Dynamics of the antiferromagnetic Heisenberg spin–1/2 chain

Master’s thesis

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Abstract

In magnetic systems, interactions between electrons can be described by an effective spin-spin interaction. When the wavefunctions of the electrons overlap mainly in one direction, the system behaves as an effectively one-dimensional spin chain. A special class of such a spin chain is the anisotropic Heisenberg model, also called the XXZ model. Exact wavefunctions for the (gapped) antiferromagnetic XXZ model are obtained using the (algebraic) Bethe Ansatz. A new result is a classification of two-spinon excitations (low energy states) in case of zero magnetic field. Using this classification the leading (two-spinon) part of the transverse dynamical structure factor (which is the Fourier transform of space and time dependent spin-spin correlation functions) is computed, thereby obtaining predictions for inelastic neutron scattering experiments.
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1. Introduction

1.1. Historical overview

Since the discovery of ferromagnetism, approximately 4000 BC, people have been fascinated by the phenomenon. One of the metaphysical explanations that Greek scientists gave was: “there is such a thing as the ‘humidity’ of iron upon which the ‘dryness’ of the magnet feeds”. This was a long held superstition that survived until the sixteenth century, when the research of ferromagnetism became scientific; most important were Gilbert in 1600 and Decartes in 1650. The key to understanding magnetism turned out to be quantum mechanics, with most notably the discovery of spin in 1925. Based on the principle of overlapping wavefunctions, Heisenberg (1928) [1] (and almost simultaneously Dirac) introduced a model, now called the Heisenberg model, in an attempt to explain ferromagnetism. It was only three years later that Hans Bethe [2] solved the ferromagnetic one-dimensional Heisenberg model, by what is now called the Bethe Ansatz. It was the first quantum many-body problem to be solved exactly. Many attempts were made to generalize the Bethe Ansatz to two or three dimensions, but they were all unsuccessful.

In the meantime Néel introduced antiferromagnetism (1932), which, up until then, had been merely a theorists’ invention. Experimental evidence came in 1938 due to Bizette et al. and was confirmed with neutron scattering by Schull et al. in 1949. Much progress was made for the anti-ferromagnetic spin chain. The ground state energy and the low energy behavior was studied by Hulthén (1938) and des Cloizeaux (1962) using the Bethe Ansatz in the thermodynamic limit. The first experiment showing that under the right circumstances some materials behave like one-dimensional antiferromagnetic spin-1/2 chains was done by Endoh et al. (1974). Kasteleijn generalized the Heisenberg model to an anisotropic model (1952), the XXZ model, which was solved by Orbach (1958) using the Bethe Ansatz.

In the 1980s the Russian school (Faddeev, Sklyanin, Takhtajan) introduced the Algebraic Bethe Ansatz, which is an algebraic formulation of the original Bethe Ansatz. Using this Algebraic Bethe Ansatz, Korepin (1982) was the first to prove Gaudin’s conjecture for the norm of the eigenstates. A more general result is the scalar product between an eigenstate and an arbitrary state proved by Slavnov (1989). Based on this Algebraic Bethe Ansatz, dynamical correlation functions could be calculated (Maillet (1999), Caux (2005)) for finite spin chains. This provided an excellent comparison for experiments. Parallel to this development, Miwa and Jimbo (1995) derived an algebraic analysis for the infinite chain at zero field [3].

1.2. More is different\textsuperscript{1}: solving the many-body problem

When Newton discovered his gravitational law this enabled him to explain Kepler orbits by solving the two-body problem: a planet orbiting the sun. However, when he tried to solve the three-body problem, he failed. Many others tried the same, but until now the problem

\textsuperscript{1}Philip Anderson (Nobel Prize in physics 1977)
remains unsolved. This is why, although we know very well how two particles interact, one is usually lost when there are more than two.

Condensed matter physics involves by definition the study of many-body problems. When the interactions are weak, this is usually handled by making approximations. Instead of solving the Schrödinger equation for \( N \) particles, thermodynamical quantities are extracted. Successful examples are: Bose-Einstein condensation and BCS theory (low temperature superconductivity). However, if we try to apply this approach to strongly interacting problems, we are likely to fail. High temperature superconductivity is an example of a strongly interacting system of which to this day no accurate description is known.

Strongly interacting systems are interesting, not only because they are hard to solve, but also because it is reasonable to expect that these systems contain more interesting physics than weakly interacting systems.

1.3. Less is more\(^2\): strongly interaction fermions

Reducing the number of spatial dimensions of your system might appear unambitious. However, quite often the opposite is true. In one-dimensional systems the interactions between the particles are usually much stronger than in higher dimensional systems. An intuitive idea supporting this is that the less possibility particles have to pass each other by, the more they will behave as a collective; a striking example is the breakdown of the Fermi liquid in one dimension. For an overview of quantum physics in one dimension see the book of Giamarchi [4].

1.3.1. Breakdown of Fermi liquid theory

When the Coulomb force between electrons is comparable to their kinetic energy, it can usually not be treated perturbatively. However, in some cases much can be achieved by reformulating the theory in terms of quasi-particles. In Fermi liquid theory, the elementary particles are not the individual electrons, but electrons dressed by charge density fluctuations. These quasi-particles still behave as fermions and can be considered as essentially free, whereas individual electrons are strongly coupled. We expect the excitations to be close to the Fermi surface. However, since the electrons are not completely free, the quasi-particle excitations have a finite lifetime. For particles close to the Fermi surface this lifetime approaches infinity. In normal metals the Fermi energy is about \( 10^4 \text{K} \). Since experiments are usually performed at much lower temperatures, the Fermi liquid description is applicable in these cases. If we look at electron systems in one dimension the physics changes drastically. Electrons in one dimension cannot move without pushing all the other electrons out of their way, or tunnel through them. As individual motion is impossible, there can only be collective excitations. As a consequence of this collective behavior the excitations in a Luttinger liquid are described by spinons (a spin particle without charge) and holons (a charged particle without spin).

1.3.2. Exact solutions and integrability

The advantage of one-dimensional systems is that the time-independent Schrödinger equation can often be solved exactly, in contrast to higher dimensional systems. The key idea is that

\(^2\)Robert Browning (English poet)
1.4 Spin-spin interaction

when two particles scatter in one dimension, their momenta and energies should either remain unchanged, or be interchanged. So if two particles scatter the only thing that can happen is that the wavefunction gains a phase shift. In general, momenta are not necessarily conserved in case of an $N$–body scattering. However, when an $N$–body scattering factorizes into two-body scatterings, we are again in the situation that scatterings only give rise to a phase shift. This is usually not the case in higher dimensional systems.

A more general concept related to this factorization of scatterings is *integrability*. We will examine this in detail in chapter 6. Integrable models have a good chance of being solved by means of the Bethe Ansatz. Examples are: the Heisenberg spin chain (the focus of this thesis), the interacting Bose-gas and the Hubbard model.

The concepts of being exactly solvable and being integrable are easily confused. In general, if a model is integrable it does not mean that an exact solution can be found, and vice versa. Whether or not a model is exactly solvable only tells us something about the mathematics that are involved. For example, any model defined on a finite lattice can be solved exactly. One ‘only’ needs to represent the Hamiltonian as matrix, and obtain all eigenstates and energy levels by diagonalization. On the other hand, integrability tells us something about the dynamics of the system. Quite often, integrable models can be solved in the thermodynamic limit (sending the number of particles to infinity).

1.4. Spin-spin interaction

Consider a crystal in which the constituent ion cores are separated by a distance that is much larger than the Bohr radius of the conduction electrons. In this case, the wavefunctions of the electrons are fixed around the nucleus: the lattice sites. This is a called a *tight-binding model*, where the movement of electrons is approximated by hopping from one lattice site to another. When the orbital overlap between electrons is very weak, only nearest neighbor hopping contributes. The tight-binding model can be improved by taking the Coulomb repulsion between two electrons at the same site into account. In second quantized notation we arrive at the Hubbard model:

$$H = -t \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle ij \rangle} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}.$$  

The operator: $a_{i\sigma}^\dagger$ creates an electron at position $i$ with spin $\sigma$. The operator $n_{i\uparrow}$ is the number (0 or 1) of electrons with up-spin at site $i$. The hopping parameter $t$ is proportional to the effective overlap of the wavefunctions of neighboring atoms and $U$ is the Coulomb repulsion between two electrons at the same site. The $\langle ij \rangle$ denotes a sum over adjacent sites. A special case of the Hubbard model is when it is *half-filled* where the average site occupancy is one, for a very strong interaction: $U/t \gg 1$. In this case no double occupancy is expected in the ground state. Furthermore, there are no fluctuations in charge, but spin-spin interactions are possible. It suffices to study a two site problem, as depicted in fig. 1.1. When we have parallel spins, Pauli’s exclusion principle forbids double occupancy. In case of anti-parallel spins, one electron can hop to an adjacent site. In this situation there is an extra energy cost $U$, which makes this state very short lived. Subsequently, either the down or upspin can hop to the empty site. In the former case nothing has effectively happened. In the second case, however, the up and down spin have changed position. This process is called *superexchange*, after Anderson [5].
In the limit $U/t \gg 1$, Anderson derived a Hamiltonian just for the spins with an effective coupling: $J \sim t^2/U$, also called the antiferromagnetic Heisenberg model:

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j.$$  \hspace{1cm} (1.2)

The crystal structure as well as the wavefunctions of the electrons can be highly anisotropic. There are many examples where the wavefunctions of the conduction electrons interact in only one spatial dimension. In these cases it is plausible that such a model can be described as an effective one-dimensional theory, usually called a spin chain. Experimental realizations of spin chains include CsCoCl$_3$ [6, 7] and CsCoBr$_3$ [8, 9]. The Heisenberg model can be generalized by introducing an anisotropy parameter $\Delta$ due to Kasteleijn [10]:

$$H_{XXZ} = J \sum_{\langle ij \rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z.$$  \hspace{1cm} (1.3)

This is also called the XXZ model, since the coupling in the $x$ and $y$—direction are equal whereas the coupling in the $z$—direction is different. The one-dimensional XXZ model is the one studied in this thesis.

