned on.

For the many-body system, the physical relevance of the lowest excited state is that it can - for a sufficiently large perturbation with the transverse field - replace the ground-state as the energetically most favourable state. Hence, the energy differences of the topological and trivial
excitation to the ground-state energy after perturbation with the transverse field, the energy gaps, are of interest.

Fig. 5.2 shows the gaps as a function of $\lambda$ for the topological excitation on the left hand side and the trivial on the right hand side for different $\alpha$.

For the topological gap the linear term in $\lambda$ from first-order perturbation theory dominates over the quadratic term from second-order in Eq. (4.20). Also, the graph shifts downwards for increasing $\alpha$. This is due to the zeroth order, in which the contributions from the spins, that are antiferromagnetically linked across the domain wall are added up. For the topological excitation the number of bonds increases by the bond length. Therefore, the energy of the system increases drastically for $\alpha \to 2$ (Fig. 3.1 of unperturbed energy $E_1$).

As seen in Sec. 4.2.3 the first order vanishes for the trivial excitation, hence the gap approaches the $x$-axis quadratically. Although both plots do not include any third or higher-order terms in $\lambda$ a tendency of the gaps to approach zero for large enough $\lambda$ can be concluded from it.

Comparing the two gaps for fixed $\alpha$ (Fig. 5.3) reveals what has already been seen in Fig. 5.1. Whereas for $\alpha \lesssim 2.5$ the 1DW mode remains energetically above the 2DW upon varying $\lambda$, for $\alpha \gtrsim 2.5$ the 1DW mode drops under the 2DW mode in a region where $\lambda$ is small enough. It is also important to emphasize again that the graphs in Fig. 5.2 and Fig. 5.3 only include perturbation up to second-order making the graphs only valid for $\lambda \ll 1$. Any values for greater $\lambda$ need to be considered as an extrapolation from this and should be treated with special care.

As previous work from the high-field limit to the lrTFIM yields [5], [6], the second-order phase transition of the nearest-neighbour TFIM from a polarized phase with $\mathbb{Z}_2$-symmetry for high fields to a symmetry-broken ordered phase for low fields at $\lambda_c = 1$ can also be observed in the long-range model but with varying critical $\lambda$ dependent on $\alpha$. This is shown in Fig. 5.4.

The critical parameter there corresponds to $(J/2h)_c$. A conversion of these high-field values into the low-field units gives the $\lambda_c^{(hl)}$ stated in Table 5.1. The comparison of the $(J/2h)_c$ with
Table 5.1: Comparison of the critical parameter $\lambda_c = (h/J)_c$ in the low-field ($\lambda_c^{(lf)}$) and high-field ($\lambda_c^{(hf)}$) approach. The values $(J/2h)_c$ are obtained from Fig. 5.4 [6].

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\lambda_c^{(lf)}$</th>
<th>$\lambda_c^{(hf)}$</th>
<th>$(J/2h)_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>2.99</td>
<td>2.523</td>
<td>0.198</td>
</tr>
<tr>
<td>2.5</td>
<td>1.84</td>
<td>1.78</td>
<td>0.283</td>
</tr>
<tr>
<td>3</td>
<td>1.41</td>
<td>1.42</td>
<td>0.351</td>
</tr>
<tr>
<td>5</td>
<td>1.06</td>
<td>1.067</td>
<td>0.468</td>
</tr>
</tbody>
</table>

Figure 5.3: Comparison of the gaps from second-order perturbation theory of the 1DW and the 2DW excitation.

Figure 5.4: Results for the critical parameter $\lambda_c = (J/2h)_c$ and the critical exponents $\nu$ of the IrT-FIM phase transition as a function of the coupling strength $\alpha$. The data corresponds to LCE/MCMC simulations in the high-field limit from Ref. [6] and data from exact diagonalization (ED) from Ref. [7].
the $\lambda_{c}^{(hf)}$ shows that the $\alpha$-region in Fig. 5.4 where the critical parameter drops from the nearest-neighbour to the mean-field universality class corresponds to an increase of the $\lambda_{c}^{(hf)}$ in the same $\alpha$-region. The critical values $\lambda_{c}^{(l)}$ in Table 5.1 are extrapolated from the second-order perturbation theory in Fig. 5.3. Therefore, the gap closure point of the lower excitation at $\lambda = 0$ is read off for fixed $\alpha$. Especially for larger $\alpha$ a good agreement with the converted values $\lambda_{c}^{(bf)}$ can be observed. In the region of small $\alpha$, however, the missing higher orders in the perturbation calculations for $\lambda_{c}^{(l)}$ seem to become more important. Nevertheless, this is a strong indication that the second-order perturbation theory done in this work already yields a good approximation for the low-energy behaviour of the lrTFIM.

### 5.2 Comparison with the numerical data

In this section, a comparison of the established results for the ferromagnetic lrTFIM with numerical data provided by the group of L.Vanderstraeten [9] will be made.

Since the results for second-order perturbation theory are only valid for small enough $\lambda$ a first comparison for fixed $\lambda = 0.25$ is made in figure 5.5.

![Comparison of energy gaps](attachment:image.png)

Figure 5.5: Comparison of the energy gaps from second-order perturbation theory with numerical data provided by [9].

