Quantum paramagnetism in the kagome and triangular transverse field Ising model
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Abstract

In this thesis the antiferromagnetic transverse field Ising model on the kagome and triangular lattice is studied. The physics of these systems is governed by the interplay of quantum fluctuations and geometrical frustration. For zero field both systems exhibit a classically disordered ground-state manifold with macroscopic degeneracy. Quantum fluctuations induced by the transverse field give rise to novel quantum ordering phenomena which are known as 'order by disorder' and 'disorder by disorder'. For the triangular lattice, existing results are indicating a quantum ordered phase arising from classical disorder. Contrary, the kagome is suggested to continue into a quantum disordered phase that is adiabatically connected to the high-field limit. Yet there is no conclusive evidence. A major goal of this thesis is to provide further evidence supporting the disorder by disorder conjecture. For this purpose, we investigate the high-field limit, where both models exhibit a gapped paramagnetic phase. A persisting paramagnetic phase, expected for the kagome lattice, requires that the excitation gap stays finite for arbitrary transverse field. We use a perturbative continuous unitary transformation to derive an effective low-energy model that allows to determine the one-particle dispersion as a high order series expansion. The resulting lowest energy band is flat up to order seven in perturbation theory indicating the existence of a localized mode. The results provide evidence for a disordered paramagnetic phase that is adiabatically connected to the low-field limit. Additionally, a consistency check is performed by means of an exact diagonalization method in the low-field regime. For the triangular lattice the perturbative approach predicts a quantum phase transition which is compatible with the 3dXY universality class.
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Chapter 1

Introduction

One of the most fundamental ideas in condensed matter theory is the concept of phase transitions. A phase describes the state of a many body system that is characterized by macroscopic physical properties emerging from its underlying constituents. Usually, the phases of a system can be associated with different symmetries that are in general conditioned by intensive parameters as temperature, pressure, magnetic or electric fields, etc. If an intensive parameter falls below a certain critical value the state of the system commonly evolves into a phase of lower symmetry. One may think of the process of freezing where the constituents of a liquid are forming a crystalline structure below a critical temperature as depicted in Figure 1.1. In this case one also speaks of a classical disorder-order transition as the crystalline structure of the solid phase manifests a certain order in contrast to the disordered liquid phase. The notion of order and disorder also plays an important role in the context of magnetism. The magnetic properties of ferromagnets for example are attributed to the ordering of the magnetic moments that are assigned to the spins of the molecules or atoms. Below the Curie temperature that is specific to the material the interactions between the spins tend to align the magnetic moments in a parallel way causing a permanent macroscopic magnetization as shown in figure 1.2. For antiferromagnets the spins instead favor an antiparallel ordering which is also known as Néel-order (see figure 1.2). Once the temperature exceeds the critical value the long-range order of the magnetic moments is destroyed by thermal fluctuations and the system evolves into a so called paramagnetic phase. Although both interactions responsible for the alignment of the spins are of quantum mechanical nature the described order-disorder transitions are purely classical phenomena as they are driven by thermal fluctuations. A fascinating equivalent of classical order-disorder phenomena occurs in the class of quantum phase
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Figure 1.1: Illustration of the phenomenon of symmetry-breaking in the case of freezing. When the temperature drops below a critical value $T_c$, the disordered liquid evolves into a solid state of crystalline structure. As a result, translational as well as rotational symmetries are broken.

Figure 1.2: Illustration of ferromagnetic and antiferromagnetic ordering. Above a critical temperature the order is destroyed by thermal fluctuations.

transitions (QPTs) [30]. In contrast to classical phase transitions, QPTs only occur for zero temperature $T = 0$. Hence, they are characterized by a nonanalyticity of the ground-state energy. Instead of thermal fluctuations this transitions are driven by quantum fluctuations arising due to the Heisenberg uncertainty principle. Quantum order may occur in a similar vein to the ordering induced by thermal fluctuations. However, it turns out that it exhibits a much richer and less trivial behaviour especially in the presence of strong quantum fluctuations where the nature of a possible ordering often remains unclear. Figure 1.3 illustrates a typical phase diagram in the vicinity of such a quantum critical point, where a quantum ordered state evolves into a quantum disordered one. In this thesis the main focus is on quantum order and disorder phenomena manifested in magnetic spin systems. In analogy to the classical
Figure 1.3: Illustration of a phasediagram in the vicinity of a quantum critical point (QCP). $g$ denotes some non-thermal parameter of the Hamiltonian driving a quantum phase transition from a quantum ordered into a quantum disordered phase. Although a QCP exists only for zero temperature $T = 0$ there are also regions of finite temperature that are effected by the QCP. This area is called quantum critical. [30]

case a quantum disordered magnetic system is refered to as a quantum paramagnet or cooperative paramagnet (see for example [29]). Because of the exponentially decaying spin correlations these systems are also called quantum spin liquids (QSLs). One of the most remarkable characteristics of a quantum spin liquid is the lack of any magnetic order down to arbitrary small temperatures due to a supression by quantum fluctuations. QSLs are of great theoretical interest as they are related to the resonating-valence-bond states proposed by Anderson as a possible description of high-temperature superconductivity [1]. Moreover, it is expected that QSLs may exhibit collective magnetic excitations featuring fractional quantum numbers [32].

An interesting mechanism that allows for the incidence of disordered phases at zero temperature is a phenomenon called frustration [36]. Frustration occurs when competing interactions of a system lead to a huge number of coequal ground-state configurations. When the system approaches zero temperature the large ground-state degeneracy supresses any ordering as there exists no distinguished ground-state. The great interest on the realization of quantum disordered states has drawn considerable attention on geometrically frustrated magnetic systems [2]. These systems are subject of intensive research especially in the context of the intriguing spin-ice phase which was first observed in pyrochlores as dysprosium titanate and holmium titanate [4]. The most astonishing feature of spin-ice is the emergence of magnetic monopoles.
This property was theoretically predicted in 2008 \[5\]. First experimental indications were found in 2009 \[3\]. The nature of spin-ice can be attributed to a geometrical frustration of magnetic moments which is effected by long range magnetic dipolar interactions.

One of the simplest magnetic models exhibiting frustration is the classical Ising model with nearest neighbour coupling providing that the spins and their interactions are arranged in a certain fashion. As an example consider the plaquettes in figure 1.4. The sign of the Ising coupling $J$ determines the favored alignment between two neighbouring spins. In both cases there is no configuration that satisfies every bond. One spin always remains frustrated. As a result the number of configurations minimizing the energy is particularly large. The frustration results only from the geometrical properties of the system. Ising models on lattices formed by frustrating plaquettes as for example the triangular or kagome lattice consequently exhibit an extensive ground-state degeneracy which results in a macroscopic entropy density at zero temperature \[38\]. The ground-state manifold of these Ising antiferromagnets is classically disordered. However, they may also give rise to quantum frustration. One could think of quantum frustration as a possible effect of introducing quantum dynamics into the highly degenerate ground-state manifold of an Ising antiferromagnet. Quantum dynamics can be induced by an additional perturbation. Naturally, an additional non-commuting term will allow quantum fluctuations within the ground-state manifold as well as fluctuations leaving the ground-state manifold. Consequently, the macroscopic ground-state degeneracy is lifted to some degree leading to a discontinuity of the entropy density for infinitesimal perturbation at zero temperature. The
singular character of the perturbation becomes manifest in a highly non-trivial problem of degenerate perturbation theory. It is clear that fluctuations within the ground-state manifold will gain the most energy due to the perturbation. Thus, particular configurations from the classical disordered ground-state manifold are selected by quantum fluctuations to compose the new ground-states of the perturbed system. The interesting question is whether the new ground-states exhibit some kind of quantum order, or whether the system continues into a quantum disordered phase. The latter statements are put together in a sketch in figure 1.5. Both scenarios are fascinating in the sense that they describe an elusive transition from a classical disorder into a non trivial quantum mechanical version of order and disorder. In the literature these phenomenas are known as 'order by disorder' and 'disorder by disorder' (see for example [20]). The first instance of order by disorder was examined by J.Villain et al. in 1980 in generalized frustrated two-dimensional Ising models [37]. In the last decade several systems were discovered to exhibit order by disorder phenomena [31, 35, 40], among others the frustrated diamond-lattice antiferromagnet [2].

The possibility of a disordered quantum phase evolving from classical disorder was first discussed by Fazekas Anderson in 1974 in the context of resonating valence-bond states [8]. A particular simple instance of disorder by disorder was found in the one-dimensional frustrated triangular Ising chain (sawtooth chain) in transverse field [25].

To date, there are not many cases of disorder by disorder known in the literature. In the recent years a number of frustrated magnetic models exhibiting this novel ordering phenomena was studied by Roderich Moessner et al. [20, 21]. Among other
things, they show that the triangular Ising antiferromagnet in transverse field exhibits an interesting order by disorder transition featuring a bond ordered phase \[15\]. Furthermore, they suggest that the kagome transverse field Ising model may provide a remarkable instance of disorder by disorder, though there is no conclusive evidence. Following up the work of Roderich Moessner, we want to study one of the antiferromagnetic Ising model in transverse field which is one the most exemplary and paradigmatic models of quantum frustration. Considering, a frustrated Ising antiferromagnet, the simplest way to induce quantum dynamics is the introduction of a transverse field. Thus, this model provides a concrete and mathematically tractable system that allows to study the effects of quantum frustration and the resulting quantum order and disorder phenomena.

The focus is on the analysis of the kagome transverse field Ising model (TFIM). Our major objective is the verification of the gapped paramagnetic phase which is expected to persist for arbitrary fields providing a new instance of disorder by disorder. For this purpose, we investigate the first excitation gap by using a quasi-particle conserving continuous unitary transformation which is performed in a perturbative fashion about the high-field limit. The resulting perturbation expansion of the gap is extrapolated with appropriate techniques which allow to estimate the energy gap for arbitrary transverse field. Furthermore we analyze the triangular lattice as an instance of order by disorder and compare our findings with recent results \[15\].

Technically our approach is related to the work of Priour et al. on the one-dimensional TFIM Ising sawtooth chain \[25\], which suggests that a perturbative treatment about the high-field limit might be an appropriate approach to examine TFIMs with disorder by disorder on higher dimensional lattices.

Indeed our findings show strong evidence for a persisting spin liquid phase in the case of the kagome TFIM implying a novel disorder by disorder transition. Furthermore, the perturbation expansion about the high-field limit reveals that the lowest energy band stays flat up to order \( n = 7 \) giving rise to a localized mode similar to localized Magnon states in related models \[28, 33\]. The locality of this mode is destroyed by quantum fluctuations in order \( n = 8 \) effecting a \( \sqrt{3} \times \sqrt{3} \)-structure. Interestingly, thermal fluctuations in the classical kagome antiferromagnet provide the same ordering behaviour \[27\].
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1.0.1 Outline

This thesis can be divided into three parts. The first part comprises chapter 2 to chapter 5 and covers all relevant methodical aspects. In chapter 2 the concept of perturbative continuous unitary transformations is introduced. This method features a linked cluster expansion which makes it particularly applicable to higher dimensional lattice models. Chapter 3 provides technical details on an automated linked cluster expansion. In chapter 4 Pade and DlogPade extrapolation techniques are presented. These tools provide important complementary methods in combination with perturbative approaches. The last methodical chapter deals with an exact diagonalization technique based the Lanczos algorithm. Chapter 6 incorporates the main part of this work. It is divided as follows.

The first sections introduce the transverse field Ising model on the kagome and triangular lattice including the current state of research as well as the mathematical and physical aspects of the model. The second part describes the explicit application of the particle-conserving perturbative continuous unitary transformation. The physical picture of the resulting effective one-particle Hamiltonian is elucidated in detail. The results for the one-particle properties are presented and discussed.

Finally, the one-particle excitation gap is investigated by means of pade and dlogpade extrapolation. In addition, an approach based on the Lanczos algorithm is used to study the low field regime on the kagome lattice. The application and the results are presented seperately for each lattice.

The last chapter provides a concluding summary on the main findings and an outlook on future perspectives.
Chapter 2

Perturbative CUT

In this section the basic concept of perturbative continuous unitary transformations (pCUT) \cite{17,18} is presented. The objective of pCUT is the derivation of an effective low-energy model that conserves the number of quasi-particles. The structure of the resulting effective Hamiltonian provides a simple and intuitive picture of the physical system and allows for the calculation of quantities as for instance the ground-state energy and the one particle dispersion. Furthermore, by calculating the excitation gap one is able to detect second order phase transitions.

The first section briefly introduces the concept of continuous unitary transformations which form the basis of the correspondent perturbative approach. The main scheme of the method and its application to a large class of problems is discussed. In the second part the cluster additivity and the linked cluster theorem as a consequence of the flow equations are examined.

2.1 Continuous Unitary Transformation

The concept of Continuous Unitary Transformations which was independently proposed by Wegner \cite{9} and Wilson and Glazek \cite{11} is based on the idea of simplifying the Hamiltonian of an examined many-body system by finding a convenient basis. Mathematically, the translation from an initial orthonormal basis into another orthonormal basis is performed by an unitary transformation. As a trivial example consider the two-dimensional $\sigma_z$- eigenbasis $|1\rangle$ and $|0\rangle$ describing a spin-$\frac{1}{2}$ system.
The spinflip operator represented by the $\sigma_x$-matrix becomes diagonal, when one performs the transformation

$$\{ |1\rangle, |0\rangle \} \rightarrow \{ |v_1\rangle, |v_2\rangle \}$$

with

$$|v_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |0\rangle) \quad |v_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |0\rangle).$$

The corresponding matrix is given by

$$U_{ij} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

This new basis would be the ideal description for a spin-$\frac{1}{2}$ system coupled to a magnetic field in the $x$ direction. In this particular case, the transformation can be regarded as a rotation of spin coordinates. Of course this example is very simple, but for most of the typical many body systems this problem is highly nontrivial. The larger the dimension of the Hilbert Space the larger may be the distance between the initial basis and the optimal one. So instead of performing the unitary transformation at once one may think of slowly rotating the basis in a controlled continuous fashion until the optimal basis is reached. For this purpose, one defines a continuous parameter $l$ such that $l = 0$ corresponds to the initial basis which transforms with increasing $l$ and finally reaches the desired basis for $l = \infty$. The unitary transformation $U(l)$ is then given by a sequence of infinitesimal unitary transforms $e^{\eta(l)dl}$ driven by the antihermitian generator

$$\eta(l) = -U^\dagger(l) \partial_l U(l).$$  \hspace{1cm} (2.1)

The change of the Hamiltonian during this transformation can then be expressed by the flow equation

$$\partial_l H(l) = [\eta(l), H(l)].$$  \hspace{1cm} (2.2)

As one can see, the flow of the Hamiltonian is determined by the choice of the antihermitian operator $\eta(l)$. Hence, the decisive step is to choose an appropriate generator so that the effective Hamiltonian $H_{\text{eff}} = H(l = \infty)$ becomes easier. A subtle choice for $\eta$, that was first proposed by Wegner [9], is given by

$$\eta^W(l) = [H_d(l), H(l)].$$  \hspace{1cm} (2.3)

where $H_d$ denotes the diagonal part of the Hamiltonian. Demanding that $H(l = \infty) = H_{\text{eff}}$, implies that the change of $H(l)$ vanishes $\Rightarrow \partial_l H(\infty) = 0$. This is equivalent to
\( \eta(l = \infty) = [H_d(l = \infty), H_{\text{eff}}] = 0 \). Provided that there is no degeneracy, \( H_{\text{eff}} \) has to be diagonal in order to satisfy this equation which was our aim in the first place. One can show that the non diagonal terms indeed vanish for \( l \rightarrow \infty \).

Another useful generator is the particle conserving generator \( \eta^Q \). In the following \( Q \) denotes the operator that counts the number of elementary excitations \( Q |n\rangle = n |n\rangle \).

Then one demands that the effective Hamiltonian commutes with \( Q \), i.e. \( [Q, H_{\text{eff}}] = 0 \).

The matrix elements of the generator in the \( Q \) eigenbasis \( \{|n\rangle |n \in \mathbb{N}\} \) are given by

\[
\eta^Q_{ij}(l) = \text{sgn}(q_i(l) - q_j(l)) H_{ij}(l).
\tag{2.4}
\]

Therefore the number of elementary excitations is a conserved quantity in the effective model. In this case the effective Hamiltonian can be written as

\[
H_{\text{eff}} = \sum_{n=0}^{\infty} H_n
\tag{2.5}
\]

where \( H_n \) is a \( n \)-particle irreducible operator, which means that the Hamiltonian is blockdiagonal in the number of elementary excitations. Figure 2.1 depicts the structure of the effective Hamiltonian in the QP basis \( \{|n\rangle |n \in \mathbb{N}\} \).

This effective Hamiltonian provides a very intuitive and substantially simplified picture of the physical system. All the \( n \)-particle energies are contained in the corresponding block \( H_n \). Consequently, \( H_0 \) comprises the physics of the ground-state manifold, whereas \( H_1 \) contains one-particle properties and so on. In this sense the
intricate many-body problem has been simplified to a few-body problem. In most cases the flow equations lead to an infinite set of differential equations as the commutator $[\eta(l), H(l)]$ generates new terms not contained in the original Hamiltonian. Therefore, one has to find an appropriate truncation scheme that captures the relevant physics. There are various methods based on CUTs that use different truncation schemes as for instance self-similar CUT [13], graph based CUT [39] and the directly evaluated CUT [19].

Besides, continuous unitary transformations also provide a basis for a perturbative treatment based on the quasi-particle conserving generator [18]. Here one choses a perturbative ansatz for the Hamiltonian and the particle conserving generator up to a certain order in a perturbation parameter. This leads to set of finite flow equations which can be solved recursively. The advantage of this method is that no truncation error is made up to the given order. Furthermore the calculations can be performed on finite clusters. Perturbative Continuous Unitary Transformations (pCUT) are an essential tool used in this thesis. A discussion on the corresponding formalism is given in the next section.

2.2 Formalism

At first let us specify the class of systems pCUT is applicable to. The models under consideration are defined on a lattice $\Gamma$. On each lattice site the dimension of the local Hilbert space is given by $d$. The interactions between this local degrees of freedom are assumed to be of finite range. Hence, the Hamiltonian is a sum of local operators acting on a finite number of sites. The model examined in this thesis is a spin system that can be completely described in terms of bosonic excitations. Therefore, only bosonic systems with symmetric states are considered, although a fermionic treatment is also possible.

The initial point is determined by a Hamiltonian that can be decomposed in the following way

$$H(x) = H_0 + xV.$$  (2.6)

The energy spectrum of $H_0$ is required to be equidistant and bounded from below. Such a system can always be represented by a Hamiltonian

$$H_0 = \sum_{i\in\Gamma,\alpha} \Delta_\alpha a_{i,\alpha}^{\dagger}a_{i,\alpha} + E_0$$  (2.7)
with the ground-state energy $E_0$ and bosonic (or fermionic) creation/annihilation operators $a_{i,\alpha}^\dagger / a_{i,\alpha}$. Information about additional quantum numbers may be encoded in $\alpha$. For simplicity, the index $\alpha$ will be dropped in the following. Furthermore, only bosonic operators $a^{(\dagger)} := b^{(\dagger)}$ are considered. Figure 2.2 illustrates an exemplary energy spectrum of $H_0$. Physically one can interpret this system as a conglomerate of quasi-particles above the vacuum. Those particles have no kinetics and do not interact, hence the problem is in principle solved for $x = 0$. For $x > 0$ the perturbation term $x V$ in general will induce kinetics and interactions leading to a non-trivial problem. The idea now is to describe the new system in terms of the quasi-particles of the unperturbed system. For this purpose, one can use a CUT that leads to an effective Hamiltonian that conserves the number of quasi-particles. This results in the following commutator equation

$$[H_{\text{eff}}, Q] = 0,$$  \hspace{1cm} (2.8)

provided that the operator $Q$ counts the number of quasi-particles. As already mentioned in [reference] this transformation can be achieved by using the particle conserving generator $\eta^Q$. Assuming that the ground-state of $H(x)$ is adiabatically connected to the one of $H(0) = H_0$, the new physical picture is valid as long as the system does not undergo a phase transition. Consequently, the initial eigenbasis of $H_0$ can be be
continuously linked to the desired optimal basis for \( H(x) \). That in turn, implies that
the transformed Hamiltonian and the generator can be expanded as a power series
in \( x \), which allows for a perturbative treatment.

The form of the transformed Hamiltonian and the generator depend on the structure
of the perturbation \( V \). In general \( V \) can be written as

\[
V = \sum_{n=-N}^{N} \, T_n, \tag{2.9}
\]

where \( T_n \) stands for an operator that decrements or increments the number of particles
by \( n \):

\[
[T_n, Q] = nT_n. \tag{2.10}
\]

In order to ensure the existence of a series expansion in \( x \) one has to restrict to fi-
nite \( N \), which means that states are connected by the perturbation, if their particle
number differs by \( \Delta n \leq N \).