1.5. Experimental realization: inelastic neutron scattering

One of the best methods to study magnetic systems is by inelastic neutron scattering experiments. Because a neutron is charge neutral, it can penetrate deep into the material. Two possible interactions can occur: it can either collide with the nuclei in the lattice or have a dipole-dipole interaction with the spins of the electrons. Because for an antiferromagnet the size of the unit cell is twice the distance between the lattice points, these types of interactions can be distinguished. In fig. 1.2 a neutron scattering experiment is illustrated. As the neutron scatters, it loses energy and momentum to the spin chain. The transferred momentum is determined by the scattering angle $\theta$, and the transferred energy of the neutron is measured.
1.6 Numerical methods for solving lattice models

Figure 1.2.: Simplistic picture of how inelastic neutron scattering experiments are performed. An incoming spin-up neutron with energy $E$ and momentum $k$ scatters with the sample. A spin-down neutron emerges with a lower energy and different momentum.

by its time of flight, measured between the source and the detector. The cross section for magnetic scattering by nuclear spins is proportional to [11]:

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \frac{k'}{k} \sum_{\alpha,\beta \in \{x,y,z\}} (\delta_{\alpha,\beta} - \frac{k_\alpha k_\beta}{|k|^2}) S^{\alpha\beta}(q,\omega)$$  \hspace{1cm} (1.4)

where $q = k - k'$ is the transferred momentum and $\omega = E - E'$ the transferred energy. $S^{\alpha\beta}$ is called the dynamical structure factor, which is the Fourier transform of the dynamical spin-spin correlation function:

$$S^{a\bar{a}}(q,\omega) = \frac{1}{N} \sum_{j,j'=1}^N e^{i q(j-j')} \int_{-\infty}^{\infty} dt e^{i \omega t} \langle S^a_j(t) S^{\bar{a}}_{j'}(0) \rangle .$$  \hspace{1cm} (1.5)

The pair $(a, \bar{a})$ denotes either the longitudinal component $(z,z)$ or the transverse components $(+, -)$ and $(-, +)$. In an experiment with unpolarized neutrons one cannot distinguish between the longitudinal and transverse components. However, in case of a polarized neutron beam the longitudinal and transverse components can be measured separately.

1.6. Numerical methods for solving lattice models

For one-dimensional quantum mechanical systems there are quite a lot of numerical methods available. We will discuss some of the most important numerical techniques. Extra attention will be paid to whether or not these methods are suitable for achieving our goal, which is: extracting the dynamics of the XXZ model.

1.6.1. Exact diagonalization

The simplest method is to exactly diagonalize the Hamiltonian. The eigenvalue-eigenvector pairs are the energy wavefunction pairs. However, there is one drawback: for the spin chain, the number of states per site is two (spin up and -down). So we have to deal with a $2^N \times 2^N$ matrix. For only ten sites the dimensions of this matrix will already be $1024 \times 1024$. Since
diagonalizing a matrix requires $O(N^3)$ operations, adding just a few more sites will be very difficult. In case of only nearest neighbor interactions, the Hamiltonian is a very sparse matrix. With some clever tricks, the number of sites can be slightly expanded. A system of thirty-six sites seems to be the ultimate maximum that computers can currently handle. Even if one is interested in a particular set of states, all other states have to be calculated as well.

1.6.2. Monte Carlo methods

The Quantum Monte Carlo method is efficient for simulating any quantum lattice model, see for example [12]. One of the advantages is that rather large system sizes can be dealt with. However, it is necessary to map a $1 + 1$ dimensional quantum model to a two dimensional classical model by going over to imaginary time. Therefore, calculated results should be converted back into physical quantities. In many cases it is not known how to perform such a conversion. Another disadvantage is that the calculation time is inversely proportional to temperature, which means that very low temperature calculations cannot be done.

1.6.3. DMRG

DMRG, invented by White in 1993 [13], is a numerical Renormalization Group procedure formulated in terms of density matrices. Using DMRG, low-energy properties can be computed very accurately for rather large one-dimensional systems. Because it is quite a new method, very little is known about how to compute dynamical quantities or temperature dependent ones. However, as it is still under development, it might become possible in the future.

1.6.4. ABACUS

The ABACUS method, developed by Caux [14], is tailor made for our purposes. It is designed for lattice models that can be solved exactly by means of the Bethe Ansatz. Dynamical quantities can be efficiently calculated at machine precision for large systems. However, finite temperature calculations still need to be implemented. For our purpose this method is the obvious choice.

1.7. Thesis outline and research questions

In chapter two, we obtain the exact wavefunctions of the time-independent Schrödinger equation for both the isotropic and anisotropic Heisenberg spin chain using the Bethe Ansatz. We also derive the Bethe equations which enable us to explicitly construct the eigenstates. Solving these Bethe equations is a mathematical challenge on its own. One of the main objectives is to solve these equations for the ground state and obtain two-spinon (low energy) excitations. In chapter three the author presents a new method to classify the states of the gapped anisotropic Heisenberg spin chain ($\Delta > 1$). This classification is important for later results, since it tells us which are the low energy states, and it enables us to construct every state exactly once. A physical interpretation of the two-spinon excitations is given in chapter four. In chapter five we derive the Bethe equations in the thermodynamical limit (sending the number of lattice sites to infinity while keeping the ratio between up and down spins fixed). In chapter six integrability is used to rederive the Bethe Ansatz in an algebraic way.
1.7 Thesis outline and research questions

In this algebraic formulation the norm of the eigenstates and transition rates between different eigenstates can be computed. Based on these results, the dynamical spin-spin correlation function, the main objective of this thesis, is computed in chapter seven. We round off in chapter eight with a conclusion and give an overview of several possible directions in which the research may be continued. To summarize, the two main research objectives in this thesis are:

1. Classification of the solutions of the Bethe equations for the gapped antiferromagnetic XXZ spin chain.

2. Obtaining the two-spinon transverse dynamical structure factor of the gapped antiferromagnetic XXZ spin chain using the (Algebraic) Bethe Ansatz.
2. Exact eigenstates of the XXZ model

In this chapter we start by studying the most important properties of the XXZ model. We proceed by building up an intuition for solving one-dimensional models exactly. With this picture in mind we obtain the exact wavefunctions of the XXZ model using the Bethe Ansatz. Then we derive the Bethe equations, which are a set of transcendental equations for the momenta of the wavefunctions. We study also complex solutions in the form of strings in the complex plane.

2.1. Anisotropic Heisenberg chain: XXZ model

The Heisenberg chain \[1\] is a model for nearest neighbor interactions between spin \(-\frac{1}{2}\) particles in one dimension. The on-site spin operators \(S^\alpha_j\) (\(j\) is the site index and \(\alpha = x, y, z\) are the coordinates of the internal space) are defined in terms of Pauli matrices: \(S^\alpha = \sigma^\alpha / 2\). The spin operators obey the canonical commutation relations \([S^\alpha_j, S^\beta_k] = i\delta_{jk}\epsilon^{\alpha\beta\gamma}S^\gamma_j\). The generalized Heisenberg chain, also called the XYZ model, for \(N\) spins is:

\[
H_{\text{XYZ}} = \sum_{j=1}^{N} \left[ J^x_j S^x_j S^x_{j+1} + J^y_j S^y_j S^y_{j+1} + J^z_j S^z_j S^z_{j+1} \right].
\] (2.1)

Periodic boundary conditions are imposed: \(S_{N+1} = S_1\). The real constants \(J^x, J^y, J^z\) are the interaction strengths between the various spin components. Two special cases, \(J^x = J^y = J^z\) and \(J^x = J^y \neq J^z\), are called the XXX and XXZ models, respectively. In this thesis we are mainly interested in the XXZ model. We replace the three \(J^x, J^y, J^z\) by \(J\) and introduce the anisotropy parameter \(\Delta \in \mathbb{R}\). It is convenient to introduce ladder operators: \(S^\pm_j = S^x_j \pm iS^y_j\) with commutation relations: \([S^\pm_j, S^\pm_k] = \pm \delta_{jk}S^\pm_j\) and \([S^z_j, S^\pm_k] = 2\delta_{jk}S^\pm_j\). With orthonormal basis states:

\[
S^+_j |\uparrow\rangle_j = |\downarrow\rangle_j, \quad S^-_j |\downarrow\rangle_j = |\uparrow\rangle_j,
S^+_j |\downarrow\rangle_j = |\downarrow\rangle_j, \quad S^-_j |\downarrow\rangle_j = 0,
S^+_j |\uparrow\rangle_j = |\uparrow\rangle_j, \quad S^-_j |\uparrow\rangle_j = 0.
\] (2.2)

With these substitutions the Hamiltonian of the XXZ model in a magnetic field is given by:

\[
H_{\text{XXZ}} = \sum_{j=1}^{N} J^x \left[ S^+_j S^-_{j+1} + S^-_j S^+_{j+1} \right] + \Delta \left( S^z_j S^z_{j+1} - \frac{1}{4} \right) - \hbar S^z_j.
\] (2.3)

The first two terms of the Hamiltonian are hopping terms: if a spin-up particle is next to a spin-down particle, the two particles interchange position. These terms are interpreted as the kinetic part of the Hamiltonian. The last two terms can be interpreted as the potential part.
2.1 Anisotropic Heisenberg chain: XXZ model

Figure 2.1.: Phase diagram of the XXZ model. With anisotropy $\Delta$ on the horizontal axis. And external field $h$ on the vertical axis.