It is noticeable that whereas the data for the trivial excitation shows a perfect agreement with the analytic formulae, the topological excitation seems to be handled differently by the numeric algorithm. One explanation might be that the sum of exponentials describing the long-range interaction in the numerical approach needs to get approximated by a finite number of terms. This corresponds to a neglect of high interaction distances in the algebraically decaying interaction energy. Yet, the large distances become significant for $\alpha \to 2$ for the energy of the topological excitation (see derivation for $E_1$ Eq. (3.4)), which would explain the deviations in Fig. 5.5 as $\alpha \to 2$. This notion has been checked by approximating the infinite sums for the 1DW (Eq. (4.20)) and the 2DW gap (Eq. (4.31)) with the first $N$ summands. Fig. 5.6 shows the result.

To reach the displayed agreement, the number of summands $N$ has been estimated by eye and continuously varied from 5000 for $\alpha = 2.1$ to 1000 for $\alpha > 2.5$. For the 2DW gap the same
approximation with $N = 1000$ does not change the result. This is due to the fact that the energy corresponding to this excitation diverges only for $\alpha \to 1$.

The total result of comparing the analytic results with the numerical data is illustrated in Fig. 5.7. Apart from the shift for the topological excitation, which may be explained with the use of the described approximation, the data stands in good agreement with each other.

Figure 5.7: Comparison of data from second-order perturbation theory with numerical data by L. Vanderstraeten [9] for $\alpha = 2.0, 2.25, 2.5$. 

Figure 5.6: Comparison of the adjusted formulae for the 1DW and 2DW gap (Eq. (4.20) and Eq. (4.31)), where the sums have been cut off after $N$ summands, with the numerical data.
6 Summary and Outlook

In this Bachelor thesis, the low-energy behaviour of the long-range transverse field Ising chain at zero temperature has been investigated (Eq. (2.2)). In the first part, the long-range Ising term has been considered in isolation leading to an exact description of the excitation energies both for the ferromagnetically and the antiferromagnetically interacting chain (Sec. 3). The developed iterative scheme works such that the excitations are classified according to the number of domain walls their respective eigenstate exhibits. For \( \geq 2 \) domain walls, the relative distance between the domain walls accounts for different corresponding eigenenergies. It has also been seen, that the excitation energies for the ferromagnetic chain diverge for an interaction constant of \( \alpha \leq 1 \) for an even number of domain walls and \( \alpha \leq 2 \) for an odd-DW excitation regarded with respect to the ground-state energy. In the antiferromagnetic case, in contrast, it is possible to obtain reasonable values of the excited energies also in the regime of \( 0 < \alpha < 1 \) (Sec. 3.6). In the all-to-all interacting case of \( \alpha = 0 \), it is possible to define a macroscopic spin incorporating any spins of the chain which determines the energy of the system in this limiting case. For the 1DW excitation, however, this approach seems to conflict with the evaluation of the expression that has been deduced from the ferromagnetic case at \( \alpha = 0 \).

In the further course of this work, the expressions for the excitation energies have been used to apply degenerate perturbation theory with regard to small transverse fields to the ferromagnetic long-range Ising chain. There, the energy gaps of the two lowest excitations of the system, one of which corresponding to the 1DW state with two ground-state configurations left- and rightwards of the domain wall and the other one corresponding to one spin flip in the chain, have been evaluated (Sec. 4). In second order perturbation theory both of these gap energies approach zero for a sufficiently large perturbation that depends on the interaction constant \( \alpha \) (Fig. 5.3). The evaluation of the local and non-local quantum fluctuation processes occurring in first- and second-order perturbation reveal that the 1DW gap closes linearly and the 2DW gap quadratically. Furthermore, the two excitation energies are crossing for \( 2.4 \lesssim \alpha \lesssim 2.5 \), if the field is fixed at a small value (Fig. 5.1). This outcome can be put into context with the phase transition that the lrTFIM exhibits from the polarized phase at large fields to the \( \mathbb{Z}_2 \) symmetry-broken ordered phase at low fields. As already indicated, a change of the low-energy excitation form the 1DW to the 2DW excitation affects the gap closure behaviour and hence the critical exponent at the phase transition. Therewith, it provides an explanation of the change of critical exponents upon varying \( \alpha \) that has been revealed in the course of recent research considering the high-field approach to the lrTFIM ([5], Fig. 5.4).

Another verification of the found results has been conducted via comparing them with numerical data that has been generated for the lrTFIM using tensor network techniques (Sec. 5.2). Here, it has been shown that the numerical model runs into accuracy problems if the 1DW gap is considered close to the divergence of the 1DW excitation at \( \alpha = 2 \). This has been demonstrated by approximating the infinite sums in the expression for the 1DW gap with a certain finite number
of summands (Fig. 5.6).

In summary, the results of this work show a deeper insight into the ferromagnetic interacting long-range spin chain. Apart from the unperturbed Ising energies, the perturbation theory calculations for the antiferromagnetic Ising chain are still missing. As Fig. 3.2 shows, the two interesting low-energy excitations in the pure Ising chain are in that case the 1DW excitation and the 2DW excitation with distance $d = 2$. They crossover at $\alpha \approx 0.4$ which might affect the nature of a phase transition in the AF-lrTFIM.

Additionally, it is possible to pursue the strong coupling expansion (Eq. 4.1) of the ferromagnetic 1DW and 2DW gaps to higher orders in the transverse field. Any contributions from further different quantum fluctuations that will occur there can be evaluated with the formulae given in Sec. 3. However, it might be recommendable to automatize the combinatorics leading to the different contributions of higher orders.
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