With this setup the general form of the Hamiltonian during the unitary transforma-
tion is given by

\[
H(x, l) = H_0 + \sum_{k=1}^{\infty} \, \sum_{|m|=k} x^k \, F(l, m) T(m), \tag{2.11}
\]

introducing the notation

\[
m = (m_1, m_2, \ldots, m_k) \tag{2.12}
\]
\[
m_i \in \{ -N, N \} \vee m \in \mathbb{Z} \tag{2.13}
\]
\[
|m| = k \tag{2.14}
\]
\[
T(m) = \prod_{i=1}^{k} T_{m_i} \tag{2.15}
\]
\[
M(m) = \sum_{i=1}^{k} m_i. \tag{2.16}
\]

This ansatz in principle follows from common perturbation theory, which states that
the correction in order \( k \) is given by a term proportional to \( V^k \). With \( 2.9 \) this results in
a sum of all possible sequences of \( T_n \) operators weighted by real functions \( F(l, m) \). To
determine the \( F(l, m) \) one solves the flow equation \( 2.2 \) by using the particle conserving
generator \( 2.4 \) that reads

\[
\eta(x, l) = \sum_{k=1}^{\infty} \, \sum_{|m|=k} x^k \, \text{sgn}(M(m)) \, F(l, m) T(m). \tag{2.17}
\]
For this generator one can show that functions $F(l, m)$ with $M(m) \neq 0$ vanish in the limit $l \to \infty$, so that in the end only the particle conserving terms with $M(m) \neq 0$ remain. The corresponding functions are determined by a set of recursive differential equations with initial conditions $F(0, m) = 1$ for $|m| = 1$ and $F(0, m) = 0$ for $|m| = 0$. Those equations can be solved analytically order by order, finally leading to the coefficients $C(m) := F(l \to \infty, m)$. Since the computational effort increases with higher order the maximum obtainable order $n_{\text{max}}$ is limited by the available computational resources. The resulting effective Hamiltonian reads

$$H_{\text{eff}}^{n_{\text{max}}} = H_0 + \sum_{k=1}^{n_{\text{max}}} x^k \sum_{|m| = k, \sum m_i = 0} C(m) T(m). \quad (2.18)$$

Because of the restriction $\sum m_i = 0$, $H_{\text{eff}}$ is blockdiagonal in the number of quasi particles (see figure 2.1). Hence, $H_{\text{eff}}$ can be written as the sum of $n$-irreducible operators $H_n$ (see eq. (2.5)). In second quantization those operators read

$$H_0 = E_0 I \quad (2.19)$$
$$H_1 = \sum_{i,j} t_{j,i} b_j^\dagger b_i \quad (2.20)$$
$$H_2 = \sum_{i_1,j_1,j_2} t_{j_1,j_2,i_1,i_2} b_{j_1}^\dagger b_{j_2}^\dagger b_{i_1} b_{i_2} \quad (2.21)$$
$$\vdots$$
$$H_n = \sum_{i_1,\ldots,i_n,j_1,\ldots,j_n} t_{j_1,\ldots,j_n,i_1,\ldots,i_n} b_{j_1}^\dagger \ldots b_{j_n}^\dagger b_{i_1} \ldots b_{i_n} \quad (2.22)$$

with the identity operator $I$ and local bosonic operators $b_i^{(\dagger)}$ annihilating (creating) a quasi particle at site $i$. This structure allows to calculate $n$-particle energies by diagonalizing the corresponding $n$-particle blocks. To determine the $n$-particle block in the spatial domain one has to apply the effective Hamiltonian on the eigen-states of the particle number operator $Q$:

$$|0\rangle \quad \text{ground-state (particle vacuum)} \quad (2.24)$$
$$|i\rangle \quad \text{state with one particle located on site } i$$
$$|i_1 i_2\rangle \quad \text{state with two particles located on site } i_1 \text{ and } i_2$$
$$\vdots$$
Due to the normal ordering of the bosonic operators in (2.23), $H_n$ only acts on states with $m \geq n$ particles: $H_n |i_1i_2 \ldots i_m\rangle = 0$ for $m < n$. The true $n$-particle contributions can be extracted by

$$P_0 H_0 P_0 := P_0 H_{\text{eff}} P_0$$

$$P_1 H_1 P_1 := P_1 H_{\text{eff}} P_1 - P_1 H_0 P_1$$

$$P_2 H_2 P_2 := P_2 H_{\text{eff}} P_2 - P_2 H_0 P_2 - P_2 H_1 P_2$$

$$\vdots$$

$$P_n H_n P_n := P_n H_{\text{eff}} P_n - \sum_{i=0}^{n-1} P_n H_i P_n$$

with projectors on the $n$-particle subspace $P_n = \sum_{\langle j_1 \ldots j_n \rangle} |j_1j_2 \ldots j_n\rangle \langle i_1i_2 \ldots i_n|$. Although $H_n$ acts on the full many-particle Hilbert space, it is sufficient to know its action on the $n$-particle Hilbert space to determine the relevant matrix elements.

For the sake of completeness, it should be noted that observables can be treated by the same unitary transformation which allows to calculate arbitrary $n$-particle quantities and correlation functions. For further details see [17].

### 2.3 Cluster decomposition

Next, one can analyze the general structure of the effective Hamiltonian in (6.17). As already discussed the $n$-th order term is a sum of all possible products of $n$ $T_m$ operators conserving the number of particles weighted by $C(m)$. These sequences can be further split into local sequences using the decomposition

$$T_m = \sum_k \tau_{m,k}$$

with $\tau_{m,k}$ creating or annihilating $m$ quasi particles in a local area labeled by the index $k$. The action of $\tau_{m,k}$ depends on the explicit structure of the interaction induced by the perturbation $V$. In the case of a nearest neighbour Ising coupling the sum runs over all corresponding nearest neighbour bonds and the index is replaced by $k = \langle i,j \rangle$. For general $n$-site interactions the sum runs over all local $n$-site bonds. In every order $n$ one has virtual fluctuations of length scale $n$ (the exact number of sites involved depends on the order and the interaction) determined by the $\tau$ sequences.

By reorganizing these terms the effective Hamiltonian can be decomposed into a sum.
of finite clusters

$$H_{\text{eff}} = \sum_{n} x^n \sum_{m : \sum m_i = 0} C(m) \sum_{\{k_1, k_2, \ldots, k_n\}} \tau_{m_1, k_1} \tau_{m_2, k_2} \cdots \tau_{m_n, k_n}$$  \hspace{1cm} (2.27)$$

$$= \sum_{n} x^n \sum_{\{C_n\}} T(C_n)$$  \hspace{1cm} (2.28)$$

with

$$T(C_n) = \sum_{m : \sum m_i = 0} C(m) \left( \sum_{\{\bigcup k_i = C_n\}} \tau_{m_1, k_1} \tau_{m_2, k_2} \cdots \tau_{m_n, k_n} \right).$$  \hspace{1cm} (2.29)$$

The clusters $C_n$ are defined by the union of the sites comprised in $k_1 \cup k_2 \ldots \cup k_n := C_n$. The second sum in (2.28) runs over all possible clusters appearing in order $n$. Since the $\tau_n$ are of finite range the number of topological different clusters is limited. It is clear, that $\{C_{n-1}\} \subset \{C_n\}$. In general the sum comprises all types of clusters i.e. it consists of connected and disconnected clusters. However, one finds that all contributions of disconnected clusters cancel out for the effective pCUT Hamiltonian (6.17). This is due to a property called cluster additivity, which is the topic of the next section.

### 2.4 Cluster additivity and linked cluster theorem

An essential and very utile feature of pCUT is the fact that the flow equations conserve the cluster additivity of operators. According to Gelfand, cluster additive quantities do possess a linked cluster expansion which is stated in the linked cluster theorem. This allows in principle to compute the entire elementary excitation spectrum in the thermodynamic limit on finite clusters. In the following the cluster additivity of the effective Hamiltonian and the resulting linked cluster expansion is discussed.

Consider an operator $O^C$ that acts on a finite cluster $C$. This operator is then defined to be cluster additive, if there are two subclusters $A$ and $B$ with $A \cup B = C$, so that $O^C$ can be decomposed into

$$O^C = O^A \otimes \mathbb{1}^B + \mathbb{1}^A \otimes O^B.$$  \hspace{1cm} (2.30)$$

Obviously, this can only be true if A and B share no sites and linking bonds i.e. they are disconnected. Moreover, this means that $O^C$ induces no entanglement between
A and B. Quantities or states defined on A do not depend on quantities defined on B. For a cluster additive Hamiltonian \( H^C = H^A \otimes I^B + I^A \otimes H^B \) one may think of two independent physical systems. Transforming \( H^C \) according to the flow equation (2.2) one finds that the resulting effective Hamiltonian \( H^C_{\text{eff}} \) is cluster additive. This implies that the irreducible matrix elements in (2.23) are also cluster additive. Using the cluster additivity of the irreducible matrix elements one can argue that only virtual processes corresponding to linked clusters can lead to a finite contribution. To see this, consider the virtual processes on a finite cluster A contributing to an irreducible one-particle hopping element \( t_{ij} \). The cluster additivity of \( t_{ij} \) implies that the value of \( t_{ij} \) with \( i,j \in A \) does not change, if one adds a disconnected cluster B (see figure 2.3). Consequently, all disconnected virtual processes acting on A and B have to cancel out. As this has to be true for arbitrary disconnected clusters A and B, one concludes that all disconnected processes have to vanish. The same argumentation holds for all irreducible matrix elements. Therefore, every irreducible \( n \)-particle block can be computed on appropriate finite clusters. The generic calculation scheme is determined by (2.26).

**Figure 2.3:** Here the consequences of the cluster additivity are illustrated. Cluster additivity implies that the hopping element \( t_{ij} \) on cluster A does not change its value, if one adds an additional isolated cluster B. Consequently, all additional disconnected virtual fluctuations occurring on the right site have to cancel out. As this has to be true for arbitrary cluster B one concludes that only linked processes can have a finite weight.

In this thesis the main focus is on the computation of one particle properties, as for instance the one-particle dispersion and first excitation gap. Considering (2.26), (2.23) and (2.25) the ground-state energy is obtained by \( E_0 = \langle 0 | H_{\text{eff}} | 0 \rangle \). For a finite order \( n_{\text{max}} \) all virtual processes in the thermodynamic limit are of finite size. Hence, one
can find a finite linked cluster $A$ with $N_A$ sites containing all this processes so that

$$\lim_{N \to \infty} \frac{1}{N} \langle 0 | H_0^{n_{\text{max}}} | 0 \rangle = \frac{1}{N_A} \langle 0 | (H_0^{n_{\text{max}}})_A | 0 \rangle_A .$$

(2.31)

The same assumptions can be made for the calculation of the hopping elements

$$t_{ij} = \langle i | H_1 | j \rangle - E_0 \delta_{ij} .$$

(2.32)

Due to the translational symmetry of the lattice the matrix $t_{ij}$ can be diagonalized by a Fourier transformation yielding the one-particle dispersion. The crucial point here is the choice of the cluster. The cluster $A$ must be selected in such a way, that all processes contributing to the matrix element of interest in the thermodynamic limit are contained in $A$. In most cases this way of computation is not efficient as the computation time and memory usage grows exponentially with the cluster size. However, the decomposition in (2.28) allows to restrict the calculation on smallest possible clusters reducing the computational effort. A further advantage is that the contribution of two topological equivalent clusters is identical, since both clusters comprise the same sequences of $\tau$ operators. Consequently, the computation has to be carried out only once for every distinct cluster. Then the essential task is to recombine the contributions of all clusters to get the correct matrix element. For this purpose, one has to calculate the number of embeddings on the lattice for every cluster and develop a correct substraction scheme to avoid double countings. A possible approach for the systematic computation of cluster weights on higher dimensional lattices is presented in the next chapter.
Chapter 3

Graph expansion

This chapter deals with some important computational aspects regarding effective Hamiltonians that meet the linked cluster theorem. Such effective Hamiltonians allow to restrict the calculations to finite clusters or graphs, providing a computation scheme that is related to linked cluster expansion methods [14]. The subsequent reduction of memory usage and computation time allows to enhance the maximal order of the resulting series expansions.

In the first sections the basic ideas of the computational representation, identification, and generation of graphs are briefly introduced. The essential concepts presented in the first part can be found in more detail in [24]. In the last sections the main focus is on the calculation of graph weights. The concept of graph decomposition for more dimensional lattices and the combinatorical issues concerning the embedding of a certain graph are elucidated in detail. For simplicity, only models with one link type are considered. However, a generalization for Hamiltonians with different couplings is also possible.

3.1 Graph representation

The clusters for the models under consideration can be represented by simple undirected graphs. A simple undirected graph is defined by a set of vertices and edges representing the sites and links of the cluster. Therefore both terms 'graph' and 'cluster' are often used on equal footing. 'Simple' means that for any two vertices there exists at least one path connecting both vertices. In the following those graphs
are also called connected graphs. Figure 3.1 shows a graphical representation of a simple undirected graph.

![Graph](image)

**Figure 3.1:** Illustration of a simple undirected graph. The numbered circles represent the vertices. The bonds are represented by the links.

The information of a graph with $n$ vertices can be stored in an adjacency matrix $A$ with $A_{ij} = 1$, if the vertices $i$ and $j$ are linked and $A_{ij} = 0$ otherwise. The diagonal entries $A_{ii}$ are set to zero, but they may also contain additional information. For example the order of the $i$-th vertex which is the number of outgoing links. As the links are nondirectional $A$ has to be symmetric. An efficient way to store a graph in a computer is by interpreting the off diagonal upper or lower matrix elements as a binary number. Therefore, the graph can be identified by an integer number. This number or graph key then completely determines the adjacency matrix. As an example consider the graph in figure 3.2. In general a graph can be represented by more than one adjacency matrix, due to the fact that one may renumber the vertices. More precisely, there are $\frac{n!}{S}$ different adjacency matrices with $S$ denoting the symmetry factor of the corresponding graph. In order to find a unique representation one chooses the labeling that maximizes the graph key. In the following, this maximum key is called graph number.

### 3.2 Graph generation

The next question is how to generate all distinct graphs required for the cluster expansion. In principle one needs a straightforward enumeration algorithm that creates all possible graphs and an efficient identification scheme to discard topologically equivalent graphs. Here, the main ideas and associated issues concerning the creation of linked undirected graphs are discussed briefly. The concepts presented in this section
are mainly based on the diploma thesis of Kris Coester [6]. A more general treatise is presented in [24]. The creation of graphs is strongly related to common combinatorical problems. A possible approach to create all topological distinct graphs with \( n \) vertices and \( m \) edges is to start with \( n \) isolated points, and to add \( m \) bonds in all possible ways. This is related to the problem of placing \( m \) different pegs in \( \frac{1}{2}n(n - 1) \) holes regarding the pegs as bonds and the holes as all possible links between pairs of vertices as shown in figure 3.3. An useful enumeration procedure performing this task is the so called 'pegs in holes' algorithm. After the complete set of graphs up to a certain number of vertices is created one has to identify and remove all topologically equivalent and redundant graphs. The identification comprises the allocation of the graph number. An efficient algorithm that performing this job is described in [6]. The rejection of redundant graphs of course depends on the specifications of the graphs of interest. Here, only connected graphs are considered, so one has to discard all disconnected graphs. One may also take into account information about the lattice the graphs have to be embedded on, as for the example the order of a vertex must not exceed the coordination number of the considered lattice. It is reasonable to a priori avoid
the generation of redundant graphs. Therefore, one may choose a slightly different approach. Instead of starting with \( n \) isolated vertices, only a single vertex is considered as the initial point. Then one adds new bonds by generating a new link between unlinked vertices or linking an additional vertex to the graph. As a result, only connected graphs are generated. Moreover, this approach allows to control the maximum coordination number of all vertices very easily.

Once all relevant graphs are generated, the computation of \( n \)-particle quantities as the ground-state energy (\( n = 0 \)) or hopping elements (\( n = 1 \)) can be performed on the corresponding clusters. In principle, this can be done by applying the effective pCUT Hamiltonian to the relevant \( n \)-particle states. For a given cluster \( C \) one has

\[
\frac{1}{N_C} \langle 0 | H_{\text{eff}}^C | 0 \rangle = \frac{\bar{E}_0^C}{N_C} := \bar{\epsilon}_0^C
\]

with \( N_C \) denoting the number of sites of \( C \) and

\[
\bar{E}_{ij}^C = \langle i | H_{\text{eff}}^C | j \rangle - \delta_{ij} \bar{\epsilon}_0^C.
\]
As already mentioned, the Hamiltonian $H_{\text{eff}}^C$ also comprises contributions of smaller subclusters $C' \subset C$. In order to avoid double countings one has to subtract those contributions. The pure graph contributions are then given by

$$
\varepsilon_0^C = \tilde{\varepsilon}_0^C - \sum_{C' \subset C} \varepsilon_0^{C'} \quad t_{ij} = \tilde{t}_{ij} - \sum_{C' \subset C} t_{ij}^{C'}.
$$

(3.3)

Figure 3.4 shows an example of this subtraction. Another approach is to take only those terms of $H_{\text{eff}}^C$ into account that are touching every site of $C$ at least once. This way all subcontributions are automatically discarded and the computation yields the pure contribution. The number of subsequences is drastically reduced. A more detailed description on how to efficiently execute the pCUT calculations on those graphs is given in [6].

The last step is to combine all the graph contributions in order to get the correct results in the thermodynamic limit. The calculation of graph weights for more dimensional lattices is the main topic of the next section.

### 3.3 Graph embedding

Due to the decomposition (2.28) every $n$-particle quantity on a given lattice $\Gamma$ can be decomposed into a sum of pure graph contributions. Considering the series expansion of the effective Hamiltonian with maximum order $m$ the corresponding decomposition
can be written as
\[
H^{(m)}_{\text{eff}} = \sum_{n} x^{n} \sum_{\{C_n\}} T(C_n) B(C_n)
\]
with \( T(C_n) \) comprising all virtual fluctuations covering the cluster \( C_n \). The second sum runs over all clusters \( C_n \) occurring in order \( n \). \( B(C_n) \) denotes the so called embedding factor of \( C_n \) which is just the number of embeddings for \( C_n \) in \( \Gamma \). In the thermodynamic limit of course the number of embeddings \( B(C_n) \to \infty \). Therefore, one defines \( B(C_n) = B(C_n)/N_e \) with \( N_e \) denoting the number of unit cells. The \( B(C_n) \) can be seen as the number of distinct embeddings that can not be mapped on each other by a lattice translation.

This section provides a scheme that allows to systematically compute embedding factors for linked undirected graphs on arbitrary lattices. First of all, the specific problems and difficulties concerning the systematic embedding of graphs are discussed. Some important predefinitions are stated that are essential for the further understanding of the algorithm. Subsequently, the explicit procedure is presented.

The difficulties associated with the embedding of graphs are mainly based on the huge variety of different topologies and complexity arising in graphs with increasing vertex number. For example consider the graph shown in figure 3.5 and try to envision all possible embeddings on a triangular lattice. The huge number of different embeddings as well as the vast combinations of loops and branches make it very difficult to develop a systematic embedding scheme.

![Figure 3.5: Illustration of an arbitrary graph with six loops. The right-hand side shows an embedding of the corresponding graph on a triangular lattice.](image)

In order to get a first overview let us start with topologically simple graphs. The simplest graphs one may think of are chains. Fig. 3.6 shows an example of a chain graph.
The embedding procedure for such graphs is quite simple. To every bond \( i \) one assigns a counter \( c_i \). On a lattice with coordination number \( q \) every counter can take a positive integer number from 1 to \( q \). The \( c_i \) can be regarded as orientations of the corresponding bonds with the first site of \( c_1 \) as a fixed pivot. The numbering \( i \) of the bonds has to ascend with increasing distance to the pivot. Furthermore, one has to define an embedding or master cluster with master sites \( M_i \) representing the lattice. The \( M_i \) contain information about their occupation (by graph sites) as well as their neighbouring master sites. For an arbitrary fixed graph site (=pivot) every combination of the \( c_i \) corresponds to a certain embedding which is depicted in Fig. 3.7. Consequently, the correct embeddings can be obtained by enumerating all combinations of the \( c_i \) for a given fixed graph site and discarding all embeddings where a master site is occupied by more than one graph site. A systematic realization of all allowed combinations is provided by the following approach:
Chapter 3 Graph expansion

- Initial setting: All counters $c_1, \ldots, c_m$ are set to an initial value $c_i = 0$. One master site is occupied by the pivot. In order to place the other graph sites the following steps must be performed.

- A graph site is placed on the master cluster according to its correspondent counter $c_i$ that determines the direction of the linking bond.

- If the graph site is placed on a valid (not occupied) master site go to $c_i+1$. Else increment the counter $c_i$ and try the next position.

- If the counter exceeds $c_i = q - 1$ (all possible values of $c_i$ have been passed) set $c_i = 1$ and go to $c_{i-1}$.

- Once the positioning of the last counter $c_m$ is approved, the corresponding embedding is valid. Continue by incrementing $c_m$.

- The algorithm terminates for $c_1 = q$.

In order to realize all possible embeddings with respect to a fixed master site $M_i$, the enumeration has to be done for each graph site fixed to this $M_i$. If the unit cell contains more than one lattice site, one has to enumerate for all $M_i$ inside a fixed unit cell. Finally, the resulting number of embeddings has to be divided by the symmetry factor $S$ of the graph (which in this case is $S = 2$) in order to avoid double countings. Of course the set of chain graphs covers only a small subset. However, this approach already forms the basis for the final embedding scheme for arbitrary connected graphs. The important step is the generalization to include the so-called tree graphs, which are the main topic of the next section.

3.4 Tree graphs

This section is intended to describe how tree graphs can be used to compute embedding factors for arbitrary linked graphs. It will turn out that every linked graph can be decomposed into a tree graph, which allows to establish a general embedding scheme.

There are many ways to define the set of tree graphs. A tree graph $T$ is determined by the following equivalent conditions.

- $T$ is connected and has no loops/cycles
• $\mathcal{T}$ is connected. The removal of any edge results in a disconnected graph.