The constant $1/4$ is introduced for convenience, so that $(S_j^z S_{j+1}^z - 1/4)$ only gives a nonzero contribution if the two sites have opposite spin. The interaction strength $J > 0$ is chosen such that the ground state is antiferromagnetic for $\Delta > 0$. The phase diagram of the XXZ model in a magnetic field is shown in fig. 2.1. Region $A$ has a ferromagnetic ground state and $C$ an anti-ferromagnetic one. In regions $A$ and $C$ the spectrum of elementary excitations is gapped; the energy gaps dependent on $h$ and $\Delta$. $B$ is the quantum critical phase which is gapless. For a more detailed survey see [15]. These three different regimes usually require a separate treatment. In this thesis we will study the basic properties of all these cases, but eventually we will focus on the gapped regime at zero field ($\Delta > 1$). It is worth to mention two special cases. The first one is: $\Delta = 0$; this is also called the $XY$-model and is the only non-trivial case in which all the eigenstates and eigenvalues are known. The second is: $\Delta \to \infty$ which is called the Ising model.

2.1.1. Rotational symmetry

The spin chain is invariant under rotations about the $z$–axis. Define the total spin operator:

$$S_{\text{tot}}^a = \sum_{j=1}^{N} S_j^a \quad a \in \{x, y, z\}.$$ (2.4)

We see that $[H_{XXZ}, S_{\text{tot}}^a] = 0$. Hence the spin in the $z$–direction is conserved so the Hilbert space separates into disjunct subspaces of fixed magnetization. We will label the subspaces by the number of down spins:

$$M = \frac{N}{2} - \left\langle \sum_{j=1}^{N} S_j^z \right\rangle.$$ (2.5)

The term $\langle \ldots \rangle$ is the average magnetization which ranges from $-N/2, -N/2 + 1, \ldots N/2$. For every subspace $M$ we have: $[H_{XXZ}, S_{\text{tot}}^a] = [H_{XXZ}, S_{\text{tot}}^y] = 0$ iff $\Delta = 1$. We therefore conclude
Exact eigenstates of the XXZ model

that the XXX model has an $SU(2)$ symmetry, while the XXZ model for $\Delta \neq 1$ has only a $U(1)$ symmetry.

2.1.2. Translational symmetry

When we impose periodic boundary conditions: $S_{j+N} \equiv S_j$, the Hamiltonian is invariant under translations $T$, e.g. shifting all spins one site (to the left or right). We begin with the permutation operator: $Q_{ij}$ which permutes the spins on sites $i$ and $j$. Then, the translation operator can be written as:

$$T = Q_{12}Q_{23}\ldots Q_{N-1,N}. \quad (2.6)$$

Since $T^N = 1$ the eigenvalues of $T$ are $e^{iP}$, where $P \equiv 2\pi n/N$ with $n = 0, 1, \ldots, N - 1$. We will construct $T$ explicitly in chapter 6 and prove that indeed $[H_{XXZ}, T] = 0$.

2.1.3. Symmetries in $\Delta$ and $h$

In case of even $N$ we consider the following unitary transformation:

$$U_1H(J,\Delta,h)U_1^{-1} = H(-J,-\Delta,h), \quad U_1 = \prod_{l=1}^{M/2} 2S_l^z, \quad (2.7)$$

so for $\Delta < 0$ we are dealing with the ferromagnetic Heisenberg chain. If the Hamiltonian was defined with a minus sign all we have to do is send $\Delta \rightarrow -\Delta$ and obtain the same system (up to a shift of $\pi$ in the momenta). Using another unitary transformation:

$$U_2H(J,\Delta,h)U_2^{-1} = H(J,\Delta,-h), \quad U_2 = \prod_{l=1}^{M} 2S_l^x, \quad (2.8)$$

we see that it is sufficient to consider the case $h > 0$ hence only the case $0 \leq M \leq N/2$ needs to be considered.

2.2. The Bethe Ansatz for the XXZ model

Before trying to solve the XXZ model exactly, we will sharpen our intuition about the dynamics of one-dimensional systems which are fundamentally different from higher dimensional ones. When two identical particles scatter elastically in one dimension, conservation of energy and momentum tells us that the momenta of the particles either are interchanged or remain unchanged. When we are dealing with a quantum mechanical system the wavefunctions of the particles can only pick up a phase shift, also called a scattering phase. In case of an $N$-body scattering, the individual momenta can generally change. However, if an $N$-body scattering is a sequence of 2-body scatterings, the momentum distribution will remain unchanged after an arbitrary number of scatterings. This condition is most likely met when all the particles are well separated. If we label the particles $j_1, \ldots, j_N$, the momenta can be distributed over the particles in $N!$ ways. An Ansatz (educated guess) for such a system would be a product of free particle wavefunctions $\psi_1$ accompanied by an amplitude $A_\mathcal{P}$, related to the scattering phase, and summed over all the $N!$ possible permutations $\mathcal{P}$ of the momenta.

$$\psi_N(j_1, \ldots, j_N) = \sum_\mathcal{P} A_\mathcal{P} \prod_{i=1}^{N} \psi_1(j_i, k_{\mathcal{P}_i}). \quad (2.9)$$
2.2 The Bethe Ansatz for the XXZ model

Instead of finding a complete wavefunction, our problem is reduced to finding all the scattering phases. At this stage it is not clear if the spins of the XXZ model interact like a sequence of elastic two-body scatterings. Therefore we will first study some special cases, before we turn to the Bethe Ansatz [2]. That it will work is not a surprise, since the first model solved with the Bethe Ansatz was the XXX model.

2.2.1. Wavefunction for down spins

If we introduce a reference state with all the spins up:

\[ |0\rangle = \bigotimes_{j=1}^{N} |\uparrow\rangle \]

we can write the eigenstates of \( S_{\text{tot}}^{z} \) as:

\[ |j_1, j_2, \ldots, j_M\rangle \equiv \prod_{k=1}^{M} S_{mk}^{-} |0\rangle \]

with eigenvalues \((N/2 - M)\). It is sufficient to have \( M \leq N/2 \). For \( M > N/2 \) we should use a reference state with all spins down. Since \([H_{XXZ}, S_{\text{tot}}^{z}] = 0\) we can write the wavefunctions for the XXZ model like:

\[ |\Psi_{M}\rangle = \sum_{\{j\}} \psi_{M}(j_1, \ldots, j_M) |j_1, \ldots, j_M\rangle \]

where the sum is over all possible configurations \( \{j\} \) of the down spins.

2.2.2. Eigenvalue equation

Using the Schrödinger equation \( H_{XXZ} |\Psi_{M}\rangle = E_{M} |\Psi_{M}\rangle \), we get:

\[ (E_{M}/J) |\Psi_{M}\rangle = \sum_{\{j\}} \psi_{M}(j_1, \ldots, j_M) \left( -\Delta(M - \sum_{n=1}^{M} \delta_{j_{n+1}, j_{n+1}}) |j_1, \ldots, j_M\rangle + \frac{1}{2} \sum_{n=1}^{M} \left( 1 - \delta_{j_{n+1}, j_{n+1}} \right) \{ |\ldots, j_{n+1}, j_{n+1}+1, \ldots\rangle + |\ldots, j_{n}, j_{n+1}-1, \ldots\rangle \} \right) \]

The first term between the big parentheses comes from: \( \Delta(S_{j}^{z}S_{j+1}^{z} - \frac{1}{4}) \), which is zero for neighboring sites with parallel spin and \(-\Delta/2\) for the \(2(M - \sum_{n} \delta_{j_{n+1}, j_{n+1}})\) neighboring sites with opposite spin. The second term comes from: \( \frac{1}{2}(S_{j}^{+}S_{j+1}^{-} + S_{j}^{-}S_{j+1}^{+}) \). It does not contribute for adjacent down spins: \( j_{n} + 1 = j_{n+1} \). Projecting this equation onto the position state \( \langle \{j\} | \) gives the equation for the wavefunction:

\[ (E_{M}/J) \psi_{M}(j_1, \ldots, j_M) = -\Delta(M - \sum_{n=1}^{M} \delta_{j_{n+1}, j_{n+1}}) \psi_{M}(j_1, \ldots, j_M) + \frac{1}{2} \sum_{n=1}^{M} \left( 1 - \delta_{j_{n+1}, j_{n+1}} \right) \{ \psi_{M}(\ldots, j_{n+1}, j_{n+1}+1, \ldots) + \psi_{M}(\ldots, j_{n}, j_{n+1}-1, \ldots) \} \]

\[ j_{M+1} \equiv j_{1} \]
2.2.3. A single down spin

In case of a single down spin the eigenvalue equation (2.14) becomes:

\[
\frac{(E_1/J)}{\psi(j_1)} = \frac{1}{2} \psi_1(j_1 + 1) + \frac{1}{2} \psi_1(j_1 - 1) - \Delta \psi_1(j_1).
\]  

(2.15)

An equation of this kind is called a second-order homogeneous difference equation. The equation can be solved in a way very similar to an ordinary differential equation. The characteristic equation is: \( \lambda^2 + c\lambda + 1 = 0 \). Until this point we can choose \( c \), as long it is any real number.