• Any two vertices in $\mathcal{T}$ are connected by a unique simple path.

• $\mathcal{T}$ is a connected graph with $n$ vertices and $n - 1$ edges.

Fig. 3.8 shows an example of a tree graph. Notice that the chain graphs described in the previous section are a subset of tree graphs. The same enumeration procedure described for the chains can be easily applied to tree graphs. The crucial point is just the numbering of the bonds. Similar to the first example, one vertex is chosen to be the fixed pivot denoted by $p_0$. Now, the bonds have to be numbered in such a fashion, that for any simple path the bond number ascends with increasing distance to $p_0$. For such labelings one finds, that the described enumeration scheme indeed realizes all possible embeddings.

Moreover, tree graphs can be used to represent any linked cluster. Consider an arbitrary connected graph $\mathcal{G}$ with $n_\mathcal{G}$ vertices and $l_\mathcal{G}$ bonds. One always finds an appropriate tree graph $\mathcal{T}$ with $l_\mathcal{T} = l_\mathcal{G}$ bonds that can cover all bonds in $\mathcal{G}$. Necessarily, some of the $n_\mathcal{T} > n_\mathcal{G}$ vertices of $\mathcal{T}$ have to overlap due to the covering. In the following all vertices in $\mathcal{T}$ covering one vertex in $\mathcal{G}$ are called doubleganger. Figure 3.9 shows an example of such a covering. This type of representation is a crucial point of the final embedding algorithm. The main idea is to decompose a graph into the corresponding representative tree graph including the information about the doublegangers. Then one iterates all possible embeddings of the representative tree graph enumerating every embedding, where all doublegangers are occupying the same master site. In order to establish an efficient embedding scheme the computational representation of such a tree graph has to meet the following demands:
Chapter 3 Graph expansion

A representative tree graph $\mathcal{T}$ is a set of $n_\mathcal{T} + d_\mathcal{T}$ graph sites $t_i$ with $d_\mathcal{T}$ doublegangers and $l_\mathcal{T}$ bonds linking pairs of graph sites. Every bond is labeled by a counter $c_k$.

Let $|(t_{i_1}) - (t_{i_2})|$ denote the distance between site $t_{i_1}$ and $t_{i_2}$. The graph site which is chosen to be the fixed pivot is denoted by $t_0 := p_0$. The numbering of the other graph sites has to be such, that any two graph sites $t_{i_1}$ and $t_{i_2}$ in a simple path starting at $p_0$ obey

$$|t_{i_1} - p_0| < |t_{i_2} - p_0| \iff i_1 < i_2.$$  \hspace{1cm} (3.5)$$

The labeling of the counters $c_k$ has to be such, that

$$\max(i_1, j_1) < \max(i_2, j_2) \iff k_1 < k_2.$$  \hspace{1cm} (3.6)$$

For any two counters $c_{k_1}$ and $c_{k_2}$ linking the graph sites $\{i_1, j_1\}$ and $\{i_2, j_2\}$. This is in accordance to the rule, that the numbering of a counter ascends with increasing distance to $p_0$ on any simple path.

Every graph site $t_i$ is associated to its doublegangers $t_j$ with $j < i$.

In the following sections the general procedure of the relevant algorithms is presented including the decomposition of arbitrary graphs and the final computation of the effective matrix elements.
3.5 Decomposition into tree graphs

This section provides an approach that allows to decompose arbitrary undirected graphs into their correspondent tree graphs. The resulting tree graph can be seen as an instruction that determines in which order the graph has to be iterated through during the embedding procedure. The initial point is given by an arbitrary connected graph $\mathcal{G}$ in form of a graph number or an adjacency matrix. The aim is to construct a representative tree graph $\mathcal{T}$ that covers $\mathcal{G}$. Due to the structure of tree graphs it is reasonable to do a recursive tree traversal and to successively number all sites. In order to obtain a numbering according to equation [3.5] one has to do a so called depth-first traversal starting at a certain pivot site. Following operations have to be performed recursively assuming that every site $g_i$ in $\mathcal{G}$ has a maximum of $q$ outgoing links.

- 1. evaluate current site
- 2. go 1st neighbour
- 3. go to 2nd neighbour
  ...
- $q + 1$. go to $q$-th neighbour

As $\mathcal{G}$ in general is no tree graph, such a traversal would end up in cycles. Therefore, every time a link is traversed it is removed from $\mathcal{G}$. Moreover, one needs a counter that enumerates all traversed sites. The evaluation of the current site in the first step comprises the following instructions.

- The current site is labeled as 'already traversed'.
- Insert the current site into the tree graph $\mathcal{T}$, by linking it to the site of the previous function call. The new site in $\mathcal{T}$ is denoted by the actual value of the counter.
- Increment the counter by one.
- Remove the traversed link from $\mathcal{G}$

The traversals to the neighbouring sites are only performed for available links. One also has to check if the actual site was already traversed. In that case only the
evaluation of the site is performed. In addition, the actual site is identified as the
doubleganger of the correspondent sites in $T$. Figure 3.10 depicts an exemplary
decomposition of a topologically simple graph.

1. \[ \begin{array}{c}
   4 \quad 1 \\
   3 \quad 2 \\
   \end{array} \]
   \[ \begin{array}{c}
   1 \\
   \end{array} \]

2. \[ \begin{array}{c}
   4 \quad 1 \\
   3 \quad 2 \\
   \end{array} \]
   \[ \begin{array}{c}
   1 \quad 2 \\
   \end{array} \]

3. \[ \begin{array}{c}
   4 \quad 1 \\
   3 \quad 2 \\
   \end{array} \]
   \[ \begin{array}{c}
   1 \quad 2 \quad 3 \\
   \end{array} \]

4. \[ \begin{array}{c}
   4 \quad 1 \\
   3 \quad 2 \\
   \end{array} \]
   \[ \begin{array}{c}
   1 \quad 2 \quad 3 \quad 4 \\
   \end{array} \]

5. \[ \begin{array}{c}
   4 \quad 1 \\
   3 \quad 2 \\
   \end{array} \]
   \[ \begin{array}{c}
   5 = 1 \\
   \end{array} \]

6. \[ \begin{array}{c}
   4 \quad 1 \\
   3 \quad 2 \\
   \end{array} \]
   \[ \begin{array}{c}
   5 = 1 \\
   \end{array} \]

Figure 3.10: Example of the graph decomposition of $G$ into its representa-
tive tree graph $T$ (right). The left-hand side shows the traversal of $G$. The red
dashed circle designates the actual site that is inserted into $T$ on the right-hand
side.

### 3.6 Computation of hopping elements

This section explains how to compute hopping elements $t_{ij}$ of an effective Hamiltonian
in the thermodynamic limit using the previously introduced embedding procedure.
One may assume that the pCUT calculations have been already performed on the
required linked clusters up to a certain order $m$. The pure $n$-th order contributions
resulting on the cluster $C$ are denoted by $t_{ij}^{(m)}|_C$. The exact result up to order $m$ can be written as

$$t_{ij}^{(m)} = \sum_{n=0}^{m} x^n \sum_{C} \sum_{\alpha,\beta} B^{ij}_{\alpha\beta}(C) t^{C}_{\alpha\beta} \quad . \tag{3.7}$$

$B^{ij}_{\alpha\beta}(C)$ stands for the number of embeddings of $C$ with $\alpha, \beta \in C$ covering $i, j \in \mathcal{M}$. In order to determine the embedding factors $B^{ij}_{\alpha\beta}(C)$ one may use a modification of the enumeration algorithm described in \[3.3\] taking into account the additional information on the doublegangers. Due to the recursive numbering of links and sites, this can be done efficiently by modifying the occupancy check in the third step:

- If the graph site $\mu$ is placed on a master site occupied by all doublegangers $d(\mu)$ with $d(\mu) < \mu$ the corresponding counter is approved and one may move to the next counter. Else the counter is incremented.

This way, illegal embeddings are rejected as early as possible.

The final computation of the $B^{ij}_{\alpha\beta}(C)$ can be performed by the following approach.

1. The first step is the choice of an sufficiently large master cluster $\mathcal{M}$ in order to avoid finite size effects. More precisely, $\mathcal{M}$ has to contain all possible embeddings of $C$ (covering $i$ and $j$) with respect to a fixed unit cell. The explicit form and size of $\mathcal{M}$ depends on the order and the considered model.

2. Decompose the graph $C$ into its representative tree graph $\mathcal{T}$ by starting at a given site $\delta \in C$ assigning the pivot to $\delta$.

3. Enumerate all relevant embeddings of $C$ in $\mathcal{M}$ with respect to a fixed unit cell $U_\mathcal{M}$. For that purpose, the pivot in $C$ has to be assigned once to each master site in $U_\mathcal{M}$. In order to obtain the $B^{ij}_{\alpha\beta}(C)$, one has to count all embeddings with $\alpha, \beta \in C$ occupying $i, j \in \mathcal{M}$. Note that either $i$ or $j$ has to be comprised by $U_\mathcal{M}$.

4. Repeat the 2. and 3. step for every $\delta$ in $C$ so that at the end every site in $C$ was chosen to be the pivot once. Alternatively: One may also use the translational invariance of the lattice. Instead of enumerating for each pivot one may count all valid translations of an approved embedding. In this case only one pivot has to be taken into account.

5. Divide the resulting number of embeddings by the symmetry factor of $C$. 


Chapter 4

Extrapolation

This chapter presents some extrapolation methods, that are essential for the further treatment and analysis of the results obtained by the perturbative continuous unitary transformation methods. The physical quantities of interest are given as high order series expansions in a certain perturbation parameter. Consequently, the validity of the approximation is restricted to sufficiently small parameters. Though, one usually is interested in a physical description for larger values of the parameter, especially if one wants to detect possible phase transitions. In order to obtain reliable results one has to use appropriate extrapolation techniques. In the following the two established extrapolation tools Padé and dlogPadé extrapolation are presented.

A more detailed introduction on these tools can be found in the review article of Guttman [7].

4.1 Padé extrapolation

As a starting point consider a physical quantity given by the series expansion

\[ F(x) = \sum_{n=0}^{m} a_n x^n = a_0 + a_1 x + a_2 x^2 + \ldots + a_m x^m \]  

(4.1)

with the perturbation parameter \( x \in \mathbb{R} \) where the order of the series is denoted by \( m \) and the coefficient of the \( n \)-th order term by \( a_n \). The basic concept of Padé extrapolation is to interpret the plain series (4.1) as a Taylor expansion of a rational function

\[ P_{L/M}^{[F]} := \frac{p_0 + p_1 x + \ldots + p_L x^L}{q_0 + q_1 x + \ldots + q_M x^M} \]  

(4.2)
with real coefficients \( p_i \) and \( q_i \). Those coefficients can be obtained by requiring that the first \( m \) coefficients of the Taylor expansion are equal to the \( a_i \) in (4.1). With \( m = M + L \) a comparison of the coefficients yields a system of linear equations determining the \( p_i \) and \( q_i \). One may assume that the extrapolation provides a good approximation of the sought quantity within an interval \( I \) if several extrapolants yield similar results in \( I \). One has to be careful with extrapolants that exhibit zeros in the denominator within \( I \) or zeros which lie close to \( I \) in the complex plane. This behaviour might be of physical nature, e.g. indicating a phase transition. If this is not the case, the pole is called 

**spurious** and one has to exclude the corresponding extrapolant. Such extrapolants are called **defective**. Usually, extrapolants with \( L \approx M \) show better results. Therefore, it is reasonable to exclude extrapolants with \( L = 1 \) and \( M = 1 \), especially if those extrapolants show a large deviation.

As the extrapolants \( P[L/M]_F \) behave like \( x^{L-M} \) for large \( x \), one is able to built in additional information about the asymptotic behaviour for \( x \to \infty \). It should be noted, that the use of Padé-extrapolation is not restricted by sign changes of the sought quantity.

### 4.2 DlogPadé extrapolation

In contrast to Padé-extrapolation the dlogPadé-extrapolation method is only applicable to quantities with definite sign. However, it usually provides the most reliable results and is very sensitive to real poles and complex poles close to the real axis. Therefore, it is particular suitable for quantities like excitation gaps and the detection of phase transitions.

Just as in the previous section the initial point is given by a plain series. Without loss of generality the series is normalized in the sense that the first coefficient is set to \( a_0 = 1 \):

\[
F(x) = 1 + a_1 x + a_2 x^2 + \ldots + a_m x^m. \tag{4.3}
\]

The dlogPadé-extrapolation is based on the Padé-extrapolation of the logarithmic derivative of \( F(x) \)

\[
\frac{d}{dx} \ln F(x) = \frac{F'(x)}{F(x)} := P[L/M]_{\ln F} = \frac{P_L(x)}{Q_M(x)} \tag{4.4}
\]

where \( P_L(x) \) and \( Q_M(x) \) are again polynomials of order \( L \) and \( M \). Due to the derivative of the numerator in Eq. \( 4.4 \) one requires \( L + M = m - 1 \). The dlogPadé extrapolant
can now be interpreted as the solution of the differential equation

\[ Q_M(x) \frac{dF(x)}{dx} = P_L(x) F(x). \] (4.5)

Consequently, the extrapolant is given by

\[ dP \left[ \frac{L}{M} \right]_F (x) = \exp \left( \int_0^x \frac{P_L(x')}{Q_M(x')} dx' \right). \] (4.6)

As already mentioned the extrapolant is very susceptible to poles and can be used to determine phase transition points. However, one has to be careful as the pole also might be spurious. In the case of a physical pole at \( x_0 \) one is able to determine the dominant power-law behaviour \( |x - x_0|^\alpha \) near \( x_0 \). For sufficiently small \( |x - x_0| \) one has

\[ dP \left[ \frac{L}{M} \right]_F (x) \approx \exp \left( \int_0^x \frac{\alpha}{x' - x_0} dx' \right) = \exp \alpha \left[ \ln |x' - x_0| \right] = |x - x_0|^\alpha. \] (4.7)

The exponent \( \alpha \) is given by the residuum of \( P_L/Q_M \) at \( x = x_0 \)

\[ \alpha = \frac{P_L(x)}{\frac{d}{dx} Q_M(x)} \bigg|_{x=x_0}. \] (4.8)

So this extrapolant is especially suited for the calculation of critical exponents.

### 4.3 Biased dlogPadé extrapolation

In many cases additional information about the function \( F(x) \) is available. This information might comprise phase transition points, critical exponents, or the asymptotic behaviour for \( x \to \infty \). The structure of the dlogPadé-extrapolation allows to implement this additional information in order to enhance the physical validity of the results.

Lets assume that there is a phase transition point at \( x_0 \) with a dominant power-law behaviour \( |x - x_0|^\alpha \) near \( x_0 \). This behaviour can be built in by modifying the logarithmic derivative

\[ G(x) = \left( \frac{d}{dx} \ln F(x) \right) (x - x_0) + Ax^m. \] (4.9)
Then one determines the constant $A$ by demanding that the Padé approximant of $G(x)$ satisfies the condition

$$P[L/M]_{G} |_{x=x_{0}} \equiv \alpha,$$  \hspace{1cm} (4.10)

which implies $dP[L/M]_{G} |_{x=x_{0}} = |x - x_{0}|^{\alpha}$. Finally, the biased dlogPadé extrapolant of $F$ can be written as

$$dP[L/M]_{F} = \exp \left( \int_{0}^{x_{0}} \frac{P[L/M]_{G}}{x' - x_{0}} \, dx' \right).$$  \hspace{1cm} (4.11)

Another important point is the incorporation of the asymptotic behaviour for $x$ approaching infinity. Similar to the latter approach one modifies (4.4) by adding a term to the logarithmic derivative

$$G(x) = \left( \frac{d}{dx} \ln F(x) \right) + Ax^{m}. \hspace{1cm} (4.12)$$

Now it is useful to map the whole positive parameter axis on a finite interval. Therefore, one applies an Euler transformation which is defined by

$$G(x) \rightarrow \tilde{G}(u) = \sum_{n=0}^{m} \tilde{a}_{n}u^{n} \text{ with } x = \frac{u}{1-u}. \hspace{1cm} (4.13)$$

The function $\tilde{G}(u)$ is obtained by replacing the parameter $x$ in $G(x)$ with $x = \frac{u}{1-u}$ and a subsequent Taylor expansion in $u$ up to order $m$. To achieve the desired asymptotic behaviour one requires

$$P[L/M]_{\tilde{G}} |_{u=1} \equiv \alpha.$$  \hspace{1cm} (4.14)

The final biased biased dlogPadé incorporating the correct asymptotic behaviour is given by

$$dP[L/M]_{F} = \exp \left( \int_{0}^{\frac{1}{1-u}} \frac{P[L/M]_{G}}{1-u} \, du \right).$$  \hspace{1cm} (4.15)
Chapter 5

Exact diagonalization

Many mathematical problems arising in physics can be formulated as an eigenvalue problem, e.g. the Schroedinger equation in quantum mechanics or the vibration analysis in classical mechanics. The general eigenvalue equation for a given $n \times n$ matrix $M$ can be expressed as

$$ Mx - \lambda Ix = 0 \quad (5.1) $$

with unknown vectors $x \in \mathbb{C}^n$ and unknown $\lambda \in \mathbb{C}$. All nontrivial vectors $x \neq 0$ satisfying this equation are called eigenvectors. The corresponding values of $\lambda$ are termed eigenvalues. They can be also seen as the roots of the characteristic polynomial

$$ \det(M - \lambda I) = 0 \quad . \quad (5.2) $$

There exists no universal solution for the eigenvalue equation [5.1] with $n > 4$ as there are no analytical expressions for the roots of an arbitrary polynomial of order $n > 4$. For large systems with $n \gg 1$ one is reliant on appropriate diagonalization tools. In the course of time a variety of different diagonalization methods were developed and each one is suited for different types of problems. Most of them are based on two major steps. The first step comprises the reduction of the matrix $M$. Due to its simplified form the matrix can be finally diagonalized in the second step. In the following a diagonalization technique is presented that is especially suited for problems where one is interested in particular eigenvalues of a very large sparse matrix. The general procedure of the so called Lanczos algorithm is discussed in this chapter, which is mainly based on the corresponding section in the book on numerical mathematics by Stoer and Bulirsch [34]. The explicit application and implementation
for the transverse field Ising model in the low field limit and further details can be found in section 6.6.2.

5.1 Lanczos algorithm

The main idea of the lanczos algorithm is to construct an orthonormal basis \( \{ q_1, q_2, \ldots, q_m \} \) such that the representation of a hermitian \( n \times n \) matrix \( A \) in this basis has a tridiagonal form

\[
q_i^\dagger A q_j = A_{ij} = 0 \quad \text{for} \quad |i - j| \geq 2.
\]  

(5.3)

The orthonormal vectors are spanning a so called Krylov space defined by

\[
K_i(q, A) := \text{span} \left[ q, Aq, \ldots, A^{i-1}q \right], \quad i \geq 1, \quad K_0(q, A) := \{0\},
\]  

(5.4)

with \( m \leq n \) denoting the largest index satisfying \( \text{dim} \left[ K_m(q, A) \right] = m \). This Krylov space is \( A \)-invariant which means that \( A^m K_m(q, A) \subseteq K_m(q, A) \). For an arbitrary vector \( q \in K_m(q, A) \) with \( \| q \| = 1 \) the \( q_i \) are determined by the following recursive equations

\[
q_1 := q, \quad \gamma_1 q_0 := 0, \\
\gamma_{i+1} q_{i+1} = A q_i - \delta_i q_i - \gamma_i q_{i-1}
\]  

(5.5)

with

\[
\delta_i := q_i^\dagger A q_i, \\
\gamma_{i+1} := \| r_i \| \quad \text{and} \quad r_i = A q_i - \delta_i q_i - \gamma_i q_{i-1}, \\
q_{i+1} := \frac{r_i}{\gamma_{i+1}}, \quad \text{if} \quad \gamma_{i+1} \neq 0.
\]  

(5.6)

Once, the vectors \( q_i \) are spanning the full Krylov space no further basis vectors can be generated. For \( i = m \) this procedure automatically aborts as \( \gamma_{m+1} = 0 \). An additional feature of this algorithm is that quantities \( O_l \) with \( [A, O_l] = 0 \) are conserved during the whole procedure. Therefore, if the starting vector \( q \) describes a physical state with quantum numbers \( o_l \in \mathbb{R} \) with \( (O_l q = o_l q) \), all other basis vectors will have the same quantum numbers \( Q_l q_i = o_l q_i \) for \( 0 < i \leq m \). This can be easily shown by
mathematical induction. Per definition, the first basis vector satisfies
\[ O_lq_1 = O_lq = o_lq. \] (5.7)

As one needs the two previous vectors for the induction one additionally has to show that
\[ O_lq_2 = O_l(Aq_1 - \delta_1q_1) = o_lAq_1 - o_l\delta_1q_1 = o_lq_2. \] (5.8)

Finally, assuming that \( O_lq_i = o_lq_i \) and \( O_lq_{i-1} = o_lq_{i-1} \) the induction step is given by
\[
O_lq_{i+1} = O_l \frac{1}{\|r_i\|} (Aq_i - \delta_iq_i - \gamma_iq_{i-1}) = \\
= \frac{1}{\|r_i\|} (AO_lq_i - \delta_iO_lq_i - \gamma_iO_lq_{i-1}) = \\
= \frac{1}{\|r_i\|} (Ao_lq_i - \delta_io_lq_i - \gamma_io_lq_{i-1} = o_lq_{i+1} \quad \Box.
\]

The corresponding tridiagonal matrix \( A_{tri} \) can be written as
\[
A_{tri}^{(i)} = \begin{pmatrix}
\delta_1 & \gamma_2 & 0 \\
\gamma_2 & \delta_2 & \ddots \\
\ddots & \ddots & \ddots \\
0 & \gamma_i & \delta_i
\end{pmatrix}.
\] (5.9)

For \( i = m \) the procedure aborts and the resulting matrix \( A_{tri}^{(m)} \) has the same eigenvalue spectrum as \( A \). One can show that the largest and smallest eigenvalues are converging very fast. If one is only interested in the extremal eigenvalues (which is often the case) one needs significantly less Lanczos steps \( i \ll m \) to get a good approximation. Another advantage of this algorithm is that one does not need to store all basis vectors to compute the eigenvalues, since only two vectors are required to calculate the next lanczos step. Consequently, one can save a lot of memory by storing only the last two vectors.

The next section describes a technique that diagonalizes a matrix of the form (5.9).

### 5.2 Diagonalization of a tridiagonal matrix

The next step comprises the diagonalization of a tridiagonal matrix. There are many different tools performing this task. Here, a technique is presented, that is especially
suited for problems where one is interested in single eigenvalues. The method is based on Sylvester’s law of inertia which states that the number of positive, negative, and vanishing eigenvalues of a matrix is conserved for arbitrary similarity transformations. More precisely, it says that two matrices $A$ and $B$ have the same number of positive, negative and vanishing eigenvalues, if there exists a regular matrix $S$ with

$$A = S^T BS.$$  \hspace{1cm} (5.10)

This can be used to determine the number $n_\lambda$ of eigenvalues $\lambda_1 \leq \ldots \leq \lambda_j$ of a tridiagonal matrix $A_{\text{tri}}$ with $\lambda_1 \leq \ldots \leq \lambda_j < \lambda$ for arbitrary $\lambda \in \mathbb{R}$. For this purpose, one performs a decomposition

$$A_{\text{tri}} - \lambda I = LU = LDL^T$$  \hspace{1cm} (5.11)

with lower triangular and upper triangular matrices $L$, $U$ and a diagonal matrix $D$. The diagonal matrix $D$ can be determined by Gaussian elimination. For regular $A_{\text{tri}} - \lambda I L$ has to be regular as well and Sylvester’s law of inertia holds. Consequently, the number of negative diagonal elements $d_i$ equals the number $n_\lambda$ of eigenvalues $\lambda_j$ of $A_{\text{tri}}$ with $\lambda_j < \lambda$. A simple algorithm computing all eigenvalues of $A_{\text{tri}}$ that are smaller than $\lambda$ is given by

$$n_\lambda := 0; \quad d_1 := \delta_1 - \lambda; \quad (5.12)$$

$$\text{if } d_1 < 0 : \quad n_\lambda := 1; \quad (5.13)$$

$$\text{for } i := 2 : n$$

$$d_i := \delta_i - \frac{(\gamma_i)^2}{d_{i-1}} - \lambda; \quad (5.14)$$

$$\text{if } d_i < 0 : \quad n_\lambda := n_\lambda + 1.$$

One uses this algorithm to determine an intervall $[\lambda_l, \lambda_r]$ that comprises a particular eigenvalue e.g. the smallest eigenvalue. Finally, the eigenvalue can be computed by a simple bisectional procedure.
Chapter 6

Antiferromagnetic Ising model in transverse Field

The technological progress in low temperature physics and the observation of quantum criticality [26] have aroused great interest on the theoretical understanding of quantum phase transitions, drawing considerable attention on one- and higher dimensional spin systems in transverse field. Those systems provide exemplary models that exhibit continuous quantum phase transitions. Due to their simplicity and richness they play an essential role in the investigation of quantum critical behaviour.

One of the simplest models in this context is the antiferromagnetic Ising model in transverse field. Despite its simplicity, it provides a wide range of interesting features e.g. continuous quantum phase transitions, exotic ground-state properties and non-trivial quantum dynamics due to quantum frustration [4, 5].

In this chapter the main focus is on the 2d antiferromagnetic transverse field Ising model (TFIM) defined on the kagome and triangular lattice. Without transverse field both systems are classically disordered antiferromagnets with a macroscopic ground-state degeneracy exhibiting a finite entropy at zero temperature [16, 38]. When exposed to a transverse field they are endowed with non-trivial quantum dynamics leading to two categories of novel phase transitions which in the literature are known as 'order by disorder' and 'disorder by disorder' [20]. These type of models were intensively studied by Moessner et al. in 2001 using a Landau-Ginzburg-Wilson approach and variational methods [20] as well as quantum Monte Carlo simulations [15]. They were able to obtain a complete phasediagram of the triangular TFIM by means of quantum Monte Carlo simulations featuring a quantum ordered phase that gives rise to a 'order by disorder' transition. In contrast, the kagome TFIM turns out to
be a system that is extremely disinclined to order. It is suggested that the kagome
TFIM may be a disordered quantum paramagnet providing an notable instance of
‘disorder by disorder’ that so far was only found in the one-dimensional sawtooth
TFIM [25]. In 2005 Nikolic and Senthil carried out further investigations analytically
demonstrating a possible disordered zero temperature phase that is consistent with
quantum Monte Carlo results [23]. However, they also show the possibility of ordered
phases in the weak transverse field limit. As there was so far no conclusive evidence
that excludes a possible ordering in the kagome TFIM the existence of a disorder by
disorder transition in two dimensions remained an open issue to date. In this thesis
the excitation gap of the kagome TFIM is studied for the whole transverse field axis
using the methods introduced in the previous chapters. The results yield strong ev-
idence for a gapped paramagnetic phase that persists for arbitrary transverse fields
implying a novel ‘disorder by disorder’ transition. In order to confirm the significance
of the results the same treatment is applied to the triangular TFIM which allows a
comparison to the already existing quantum Monte Carlo results [15].

The first section provides a basic discussion on the mathematical and physical as-
pects of the antiferromagnetic transverse field Ising model including a brief outline
of the already known results concerning the kagome and triangular TFIM. Then the
focus is laid on the high field limit and the mapping to a hardcore bosonic picture
which forms the initial point of the subsequent perturbative treatment on the basis
of perturbative continuous unitary transformations. The structure of the resulting
effective Hamiltonian and the physical aspects of the 1QP mode are elucidated in
detail. It is shown that the kagome TFIM gives rise to a localized mode exhibiting
an energy band that is flat up to order $n = 8$. This behaviour can be understood by a
destructive interference of quantum fluctuations with a certain topology. A heuristic
method is described that allows to predict localized modes as well as the order for
which the locality is destroyed.

The central issue of the last sections is the analysis of the gap for the kagome and tri-
angular TFIM. The extrapolation schemes described in chapter 4 are used to obtain
significant results for the whole transverse field parameter axis. In addition, we ana-
lyze a possible opening of the gap on the kagome TFIM for finite systems in the low
field limit using degenerate perturbation theory and exact diagonalization methods,
which allows a consistency check with the results obtained by the extrapolation.
6.1 Model

The model under investigation is a system of spins carrying $S = 1/2$ located on the sites of a kagome or triangular lattice. The spins are interacting via an antiferromagnetic nearest neighbour Ising coupling. Additionally, all spins are coupled to a uniform transverse magnetic field. The corresponding Hamiltonian reads

$$H = J \sum_{\langle i, j \rangle} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x$$

(6.1)

with Pauli matrices $\sigma_i^z$ and $\sigma_i^x$ acting on the Hilbert space of the $i$-th spin, a parameter $J > 0$ specifying the Ising exchange and the magnetic field strength $h$. The sum in the Ising term comprises all nearest neighbours. A graphical representation of the models is shown in figure 6.1. For the zero field case $h = 0$ the Hamiltonian describes a classical antiferromagnet. Every spin can be in one of two states `up`(+1) or `down`(-1). Hence, the eigenstates of the system are given by all possible product states with $|\psi\rangle = \bigotimes_i |s_i\rangle$ and $s_i = \pm 1$. In order to minimize the energy, the antiferromagnetic coupling requires two neighbouring spins to be aligned antiparallelly. However, there exists no state with all bonds satisfying the antiferromagnetic condition due to the frustrated geometry of the lattices. On a triangular plaquette with two antiferromagnetically ordered spins the third one remains uncertain as shown in figure 6.2. Both possible configurations result in a plaquette with one ferromagnetic and two antiferromagnetic bonds. This effect is called frustration. A ground-state is given by a configuration where every plaquette on the lattice has two antiferromagnetic ordered bonds. In the thermodynamic limit the number of configurations satisfying
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Figure 6.2: Visualization of a frustration on a kagome lattice. The third spin on the plaquette may point either up or down.

this condition is infinitely large. This results in an extensive ground-state degeneracy that gives rise to a finite entropy at zero temperature, which is a main characteristic of frustrated models. In the following, the ground-states of frustrated systems are called spin-ice states due to their close connection to the frustrated ground-states in spin-ice [10]. Note, that the frustration in spin-ice materials, however, is induced by long-range dipolar magnetic interactions (in contrast to the nearest neighbour interactions in the considered Ising model). Figure 6.3 shows a spin-ice state on a kagome lattice. The kagome Ising antiferromagnet has a ground-state entropy per site of $S = 0.502k_b$ with short-ranged spin-spin correlations [16]. Its ground-state manifold is classically disordered.

Next, consider applying a small but finite transverse field with $h/J \ll 1$. This perturbation induces quantum fluctuations by slightly tilting the spins from the $z$-direction.

Figure 6.3: Two illustrations of the same spin-ice state on a kagome lattice. The green spheres and blue arrows represent spins pointing 'up' or 'down'. The red highlighted links specify the ferromagnetic bonds.
For any infinitesimal field $0 < h < \epsilon$ the fluctuations will lift the macroscopic ground-state degeneracy giving rise to a discontinuity in the entropy at zero field $h = 0$ and zero temperature $T = 0$. Such singular perturbations lead to a non-trivial problem in degenerate perturbation-theory as any linear combination from the classical macroscopic ground-state manifold may compose a possible quantum ground-state. This type of problems is typical for classical frustrated systems perturbed by a non-commuting term that induces quantum fluctuations. Considering classical disordered systems, the incorporation of quantum fluctuations leads to the following two generic scenarios.

The first instance is called order by disorder. In this scenario quantum fluctuations are selecting a certain state (or a subset of states) from the classically disordered ground-state manifold exhibiting a non-trivial ordering pattern that breaks the symmetry of the system. Moessner and Sondhi proposed a heuristic approach to identify potential states that may form the basis for a symmetry-breaking ground-state [20]. Their main idea is to find those configurations that allow the softest fluctuations and thus gain the most energy from the perturbation. A composition of these states then forms the basis for a variational analysis. In the case of the TFIM the corresponding configurations are given by the states with the largest number of flippable spins. As the fluctuations induced by the transverse field are single spin flips along the $z$-axis, the configurations with all flippable spins pointing into $x$-direction gain the most energy. Figure 6.4 shows the maximally flippable state on the triangular lattice providing a bond-ordered pattern. Monte Carlo simulations carried out by Moessner and Isakov indeed confirmed that the triangular TFIM gives rise to such a bond-ordered phase that occurs for infinitesimal transverse field and persists up to a
quantum critical point [15]. A sketch of their resulting phase diagram is depicted in figure 6.5.

![Phase Diagram](image)

**Figure 6.5:** Sketch of the triangular TFIM phase diagram obtained by Monte Carlo simulations [15] for finite temperature $T$ and transverse field $h$ in units of $J$.

The second scenario is called *disorder by disorder* and was first proposed by Anderson and Fazekas as a mechanism to construct resonating valence-bond states [8]. Here, the disordered ground-state manifold continues into a quantum disordered phase with short-range correlations leading to a possible opening of a gap.

There are reasonable assumptions that the kagome TFIM is a candidate for such a scenario. The analysis of the maximally flippable states yields exponentially many candidates which do not provide any ordering pattern [20]. A low-order Landau-Wilson-Ginzburg analysis for infinitesimal fields also fails to predict an ordering pattern [21]. Moreover, Monte Carlo simulations indicate that there are exponentially decaying short-range correlations for high fields $\frac{h}{J} \gg 1$ [15]. Figure 6.6 shows the phase diagram for the kagome TFIM proposed by Moessner et al. [21]. Altogether, it is suggested that the kagome TFIM may be a rare spin liquid (cooperative paramagnet) on the whole $h$-axis featuring a novel disorder by disorder transition. However, despite all these indications, it is still an open question whether the kagome TFIM in fact exhibits disorder by disorder. In the following sections an approach is presented that was so far not considered and that might provide conclusive evidence. The idea is to tackle the problem in a perturbative fashion starting at the high field limit.
In this limit with $J = 0$ all spins are polarized along the positive $x$-direction. The system has a unique disordered ground-state with elementary excitations given by single spin flips with an energy gap $\Delta = 2h$. Thus, the system can be classified as a simple gapped paramagnet. Common perturbation theory states that turning on the Ising term will change the energy spectrum in a continuous way. As the system has a unique ground-state and a finite gap one concludes that for sufficiently small perturbation $0 < J < \epsilon$ the system has to stay in a paramagnetic phase. Disorder by disorder, however, implies that the paramagnetic phase continues for arbitrary $J/h$ i.e. all excitation gaps do not close. On the other hand a closing of the gap would indicate a second order phase transition contradicting the previously stated assumptions. As there are no indications for first order phase transitions, the analysis of the gap provides a practical way to verify the disorder by disorder conjecture.

Further motivation for this approach was provided by Priour, Gelfand and Sondhi who did a perturbative expansion about large transverse field for the TFIM on a 1d triangular chain [25]. They showed that the introduction of quantum fluctuations...
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opens a gap but leaves the ground-state disordered for arbitrary values of the transverse field. Figure 6.7 depicts their results of the excitation gap obtained by dlogPadé extrapolation and exact diagonalization methods. The consistency between perturbative results and exact diagonalization suggests that a perturbative approach could be also applied to higher dimensional lattices, as the high field limit of the TFIM offers the ideal setting for a perturbative treatment. The perturbative continuous unitary transformations method introduced in chapter 2 is perfectly suited to this type of problems especially considering higher dimensional systems. It allows to compute \( n \)-particle quantities analytically as high order series expansions in the perturbation parameter. In combination with the extrapolation techniques described in chapter 4, pCUT provides a powerful tool to determine the excitation gap of the kagome and triangular TFIM. Moreover, one is able to calculate the one-particle dispersion and the momentum of the lowest excitation which provide information about a possible ordering pattern in the case of a quantum phase transition.

Additionally, the information about the momentum quantum numbers is used to determine the excitation energy in the low-field limit corresponding to the state that is adiabatically connected to the lowest excitation in the high field limit.

Figure 6.7: Illustration of the first excitation gap of the antiferromagnetic saw-tooth Ising chain in transverse field (\( \Gamma \equiv h \)). The figure shows extrapolations of the gap obtained for an perturbative approach about the high-field limit. The gap stays finite for arbitrary fields indicating a disorder by disorder transition for \( \Gamma = 0 \). Figure is taken from [25].
Before discussing the explicit application of pCUT to the TFIM a preliminary discussion on the high field limit is presented in the next section.

### 6.2 High field limit: Mapping to hardcore bosons

This section is intended to elucidate the physics of the TFIM in the high field limit that forms the initial point for the subsequent perturbative treatment. For the sake of simplicity consider the unitary transformation that performs a global rotation in spin space such that $\sigma^z_i \rightarrow \sigma^x_i$ and $\sigma^x_i \rightarrow \sigma^z_i$. The TFIM Hamiltonian (6.1) then reads

$$H = J \sum_{\langle i,j \rangle} \sigma^x_i \sigma^x_j + h \sum_i \sigma^z_i \tag{6.2}$$

For zero coupling $J = 0$ the ground-state is the fully polarized state with all spins pointing down along $z$-direction. Flipping a spin into positive $z$-direction corresponds to an elementary excitation that costs an energy of $\Delta = 2h$ as depicted in Figure 6.8. The energy spectrum of a finite system with $N$ spins is given by $\{ E_n = h(2n - N) | n \in \mathbb{N} | 0 < n < N \}$. It is has a equidistant spacing of $\Delta = 2h$. It is reasonable to shift the spectrum by a constant energy so that the ground-state energy has a finite value $E_0$ in the thermodynamic limit $N \rightarrow \infty$. As described in chapter 2 it is expedient to interpret the elementary excitations as quasi-particles above the vacuum which is denoted by the state $|0\rangle$. Therefore, the spin flips are described in terms of hardcore bosons with creation and anihilation operators $b_i$ and $b_i^\dagger$ creating...
or anihilating a boson on site \( i \)

\[
\begin{align*}
&b_i^\dagger b_i \ldots b_i^\dagger \ldots \ldots b_n^\dagger |0\rangle = |i_1i_2\ldots i_n\rangle \quad \text{with} \quad i_1 \neq i_2 \neq \ldots \neq i_n \\
&b_i b_i \ldots b_n |i_1i_2\ldots i_n\rangle = |0\rangle \quad \text{with} \quad i_1 \neq i_2 \neq \ldots \neq i_n
\end{align*}
\]

according to the notation in [2.25]. Besides the usual bosonic commutation relations

\[
\left[ b_i, b_j^\dagger \right] = \delta_{ij} \quad \left[ b_i^\dagger, b_j^\dagger \right] = [b_i, b_j] = 0 \quad (6.3)
\]

these operators have to fulfill the hardcore constraint

\[
b_i b_i = b_i^\dagger b_i^\dagger = 0 \quad (6.4)
\]

This means that every site \( i \) can be occupied by maximal one boson as every spin can take only the two states ‘up’ or ‘down’ (or in bosonic language: ‘occupied’ and ‘empty’). For zero coupling \( J = 0 \) the Hamiltonian just counts the number of hardcore bosons

\[
H = 2h \sum_i b_i^\dagger b_i + E_0 = 2hQ + E_0 \quad (6.5)
\]

Consequently, the eigenbasis of \( H \) is given by the eigenbasis of the particle number operator \( Q \) [2.25].

Next, consider switching on the Ising term with coupling parameter \( J > 0 \). In \( \sigma^z \) basis the pauli matrix \( \sigma^x \) is just a spin-flip operator \( \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \). Thus, the action of the Ising term comprises the spin-flip of all pairs of neighbouring spins. According to the hardcore bosonic picture one has to consider three cases. The application of \( \sigma^x_i \sigma^x_j \) on a state with two spins \( i \) and \( j \) both pointing down (or up) corresponds to the creation (or anihilation) of two hardcore bosons. If both spins are aligned antiparallely, the Ising term that leads to a nearest neighbour hopping of the hardcore boson. All three cases are depicted in Figure 6.9 and 6.10.

Altogether, the mapping of the TFIM Hamiltonian to hardcore bosons yields

\[
H = 2h \sum_i b_i^\dagger b_i + J \left( \sum_{\langle i,j \rangle} b_i^\dagger b_j + b_i b_j^\dagger + b_j b_i^\dagger + b_j b_i \right) \quad (6.6)
\]

setting \( E_0 = 0 \).

The next step comprises the transformation of [6.6] into an effective Hamiltonian by
using the pCUT method. An extensive discussion on this issue is presented in the following section.

6.3 pCUT: Structure of the effective TFIM Hamiltonian

A perturbative continuous unitary transformation is used to derive an effective Hamiltonian that conserves the number of hardcore bosons emanating from the highfield limit of the antiferromagnetic transverse field Ising model. The transformation is performed for the two subspaces, where the number of quasi-particles is fixed to
zero (0QP sector) and one (1QP sector), in order to determine the excitation gap. According to (2.23) the resulting effective one-particle Hamiltonian has the form

$$H_{\text{eff}}^{(1)} = \sum_{i,j} t_{ij} \tilde{b}_i \tilde{b}_j$$  \hspace{1cm} (6.7)

Both sectors are given as high order series expansions in the perturbation parameter. In this basis the expansions of the hopping terms $t_{ij} \tilde{b}_i \tilde{b}_j$ are composed of different sequences of the creation and anihilation operators of the unperturbed system $\tilde{b}_i$ and $\tilde{b}_j$. In physical terms, the new quasi-particles that are conserved in the perturbed system can be interpreted as conglomerates of quasi-particles of the unperturbed system. Those particles are delocalized by virtual quantum fluctuations that are induced by the perturbation.

In the following the main focus is on the analysis of the quantum fluctuations generated by the Ising term in the TFIM. The application of pCUT to the TFIM Hamiltonian is presented step by step. The structure of the resulting effective Hamiltonian and its underlying physics is elucidated in detail.

6.3.1 Method

As described in chapter 2 the generic starting point for a perturbative treatment in quantum mechanics is given by a Hamiltonian of the form

$$H = H_0 + xV$$  \hspace{1cm} (6.8)

with an exactly solvable part $H_0$ and a perturbation term $xV$. The pCUT formalism additionally requires the following two conditions

- $H_0$ has an equidistant energy spectrum that is bounded from below by an unique ground-state. The energy of an elementary excitation is given by the difference between two adjacent energy levels. The elementary excitations can be interpreted as quasi-particles above the vacuum.

- The perturbation can be decomposed into $V = \sum_{n=-N}^{N} T_n$ with operators $T_n$ incrementing or decrementing the number of quasi-particles by $n$.