The roots of the characteristic equation separates into three solutions:

\[
\psi(x) = \begin{cases} 
  a\lambda_1^x + b\lambda_2^x & \text{\( \lambda_1 \) and \( \lambda_2 \) are real and distinct}, \\
  (a + bx)(\pm 1)^x & \lambda_1 = \lambda_2 = \pm 1, \\
  ae^{ikx} + be^{-ikx} & \lambda_{1,2} = e^{\pm ikx}.
\end{cases}
\]  

(2.16)

If we impose periodic boundary conditions, only the third case is relevant, so we try the plane wave: \( \psi_1(j_1) = e^{ik_1j_1} \). Plugging this into (2.15) gives the energy:

\[
E_1/J = \cos k_1 - \Delta.
\]  

(2.17)

2.2.4. Two neighboring down spins

We start with the case of only two downspins. There are now two different cases to consider, when the down spins are separated and when they are next to each other:

\[
(E_2/J)\psi_2(j_1, j_2) = -2\Delta \psi_2(j_1, j_2) + \frac{1}{2} \left\{ \psi_2(j_1+1, j_2) + \psi_2(j_1, j_2+1) + \psi_2(j_1-1, j_2) + \psi_2(j_1, j_2-1) \right\} \quad j_1 + 1 < j_2
\]

(2.18a)

\[
(E_2/J)\psi_2(j_1, j_2) = -\Delta \psi_2(j_1, j_2) + \frac{1}{2} \left\{ \psi_2(j_1, j_2+1) + \psi_2(j_1-1, j_2) \right\} \quad j_1 + 1 = j_2
\]

(2.18b)

In the spirit of (2.9) we try:

\[
\psi_2(j_1, j_2) = A_{12}e^{ik_1j_1+ik_2j_2} + A_{21}e^{ik_2j_1+ik_1j_2}.
\]  

(2.19)

Plugging this wavefunction into (2.18a) gives:

\[
E_2/J = \cos k_1 + \cos k_2 - 2\Delta.
\]  

(2.20)

Substituting this result into (2.18b) yields:

\[
\left( \cos k_1 + \cos k_2 - \Delta \right) \left( A_{12}e^{ik_1j_1+ik_2j_2} + A_{21}e^{ik_2j_1+ik_1j_2} \right) =
\]

\[
+ \frac{1}{2} \left\{ A_{12}e^{ik_1j_1+ik_2j_2}e^{ik_2} + A_{21}e^{ik_2j_1+ik_1j_2}e^{ik_1} + A_{12}e^{ik_1j_1+ik_2j_2}e^{-ik_1} + A_{21}e^{ik_2j_1+ik_1j_2}e^{-ik_2} \right\}
\]  

(2.21)

Recalling that \( j_2 = j_1 + 1 \), and after cancelling common factors, we get:

\[
A_{12} \left( 1 + e^{i(k_1+k_2)} - 2\Delta e^{ik_2} \right) + A_{21} \left( 1 + e^{i(k_1+k_2)} - 2\Delta e^{ik_1} \right) = 0.
\]  

(2.22)
2.2 The Bethe Ansatz for the XXZ model

When $k_1 = k_2$ it follows that $A_{12} + A_{21} = 0$, hence the wavefunction vanishes. Thus only states with noncoinciding momenta should be considered. This agrees with our intuition based on Pauli’s principle for spin–1/2 particles. The next step is to relate $A_{12}$ and $A_{21}$ to a scattering phase.

\[
\frac{A_{12}}{A_{21}} = -\frac{1 + e^{i(k_1 + k_2)} - 2\Delta e^{ik_1}}{1 + e^{i(k_1 + k_2)} - 2\Delta e^{ik_2}} \equiv -e^{-i\phi(k_1,k_2)}, \quad (2.23)
\]

where the two particle scattering phase $\phi$ is defined as:

\[
\phi(k_1, k_2) = \frac{1}{i} \ln \left( \frac{\cos \frac{k_1 + k_2}{2} - \Delta \cos \frac{k_1 - k_2}{2} + i \Delta \sin \frac{k_1 - k_2}{2}}{\cos \frac{k_1 + k_2}{2} - \Delta \cos \frac{k_1 - k_2}{2} - i \Delta \sin \frac{k_1 - k_2}{2}} \right)
= 2 \arctan \frac{\Delta \sin \frac{k_1 - k_2}{2}}{\cos \frac{k_1 + k_2}{2} - \Delta \cos \frac{k_1 - k_2}{2}}. \quad (2.24)
\]

In the last step we used: $\arctan x = \frac{i}{2} (\ln(1 - ix) - \ln(1 + ix))$. There is a branch cut starting at $\cos \frac{k_1 + k_2}{2} - \Delta \cos \frac{k_1 - k_2}{2} = 0$. The branch is chosen such that $\phi(0,0) = 0$ and $\phi(k_1, k_2) = -\phi(k_2, k_1)$.

We can generalize this result for $M$ down spins. The derivation goes completely analogous to the $M = 2$ case. The following two cases needed to be considered. Namely, when all down spins are isolated $j_n + 1 < j_{n+1} \forall n$:

\[
(E_M/J)\psi_M(j_1, \ldots, j_M) = -\Delta(M-1)\psi_M(j_1, \ldots, j_M)
+ \frac{1}{2} \sum_{n=1}^{M} \{ \psi_M(\ldots, j_n - 1, \ldots) + \psi_M(\ldots, j_n + 1, \ldots) \} \quad j_n + 1 < j_{n+1} \forall n \quad (2.25)
\]

and for one nearest neighbor pair: $j_l + 1 = j_{l+1}$ and $j_n + 1 < j_{n+1} \ n \neq l$

\[
(E_M/J)\psi_M(j_1, \ldots, j_M) = -\Delta(M-1)\psi_M(j_1, \ldots, j_M)
+ \frac{1}{2} \sum_{n \neq l, l+1}^{M} \{ \psi_M(\ldots, j_{n-1}, \ldots) + \psi_M(\ldots, j_{n+1}, \ldots) \}
+ \frac{1}{2} \{ \psi_M(\ldots, j_{l-1}, j_{l+1}, \ldots) + \psi_M(\ldots, j_{l}, j_{l+2} \ldots) \} 
\quad j_l + 1 = j_{l+1}. \quad (2.26)
\]

Our Bethe Ansatz wavefunction is:

\[
\psi_M(j_1, \ldots, j_M) = \sum_{\mathcal{P}} A_{\mathcal{P}} e^{i \sum_{n=1}^{M} k_{\mathcal{P}_n} j_n}. \quad (2.27)
\]

Similar as in the $M = 2$ case we can plug this wavefunction into (2.25) to obtain:

\[
E_M/J = \sum_{n=1}^{M} (\cos k_n - \Delta). \quad (2.28)
\]
If we now substitute this into (2.26) we obtain:

\[
\sum_{\mathcal{P}_{even}} \left( \cos k_{\mathcal{P}_i} + \cos k_{\mathcal{P}_{i+1}} - \Delta \right) \left( A_p e^{i k_{\mathcal{P}_i} j_i + i k_{\mathcal{P}_{i+1}} j_{i+1}} + A_{p'} e^{i k_{\mathcal{P}'_i} j_i + i k_{\mathcal{P}'_{i+1}} j_{i+1}} e^{i \sum_{a \neq i, i+1} k_{\mathcal{P}_a} j_a} \right)
\]

\[
= \sum_{\mathcal{P}_{even}} \frac{1}{2} \left( A_p e^{i k_{\mathcal{P}_i} j_i + i k_{\mathcal{P}_{i+1}} j_{i+1}} (e^{-i k_{\mathcal{P}_i}} + e^{i k_{\mathcal{P}_{i+1}}}) + A_{p'} e^{i k_{\mathcal{P}'_i} j_i + i k_{\mathcal{P}'_{i+1}} j_{i+1}} (e^{-i k_{\mathcal{P}'_i}} + e^{i k_{\mathcal{P}'_{i+1}}}) \right) e^{i \sum_{a \neq i, i+1} k_{\mathcal{P}_a} j_a}. \quad (2.29)
\]

The summation is only over the even permutations because the odd permutations are being included explicitly by the \(A_{p'}\) terms. Given that (2.26) is supposed to be valid for every configuration \(\{j_a\}\), the LHS and the RHS should be equal for every term that is summed over. Hence (2.29) reduces to the two-body scattering (2.22), namely:

\[
A_p \left( 1 + e^{ik_{\mathcal{P}_i + k_{\mathcal{P}_{i+1}}}} - 2\Delta e^{i k_{\mathcal{P}_{i+1}}} \right) + A_{p'} \left( 1 + e^{ik_{\mathcal{P}'_i + k_{\mathcal{P}'_{i+1}}}} - 2\Delta e^{i k_{\mathcal{P}'_{i+1}}} \right) = 0. \quad (2.30)
\]

We can recast this as:

\[
\frac{A_p}{A_{p'}} = -e^{-i \phi(k_{\mathcal{P}_i}, k_{\mathcal{P}'_i})}. \quad (2.31)
\]

**2.2.5. General case**

For a general configuration of down spins, we get (2.30) for every pair of neighboring down spins. To find an expression for \(A_{\mathcal{P}}\) we use that every permutation \(\mathcal{P}\) can be written as a product of transpositions acting upon the identity permutation. So if we have an expression for the identity permutation, all other permutations can be expressed in terms of the identity permutation and a product of scattering phases:

\[
A_{\mathcal{P}} = e^{-\frac{i}{2} \sum_{1 \leq a < b \leq M} \phi(k_{\mathcal{P}_a}, k_{\mathcal{P}_b})} \quad (2.32)
\]

resulting in the complete Bethe ansatz for \(j_1 < j_2 < \ldots < j_M\):

\[
\psi_M(j_1, \ldots, j_M) = \sum_{\mathcal{P}} (-1)^{[\mathcal{P}]} e^{i \sum_{a=1}^{M} k_{\mathcal{P}_a} j_a - \frac{i}{2} \sum_{1 \leq a < b \leq M} \phi(k_{\mathcal{P}_a}, k_{\mathcal{P}_b})}. \quad (2.33)
\]

The factor \((-1)^{[\mathcal{P}]}\) comes from the minus sign in front of (2.31), where \([\mathcal{P}]\) denotes the parity of the permutation. The energy and total momentum are:

\[
E_M = J \sum_{a=1}^{M} (\cos k_a - \Delta) - \frac{Jh}{2} (N - 2M), \quad P = \sum_{a=1}^{M} k_a. \quad (2.34)
\]

**2.2.6. Consistency relations**

We note that the \(A_{\mathcal{P}}\) should obey a consistency relation. For example in the case \(M = 3\), there are two ways of going from \(A_{123}\) to \(A_{321}\):

\[
A_{123} \rightarrow A_{213} \rightarrow A_{231} \rightarrow A_{321}, \quad A_{123} \rightarrow A_{132} \rightarrow A_{312} \rightarrow A_{321}. \quad (2.35)
\]

Both ways should yield the same result; this is easy to check using (2.31) and (2.32). For the moment it is enough to note that (2.32) indeed satisfy this consistency relation. In chapter six this consistency relation will play a crucial role.
2.3 The Bethe equations

Imposing periodic boundary conditions, we should have:

$$\psi_M(j_1,\ldots,j_M) = \psi_M(j_2,\ldots,j_M,j_1 + N).$$ (2.36)

This can be easily interpreted as: sending the $j_1$ down spin through the system, picking up $M - 1$ scattering phases, and then returning it to its original position. We identify: $j_n + N \equiv j_n$. Imposing these conditions on the Bethe wavefunction:

$$\sum_{\mathcal{P}} (-1)^{|\mathcal{P}|} A_P e^{i \sum_a k_{Pa} j_a} = \sum_{\mathcal{P}} (-1)^{|\mathcal{P}|} A_P e^{i \sum_a k_{Pa} j_{a+1}} e^{ik_{\mathcal{P}}M N}. \quad (2.37)$$

For every term with $A_P$ on the LHS we should take $A_Q$ on the RHS with $Q = (P_2,\ldots,P_M,P_1)$, such that $e^{i \sum_a k_{Pa} j_a} = e^{i \sum_a k_{Qa} j_{a+1}}$. This gives:

$$(-1)^{|\mathcal{P}|} A_P = (-1)^{|Q|} A_Q e^{ik_{P_1} N} \Leftrightarrow e^{ik_{P_1} N} = (-1)^{M-1} \frac{A_P}{A_Q}. \quad (2.38)$$

Using (2.32) we have:

$$A_P = e^{-\frac{i}{2} \sum_{b>1} \phi(k_{P_1},k_{P_b})} e^{-\frac{i}{2} \sum_{1<a<b<M} \phi(k_{Pa},k_{Pb})},$$

$$A_Q = e^{\frac{i}{2} \sum_{a>1} \phi(k_{P_1},k_{Pa})} e^{-\frac{i}{2} \sum_{1<a<b<M} \phi(k_{Pa},k_{Pb})}.$$\[These equations must hold for all permutations $\mathcal{P}$, and therefore we obtain the Bethe equations:

$$e^{ik_{P_1} N} = (-1)^{M-1} e^{i \sum_{b\neq a} \phi(k_a,k_b)}. \quad (2.39)$$\]

This is a set of $M$ coupled equations for $M$ unknown $k_j$. These equations are transcendental, due to form of the scattering phase $\phi$, which makes it impossible to have one of the $k_j$ on the LHS and all the other ones on the RHS. Therefore, to find a solution of these equations, an algorithm, Newton-Raphson for instance, is needed. A solution of this set of equations corresponds to an eigenstate of the XXZ model from which we can compute its energy and total momentum. It is convenient to take the the logarithm of the Bethe equations (2.39):

$$k_j - \frac{1}{N} \sum_{i \neq j} \phi(k_j,k_i) = 2\pi \tilde{I}_j \mod 2\pi. \quad (2.40)$$

The factor $\log(-1)^{M-1}$ in the first equation is represented by the $\tilde{I}_j$. Where $\tilde{I}_j$ are half-odd integers if $M$ is even and integers for odd $M$. Since $k$ is defined mod$(2\pi)$ we should define the $\tilde{I}_j \mod(N)$. We can now parametrize different solutions of the Bethe equations by different choices for $\tilde{I}_j$.

2.3.1. Bethe Ansatz for other models

Althought we derived the Bethe wavefunction (2.33) and the Bethe equations (2.39) for the XXZ model, their structure remains the same for other exactly solvable models in one dimension. What is different is, of course, the two particle scattering phase $\phi(k_1,k_2)$ and the choice for the quantum numbers $\tilde{I}_j$.  

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2.4. Parametrization

At this point it is convenient to reparametrize the Bethe equations, due to Orbach [16], in terms of $\lambda$ called rapidities. The motivation for this is that the new scattering phase $\theta(\lambda_j, \lambda_l)$ is only a function of the difference: $\lambda_j - \lambda_l$. The parametrization will be different for the three classes of $\Delta$.

2.4.1. Gapped anisotropic case: $|\Delta| > 1$

We start with the parametrization for the $|\Delta| > 1$ case, since this the one we will mostly work with and it is also the most subtle one. Using the parametrization,

$$e^{ik} = \frac{\sin(\lambda + i\eta/2)}{\sin(\lambda - i\eta/2)}, \quad \eta = \text{arccosh}(\Delta), \quad (2.41)$$

the RHS of the Bethe equations become:

$$e^{-i\phi(k_1, k_2)} = \frac{1 + e^{i(k_1 + k_2)} - 2\Delta e^{ik_1}}{1 + e^{i(k_1 + k_2)} - 2\Delta e^{ik_2}} = -\frac{\sin(\lambda_1 - \lambda_2 + i\eta)}{\sin(\lambda_1 - \lambda_2 - i\eta)}. \quad (2.42)$$

The Bethe equations (2.39) become:

$$\left(\frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)}\right)^N = \prod_{k \neq j}^M \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k - i\eta)}. \quad (2.43)$$

Taking the logarithm of (2.41):

$$k(\lambda) = -i \ln \left(\frac{\sin(\lambda + i\eta/2)}{\sin(\lambda - i\eta/2)}\right) = \pm \pi - i \ln \left(\frac{\tanh(\eta) - i \tan(\lambda)}{\tanh(\eta) + i \tan(\lambda)}\right) = \pi - 2 \arctan \left(\frac{\tan(\lambda)}{\tanh(\eta/2)}\right) - 2\pi \left[\frac{\lambda}{\pi} + \frac{1}{2}\right] \mod 2\pi$$

$$\equiv \pi - \theta_1(\lambda) \mod 2\pi. \quad (2.44)$$

In the first step we used: $\ln(-1) = \pm \pi$ together with (B.14), in the second step: (B.17) with $\arctan(-x) = \pi - \arctan(x)$. The floor function: $\lfloor x \rfloor = \{ n \in \mathbb{Z} | n \leq x \}$ was introduced to guarantee that we stay in the same branch of the logarithm. We chose the branch of the logarithm such that $0 \leq \Re k < 2\pi \leftrightarrow -\pi/2 < \Re \lambda \leq \pi/2$. The scattering phase can now be brought into an appealing form:

$$\phi(k(\lambda_1), k(\lambda_2)) = i \ln \left(\frac{-\sin(\lambda_1 - \lambda_2 + i\eta)}{\sin(\lambda_1 - \lambda_2 - i\eta)}\right) = 2 \arctan \left(\frac{\tan(\lambda_1 - \lambda_2)}{\tanh(\eta)}\right) + 2\pi \left[\frac{\lambda_1 - \lambda_2}{\pi} + \frac{1}{2}\right] \equiv \theta_2(\lambda_1, \lambda_2). \quad (2.45)$$