This approach is valid if the ground-state of $H_0$ is adiabatically connected to the ground-state of $H(x)$. As shown in the previous section the pure transverse field
term actually conforms to the specifications of $H_0$. Therefore, the pure transverse field term can be identified as the unperturbed system. For this purpose, the TFIM Hamiltonian is reformulated by

$$H(x) = \frac{H}{2\hbar} = \sum_i \sigma_i^z + \frac{J}{2\hbar} \sum_{(i,j)} \sigma_i^z \sigma_j^z$$

$$= \sum_i b_i^\dagger b_i + \frac{J}{2\hbar} x \left( \sum_{(i,j)} b_i^\dagger b_j + b_j^\dagger b_i^\dagger + \text{h.c.} \right) .$$  \hspace{1cm} (6.9)$$

The factor $\frac{1}{2}$ is integrated into the perturbation parameter $x$ in order to obtain a normalized excitation gap $\Delta(x = 0) = 1$ in units of $\hbar$. The Ising term is treated as the perturbation. According to the requirements of $V$, one has to identify the $T_n$ operators comprised by the Ising term. Due to the mapping to hardcore bosons the substitutions are apparent. One defines

$$T_0 := \sum_{(i,j)} b_i^\dagger b_j$$ \hspace{1cm} (6.10)$$

$$T_{+2} := \sum_{(i,j)} b_j^\dagger b_i^\dagger$$ \hspace{1cm} (6.11)$$

$$T_{-2} := \sum_{(i,j)} b_j b_i$$ \hspace{1cm} (6.12)$$

as $b_j^{(t)} b_i^{(t)}$ annihilates (or creates) two hardcore bosons and $b_j^\dagger b_i$ corresponds to a shift that does not change the number of particles.

Formally, one has to verify the relation $[Q, T_n] = nT_n$ by using the commutation relations (6.3). With the particle counting operator $Q = H_0 = \sum_i b_i^\dagger b_i$ one finds

$$[Q, T_{-2}] = \sum_{(k,l)} \sum_i \left[ b_i^\dagger b_i, b_k b_l \right]$$

$$= \sum_{(k,l)} \sum_i \left[ b_i^\dagger b_i, b_k b_l \right]$$

$$= -2 \sum_{(k,l)} b_k b_l = -2 \cdot T_{-2}$$ \hspace{1cm} (6.13)$$

For the $T_{+2}$ operator one proceeds in a similar way. For this case the remaining commutators in the third line yield $+\delta_{ik}$ instead of $-\delta_{ik}$. For the $T_0$ operator one
obtains

\[
[Q, T_0] = \sum_{i\langle k,l \rangle} \sum_{\langle j,l \rangle} \left[ b_i^\dagger b_i, b_{k,j}^\dagger b_j \right] = \sum_{i\langle k,l \rangle} \sum_{\langle j,l \rangle} \left[ b_i^\dagger b_i, b_{k,j}^\dagger b_j \right] + \left[ b_i^\dagger b_i, b_{k,j}^\dagger b_j \right] = 0 \quad (6.14)
\]

Thus, the TFIM Hamiltonian in the highfield limit meets all conditions required for the application of the pCUT method.

Next, let us outline the crucial steps for the determination of the effective Hamiltonian. The flow equations

\[
\frac{\partial}{\partial \ell} H(x, \ell) = [\eta^Q(x, \ell), H(x, \ell)] \quad (6.15)
\]

are solved in a perturbative fashion using the particle conserving generator \( \eta^Q(x, \ell) \).

In the \( Q \) eigenbasis the matrix elements of this operator read

\[
\eta_{ij}^Q(x, \ell) = \text{sgn}(q_i - q_j) H_{ij}(x, \ell). \quad (6.16)
\]

The resulting particle conserving effective Hamiltonian has the form

\[
H_{\text{eff}}^{n_{\text{max}}} = H_0 + \sum_{k=1}^{n_{\text{max}}} x^k \sum_{|m| = k} \sum_{m_i = 0} C(m) T(m) \quad (6.17)
\]

For the TFIM the operator sequences are given by \( T(m) = T_{m_1} T_{m_2} \ldots T_{m_k} \) with \( m_i \in \{-2, 0, 2\} \). The coefficients \( C(m) \) are corresponding to a certain operator sequence and do not depend on the considered model. The pCUT coefficients are available in electronical form in our database. In order to compute the matrix elements \( t_{ij} \) in (6.7) one has to apply the operator sequences to the corresponding states on an appropriate cluster. This routine is performed by a program provided by Kai Schmidt, which allows to compute matrix elements of the 0QP, 1QP and 2QP sectors on arbitrary clusters. The correct choice of the clusters in dependency of the desired order and matrix element is discussed in the next section. Using this approach the maximally obtained order for the calculation of the 1QP sector is limited to \( n_{\text{max}} = 8 \).
as the computation time and memory usage grows exponentially with the system size. In order to enhance the efficiency, the calculations are carried out on minimal graphs using the graph expansion method introduced in\[3\]. A modified code provided by Kris Coester is used to obtain a list of all relevant graphs and the corresponding amplitudes resulting from the pCUT calculations. The final step comprises the recombination of the particular graph contributions in order to obtain the correct results in the thermodynamic limit. The embedding scheme described in chapter 3 forms the basis for the latter procedure. With this approach the gap can be calculated up to order $n_{\text{max}} = 13$ on the kagome lattice and $n_{\text{max}} = 11$ on the triangular lattice.

Note, that the routines of graph generation and graph embedding are working independently from one another. This makes this approach very versatile and efficient at the same time. Once, a database of graphs and corresponding hopping elements is established, the embedding scheme allows to compute the effective matrix elements for arbitrary lattices and clusters. Moreover, this approach can be applied to other methods that provide a linked cluster expansion.

In the next section the attention is turned on the structure of the effective Hamiltonian and the characteristics of the quantum fluctuations arising in the TFIM. The linked cluster expansion allows an analysis of particular contributions of virtual fluctuations in the spatial domain and delivers insight into some interesting effects.

### 6.3.2 Quantum fluctuations in the TFIM

Here a detailed discussion on the explicit shape and structure of the virtual fluctuations arising in the effective Hamiltonian is given. The following analysis elucidates further aspects concerning the optimal choice of master clusters and the determination of relevant graphs. Furthermore, it provides an illustrative depiction of the physical processes governing the characteristics and dynamics of one-particle states. As will be shown in the subsequent sections, the TFIM on the kagome lattice gives rise to a localized mode similar to the magnon states that are especially known in the context of macroscopic magnetization jumps\[33\]. The definitions and ideas presented in this section play an essential role for the further discussion on local modes in the TFIM.

It was shown that the effective Hamiltonian of the TFIM is a series of monomials of the operators $T_{-2}$, $T_{+2}$ and $T_0$. All processes in order $n$ are encoded in monomials of $n$-th degree. In order to analyze the resulting local processes, consider the
The local operators $\tau_{m,k}$ can be identified in the following way:

\begin{align}
\tau_{-2,k} &= b_i b_j \\
\tau_{+2,k} &= b_i^\dagger b_j^\dagger \\
\tau_{0,k} &= b_i^\dagger b_j
\end{align}

with the local bond index $k = i, j$. Consequently, the virtual fluctuations are given by all possible combinations of two-particle creation or anihilation processes and one-particle shifts with respect to particle conservation:

$$H_{\text{eff}} = H_0 + \sum_k x^k \sum_{\{\sum m_i = 0\}} \sum_{\{(i_1,j_1) \ldots (i_k,j_k)\}} \tau_{m_1,(i_1,j_1)} \tau_{m_2,(i_2,j_2)} \ldots \tau_{m_k,(i_k,j_k)}$$

$$\text{with } m_i = \{-2, 0, +2\}$$

As we are interested in the physics of one-particle states, only the one-particle irreducible matrix $H_1 = \sum_{\langle i,j \rangle} \langle i | H_{\text{eff}} | j \rangle \langle j | - E_0 \delta_{ij}$ is considered. The aim is to identify those virtual processes that are contributing to the irreducible matrix elements $t_{ij}$.

Due to the linked cluster theorem only linked processes can have a finite contribution. Linked processes are defined by operator sequences $\tau_{m_1,(i_1,j_1)} \tau_{m_2,(i_2,j_2)} \ldots \tau_{m_k,(i_k,j_k)}$ acting on linked subclusters $C = i_1 \cup j_1 \cup \ldots \cup i_k \cup j_k$. Hence, every process on a linked subcluster $C$ transferring a particle from site $i \in C$ to $j \in C$ may contribute to the hopping element $t_{ij}$. Figure 6.11 shows an example of different virtual fluctuations of order $n = 4$ on a fixed subcluster contributing to $t_{ij} = \langle i | H_1 | j \rangle$.

**Figure 6.11:** Illustration of two different order $n = 4$ processes on the same subcluster contributing to $t_{ij}$. The red highlighted circles denote occupied sites. Due to simplicity the spatial index of the $\tau$ operators is neglected. The first process corresponds to the sequence $\tau_{+2} \tau_{-2} \tau_{+2} \tau_{-2}$. The second sequence is given by $\tau_{+2} \tau_{-2} \tau_{+2} \tau_{-2} \tau_{+2} \tau_{-2}$.

In this context it is useful to introduce the notion of hopping graphs.
The set of all virtual fluctuations on a certain subcluster $C$ transferring a particle from site $i$ to site $j$ is represented by a hopping graph $G_{C}^{\alpha\beta}$. A hopping graph $G_{C}^{\alpha\beta}$ is a graph $G$ with two selected sites $\alpha, \beta \in G$ defining an initial- and end site. Furthermore, there exits a bijective mapping $G_{C}^{\alpha\beta} \rightarrow C$ such that $\alpha$ and $\beta$ are covering $i$ and $j$. $G_{C}^{\alpha\beta}$ thus denotes the contribution to $t_{ij}$ of the corresponding embedding of $G$. A certain embedding is refered to as the virtual hopping process from $i$ to $j$ on $C$. The particular $\tau$ sequences acting in $C$ are called subprocesses of $G_{C}^{\alpha\beta}$. Note, that two different virtual hopping processes that are represented by the same hopping graph yield the same contribution as they comprise identical sub processes. (As described in chapter 3 this is the essential point of the embedding scheme.) In other words, they are topologically equivalent. Figure 6.12 shows two distinct virtual hopping processes of $t_{ij}$ that are represented by an identical hopping graph.

![Figure 6.12](image)

**Figure 6.12:** (1) Two different virtual hopping processes contributing to $t_{ij}$. Both have the same hopping graph shown in (2).

Next, let us examine the relation between the shape and the size of virtual hopping processes considering a certain order. The question is whether a particular hopping
graph actually has a non-vanishing contribution for a given order. This allows to determine the maximal size of the relevant graphs determining the minimal size of the master cluster. First, note that the number of $\tau$ operators in a particular sequence equals the considered order. As the $\tau$ operators are acting on single bonds all graphs in order $n$ can have at maximum $n$ bonds. However, the minimal order of a virtual hopping process of fixed size also depends on the starting and end point of the quasiparticle. For certain hopping processes some bonds have to be touched more than one time in order to connect the initial state with the desired final state. The TFIM (or more general: effective models composed of sequences with $\tau_m |m = \{-2, 0, +2\}$) provide a very illustrative scheme that allows to construct hopping processes for a given order. One finds that all virtual fluctuations of $t_{ij}$ are related to a hypothetical process where the particle is hopping from site to site starting at $i$ and finally arriving at $j$. Such a process corresponds to a pure $\tau_0$ sequence shifting the quasi-particle from site to site. To see this, consider an arbitrary $\tau$-sequence in order $n$ transfering a particle from site $i$ to site $j$

$$\tau_{m_1,(i_1j_1)} \tau_{m_2(i_2,j_2)} \cdots \tau_{m_n(i_n,j_n)} |i\rangle = |j\rangle \quad (6.22)$$

on a given linked subcluster $C = i_1 \cup j_1 \cup \ldots i_n \cup j_n$. During this process the states on every site in $C$ are flipped between 'occupied' and 'empty'. At the beginning, site $i$ is occupied and all other sites are empty. After the fluctuation process only site $j$ is occupied. Note, that every $\tau$ operator can be seen as a flip $f_{i_1}f_{j_1}$ of two neighbouring sites $i_1$ and $j_1$. Hence, the hopping process corresponds to a sequence of state flips $f_k$ that are applied in a certain succession. If the initial and the final state on a site $p$ are identical, the number of flips $f_p$ must to be even. Else if $i \neq j$, the number of flips $f_i$ and $f_j$ must be odd. It is clear that the final state does not depend on the particular sequence of flip operators, since the flip operators commute. Thus, any permutation of flips will lead to the same final state $|j\rangle$. As every $\tau$-sequence of given order $n$ on a subcluster $C$ can be written as a succession of flips, one concludes that all $n$-th order $\tau$-sequences transfering a particle from $i$ to $j$ on $C$ are related by a certain permutation of their corresponding flip representation. As an example consider the processes shown in figure 6.13.

In a final step one has to exclude the existence permutations of order $m < n$ giving rise to a distinguished $\tau$-sequence that is not related to a pure $\tau_0$ sequence. For this purpose one may argue as follows. Consider a hopping process from site $i$ to $j$ on a subcluster $C$ and the corresponding $\tau_0$-sequence $T_n$ with minimal order $n$. In this
Figure 6.13: All $\tau$ sequences for a chain of order $n = 3$. The processes are related to each other by a permutation of neighbouring state flips.

context minimal order means that there are no $\tau_0$-sequences on $C$ transferring from $i$ to $j$ with order $m < n$. Now, assume that there is an $\tau$-sequence $T_m$ of order $m < n$ that is not related to a pure $\tau_0$-sequence but is acting on the same subcluster $C$. All flips in $T_m$ must be a comprised by $T_n$. Removing a pair of flips $f_a f_b$ from $T_n$ with neighbouring sites $a$ and $b$ corresponds to the creation of two particles on $a$ and $b$ (or the shift of a particle if $a = j$ or $b = j$). Hence, the operators $f_a f_b$ has to be removed twice leading to two different cases.

1. Removing $f_a f_b f_a f_b$ from $T_n$ corresponds to a removal of the bond $(a, b)$ from $C$. Consequently, $T_m$ does not act on the full subcluster $C$.

2. $T_m$ still comprises flip operators $f_a f_b$. From this follows that $T_m$ is a pure $\tau_0$ sequence with order $m < n$ contradicting the first assumption.

One concludes that there are no distinguished $\tau$-sequences that are not related to $\tau_0$-sequences.

It should be noted that the pCUT coefficients of pure $T_0$ sequences of order $n \geq 2$ vanish and that these processes therefore do not contribute. However, they are a great help to envision virtual hopping processes of a certain order.

In the next section the pCUT results of the triangular and kagome TFIM are presented and discussed.
6.4 One-particle properties of the kagome and triangular TFIM

In this section the one-particle properties of the kagome and triangular TFIM are determined by means of the effective Hamiltonian obtained with pCUT. First, both systems are considered separately. A subsequent comparison and general discussion is presented in the last subsection.

6.4.1 Triangular lattice

The pure one-particle contributions obtained by the perturbative unitary transformation are the matrix elements $t_{ij}$ of the irreducible one-particle Hamiltonian $H_1$ in (6.7) that is defined on a triangular lattice $\Gamma_{tri}$. As already discussed, the $t_{ij}$ denote the amplitudes of a quasi-particle hopping from site $i$ to site $j$. The locations on the triangular lattice can be assigned to position vectors $\vec{r}_i$ and $\vec{r}_j$ as shown in figure 6.14. According to 2.25, the one-particle basis states are denoted by $|i\rangle := |\vec{r}_i\rangle$. In this sense, one defines

$$t_{ij} := t(\vec{r}_i, \vec{r}_j) = t(\vec{r}_i, \vec{r}_i + \vec{d})$$

(6.23)

with a corresponding hopping vector $\vec{d} = \vec{r}_j - \vec{r}_i$. The considered Hamiltonian is

![Figure 6.14: Illustration of the triangular lattice. The vectors $\vec{e}_1$ and $\vec{e}_2$ are elementary lattice translations of length $(\vec{e}_i)^2 = 1$. The vectors $\vec{r}_i$ denote locations on the lattice.](image)
invariant under lattice translations implying the following relation:

\[ t(\vec{r}_i, \vec{r}_i + \vec{d}) = t(\vec{r}_i + \vec{a}, \vec{r}_i + \vec{d} + \vec{a}) \quad \forall \, \vec{a} = n\vec{e}_1 + m\vec{e}_2 \mid n, m \in \mathbb{Z} \quad (6.24) \]

Consequently, the hopping elements only depend on the hopping vector \( \vec{d} \)

\[ t(\vec{r}_i, \vec{r}_i + \vec{d}) := t_{\vec{d}} \quad \forall i, j \in \Gamma_{\text{tri}} \quad (6.25) \]

Note, that the number of distinct hopping elements \( t_{\vec{d}} \) is limited due to the finite range of the considered processes in \( H_{\text{eff}} \).

In order to determine the eigenenergies of \( H_1 \), one has to perform a basis transformation from the spatial domain into momentum space. The momentum basis states are obtained by the Fourier transform

\[ |\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_j e^{-i\vec{k}\vec{r}_j} |r_j\rangle \quad (6.26) \]

whereas \( N \) is the number of sites in \( \Gamma_{\text{tri}} \). The correspondent matrix elements of \( H_1 \) can be obtained by

\[ \langle k' | H_1 | k \rangle = \langle k' | \frac{1}{\sqrt{N}} \sum_{d} \sum_j e^{-i\vec{k}\vec{r}_j} t_{\vec{d}} |r_j + \vec{d}\rangle \quad (6.27) \]

\[ = \langle k' | \frac{1}{\sqrt{N}} \sum_{d} \sum_j e^{-i\vec{k}(\vec{r}_j - \vec{d})} t_{\vec{d}} |r_j\rangle \quad (6.28) \]

\[ = \langle k' | \sum_{\vec{d}} e^{-i\vec{k}\vec{d}} t_{\vec{d}} \frac{1}{\sqrt{N}} \sum_j e^{-i\vec{k}\vec{r}_j} |r_j\rangle \quad (6.29) \]

\[ = \delta_{k'k} \sum_{\vec{d}} e^{i\vec{k}\vec{d}} t_{\vec{d}} \quad (6.30) \]

\[ = \delta_{k'k} \omega(\vec{k}, x) \quad (6.31) \]

In momentum space the irreducible one-particle Hamiltonian becomes diagonal. The dispersion \( \omega(\vec{k}, x) = \sum_{\vec{d}} e^{i\vec{k}\vec{d}} t_{\vec{d}(x)} \) represents the one-particle excitation energies in dependence of the momentum \( \vec{k} \) and perturbation parameter \( x \). Note, that the hopping elements \( t_{\vec{d}} \) are polynomials in \( x \). The sum runs over all hopping vectors \( \vec{d} \) occurring up to order \( n_{\text{max}} \). Due to inversion symmetry \( t_{\vec{d}} = t_{-\vec{d}} \) the sum can be restricted to positive hopping vectors \( \vec{d}^+(\vec{d}^+) = n\vec{e}_1 + m\vec{e}_2 \) with \( n, m \in \mathbb{N} \) and order\( (\vec{d}) \leq n_{\text{max}} \).
yielding the one-particle dispersion

\[ \omega(\vec{k}, x) = t_0 + 2 \sum_{d^+} t_d \cos(\vec{k}d). \quad (6.32) \]

The coefficients of the dispersion up to order \( n = 4 \) are listed in Appendix C. A contour plot of the resulting one-particle dispersion for \( x = \frac{1}{8} \) is depicted in figure 6.15. The

![Contour plot of the one-particle dispersion \( \omega(\vec{k}) \) for the triangular TFIM with \( x = \frac{1}{8} \) in units of \( \hbar \). All processes up to order \( n = 11 \) are taken into account.](image)

minima of the dispersion are located at \( \vec{k}_{\text{min}} = \pm(\frac{4}{3}\pi, \frac{2}{3}\pi) \), \( \vec{k}_{\text{min}} = \pm(\frac{2}{3}\pi, -\frac{2}{3}\pi) \), and \( \vec{k}_{\text{min}} = \pm(\frac{4}{3}\pi, -\frac{4}{3}\pi) \). They are identifying the momentum and energy of the one-particle excitation gap. Up to order \( n = 11 \) the resulting gap is given by

\[
\omega(\vec{k}_{\text{min}}) = 1 - 3x + \frac{3}{2}x^2 - \frac{15}{2}x^3 + \frac{243}{8}x^4 - \frac{1671}{8}x^5 + \frac{22275}{16}x^6 - \frac{162855}{16}x^7 + \frac{9700617}{128}x^8 - \frac{595490847}{1024}x^9 + \frac{2010551941313}{442368}x^{10} - \frac{1777064899901}{49152}x^{11}. \quad (6.33)
\]
In general the momentum of the gap defines a favoured ordering structure of the considered system. As will be shown, the order is strongly influenced by frustration which often leads to non-trivial ordering structures. The triangular TFIM provides a vivid example for the connection between frustration and order which is illustrated in the following.