It is clear that $\theta_2(\lambda_1, \lambda_2) = -\theta_2(\lambda_2, \lambda_1)$. Taking the logarithm of the Bethe equations:
2.4 Parametrization

![Graph of the scattering phase θ₂(λ) for Δ = 1.05 (solid line), Δ = 1.2 (small dashes), Δ = 4 (large dashes).](image)

Figure 2.2.: The scattering phase θ₂(λ) for Δ = 1.05 (solid line), Δ = 1.2 (small dashes), Δ = 4 (large dashes).

\[
2 \arctan \left( \frac{\tan(\lambda_j)}{\tanh(\eta/2)} \right) + 2\pi \left( \frac{\lambda_j}{\pi} + \frac{1}{2} \right) = \frac{2\pi I_j}{N} + \frac{1}{N} \sum_{l=1}^{M} 2 \arctan \left( \frac{\tan(\lambda_j - \lambda_l)}{\tanh(\eta)} \right) + 2\pi \left( \frac{\lambda_j - \lambda_l}{\pi} + \frac{1}{2} \right)
\]

or in a more compact notation:

\[
\theta_1(\lambda_j) = \frac{2\pi I_j}{N} + \frac{1}{N} \sum_{l=1}^{M} \theta_2(\lambda_j - \lambda_l).
\]

The energy in terms of rapidities:

\[
E = J \sum_{j=1}^{M} \left( \cos(2 \arctan \frac{\tan \lambda_j}{\tanh \eta}) - \cosh(\eta) \right) - h\left( \frac{N}{2} - M \right)
\]

\[
= J \sum_{j=1}^{M} - \frac{\sinh^2 \eta}{\cosh \eta - \cos 2\lambda_j} - h\left( \frac{N}{2} - M \right).
\]

In the last step we used: \( \cos(2 \arctan(x)) = \frac{1-x^2}{1+x^2} \). The momentum in terms of the rapidities:

\[
P = \sum_{j=1}^{M} \frac{1}{i} \ln \left( \frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)} \right) = \sum_{j=1}^{M} (\pi - \theta_1(\lambda_j)) = \pi M - \frac{2\pi}{N} \sum_{j=1}^{M} I_j \mod 2\pi.
\]

The last equality follows from the Bethe equations.

2.4.2. Isotropic case: \( \Delta = 1 \)

As one might expect, the parametrization for the isotropic case is the easiest one:

\[
e^{ik} = \frac{\lambda + i/2}{\lambda - i/2}.
\]
The Bethe equations in this parametrization are:

\[
\left( \frac{\lambda_j + i/2}{\lambda_j - i/2} \right)^N = \prod_{k \neq j} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}
\]

and in logarithmic form:

\[
2 \arctan(2\lambda_j) = 2\pi I_j N + \frac{1}{N} \sum_{k=1}^{M} \arctan(\lambda_j - \lambda_k).
\]

### 2.4.3. Gapless anisotropic case: $|\Delta| \leq 1$

For completeness we also give the parametrization for the gapless case:

\[
e^{ik} = \frac{\sinh(\lambda + i\zeta/2)}{\sinh(\lambda - i\zeta/2)}, \quad \zeta = \arccos(\Delta),
\]

resulting in the Bethe equations:

\[
\left( \frac{\sinh(\lambda_j + i\zeta/2)}{\sinh(\lambda_j - i\zeta/2)} \right)^N = \prod_{k \neq j} \frac{\sinh(\lambda_j - \lambda_k + i\zeta)}{\sinh(\lambda_j - \lambda_k - i\zeta)}.
\]

Taking the logarithm:

\[
2 \arctan \frac{\tanh \lambda_j}{\tan \zeta/2} = 2\pi I_j N + \sum_{k=1}^{M} 2 \arctan \frac{\tanh \lambda_j - \lambda_k}{\tan \zeta}.
\]

### 2.4.4. General expressions

We can summarize the Bethe equations for all $\Delta$ as in terms of:

\[
e^{ik} = \varphi(\lambda + i\eta/2) \varphi(\lambda - i\eta/2),
\]

\[
k(\lambda) = \pi - \theta_1(\lambda),
\]

and the Bethe equations become:

\[
\left( \frac{\varphi(\lambda_j + i\eta/2)}{\varphi(\lambda_j - i\eta/2)} \right)^N = \prod_{k \neq j} \frac{\varphi(\lambda_j - \lambda_k + i\eta)}{\varphi(\lambda_j - \lambda_k - i\eta)}.
\]
2.5 Complex solutions: bound states

The logarithmic Bethe equations are:

\[ \theta_1(\lambda_j) = \frac{\pi}{N} I_j + \frac{1}{N} \sum_{l=1}^{M} \theta_2(\lambda_j - \lambda_l), \quad (2.59) \]

and the total energy and momenta are:

\[ E = -J\pi \sum_{l} a_1(\lambda_l) \varphi(i\eta) - \hbar\left(\frac{N}{2} - M\right), \quad (2.60) \]

\[ P = \sum_{j=1}^{M} (\pi - \theta_1(\lambda_j)) = \pi M - \frac{2\pi}{N} \sum_{j=1}^{M} I_j \quad \text{mod} \ 2\pi. \quad (2.61) \]

Note the symmetry between the equations for \(|\Delta| < 1\) and \(|\Delta| > 1\):

\[ \eta|\Delta| < 1 = i\eta|\Delta| > 1 \]

\[ \lambda|\Delta| < 1 = -i\lambda|\Delta| > 1. \]

Of course, starting with the equations for the \(|\Delta| > 1\), we can take the limit \(\Delta \to 1\) and end up with the isotropic case by \(\lambda|\Delta| = 1 = \lim_{\eta \to 0} \lambda|\Delta| > 1/\eta\). The limit can also be done starting from \(|\Delta| < 1\) case. The Bethe equations in this generic form, allow us to do many calculations simultaneously for all three parametrizations. However, the solutions in terms of rapidities are quite different for all three cases. In the XXX model the rapidities lie in the entire complex plane. For the XXZ gapless case the rapidities are restricted to the strip \(-\pi/2 < \text{Im} \ \lambda \leq \pi/2\) in the complex plane, due to the periodicity of the sinh function in the complex plane. And for the XXZ gapped case the rapidities are restricted in the real direction: \(-\pi/2 < \text{Re} \ \lambda \leq \pi/2\).

2.5. Complex solutions: bound states

In the next chapter we will see that the real solutions do not span the complete Hilbert space, so complex solutions of the Bethe equations should also exist. A general approach for finding complex solutions is not known due to the immense complexity of the problem. However, in special cases complex solutions can be studied.

For a complex root \(\lambda\) with \(\text{Im} \ \lambda > 0\) the LHS of the Bethe equations goes to infinity when \(N \to \infty\). We can distinguish two cases the RHS can go to infinity:

- In case of finite \(M\), only a finite number of terms on the RHS can blow up. This case can be dealt with using the string hypothesis discussed below.

- When \(M/N\) is fixed, either a finite number terms on the RHS can blow up. Or the product of many finite terms can diverge. This case is much more complicated, but low-energy excitations can be studied in the thermodynamic limit.

Complex rapidities, and therefore complex momenta, sound rather unphysical. However, they can be interpreted as bound states: a group of down spins with the same real momenta that are bound together. We will explain this a bit more later on.

2.5.1. Self-conjugacy of the Bethe-wavefunctions

Before turning to the string hypothesis, we first mention an important property of the Bethe-solutions: they are self-conjugate. Having a solution \(\{\lambda_j\}\) is easy to see that \(\{\bar{\lambda}_j\}\) is also a solution: by taking the complex conjugate and inverting both sides of (2.58). Less obvious is that \(\{\bar{\lambda}_j\} = \{\lambda_j\}\), proven by Vladimirov [17].
2.5.2. String hypothesis: $|\Delta| > 1$ and $|\Delta| = 1$

In this section we consider the string hypothesis for the $|\Delta| = 1$ case which already appeared in Bethe’s paper [2] and was further developed by Takahashi [18]. Simultaneously we deal with the $|\Delta| > 1$ case [19], since in both cases the imaginary part of the rapidities lie in the interval $(-\infty, \infty)$.