As one can see, the maximum of the one-particle excitation energy is located at $\vec{k} = \vec{0}$. Interpreting the phase $e^{i\vec{k}\vec{r}}$ of a one-particle state $|\vec{r}\rangle$ as a classical two dimensional vector, the $\vec{k} = \vec{0}$ state corresponds to a superposition of one-particle states with parallelly aligned phase vectors. This configuration is energetically unfavourable as a result of the antiferromagnetic coupling. Instead, quantum fluctuations induced by the perturbation favour an antiparallel alignment of phase vectors. For non-frustrating lattices, e.g. the square lattice, the antiferromagnetic Ising term consequently induces a Neel order with $\vec{k} = (\pi, \pi)$. However, the triangular lattice does not provide a global antiparallel alignment due to frustration. Figuratively speaking, the minima of the one-particle dispersion identifying the locations of the gap are displaced by the frustration. This effect can be visualized as follows. Consider the system in figure 6.16 that adiabatically connects the triangular TFIM with the square TFIM by a parameter $\delta \in [0, 1]$. The parameter $\delta$ indicates the degree of frustration with $\delta = 1$ corresponding to the fully frustrated triangular antiferromagnet and $\delta = 0$ yielding the non-frustrated square antiferromagnet. In both cases the one-particle energy starts to disperse in first order in $x$. Thus, it is sufficient to consider first order processes given by nearest neighbour hopping. The corresponding one-particle dispersion then reads

$$\omega_{\delta}(\vec{k}) = 1 + xt_1 (2 \cos (k_1) + 2 \cos (k_2) + \delta 2 \cos (k_2 - k_1)) \quad (6.34)$$

with $x = \frac{J}{h}$ and $t_1 = 1$. Figure 6.17 shows the dispersion $\omega_{\delta}(\vec{k})$ for different parameters $\delta$ and $x = \frac{1}{8}$. For zero frustration ($\delta = 0$) there is a single gap located at $\vec{k} = (\pi, \pi)$. For small but finite frustration ($\delta = 0.3$) the gap is still located at $\vec{k} = (\pi, \pi)$ but the excitation energy is slightly raised and less dispersive due to the frustration. Above a critical value $\delta_c < \delta = 0.65$ the dispersion yields two gaps that are symmetrically displaced from the original minimum. As a result of the newly formed structure the energy gaps are lowered again. Note, that the energy at $\vec{k} = 0$ is constantly increasing as $\delta$ introduces additional antiferromagnetic couplings. For $\delta = 1$ one obtains the primarily considered triangular TFIM. Its ordering structure
Figure 6.16: Illustration of the TFIM on a square lattice with an additional antiferromagnetic coupling connecting spins on a diagonal with coupling strength $\delta J$. For $\delta = 0$ the system is a simple square TFIM. For $\delta = 1$ one obtains the triangular TFIM. Thus, $\delta$ can be seen as a parameter that indicates the degree of frustration. The elementary lattice translation vectors are denoted by $\vec{e_1}$ and $\vec{e_2}$.

is illustrated in figure 6.18. Compared to the ordering structure on the square lattice for $\delta = 0$, the triangular lattice provides a more orderly structure with lower symmetry. Apparently, the frustration driven by $\delta$ induces a further ordering for $\delta > \delta_c$. A curve sketching of $\omega_\delta(\vec{k})$ yields a critical value of $\delta_c = 0.5$. Note, that the previous considerations are concerning the first excitation gaps and not the ground state. In this sense, the transition at $\delta_c$ does not describe a quantum phase transition. However, it provides an indication of possible ordering patterns induced by quantum phase transitions at higher values of $x$ (low transverse field). The closing of the excitation gap for a critical $x_c$ indicates the condensation of a whole branch of high energy modes forming a new ground state. The symmetry of the new ground state is determined by the energetically favoured ordering of the lowest excitation. As both systems, the triangular TFIM and square TFIM, exhibit quantum order at low transverse field [20, 22] a tuning of $\delta$ for $x > x_c$ could give rise to a quantum phase
Figure 6.17: Contour plots for the dispersion $\omega_\delta(k)$ at different values of $\delta$. The corresponding plots on the bottom show the dispersion parametrized with $k_1 = 2\pi - k_2$. 
transition between two quantum ordered phases, providing an interesting subject for future work.

In the next section the focus is on the one-particle properties of the kagome TFIM.

### 6.4.2 Kagome lattice

The calculation of the dispersion on the kagome lattice is done in an analogous fashion to the triangular lattice. Though, one has to consider that the kagome lattice is no regular bravais lattice. The kagome structure can be defined as an arrangement of triangular unit cells located at the sites of an effective triangular lattice as shown in figure 6.19. According to this, the one-particle states in the spatial domain are defined as $|\vec{r},\alpha\rangle$ with $\vec{r}$ denoting the position of the unit cell and $\alpha$ specifying the location of the particle within the unit cell. The Fourier-transform of the basis states then reads

$$|\vec{k},\alpha\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} |\vec{r},\alpha\rangle$$  \hspace{1cm} (6.35)

with complex coefficients $C_\alpha$ and $N$ denoting the total number of unit cells. The translational symmetry of the Hamiltonian requires

$$\langle \vec{r}, \beta | H_1 | \vec{r}, \alpha \rangle = t^{\alpha\beta}_d$$  \hspace{1cm} (6.36)
Figure 6.19: Illustration of the kagome lattice defined by a triangular unit cell which is depicted on the left-hand site. The unit cells are located at the sites of an effective triangular lattice as shown on the right-hand side. The elementary lattice translations vectors are denoted by $\vec{e}_1$ and $\vec{e}_2$.

for arbitrary unitcells $i$ and $j$. Consequently, the action of the irreducible one-particle Hamiltonian on $|\vec{k},\alpha\rangle$ yields

$$H_1 |\vec{k},\alpha\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{d},\beta} \sum_{\vec{r}} e^{-i\vec{k}\vec{r}} t_{\alpha\beta}^{\vec{d}} |\vec{r} + \vec{d},\beta\rangle \quad (6.37)$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{r}} \sum_{\vec{d}} e^{-i\vec{k}(\vec{r}-\vec{d})} t_{\alpha\beta}^{\vec{d}} |\vec{r},\beta\rangle \quad (6.38)$$

$$= \sum_{\vec{d}} e^{-i\vec{k}\vec{d}} t_{\alpha\beta}^{\vec{d}} \left\{ \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{k}\vec{r}} |\vec{r},\beta\rangle \right\} \quad (6.39)$$

$$= \sum_{\vec{d},\alpha} e^{-i\vec{k}\vec{d}} t_{\alpha\beta}^{\vec{d}} |\vec{k},\beta\rangle \quad (6.40)$$

$$= \Omega \vec{C} \quad (6.41)$$

$\Omega$ is a hermitian $3 \times 3$-matrix with matrix elements $\Omega_{\alpha\beta} = \sum_{\vec{d},\alpha} e^{i\vec{k}\vec{d}} t_{\alpha\beta}^{\vec{d}}$ representing the one-particle Hamiltonian in momentum space. The matrix elements up to order $n = 4$ are listed in Appendix C. Due to lattice symmetries it is sufficient to calculate $\Omega_{11}(k_1,k_2)$ and $\Omega_{12}(k_1,k_2)$. The other matrix elements can be obtained by the
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The following relations

\[
\begin{align*}
\Omega_{22}(k_1, k_2) &= \Omega_{11}(k_2, k_1) \\
\Omega_{33}(k_1, k_2) &= \Omega_{11}(-k_2, k_1 - k_2) \\
\Omega_{13}(k_1, k_2) &= \Omega_{12}(k_1 - k_2, -k_2) \\
\Omega_{23}(k_1, k_2) &= \Omega_{12}(k_2 - k_1, -k_1)
\end{align*}
\]  
\tag{6.42}

\[
\Omega_{\alpha\beta} = (\Omega_{\beta\alpha})^*
\]  
\tag{6.43}

Diagonalizing the Hamiltonian finally yields three one-particle energy bands. The resulting three one-particle energy bands for \(x = \frac{1}{10}\) are depicted in figure 6.20, 6.21 and 6.22. There are two dispersive high-energy bands and a low-energy band that stays flat up to and including order \(n = 7\)

\[
\omega^{(7)}_{\text{low}}(\vec{k}) = 1 - 2x + 2x^2 - 3x^5 + \frac{243}{8}x^6 + \frac{2609}{8}x^7.
\]  
\tag{6.44}

Figure 6.20: Illustration of both high 1QP energy bands of the kagome TFIM for \(x = 0.1\).

In the following, the focus is on the low-energy band. Note, that in general the \(\vec{k}\) independence of an one-particle energy band indicates the existence of a localized one-particle mode as any superposition of momentum basis states \(|\vec{k}\rangle\) provides an eigenstate of \(H_1\). A uniform superposition in momentum space corresponds to a state that is completely localized in the spatial domain. One concludes that the effective Hamiltonian \(H^{(7)}_1\) of the kagome TFIM gives rise to a local one-particle eigenmode.
Figure 6.21: Lowest one-particle energy band of the kagome TFIM for $x = 0.1$.

Figure 6.22: One-particle energy bands of the kagome TFIM for $x = 0.1$ against $k_1 = 2\pi - k_2$. 
Interestingly, this mode starts to disperse in order $n = 8$, which means that quantum fluctuations occurring in order $n = 8$ are lifting the degeneracy in momentum-space and select a specific gap to be energetically more favourable. The locations of the energy gap are $\vec{k}_{\text{min}} = \pm(\frac{4}{3}\pi, \frac{2}{3}\pi)$, $\vec{k}_{\text{min}} = \pm(\frac{2}{3}\pi, -\frac{4}{3}\pi)$ and $\vec{k}_{\text{min}} = \pm(\frac{4}{3}\pi, -\frac{4}{3}\pi)$. The form of the resulting eigenvector (up to a global phase shift) is given by

$$\vec{C} = \frac{1}{\sqrt{3}} \left( 1, e^{i\frac{2}{3}\pi}, e^{-i\frac{2}{3}\pi} \right) |\vec{k}_{\text{min}}\rangle .$$

(6.45)

This corresponds to the $\sqrt{3} \times \sqrt{3}$-structure shown in figure 6.23. Note, that it is consistent with the ordering pattern in the bond ordered phase of the kagome antiferromagnet with tilted field (figure 6.6) suggested by Moessner et al. [20, 21].

Interestingly, one finds that the kagome Heisenberg antiferromagnet exhibits very similar phenomena. In 1991 Harris et al. studied the classical antiferromagnetic Heisenberg model on a kagome lattice by means of a high-temperature expansion and showed that thermal fluctuations are inducing the same $\sqrt{3} \times \sqrt{3}$-structure illustrated in figure 6.23. Similar to the kagome TFIM, this structure is generated in 8-th order in $\frac{1}{T}$ indicating considerable similarities between thermal fluctuations and virtual quantum fluctuations arising in the TFIM.

In the same work they further demonstrated that a spin wave theory of the quantum

\begin{figure}[h]
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\includegraphics[width=\textwidth]{figure6.23.png}
\caption{Illustration of the eigenstate corresponding to the gap. The state exhibits a $\sqrt{3} \times \sqrt{3}$-structure.}
\end{figure}
mechanical Heisenberg model on the kagome lattice gives rise to a local mode corresponding to an hexagonal arrangement of nearest neighbour spins with alternating phase. This mode is similar to the localized magnons in frustrated antiferromagnets which are of great interest in current research especially in the context of macroscopic magnetization jumps \cite{33}. In the following section we show that the kagome TFIM also exhibits such a localized eigenmode. The reason for the locality of this mode up to order \( n = 7 \) and the processes effecting its dispersion in higher orders are studied in detail.

### 6.4.3 Local mode in the kagome TFIM

This section provides an extensive analysis of the local mode emerging in the kagome transverse field Ising model. The existence and the properties of this local mode can be understood by means of simple geometrical considerations. In the subsequent section the concepts developed for the kagome TFIM are generalized to a larger class of models providing a heuristic method for the identification and characterization of localized modes.

As shown in the previous section, the lowest one-particle energy band of the kagome TFIM exhibits no \( \vec{k} \) dependency up to and including order \( n = 7 \) suggesting the existence of an local eigenmode that becomes dispersive in order \( n = 8 \). In general, a localized state can be defined as a superposition of one-particle states \( |r_i⟩ \) located in a restricted area \( \mathcal{L} \)

\[
|\psi_{\text{loc}}⟩ = \sum_{r_i \in \mathcal{L}} \alpha_i |r_i⟩.
\]

with some coefficients \( \alpha_i \). Locality up to order \( n = 7 \) means

\[
H_1 |\psi_{\text{loc}}⟩ = \epsilon |\psi_{\text{loc}}⟩ + O(x^8).
\]

For small perturbation \( x \ll 1 \) the corresponding true eigenstate \( |\Psi⟩ \) hence provides a very small probability density of finding an particle outside the area \( \mathcal{A} \).

Considering the kagome TFIM the local mode is given by a superposition of one-particle states located at the sites of an arbitrary hexagon similar to the localized mode in the kagome Heisenberg antiferromagnet ref\[33\]. The local mode is illustrated in figure \[6.24\]. According to the numbering of sites in figure \[6.24\] the corresponding
state can be written as

\[ |\psi_{\text{loc}}\rangle = \frac{1}{\sqrt{6}} (|1\rangle - |2\rangle + |3\rangle - |4\rangle + |5\rangle - |6\rangle) \]

(6.48)

Applying the effective Hamiltonian \( H_1 \) to this state indeed yields locality in terms of

\[ \text{equation (6.47).} \]

Based on the effective particle picture the locality can be explained by an destructive interference of virtual hopping processes which prevents the particles from escaping the hexagon. The dispersion emerging in order \( n = 8 \) must be related to non trivial processes that do not occur for \( n < 8 \).

In order to understand the essential mechanisms effecting the locality and dispersion it is useful to characterize the different processes using the concept of hopping graphs introduced in chapter \( \text{3} \). Recall that a hopping graph \( G^{\alpha\beta} \) represents the contribution of all \( \tau \)-sequences from \( \alpha \) to \( \beta \) on \( G \). Virtual hopping processes represented by the same hopping graph are topologically equivalent and hence yield the same contribution. With this picture in mind one is able to visualize the destructive interference of different hopping processes. Note that virtual fluctuations with a particle staying at the hexagon (e.g. local hopping) can not contribute to a dispersion in any order in \( x \) as they effect no kinetics.

At first, consider the fluctuations in first order which are given by a simple nearest
neighbour hopping. Figure 6.25 shows all relevant first order fluctuations leaving the hexagon. Apparently, all processes exhibit the same topology (as they are represented by the same hopping graph) providing identical hopping amplitudes. Due to the alternating phase of the particles every fluctuation is annihilated by an contrary fluctuation of a particle with opposite sign. The first order processes exemplify the incidence of opposing fluctuations which is essential for destructive interference. Note, that the illustrated nearest neighbour hopping processes on the considered hopping graph are not only canceling out for order \( n = 1 \) but also for arbitrary orders in \( x \) as the annihilation of opposing fluctuations does not depend on their comprised sub processes. It is rather the geometry of the fluctuations that constitutes the crucial point. Following the findings in the subsection 6.4.2 any process in order \( n \) can be represented by a particle hopping from site to site in \( n \) steps. In order to escape the hexagon any particle has to traverse at least one of the sites \( p^*_i \) enclosing the hexagon. Now, envision a process of a particle \('+\)' traversing the hexagon and escaping through a \( p^*_i \). The opposing process is then given by an mirrored particle \('-\)' imitating the process of \('+\)' within the hexagon (such that both \('+\)' and \('-\)' are escaping through the same \( p^*_i \)) and tracing the path of \('+\)'.

**Figure 6.25**: Illustration of all first order fluctuations leaving the hexagon corresponding to the local mode. Processes of different color have an opposite sign. Consequently all processes are annihilating each other.

A general procedure to construct a possible counter process of a certain fluctuation is given as follows:

- Consider a process from site \( i \) to site \( j \) on a cluster \( C \) represented by a hopping graph \( G^C_{\alpha \beta} \). In order to obtain a counter process, mirror a subcluster of \( C \) along
Figure 6.26: Example of two counter processes. The illustrated processes correspond to a particle ‘+’ or ‘−’ hopping to site \( j \) on the highlighted subclusters. The points \( p_{*}^{i} \) enclosing the hexagon are colored green. Note, that the particles are leaving through the same \( p_{*}^{i} \). Both processes are represented by the hopping graph shown on the right-hand side. Hence, their contributions cancel out.

This procedure is called counter graph transformation. Its principle is exemplified in figure 6.27. Every process that allows for a counter graph transformation is annihilated by a destructive interference with its counter process. Actually, one finds generic types of processes that always allow for a counter graph transformation. Those are processes with a final site \( j \) lying on a symmetry line of the lattice and processes covering only one \( p_{*}^{i} \) (particle escapes hexagon but does not return) or two \( p_{*}^{i} \) on the same symmetry line.

There are also hopping graphs that change their topology for any possible counter graph transformation as shown in figure 6.28. These graphs represent virtual fluctuations that are not completely annihilated by opposing processes yielding a finite amplitude of a particle leaving the hexagon. Hence, they correspond to processes that lead to a dispersion of the local mode. The crucial step is to identify the smallest graphs that have no counter graph in order to determine for which order the mode
Figure 6.27: Example of a counter graph transformation. A subcluster containing the initial site of the particle is mirrored along a symmetry line that crosses a touched site \( p^* \).

Figure 6.28: Example of a process that is not annihilated by a counter process. Any counter graph transformation changes the topology. Consequently, the contributions of the competing processes are differing. This leads to a finite hopping amplitude of a particle leaving the hexagon.
Figure 6.29: Illustration of the looped process that first appears in order $n = 7$ and the corresponding counter process. The particle hops to a final site $j$ lying on a symmetry line.

will start to disperse. In general those graphs are related to closed loops comprising two different $p^*_i$ that do not lie on the same symmetry line. Note, that any counter graph transformation will cut such an loop.

Following this argumentation and the results on the low-energy band, the first relevant graphs on the kagome lattice have to occur in order $n = 8$. Naively, one would expect a dispersion in order $n = 6$ since the smallest looped process is given by an enclosed hexagon that first appears in order $n = 6$. However, this hopping graph corresponds to a local process and hence does not contribute to the dispersion. The next looped process is of order $n = 7$. In this case, the occupied site of the final state is located at a symmetry line of the lattice. Thus, there exits a corresponding counter process as shown in figure 6.29. In compliance with our results, the first hopping graph that is not annihilated by an opposing fluctuation appears in order $n = 8$.

Figure 6.30 depicts the correspondent looped process. Besides this loop, there are also other processes leading to a dispersion in order $n = 8$. All of them are related to non-trivial looped processes. An interesting feature of this localized mode is the fact, that it is very robust against small external perturbations. Due to the geometry of the lattice a large majority of fluctuations is annihilated. The occurrence of localized states in other lattices and models is discussed in the next subsection.
6.4.4 Local one-particle states

This section provides a general discussion on local modes arising in other lattices. A simple heuristic scheme is described that allows the identification of local modes on different classes of models. Furthermore, possible construction schemes for systems exhibiting localized modes are presented.

As shown in section 6.4 the one-particle mode of the triangular TFIM already disperses in first order in $x$. In contrast to the kagome lattice there seems to be no localized state although both systems exhibit the same intrinsic physics. One concludes, that the emergence of such localized states is of geometrical nature. Based on the geometrical observations on the kagome lattice one could state the following criteria for a lattice exhibiting a local mode. Consider an arrangement of one-particle states located on the sites $r$ within an restricted area $\mathcal{L}$. The sites enclosing this local area are denoted by $p$. It is clear that any path leaving $\mathcal{L}$ has to pass through a $p$ which can interpreted as a gate. In order to allow destructive interference every gate $p$ has to be connected to at least two sites $r$ in $\mathcal{L}$. This restricted area provides a localized mode, if it allows for an arrangement of particles with alternating sign, such that every path between an $r_i$ and a $p$ within the restricted area is annihilated by an opposing path. The locality of the considered mode is destroyed by paths or
processes that are closing a loop between different $p$.

Considering the triangular lattice, it turns out that there is no local arrangement that complies to the stated criteria. One always finds a $p$ that is connected to only one site in $\mathcal{L}$ providing a branch that allows a particle to escape in first order.

Let us illustrate these principles by means of another frustrated lattice. For instance, consider the checkerboard lattice shown in figure 6.31. Following our criteria the localized state is given by an arrangement of particles with alternating phase located at the sites of an square plaquette. The displayed process closes a non trivial loop between two different sites $p$ and removes the particle from the plaquette. In the case of the TFIM the corresponding hopping graph first appears in order $n = 5$. Calculations for the checkerboard TFIM carried out by Kris Coester indeed show that the dispersion of the lowest one-particle mode is completely flat up to and including order $n = 4$ in accordance with the predictions. This heuristic can be also generalized to a larger class of systems. In principle it can be applied to all models providing a white graph expansion [6]. White graph expansion implies that the contribution of a certain graph only depends on its topology, which holds true for all lattice systems with uniform couplings.

Based on these rules one is able to construct a variety of different systems exhibiting localized states. A simple construction scheme is given as follows.

Consider a plaquette that meets all criteria stated above. In general such a plaquette consists of connected sites $i$ representing the location of the local mode and some enclosing sites $p$ constituting the gates of the mode. The whole system can be obtained by an arrangement of plaquettes that are connected by their gates $p$. Figure 6.32 shows an example of a two dimensional lattice that is constructed in this fashion.
The locality of the corresponding mode is destroyed by a process that is represented by the displayed hopping graph. There are also systems exhibiting modes that are expected to be local up to infinite order as for example the one dimensional chains of non-frustrated plaquettes exemplified in figure 6.33. There is no cycle process in one dimension that closes a non-trivial loop and destroys the locality. Hence, all processes allowed on these chains are are annihilating each other. The construction scheme shown above is based on an interesting physical mechanism. As already mentioned in section 6.4 the energetically favoured momentum of the one-particle modes is strongly related to the pattern induced by the perturbation. In the case of the antiferromagnetic Ising coupling the phase vectors of the one-particle modes tend to align antiparallelly in order to minimize the energy. Frustation, however, supresses a global minimization. Instead, the modes try to minimize their energy by finding a local structure that allows for a non-frustrated arrangement. These local structures are the basis of the localized mode. Note, that all discussed local modes are characterized by non-frustrated plaquettes. The emergence of localized modes can be seen as an effect of geometrically frustrated systems that capture local excitations within non-frustrated structures.

**Figure 6.32**: Example of a lattice exhibiting a localized mode. In the case of the TFIM the displayed looped process occurs in order $n = 10$. Consequently, the corresponding low-energy mode is expected to be flat up to and including order $n = 9$. 
Figure 6.33: Two example of localized modes in frustrated chain systems. For the TFIM this modes are expected to be local up to infinite order.

6.5 Order by Disorder

This section provides an analysis of the paramagnetic phase in the triangular transverse field Ising model by investigating the one-particle excitation gap from the high-field regime. Recent Monte Carlo studies are suggesting that the triangular TFIM exhibits a quantum critical point connecting the paramagnetic phase with a bond ordered phase [15, 20]. This quantum phase transition is assumed to be in the 3dXY universality class (see for example [15]).

In section 6.4 the one-particle excitation spectrum is calculated perturbatively in the high-field limit which allows to determine the excitation gap as a high order series expansion in \( x = \frac{J}{2\hbar} \). In the following Padé and dlogPadé extrapolation techniques are applied in order to detect the closing of the gap at the quantum critical point. The results are compared to existing Monte Carlo data [15]. Furthermore, the critical exponent \( \nu z \) is determined by means of the extrapolants.

Consider a quantum phase transition at a critical point \( x_c \). In the vicinity of the quantum critical point, the gap is dominated by the power-law behaviour \( \Delta(x) \propto |x - x_c|^{\nu z} \) [30] with \( z = 1 \) in the case of the triangular TFIM [15]. Hence, the critical exponent \( \nu \) can be obtained by means of the extrapolants using equation (4.8) and identifying \( \alpha = \nu \).
6.5.1 Results

According to (6.33) the series expansion of the gap up to order \( n = 11 \) in \( x \) reads

\[
\Delta(x) = 1 - 3x + \frac{3}{2}x^2 - \frac{15}{2}x^3 + \frac{243}{8}x^4 - \frac{1671}{8}x^5 + \frac{2275}{16}x^6 \\
- \frac{162855}{16}x^7 + \frac{9700617}{128}x^8 - \frac{595490847}{1024}x^9 \\
+ \frac{2010551941313}{442368}x^{10} - \frac{1777064899901}{49152}x^{11}.
\] (6.49)

dlogPadé techniques are used to determine various extrapolants \( dP[L/M]_\Delta(x) \). The critical points \( x_c \) where \( dP[L/M]_\Delta(x) = 0 \big|_{x=x_c} \) are related to poles arising at the corresponding root of the denominator \( Q_M(x) \).

Figure 6.34 shows the resulting dlogPadé extrapolants \( dP[L/M]_\Delta(x) \) as well as the bare series \( \Delta(x) \) in order \( n = 11 \). Defective extrapolants are excluded. As one can see, the extrapolants show a strong tendency to close in a narrow region around \( x \approx 0.305 \). The particular \( x_c \) and the corresponding critical exponents \( \nu \) are listed in tabular 6.1. The location of the critical point suggested by Monte Carlo simulations is given by \( x_c^{(MC)} = 0.303 \pm 0.009 \) [15]. The convergence behaviour of the critical values...
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<th>DlogPade[LL,M]</th>
<th>$x_c$</th>
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Table 6.1: Critical values $x_c$ and critical exponents resulting from DlogPade extrapolations.

$x_c$ compared to $x_c^{(MC)}$ is demonstrated in figure 6.35. Obviously, the extrapolations are in considerable agreement with the quantum Monte Carlo result suggesting a second order quantum phase transition in the vicinity of $x_c^{(MC)}$ and $x_c = 0.305$. In the following the critical value is estimated by $x_c^{\text{approx}} \approx 0.304$. Next, we investigate the critical exponent $\nu$. According to [15] there is considerable evidence that the quantum phase transition is in the $3dXY$ universality class. Existing results are suggesting $\nu_{3dXY} \approx 0.67$ [12]. In order to obtain a valid estimation for $\nu$ the estimated critical value $x_c^{\text{approx}} \approx 0.304$ is used to bias the extrapolations. Figure 6.36 shows the convergence behaviour of the resulting critical exponents $\nu_{\text{bias}}$ compared to $\nu_{3dXY}$. For higher orders the critical exponents lie very close the literature value $\nu_{3dXY} \approx 0.67$ [12] indicating a $3dXY$ quantum phase transition. According to the results in section 6.4 the momenta of the lowest excitation indicate a $\sqrt{3} \times \sqrt{3}$-structure. Consequently, the closing of the gap at $x_c \approx 0.304$ corresponds to a quantum phase transition between an disordered paramagnetic phase for $x < x_c$ and a quantum ordered phase for $x > x_c$. The symmetry of the ordered phase is reduced according to the $\sqrt{3} \times \sqrt{3}$ which is consistent with the bond ordered phase in Figure 6.4 suggested by Moessner et al. [20, 21]. One concludes that the classical disordered phase of the triangular Ising antiferromagnet continues into an ordered quantum phase for infinitesimal transverse field $h$ providing an instance of order by disorder.
Figure 6.35: Illustration of the convergence behaviour of the critical values $x_c$ resulting from the DlogPadé extrapolants $dP[L/M]$ in dependence of the considered order $r = L + M + 1$. Connected points of the same color correspond to extrapolants with constant $d = L - M$. The dashed line represents the quantum Monte Carlo result $x_c^{(MC)} = 0.303 \pm 0.009$ [15]. The light blue area indicates the corresponding margin of error.

Figure 6.36: Illustration of the convergence behaviour of the critical exponents $\nu_{bias}$ resulting from the biased DlogPadé extrapolants $dP[L/M]$ in dependence of the considered order $r = L + M + 1$. Connected points of the same color correspond to extrapolants with constant $d = L - M$. The literature value $\nu_{3dXY}$ is represented by the dashed line.
6.6 Disorder by disorder

In this section the paramagnetic phase of the kagome transverse field Ising model is studied. The kagome TFIM is expected to be in a paramagnetic spin liquid phase for arbitrary transverse fields $h$. This implies that the disordered quantum paramagnet in high fields is adiabatically connected to the low field limit. Hence, the kagome TFIM could provide a novel instance of disorder by disorder as the classical disordered antiferromagnet continues into a disordered quantum phase.

The major goal is to provide conclusive evidence that the disordered paramagnetic phase persists for any transverse field. For this purpose, the one-particle excitation gap of the kagome TFIM is investigated by applying Padé and dlogPadé extrapolation methods to the perturbative results in the high field limit obtained in section 6.4. Additionally, we study the energy splitting induced in the low field regime which opens a gap between the momentum subspaces with $\vec{k} = (\frac{2}{3}, -\frac{2}{3})$ and $\vec{k} = 0$. This is done by means of a Lanczos based algorithm carried out on appropriate finite systems. The results allow to estimate the excitation energy of the eigenmode that is expected to be adiabatically connected to the lowest one-particle mode in the high field limit. A preliminary discussion and further details on this approach are given in the first part. The results for the low field regime and the extrapolation data are presented and discussed in the subsequent part.

6.6.1 Preliminary discussion

This subsection discusses the low field regime $x \gg 1$ and its connection to the high field limit with $x \ll 1$. We describe how to determine the energy of the low field mode that is adiabatically connected to the lowest one-particle mode in the high field limit, based on the premise that the gapped paramagnetic phase persists for arbitrary transverse field.

Note, that the emergence of a phase transition corresponds to a closing of the gap or a condensation of higher bound states. However, the condensation of higher $n$-particle modes is unlikely to happen as the leading order contributions in the 2QP subspace are indicating a repulsive interaction which suppresses the emergence of bound states. (The explicit calculation is shown in Appendix B.) Consequently, one expects that the one-particle excitation gap is the relevant order parameter.

It is assumed that the gap stays finite for arbitrary $x$ with $\Delta(x \to \infty) \geq 0$ implying that the ground state and lowest one-particle mode in the high field limit can be
adiabatically traced to the low field regime. From the results obtained in section 6.4 it is known that the lowest one-particle mode in the high field limit is characterized by a momentum $\vec{k}_{\text{gap}} = (\frac{2}{3}\pi, -\frac{2}{3}\pi)$ whereas the ground state has $\vec{k} = \vec{0}$. Since the full Hamiltonian exhibits translational invariance the momentum is a conserved quantity of the system and one concludes that the corresponding energy levels in the low field regime are characterized by the same quantum numbers $\vec{k}$. A qualitative sketch of the situation is depicted in figure 6.37. In the low field regime the situation can be displayed as follows. Consider the dimensionless TFIM Hamiltonian in units of $J$:

$$H_{\text{low-field}} = \frac{H_{\text{TFIM}}}{J} = \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + \frac{h}{J} \sum_i \sigma_i^x = H_0 + yV \quad \text{with} \quad y = \frac{h}{J}. \quad (6.50)$$

For zero field $y = 0$ the Hamiltonian describes the classical kagome Ising antiferromagnet with macroscopic ground state degeneracy. An infinitesimal field $y \ll 1$ lifts this degeneracy leading to an energy splitting between states with different momenta $\vec{k}$ as shown in figure 6.38. Following the previous argumentation, the perturbation opens a gap $\tilde{\Delta}(y)$ between the ground state with $\vec{k} = 0$ and a lowest excited state with $\vec{k}_{\text{gap}} = (\frac{2}{3}\pi, -\frac{2}{3}\pi)$. The energy gap $\tilde{\Delta}(y)$ in units of $J$ and the gap $\Delta(x)$ in units of $2h$ are related by the following equation

$$\left. \frac{\partial}{\partial y} \tilde{\Delta}(y) \right|_{y=0} = 2 \lim_{x \to \infty} \Delta(x). \quad (6.51)$$

A derivation of this relation is shown in Appendix A. Thus, the gap $\delta(x \to \infty)$ can be determined by means of first order degenerate perturbation theory. The effective

\begin{figure}[h]
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\includegraphics[width=\textwidth]{figure6.37.png}
\caption{Qualitative sketch of the ground-state energy and the lowest excitation for the kagome TFIM in dependency of $\frac{J}{h}$. It is assumed that both states are adiabatically connected to the low-field limit.}
\end{figure}
Hamiltonian of the perturbed ground state manifold in first order perturbation theory is given by

\[ H_{G}(y) = \tilde{E}_{0} \mathbb{1} + yPVP \]  

where \( \tilde{E}_{0} \) denotes the ground state energy of the unperturbed system and the operators \( P \) are projectors on the unperturbed ground state manifold. The perturbation is given by \( V = \sum_{i} \sigma_{x}^{i} \). Note, that \( V \) is block diagonal in \( \vec{k} \) due to translational symmetry. From equation 6.51 one concludes that the gap \( \delta(x \rightarrow \infty) \) is given by the difference between the lowest eigenvalues of the \( \vec{k} = 0 \) and \( \vec{k}_{\text{gap}} \) subspace of \( H_{G}^{(1)} = PVP \). In principle one has diagonalize the corresponding martices \( H_{G}^{(1)}|_{k=0} \) and \( H_{G}^{(1)}|_{k=(\frac{2}{3}\pi, -\frac{2}{3}\pi)} \) in order to obtain the sought eigenvalues. Though, an exact diagonalization for the thermodynamic limit is not possible as both matrices are of infinite dimension due to of the macroscopic ground state degeneracy. The idea is to solve this problem on appropriate finite systems of different sizes in order to obtain an estimation of the energy splitting in the thermodynamic limit. One expects that the energy splitting converges to the gap \( \Delta(x \rightarrow \infty) \) with increasing system size. The procedure used in this thesis is based on the Lanczos algorithm. The physical and computational aspects of this approach are briefly discussed in the next section.

### 6.6.2 Low field regime: Lanczos algorithm

The goal is to determine the energy splitting between the lowest eigenvalues of the subspace with \( \vec{k} = 0 \) and \( \vec{k}_{\text{gap}} \) in \( H_{G}^{(1)} = PVP \) on appropriate finite systems. In order to ensure conservation of momentum the finite systems have to exhibit translational
invariance which can be realized by periodic boundary conditions. Note, that finite systems only allow for discrete values of $\vec{k}$ depending on the size and geometrical structure of the system. Hence, the choice of the cluster plays a crucial role. As we are interested in the energy of the $\vec{k}$ mode the system has to be constructed of unit cells of the $\sqrt{3} \times \sqrt{3}$-structure which contains $N = 9$ spins. The corresponding clusters considered in this thesis are shown in figure 6.39. Due to the extensive ground state degeneracy the dimension of $H_G^{(1)}$ grows exponentially with system size. However, we are only interested in the lowest eigenvalues of the particular subspaces $H_G^{(1)}|_{\vec{k}=0}$ and $H_G^{(1)}|_{\vec{k}=(\frac{2\pi}{\sqrt{3}},\frac{2\pi}{\sqrt{3}})}$. As discussed in chapter 5 the Lanczos algorithm provides a very efficient procedure to tackle such problems. The idea is to start with a ground state (or spin-ice state) with defined momentum $\vec{k}$. Since $\vec{k}$ is a conserved quantity of $PVP$, all states of the Krylov space generated by the Lanczos algorithm for $A := PVP$ (see chapter 5) will have the same momentum quantum number $\vec{k}$. This way only the

![Figure 6.39: Illustration of the periodic clusters used for the Lanczos algorithm.](image)
relevant subspace is taken into account. The most important feature of the Lanczos algorithm is the fast convergence of extremal eigenvalues. The number of Lanczos steps required for the convergence of the lowest eigenvalues is much smaller than the actual dimension of \( H^{(1)}_G |_{k=0} \) and \( H^{(1)}_G |_{k=(\frac{3\pi}{2},\frac{3\pi}{2})} \) respectively. For instance, the lowest eigenvalue for a system of size \( N = 36 \) and ground state degeneracy \( g > 10^7 \) is converged \((\epsilon < 10^{-8})\) after \( n_L = 100 \) Lanczos steps.

In the following a brief summary of the essential aspects concerning the computational representation and realization of the states and the operator \( PVP \) is given.

**Computational aspects**

A very efficient way to represent a state of \( N \) spin-\( \frac{1}{2} \) in a computer is to take the correspondent configuration in \( \sigma_z \) basis \( s_1s_2...s_N \) with \( s_i \in 0,1 \) as the binary bits of an integer number \( z \). For arbitrary but fixed labeling of spins every configuration is assigned to a unique state \( |z\rangle \). The perturbation operator \( V \) is given by a sum of bitwise flips

\[
V = \sum_i f_i. \tag{6.53}
\]

In order to realize the projection on the ground state manifold in \( PVP \) one has to discard all flipped states \( |f_i z\rangle \) that are not in the ground state manifold. Recall, that a ground state (also called spin-ice state) was defined by a configuration where any triangular plaquette satisfies two antiferromagnetic bonds. In the following we omit the operator \( P \) in our notation and take the sum in 6.53 as a sum that is restricted to allowed spin flips.

The next step is the generation of a ground state with defined momentum \( \vec{k} = 0 \) or \( \vec{k} = (\frac{2\pi}{3},\frac{2\pi}{3}) \). For this purpose, one generates a random spin-ice state \( |z\rangle \) and takes the sum of all distinct translations of \( |z\rangle \) weighted with a corresponding phase factor \( e^{-i\vec{k}\vec{r}} \). It is useful to introduce the following notation. \( \mathcal{M}(z) \) denotes the set of all distinct translations of \( |z\rangle \) weighted with a corresponding phase factor. \( m(z) \) is the number of all distinct translations of \( z \). According to this, an initial state with momentum \( \vec{k} \) can be written as

\[
|\psi(z)\rangle = \frac{1}{\sqrt{m(z)}} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}\vec{r}} T_l |z\rangle \tag{6.54}
\]

with correspondent translation operators \( T_l \). In order to safe memory usage it is expedient to represent such a state by a particular \( z \in \mathcal{M}(z) \) associated with a weight \( \alpha = 1 \). All other states in the sum are fully determined by this particular
Chapter 6 Antiferromagnetic Ising model in transverse Field

identifier \( z \). A possible way to define a unique identifier is by choosing the translated state with minimal labeling \( z = \min(\mathcal{M}(z)) \). Thus, the representation is defined as

\[
|z\rangle \Rightarrow \frac{1}{\sqrt{m(z)}} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}_l \cdot \vec{r}_l} |z\rangle .
\]

(6.55)

Next, one has to determine the accordant representation of \( PVP \). Using the translational invariance of \( PVP \) with \( [PVP, T_l] = 0 \), the action of \( PVP \) on \(|z\rangle\) yields

\[
PVP |z\rangle \Rightarrow \sum_{i \in N} f_i \frac{1}{\sqrt{m(z)}} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}_l \cdot \vec{r}_l} |z\rangle
\]

(6.56)

\[
= \frac{1}{\sqrt{m(z)}} \sum_{i \in N_1} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}_l \cdot \vec{r}_l} |f_i z\rangle .
\]

(6.57)

The first sum over all allowed spin flips \( i \in N \) can be divided into \( N_1 \) for flips resulting in \( m(f_i z) \leq m(z) \) and \( N_2 \) in the case of \( m(f_i z) > m(z) \) yielding

\[
PVP |z\rangle = \frac{1}{\sqrt{m(z)}} \sum_{i \in N_1} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}_l \cdot \vec{r}_l} |f_i z\rangle
\]

(6.58)

\[
+ \frac{1}{\sqrt{m(z)}} \sum_{i \in N_2} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}_l \cdot \vec{r}_l} |f_i z\rangle .
\]

(6.59)

In the first case the number of distinct translations of \(|f_i z\rangle\) is smaller than the number of translations in \( \mathcal{M}(z) \). Hence, the sum over \( \mathcal{M}(z) \) will generate \( \frac{m(z)}{m(f_i z)} \) identical states of translations in \( \mathcal{M}(f_i z) \). As a result one obtains

\[
\frac{1}{\sqrt{m(z)}} \sum_{i \in N_1} \sum_{l \in \mathcal{M}(z)} e^{i\vec{k}_l \cdot \vec{r}_l} = \frac{1}{\sqrt{m(z)}} \sum_{i \in N_1} m(z) \sum_{l \in \mathcal{M}(f_i z)} e^{i\vec{d}(z,f_i z) \cdot \vec{r}_l} e^{i\vec{k}_l \cdot \vec{r}_l} |f_i z\rangle
\]

\[
= \sum_{i \in N_1} \frac{\sqrt{m(z)}}{\sqrt{m(f_i z)}} e^{i\vec{d}(z,f_i z)} \frac{1}{\sqrt{m(f_i z)}} \sum_{l \in \mathcal{M}(f_i z)} e^{i\vec{k}_l \cdot \vec{r}_l} |f_i z\rangle
\]

\[
= \sum_{i \in N_1} \sqrt{\frac{m(z)}{m(f_i z)}} e^{i\vec{d}(z,f_i z)} |f_i z\rangle
\]

(6.60)

with \( \vec{d}(z,f_i z) \) denoting the translation vector which connects the two states \(|z\rangle\) and \(|f_i z\rangle\).

In the second case the sum over \( \mathcal{M}(z) \) does not generate all translations of \(|f_i z\rangle\). Yet,
it is possible to combine summands of the second sum \( \sum_{i \in \mathcal{N}^2} e^{i \vec{k} \vec{r}_i} |f_i z\rangle \) such that

\[
\frac{1}{\sqrt{m(z)}} \sum_{i \in \mathcal{N}^2} \sum_{l \in M(f_i z)} e^{i \vec{k} \vec{d}(z, f_i z)} \sqrt{m(z)} |f_i z\rangle = \\
= \sum_{i \in \mathcal{N}^2} e^{i \vec{k} \vec{d}(z, f_i z)} \sqrt{m(z)} \frac{m(z)}{m(z)} |f_i z\rangle = \\
= \sum_{i \in \mathcal{N}^2} \frac{1}{\sqrt{m(z)}} \frac{m(z)}{m(f_i z)} e^{i \vec{k} \vec{d}(z, f_i z)} \sqrt{m(z)} |f_i z\rangle.
\]

(6.61)

Note, that the considerations are valid for all periodic lattice systems. Altogether, one finds

\[
PVP |z\rangle = \sum_{i \in \mathcal{N}} \frac{\sqrt{m(z)}}{\sqrt{m(f_i z)}} e^{i \vec{k} \vec{d}(z, f_i z)} |f_i z\rangle.
\]

(6.62)

Consequently, it is sufficient to consider the spin flips for \( |z\rangle \) and to weight them with a factor \( \frac{\sqrt{m(z)}}{\sqrt{m(f_i z)}} e^{i \vec{k} \vec{d}(z, f_i z)} \). This principle allows to save a large amount of memory.

In the next section the results for the kagome TFIM are presented.