Consider a system with infinite $N$ and finite $M$. Take $\lambda_j$ with $0 < \text{Im} (\lambda_j) < \infty$. Recall the Bethe equations (2.43):

$$\left( \frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)} \right)^N = \prod_{k \neq j} \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k - i\eta)}.$$ 

The factor on the LHS of the Bethe equations:

$$\left| \frac{\sin(\text{Re} \lambda_j + i(\text{Im} \lambda_j + \eta/2))}{\sin(\text{Re} \lambda_j + i(\text{Im} \lambda_j - \eta/2))} \right|^2 = \frac{\cos(2\text{Re} \lambda_j) - \cosh(2\text{Im} \lambda_j + \eta)}{\cos(2\text{Re} \lambda_j) - \cosh(2\text{Im} \lambda_j - \eta)} > 1 \quad (2.62)$$

so the LHS goes to infinity for infinite $N$. For finite $M$ there must be a corresponding $\lambda_k$ for which the denominator on the RHS blows up: $\lambda_k = \lambda_j - i\eta$. Using this argument repeatedly, and the fact that a solution $\{\lambda_j\}$ has to be self-conjugate, we find a possible set of complex roots: $\{\lambda_j, \lambda_j - i\eta, \lambda_j - 2i\eta, \ldots, \lambda_j\}$. This leads us to the string hypothesis for a string of length $n$:

$$\lambda_{n,j} = \lambda_{n} + \frac{i\eta}{2}(n + 1 - 2j), \quad (2.63)$$

with $j = 1 \ldots n$. The string hypothesis for the XXX model goes completely analogously:

$$\lambda_{n,j} = \lambda_{n} + \frac{i}{2}(n + 1 - 2j). \quad (2.64)$$

Since $\varphi(\lambda)$ is a monotonic increasing function in the imaginary direction, we expect that all possible string lengths are allowed.

2.5.3. String hypothesis: $|\Delta| < 1$

The string hypothesis for the $|\Delta| < 1$ case is quite different from the previous ones. The imaginary part of the rapidities are now periodic in the interval $(-i\pi/2, i\pi/2]$. In contrast to the cases $|\Delta| \geq 1$ where the imaginary part stretches from minus to plus infinity. And the string can not only be centered on the real-axis but also on the $i\pi/2$ axis. So in this case the string hypothesis is:

$$\lambda_{n,j} = \lambda_{n} + \frac{i\eta}{2}(n + 1 - 2j) + \frac{i\pi}{4}(1 - v_j), \quad (2.65)$$

with the parities $v_j \pm 1$. Since $\varphi(\lambda)$ is not monotonic increasing in the imaginary direction, studying the possible string lengths for this case is much more complicated than the $|\Delta| \geq 1$ case. For a discussion see Takahashi’s book [20].

2.5.4. String hypothesis for a finite chain: deviated strings

Turning back to the problem for finite $N$ and $M \ll N/2$, it is assumed that the complex solutions have the form of deviated strings:

$$\lambda_{n,j} = \lambda_{n} + \frac{i\eta}{2}(n + 1 - 2j) + \frac{i\pi}{4}(1 - v_j) + i\delta_{n,j}, \quad (2.66)$$
where the deviations $\delta_{n,j}^{a,b}$ are exponentially suppressed with system size, i.e. $|\delta| = O(e^{-\text{const}N})$.

We can make this plausible by considering a 2-string: $\{\lambda_a = \lambda + i\eta/2 + i\delta, \lambda_b = \lambda - i\eta/2 - i\delta\}$. The Bethe equation for $\lambda_a$ is:

$$e^{ik_aN} = \varphi(\lambda_a - \lambda_b + i\eta) \prod_{l \neq a, b} \frac{\varphi(\lambda_a - \lambda_l + i\eta)}{\varphi(\lambda_a - \lambda_l - i\eta)}$$

$$= \frac{\varphi(2i\eta)}{2i\delta} \prod_{l \neq a, b} \frac{\varphi(\lambda_a - \lambda_l + i\eta)}{\varphi(\lambda_a - \lambda_l - i\eta)}$$

(2.67)

where the approximations: $\varphi(2i\eta + 2i\delta) \approx \varphi(2i\eta)$ and $\varphi(2i\delta) \approx 2i\delta$ were made. With $\text{Im} (k_a) = \text{Im} (\pi - \theta_1(\lambda + i\eta/2)) > 0$ we find:

$$|\delta| = \frac{1}{2} |\varphi(2i\eta)| e^{-aN} e^{b(M-2)},$$

(2.68)

with $a,b > 0$. Hence for $M \ll N/2$ we have indeed $|\delta| = O(e^{-\text{const}N})$. If we repeat this argument for strings with $n > 2$, (2.67) is an equation for $\delta_{n,j}^{a,b} - \delta_{n,j}^{a,b+1}$. But since $\delta_{n,j}^{a,b} = -\delta_{n,j}^{a,b-n}$ we find that $\delta_{n,j}^{a,b-n/2}$ is exponentially suppressed, hence all the other deviations are as well.

For long chains the deviations can be neglected, but we should keep in mind that they are actually there in order to have regular expressions.

### 2.5.5. Bethe equations for string solutions

For string rapidities the Bethe Equations take the form:

$$\left(\frac{\varphi(\lambda_{n,j}^a + i\eta/2)}{\varphi(\lambda_{n,j}^a - i\eta/2)}\right)^N = \prod_{(m,\beta) \neq (n,\alpha)} \prod_{k=1}^{m} \frac{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta + i\eta)}{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta - i\eta)} \times \prod_{j' \neq j} \frac{\varphi(\lambda_{n,j}^a - \lambda_{n,j'}^a + i\eta)}{\varphi(\lambda_{n,j}^a - \lambda_{n,j'}^a - i\eta)}.$$  

(2.69)

The last product is delicate because either the numerator or the denominator may become very small. We can remove the last product by multiplying the equations with the $n$ rapidities $\lambda_{n,j}^a$ which from a string. A term $\varphi(i(\delta_{n,a} - \delta_{n,b} + \eta))$ in the numerator cancels against the term $\varphi(i(\delta_{n,b} - \delta_{n,a} - \eta))$ in the denominator. The LHS gives:

$$\prod_{j=1}^{n} \frac{\varphi(\lambda_{n,j}^a + i\eta/2)}{\varphi(\lambda_{n,j}^a - i\eta/2)} = \frac{\varphi(\lambda_n + i\eta/2)}{\varphi(\lambda_n + i(n-2)\eta/2)} \frac{\varphi(\lambda_n + i(n-2)\eta/2)}{\varphi(\lambda_n + i(n-4)\eta/2)} \ldots \frac{\varphi(\lambda_n - i(n-2)\eta/2)}{\varphi(\lambda_n - i\eta/2)}$$

$$= \frac{\varphi(\lambda_n + i\eta/2)}{\varphi(\lambda_n - i\eta/2)}.$$  

(2.70)

Hence the LHS of the new Bethe equations depends only on $\lambda_n$. So we reduced the Bethe equations to:

$$\left(\frac{\varphi(\lambda_n + i\eta/2)}{\varphi(\lambda_n - i\eta/2)}\right)^N = \prod_{(m,\beta) \neq (n,\alpha)} \prod_{j=1}^{m} \prod_{k=1}^{n} \frac{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta + i\eta)}{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta - i\eta)}.$$  

(2.71)

The remaining product of the RHS is more complicated. First we do the product over $k$

$$\prod_{k=1}^{m} \frac{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta + i\eta(m+1-2k-2)/2)}{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta - i\eta(m+1-2k+2)/2)} = \frac{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta + i\eta(m+1)/2)}{\varphi(\lambda_{n,j}^a - \lambda_{m,k}^\beta - i\eta(m+1)/2)}$$

(2.72)
and introduce the notation \( \phi_i = \varphi(\lambda_i^\alpha - \lambda_i^\beta + in/2) \). The product over \( j \) gives:

\[
\frac{\varphi_{m-n}}{\varphi_{-(m-n)}} \left[ \frac{\varphi_{n-m+2}}{\varphi_{-(n-m+2)}} \right]^2 \left( \frac{\varphi_{m-n+4}}{\varphi_{-(m-n+4)}} \right)^2 \cdots \left( \frac{\varphi_{n-m-2}}{\varphi_{-(n-m-2)}} \right)^2 \frac{\varphi_{n+m}}{\varphi_{-(n+m)}}. \tag{2.73}
\]

If \( n > m \): \( n - m = |n - m| \) and the terms with the numerator in the symmetric interval: \(-|n-m|+2 \ldots |n-m|-2\) cancel against each other, using

\[
\left( \frac{\varphi_{-|n-m|+2}}{\varphi_{|n-m|-2}} \right)^2 \cdots \left( \frac{\varphi_{|n-m|-2}}{\varphi_{-|n-m|+2}} \right)^2 = 1 \tag{2.74}
\]

and

\[
\frac{\varphi_{m-n}}{\varphi_{-(m-n)}} \left( \frac{\varphi_{|n-m|}}{\varphi_{-|n-m|}} \right)^2 = \frac{\varphi_{n-m}}{\varphi_{-(n-m)}}, \tag{2.75}
\]

so we are left with:

\[
\frac{\varphi_{n+m}}{\varphi_{-(n+m)}} \frac{\varphi_{|n-m|}}{\varphi_{-(|n-m|)}} \left[ \frac{\varphi_{|n-m|+2}}{\varphi_{-(n-m+2)}} \right]^2 \left( \frac{\varphi_{m-n+4}}{\varphi_{-(m-n+4)}} \right)^2 \cdots \left( \frac{\varphi_{n-m-2}}{\varphi_{-(n-m-2)}} \right)^2 \frac{\varphi_{2n}}{\varphi_{-2n}}. \tag{2.76}
\]