### 6.6.3 Results

The resulting series expansion of the one-particle gap up to order \( n = 13 \) in \( x = \frac{J}{2h} \) is given by

\[
\Delta^{(13)}(x) = 1 - 2x + 2x^2 - 3x^5 + \frac{243}{8} x^6 - \frac{2609}{8} x^7 + \frac{28531}{16} x^8 - \frac{2609}{2} x^{10} - \frac{1340557475}{36238786560} x^{13}.
\]

(6.63)

Figure 6.40 shows the bare series of \( \Delta(x) \) in order \( n = 12 \) and \( n = 13 \) as well the resulting dlogPadé extrapolants for \( x \in [0, 2] \). Note, that the series of \( \Delta(x) \) converges very slowly as the absolute value of the coefficients is growing exponentially with ascending order. For \( x < 0.4 \) all extrapolations seem to be well converged. A closing of the the gap in this region can be excluded. But also for regions beyond the high field regime most of the extrapolants indicate a clear trend. Though isolated extrapolants exhibit instabilities, there is no tendency that the gap closes at a certain critical value.
In order to obtain more significant results for the whole parameter axis, it is appropriate to perform an Euler transformation

\[ x = \frac{u}{u - 1} \]  

(6.64)

which maps the whole parameter axis \( x \in [0, \infty] \) on a finite interval \( u \in [0, 1] \). Subsequently, the gap \( \hat{\Delta}(u) \) is expanded up to order \( n = 13 \) in \( u \) yielding

\[
\hat{\Delta}^{(13)}(u) = 1 - 2u + 2u^3 + 4u^4 + 3u^5 + \frac{187}{8}u^6 - \frac{1431}{8}u^7 + \frac{723}{16}u^8 - \frac{49639}{512}u^9 + \frac{24045959}{6144}u^{10} - \frac{208355215}{12288}u^{11} + \frac{13456372727}{294912}u^{12} - \frac{11793702839375269}{36238786560}u^{13} \]  

(6.65)

One expects that the dlogPadé extrapolants in \( u \) are more stable within a finite interval \( u \in [0, 1] \) allowing to estimate the gap for \( x \to \infty \).

The energy gaps obtained in the Lanczos computation on finite systems of size \( N = 9, N = 18, N = 27 \), and \( N = 36 \) are listed in tabular 6.2. The results for the finite systems are used to obtain an estimation of the gap in the thermodynamic limit.
Table 6.2: Results for the energy gap in the low field regime on the considered finite systems of size $N$.

Based on general considerations, one can argue that the excitation gap of a two-dimensional system scales with the reciprocal system size $\frac{1}{N}$.

In Figure 6.41 the energy gaps $\delta(N)$ are plotted against $\frac{1}{N}$.

![Graph showing the energy gap versus $1/N$.](image)

**Figure 6.41**: Resulting gaps for systems of finite size $N$. One assumes a scaling proportional to the reciprocal system size. The regression line indicates a finite gap in the thermodynamic limit.

The data are fitted by a least-squares estimation yielding the following regression line

$$\Delta_{\text{lin}}(\frac{1}{N})[2h] = 0.181 + 0.577 \frac{1}{N}.$$

Hence, the gap in the thermodynamic limit can be estimated by

$$\Delta_{\infty} \approx \Delta_{\text{lin}}(0) = 0.181.$$
The resulting dlogPadé extrapolants for $\Delta(u)$ and the results of the Lanczos approach in the low-field limit are depicted in figure 6.42. Note, that the low field limit corresponds to $u = 1$. As one can see, most of the extrapolations are approaching a finite value $\Delta_\infty \approx 0.2 \pm 0.03$ for $u = 1$ which is consistent with the exact diagonalization results obtained in the low field regime. Although isolated extrapolants deviate from the indicated trend, they show no tendency to close for $u \in [0, 1]$.

As a further consistency check, the value of the extrapolants for $u = 1$ is biased to the value calculated in the low-field regime given by $\Delta_\infty = 0.181$. The resulting extrapolants are shown in figure 6.43. The enhanced stability of the extrapolations indicates a reasonable consistency between the extrapolations and the exact diagonalization results. Altogether, the results provide considerable evidence, that the gap stays finite for all values of $x$. We conclude that the kagome TFIM exhibits a disordered paramagnetic phase that is adiabatically connected to the low-field regime.
Figure 6.43: Biased dlogPadé extrapolations with $\Delta(u = 1) = 0.181$. 
Chapter 7

Conclusion

This chapter provides a conclusive summary of the central issues and findings of this thesis. The first section is a recapitulation of the methodical aspects, the application on the transverse field Ising model and the resultant findings for the kagome and triangular lattice. The second section gives an outlook on open issues and possible future work.

7.1 Summary

In this thesis the antiferromagnetic transverse field Ising model defined on the kagome and triangular lattice is studied. Both models are exemplary models of frustrated magnets that are supposed to exhibit a quantum version of order by disorder (triangular) and disorder by disorder (kagome) [20, 21].

A combination of particle-conserving perturbative continuous unitary transformations about the high-field limit and appropriate extrapolation tools is used to examine the first excitation gap and the properties of the corresponding one-particle mode, in order to detect possible second order phase transitions. This approach is complemented by first order degenerate perturbation theory using an exact diagonalization method based on the Lanczos algorithm.

The initial point for the perturbative treatment is the high field limit of the transverse field Ising model. In this limit the ground-state is given by a fully polarized state. According to this the lowest excitation is given by a single spinflip that costs an energy of $2\hbar$. The spinflips are interpreted as quasi-particles that can be described in terms of hardcore-bosons. The Ising term is treated as a perturbation driven by
the perturbation parameter $x = \frac{J}{2h}$. The transformation is employed to derive an effective Hamiltonian for the one-particle subspace reducing the intricate many-body problem to a tractable one-particle problem. The resultant effective model is exact in the thermodynamic limit up to a certain order in the perturbation parameter $x$. The transformation is performed by means of a linked cluster expansion increasing the maximum attainable order. For this purpose, an automated computer program is developed that allows for a cluster expansion on higher dimensional lattices. The resultant Hamiltonian is a high order series expansion in $x$. Due to the truncation, the range of validity is limited to small values of the perturbation parameter. In order to enhance the reliability to higher values Padé and dlogPadé extrapolation methods are employed.

The effective one-particle Hamiltonian of the kagome TFIM is calculated up to order $n = 13$. A fourier transformation into momentum-space yields a $3 \times 3$ matrix that can be diagonalized analytically. The eigenvalues are the energy bands of the three one-particle modes originating from the three-site unit cell of the kagome lattice. It turns out that there are two dispersive high-energy bands and one low-energy band that stays flat up to and including order seven. This flat-band behaviour can be ascribed to the existence of a localized mode that is a superposition of one-particle states on a hexagon provided with an alternating phase. An analysis of the sub processes in the effective Hamiltonian provides an accurate understanding of this effect. Moreover, those processes that are responsible for the delocalization in higher orders can be identified. Based on this findings a heuristic method for arbitrary lattices is developed that allows to predict the existence of localized modes and determines their properties by means of simple geometrical considerations. The gaps of the low-energy mode are located at $\vec{k} = \pm \left(\frac{4}{3}\pi, \frac{2}{3}\pi\right)$, $\vec{k} = \pm \left(\frac{2}{3}\pi, -\frac{4}{3}\pi\right)$ and $\vec{k} = \pm \left(\frac{4}{3}\pi, -\frac{2}{3}\pi\right)$. The corresponding eigenvector indicates that the preferred ordering on the kagome TFIM manifests a $\sqrt{3} \times \sqrt{3}$-structure similar to the $\sqrt{3} \times \sqrt{3}$-structure that is induced by thermal fluctuations in the classical kagome antiferromagnet [27].

For the triangular TFIM the computations are carried out up to order $n = 11$. The energy band becomes dispersive in first order which is consistent with the developed concepts predicting that a localized mode does not exist for the triangular lattice. The momenta of the energy gap are identical to the momenta found for kagome lattice. Analogous to this, a $\sqrt{3} \times \sqrt{3}$-structure is energetically most favorable according to the ordering structure in the bond ordered phase proposed by Moessner et. al.
The extrapolation data of the excitation gap on the triangular lattice significantly suggest that the gap closes around $x_c \approx 0.304$ indicating a second order phase transition into an ordered phase. The results are in excellent agreement with Monte Carlo simulations that yield a critical value $x_c = 0.303 \pm 0.009$ [15]. In addition the extrapolants are used to estimate the critical exponent $\nu$ suggesting a value of $\nu \approx 0.67 \sim 0.68$ which is very close to the predicted critical exponent in the 3d XY universality class $\nu = 0.67$ [12].

The kagome TFIM is expected to be in a paramagnetic phase for arbitrary transverse fields which implies that the gap does not close for $x \to \infty$. Indeed the extrapolants show no tendency that the gap closes for $x$ approaching infinity. For $x \to \infty$ most of the extrapolants indicate a finite gap of $\Delta(x \to \infty) = 0.200 \pm 0.025$.

In addition, the reliability of the extrapolants for the low field limit ($x \to \infty$) is checked. For zero field the system exhibits a macroscopic ground-state degeneracy. Therefore, degenerate perturbation theory has to be employed. The introduction of a transverse field effects a splitting between the $\vec{k} = 0$ and $\vec{k}_{gap}$ mode in first order perturbation theory. In the thermodynamical limit this splitting equals the value of the energy gap in units of $\hbar$ for $x \to \infty$. Due to the extensive ground-state degeneracy only finite systems can be considered. In order to obtain an reliable estimate of the splitting, first order degenerate perturbation theory is applied to appropriate periodic clusters of finite size comprising the momentum $\vec{k}_{gap}$. The computation is performed by means of a particular adapted Lanczos algorithm on clusters of size $N = 9$, $N = 18$, $N = 27$ and $N = 36$. The resulting gaps show a systematic decrease with increasing system size ($\sim \frac{1}{N}$) indicating a gap of $\Delta \approx 0.181$ for $N \to \infty$ which is consistent with the extrapolation data. One concludes that the first excitation gap indeed stays finite.

It can be further argued that the condensation of higher modes due to binding effects is unlikely to occur as the leading order in the two-particle subspace manifests a repulsion.

Altogether, there is strong evidence that the kagome TFIM is a quantum paramagnet for the whole parameter axis exhibiting a novel disorder by disorder transition.
7.2 Outlook

This section is intended to provide a brief overview of alternative approaches and future perspectives in context of the physical systems studied in this thesis. A major detriment of perturbative continuous unitary transformations is the limitation to finite orders in the perturbation parameter. For series expansions exhibiting particularly slow convergence (e.g., when long range processes become important) this limitation could cause severe stability problems in the extrapolations. Therefore, one could use alternative CUT based methods that circumvent this problem by means of another truncation scheme. Two recently developed methods that are especially suited for gapped systems are the graph based CUT (gCUT) [39] and the directly evaluated enhanced perturbative CUT (deepCUT) [19]. In contrast to the pCUT approach which provides exact results up to a certain order this new methods are taking into account processes up to infinite order by utilizing a numerical evaluation of the flow equations.

An interesting extension of the considered transverse field Ising model is the introduction of an additional longitudinal magnetic field $h_l$. As proposed by Moessner et al. a tilted field applied to the kagome antiferromagnet might give rise to a bond ordered phase [20] in the regime of small transverse field. In order to access this regime one might employ the same perturbative approach used in this thesis considering the limit of high transverse field that is slightly tilted by a finite $h_l$. In terms of perturbative unitary transformations this would lead to a more intricate kind of quasi-particles that feature new processes including $T_{\pm 1}$ operators. However, from the technical point of view the transformation should work without difficulty. In this context one also could treat the longitudinal field as an additional perturbation.

The combined application of perturbative unitary transformation and linked graph expansion might be a promising approach for the investigation of three dimensional frustrated spin systems, as, for instance, the spin-$\frac{1}{2}$ pyrochlores. These systems are manifesting an extremely rich phase diagram exhibiting coulomb phases and spin liquid phases, both giving rise to deconfined spinon excitations and emergent quantum electrodynamics [31].
Appendix A

Energy gap in the low-field regime

In the low field regime it is convenient to measure the energy in units of the coupling $J$. The energy gap measured in this units is denoted by $	ilde{\Delta}(y)$ with $y = \frac{\hbar}{J} = \frac{1}{2x}$. In the high field regime the energy is measured in units of $2\hbar$. The corresponding gap is given by $\Delta(x)$. Note, that both quantities are dimensionless. They are related by

$$
\tilde{\Delta}(y) = \frac{1}{x} \Delta(x) = 2y\Delta\left(\frac{1}{2y}\right). \quad (A.1)
$$

We assume that the gap of the system is finite for arbitrary fields implying

$$
\lim_{x \to \infty} \Delta(x) = \Delta_\infty \geq 0. \quad (A.2)
$$

Now, consider the derivative of $\tilde{\Delta}(y)$ for $y \to 0$

$$
\left. \frac{\partial}{\partial y} \tilde{\Delta}(y) \right|_{y=0} = \lim_{y \to 0} \left. \frac{\partial}{\partial y} \left(2y\Delta\left(\frac{1}{2y}\right) \right) \right|_{y=0} \quad (A.3)
$$

$$
= \lim_{y \to 0} 2\Delta\left(\frac{1}{2y}\right) + 2y \frac{\partial}{\partial y} \left(\Delta'\left(\frac{1}{2y}\right) \right) \quad (A.4)
$$

$$
= \lim_{y \to 0} 2\Delta\left(\frac{1}{2y}\right) - \frac{2}{y} \left(\Delta'\left(\frac{1}{2y}\right) \right) \quad (A.5)
$$

$$
= \lim_{x \to \infty} 2\Delta(x) - x\Delta'(x) \quad (A.6)
$$
Appendix A.

Appendix A Energy gap in the low-field regime

with $\Delta'(x) = \frac{\partial}{\partial x} \Delta(x)$. The assumption (1) requires that $\Delta(x)$ decreases faster than $\frac{1}{x}$. One concludes that

$$\frac{\partial}{\partial y} \tilde{\Delta}(y)|_{y=0} = \lim_{x \to \infty} 2\Delta(x) - \lim_{x \to \infty} x\Delta'(x) = 0$$

(A.7)

$$= 2\Delta_{\infty} .$$

(A.8)
Appendix B

2QP contributions

The leading order contribution of the 2QP subspace in the TFIM is calculated. The first processes in the 2QP subspace occur in order $n = 2$ as the first order vanishes. The involved cluster is given by a single bond $B$. According to (2.26) the 2QP contribution on $B$ is given by

$$t_{2QP}^B = \langle i_1, j_1 | x^2 \left( C(-2, +2) \tau_+ \tau_- - C(+2, -2) \tau_+ \tau_- \right) | i_1, j_1 \rangle = x^2 . \quad (B.1)$$

The corresponding virtual fluctuations are depicted in Figure B.1. The positive value of the leading order contribution indicates a repulsive interaction. One concludes, that bound states are unlikely to emerge.

Figure B.1: Illustration of the virtual fluctuations involved in the leading order 2QP contribution.
Appendix C

Dispersion coefficients

The coefficients of the one-particle dispersion for the triangular lattice are listed up to order $n = 4$:

$$\omega_{\text{tri}}^{(0)} = 1$$
$$\omega_{\text{tri}}^{(1)}(k_1, k_2) = 2 \cos (k_1) + 2 \cos (k_1 - k_2) + 2 \cos (k_2)$$
$$\omega_{\text{tri}}^{(2)}(k_1, k_2) = -2 \cos (2k_1 - k_2) - \cos (2k_1) + 3 - 2 \cos (k_2) - 2 \cos (k_1) - 2 \cos (k_1 - 2k_2)$$
$$+ 2 \cos (k_1 - k_2) - \cos (2k_1 - k_2) - \cos (2k_2) - 2 \cos (k_1 + k_2)$$
$$\omega_{\text{tri}}^{(3)}(k_1, k_2) = 6 \cos (2k_2) + 6 \cos (2k_1 - k_2) - \cos (k_1) + 3 \cos (2k_1 - 3k_2)$$
$$- 12 + 3 \cos (3k_1 - k_2) + 3 \cos (k_1 - 3k_2) - \cos (k_1 - k_2) + 3 \cos (2k_1 + k_2)$$
$$+ 3 \cos (k_1 + 2k_2) + 6 \cos (k_1 - 2k_2) + \cos (3k_1 - 3k_2) + \cos (3k_2)$$
$$+ 3 \cos (3k_1 - 2k_2) + 6 \cos (2k_1) - \cos (k_2) + \cos (3k_1)$$
$$+ 6 \cos (k_1 + k_2) + 6 \cos (2k_1 - 2k_2)$$
$$\omega_{\text{tri}}^{(4)}(k_1, k_2) = -5 \cos (k_1 + 3k_2) + 9 \cos (k_1 - k_2) - \frac{15}{2} \cos (2k_1 - 4k_2)$$
$$- 20 \cos (2k_1 - 3k_2) - \frac{41}{2} \cos (2k_2) - \frac{41}{2} \cos (2k_1) - \frac{5}{4} \cos (4k_1)$$
$$+ \frac{207}{4} - 20 \cos (3k_1 - 2k_2) - 5 \cos (4k_1 - k_2) - \frac{5}{4} \cos (4k_1 - 4k_2)$$
$$- 20 \cos (2k_1 + k_2) - 16 \cos (2k_1 - k_2) + 9 \cos (k_1) - \frac{15}{2} \cos (2k_1 + 2k_2)$$
$$- 5 \cos (3k_1 + k_2) - 15 \cos (3k_1) - 20 \cos (k_1 + 2k_2) - 15 \cos (3k_1 - 3k_2)$$
$$- 5 \cos (3k_1 - 4k_2) - 5 \cos (k_1 - 4k_2) - 20 \cos (3k_1 - k_2) - 16 \cos (k_1 - 2k_2)$$
$$- \frac{41}{2} \cos (2k_1 - 2k_2) - 16 \cos (k_1 + k_2) - 5 \cos (4k_1 - 3k_2) - 20 \cos (k_1 - 3k_2)$$
$$+ 9 \cos (k_2) - \frac{15}{2} \cos (4k_1 - 2k_2) - \frac{5}{4} \cos (4k_2) - 15 \cos (3k_2)$$
Appendix C Dispersion coefficients

The coefficients of the matrix elements $\Omega_{11}$ and $\Omega_{12}$ up to order $n = 4$ are given by

\[ \Omega_{11}^{(0)} = 1 \]
\[ \Omega_{11}^{(1)} = 0 \]
\[ \Omega_{11}^{(2)} = 2 - \cos (k_1 - k_2) - \cos (k_1) \]
\[ \Omega_{11}^{(3)} = -4 + 2 \cos (k_2) + 2 \cos (k_1) + 2 \cos (k_1 - k_2) \]
\[ \Omega_{11}^{(4)} = \frac{5}{2} - \frac{5}{4} \cos (2k_1) - \frac{5}{4} \cos (2k_1 - 2k_2) \]
\[ \quad - \frac{15}{2} \cos (k_2) - \frac{5}{2} \cos (2k_1 - k_2) + \frac{1}{4} \cos (k_1) \]
\[ \quad - \frac{5}{4} \cos (k_1 - 2k_2) + \frac{1}{4} \cos (k_1 - k_2) - \frac{5}{4} \cos (k_2 + k_1) \]
\[ \Omega_{11}^{(0)} = 0 \]
\[ \Omega_{11}^{(1)} = 1 + \cos (k_1 - k_2) + i \cdot \sin (k_1 - k_2) \]
\[ \Omega_{11}^{(2)} = -\frac{1}{2} \cos (k_1) - \frac{1}{2} i \sin (k_1 - k_2) - \frac{1}{2} \cos (k_1 - k_2) - \frac{1}{2} i \sin (k_1) \]
\[ \quad + \frac{1}{2} i \sin (k_2) - \frac{1}{2} - \frac{1}{2} \cos (k_2) \]
\[ \Omega_{11}^{(3)} = \frac{1}{2} \cos (2k_1 - k_2) - (2i) \sin (k_1 - k_2) + \frac{1}{2i} \sin (2k_1 - 2k_2) - \frac{3}{2} + \frac{1}{2i} \sin (k_1 - 2k_2) \]
\[ \quad + \frac{1}{2} \cos (k_1 - 2k_2) + \frac{3}{2} \cos (k_1) + \frac{3}{2} \cos (k_2) + \frac{1}{2i} \sin (2k_1 - k_2) \]
\[ \quad - \cos (k_1 - k_2) + \frac{1}{2i} \sin (k_1) - \frac{1}{2} \sin (k_2) + \frac{1}{2} \cos (2k_1 - 2k_2) \]
\[ \Omega_{11}^{(4)} = -\frac{15}{8} \cos (2k_1 - 2k_2) + \frac{9}{2i} \sin (k_1 - k_2) - \frac{5}{2} \cos (k_1 - k_2) \]
\[ \quad - \frac{5}{2i} \sin (2k_1 - k_2) - 3 \cos (k_1) - \frac{5}{2} \cos (2k_1 - k_2) - \frac{5}{4} \cos (k_2 + k_1) \]
\[ \quad + \frac{3}{4} \cos (k_1 - k_2) + (2i) \sin (k_1) + \frac{5}{8i} \sin (2k_1 - 2k_2) - \frac{5}{8} \cos (2k_2) - \frac{15}{8i} \sin (2k_1 - 2k_2) \]
\[ \quad - (2i) \sin (k_2) + \frac{21}{8} - 3 \cos (k_2) - \frac{5}{8i} \sin (2k_1) - \frac{5}{8} \cos (2k_1) - \frac{5}{2i} \sin (k_1 - 2k_2) \]
Bibliography


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Eidesstattliche Versicherung

Ich versichere hiermit an Eides statt, dass ich die vorliegende Masterarbeit mit dem Titel "Quantum paramagnetism in the kagome and triangular transverse field Ising model" selbständig und ohne unzulässige fremde Hilfe erbracht habe. Ich habe keine anderen als die angegebenen Quellen und Hilfsmittel benutzt sowie wörtliche und sinngemäße Zitate kenntlich gemacht. Die Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen.

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