If \( m > n \): \( |n-m| = m-n \) nothing cancels, so we get the same expression for the \( n > m \) case. When \( n = m \) we are left with:

\[
\frac{\varphi_{2n}}{\varphi_{-2n}} \left( \frac{\varphi_{2}}{\varphi_{-2}} \right)^2 \cdots \left( \frac{\varphi_{2n-2}}{\varphi_{-(2n-2)}} \right)^2. \tag{2.77}
\]

Finally, the Bethe equations for the real parts of the strings become:

\[
\left( \frac{\varphi_{n}(\lambda_i^\alpha)}{\varphi_{-n}(\lambda_i^\alpha)} \right)^N = \prod_{(m,\beta) \neq (n,\alpha)} \Phi_{nm}(\lambda_i^\alpha - \lambda_i^\beta), \tag{2.78}
\]

\[
\Phi_{nm} = \begin{cases} 
\frac{\varphi_{n+m}}{\varphi_{-(n+m)}} \frac{\varphi_{|n-m|}}{\varphi_{-(|n-m|)}} \left[ \frac{\varphi_{|n-m|+2}}{\varphi_{-(n-m+2)}} \right]^2 \left( \frac{\varphi_{m-n+4}}{\varphi_{-(m-n+4)}} \right)^2 \cdots \left( \frac{\varphi_{n-m-2}}{\varphi_{-(n-m-2)}} \right)^2 & n \neq m \\
\frac{\varphi_{2n}}{\varphi_{-2n}} \left( \frac{\varphi_{2}}{\varphi_{-2}} \right)^2 \cdots \left( \frac{\varphi_{2n-2}}{\varphi_{-(2n-2)}} \right)^2 & n = m.
\end{cases} \tag{2.79}
\]

It is easy to check that for all \( n = 1 \) these equations reduce to the Bethe equations (2.39) for real rapidities.

**2.5.6. Bethe-Takahashi equations**

Just like we did for real solutions, we can consider the logarithmic version and obtain the *Bethe-Takahashi equations*

\[
\theta_n(\lambda_i^\alpha) = \frac{2\pi}{N} r_n^\alpha + \frac{1}{N} \sum_{(m,\beta) \neq (n,\alpha)} \Theta_{nm}(\lambda_i^\alpha - \lambda_i^\beta), \tag{2.80}
\]

\[
\theta_n(\lambda) = 2 \arctan \left( \frac{\tan \lambda}{\tanh n\eta/2} \right) + 2\pi \left( \frac{\lambda - 1/2}{\frac{1}{2}} \right),
\]

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2.5 Complex solutions: bound states

\[ Θ_{mn}(\lambda) = \begin{cases} 
\theta_{|n-m|}(\lambda) + 2\theta_{|n-m|+2}(\lambda) + \ldots + 2\theta_{n+m-2}(\lambda) + \theta_{n+m}(\lambda) & n \neq m, \\
2\theta_2(\lambda) + 2\theta_4(\lambda) + \ldots + 2\theta_{2n-2}(\lambda) + \theta_{n+m}(\lambda) & n = m,
\end{cases} \quad (2.81) \]

where \( I^m_n \) is an integer (half-odd integer) if \( N - M_n \) is odd (even) and with \( \sum_{n=1}^{M} nM_n = M \). So the Bethe equation for string solutions reduces to an equation for the real parts of the strings.

2.5.7. Energy and momentum of string solutions

First we introduce a useful sum:

\[ \sum_{a=1}^{n} \ln \left( \frac{\varphi(\lambda^{a,j}_n + i\eta/2)}{\varphi(\lambda^{a,j}_n - i\eta/2)} \right) = \ln \left( \prod_{a=1}^{n} \frac{\varphi(\lambda_n^{a} + i\eta(2n + 2 - 2a))}{\varphi(\lambda_n^{a} - i\eta(2n - 2a))} \right) = \ln \left( \frac{\varphi(\lambda_n^{a} + \frac{i\eta}{2}n)}{\varphi(\lambda_n^{a} - \frac{i\eta}{2}n)} \right) \quad (2.82) \]

from which it follows that:

\[ \sum_{j=1}^{n} a_1(\lambda^{n,j}_n) = \sum_{j=1}^{n} \frac{d}{d\lambda} \ln \left( \frac{\varphi(\lambda + i\eta/2)}{\varphi(\lambda - i\eta/2)} \right) \bigg|_{\lambda=\lambda^{n,j}_n} = \frac{d}{d\lambda} \ln \left( \frac{\lambda + \frac{i\eta}{2}n}{\lambda - \frac{i\eta}{2}n} \right) \bigg|_{\lambda=\lambda_n^{a}} = a_n(\lambda_n^{a}). \quad (2.83) \]

Hence the energy in case of string rapidities is:

\[ E_M = -\pi J \sum_{a,j,n} a_1(\lambda^{n,j}_n) \varphi(i\eta) = -\pi J \sum_{a,n} a_n(\lambda_n^{a}) \varphi(i\eta) \quad (2.84) \]

and the total momentum:

\[ P = \sum_{a,j,n} \frac{1}{i} \ln \frac{\varphi(\lambda^{n,j}_n + i\eta/2)}{\varphi(\lambda^{n,j}_n - i\eta/2)} = \sum_{a,n} \pi - \theta_n(\lambda_n^{a}) = \pi \sum_{n} M_n + \frac{2\pi}{N} \sum_{n} I^m_n. \quad (2.85) \]

2.5.8. Failure of the string hypothesis

The string hypothesis is known not to be rigorously valid, even in the sector \( M = 2 \). Vladimirov [21] showed that for the XXX model in case of \( M = 2 \) complex solutions like \( \lambda_{\pm} = N \pm i\sqrt{N} \) exist for large \( N \). Another analysis done by Essler et al. [22] also for the XXX model and \( M = 2 \), showed that there are extra real solutions in the form of strongly deviated two-strings. This analysis was repeated for the XXZ model [23, 24]. For general \( M \) this was studied for the XXX model by Hagemans et al. [25].

2.5.9. Complex solutions for \( M = N/2 \)

When \( M = N/2 \) complex solutions can be studied for low energy excitations in the thermodynamic limit without making use of the string hypothesis, see Babelon et al. [26] and Woynarovich [27]. They found solutions in the form of 2-string, wide pairs and quartets. The last two can be considered as strongly deviated strings whose deviations cannot be neglected.
2.5.10. Bound states

We should still justify that string solutions of the Bethe equation are indeed bound states. For $M = 2$ and $N \gg M$, complex rapidities take the form: $\lambda_1 = \lambda - i/2 - i\delta$ and $\lambda_2 = \lambda + i/2 + i\delta$. Using (2.44), we have: $k_1 = \kappa - i\sigma$ and $k_2 = \kappa + i\sigma$ with $\sigma > 0$. We now turn to the wavefunction (2.33)

$$\psi_M = A_{12}e^{ik_{1j_1} + ik_{2j_2}} + A_{21}e^{ik_{2j_1} + ik_{1j_2}} = A_{12}e^{ikj}e^{-\sigma x} + A_{21}e^{ikj}e^{\sigma x},$$

where $j = j_1 + j_2$ is the average position of the spins and $x = j_2 - j_1 > 0$ the distance between them. The first part of the wavefunction decays exponentially as function of $x$. Hence adjacent spins are the most probable. The second term looks concerning, since it blows up exponentially. However, since $\lambda_1$ and $\lambda_2$ form a deviated string we have: $A_{12}/A_{21} \sim 1/\delta$, hence for small deviations we can neglect the second term. In the case $N \to \infty$ this term vanishes completely.

2.6. Summary

This chapter started with a short introduction of the XXZ model. The main part was devoted to finding the exact wavefunctions (2.33) using the Bethe Ansatz which boils down to three important steps:

1. Wavefunctions are written in terms of down spins only.
2. Since the dynamics are restricted to one dimension, scattered particles only pick up a scattering phase, while the momenta are either unchanged or interchanged.
3. An M-body scattering factorizes to two body scatterings.

Next we imposed periodic boundary conditions which resulted in a restriction for the momenta: the Bethe equations (2.39). Finally, we studied complex solutions of the Bethe equations in the limit of infinite $N$ and finite $M$ to obtain the Bethe-Takahashi equations: (2.80).
3. Classification of states

Naively, one might expect the number of states for $M$ real rapidities to be: \( \binom{N}{M} \), since there are $M$ quantum numbers $I_j$ to be chosen from a set of size $N$. This turns out not to be the case; not every choice of quantum numbers represents an eigenstate. Therefore, we need a classification that tells us which sets of quantum numbers represent eigenstates. Once we have such a classification, in case the string hypothesis holds, we can try to prove completeness i.e. the solutions from the Bethe equations span the complete Hilbert space. Furthermore, when we want to actually calculate something, for example the energy spectrum using a computer program, we need a precise prescription telling us which quantum numbers we should take to be sure all eigenstates are calculated exactly once.

**Depiction of quantum numbers**
When thinking about a classification of quantum numbers, it may be useful to picture the chosen quantum numbers as particles, and the vacant quantum numbers as holes. See for example the figure. It will turn out that for a given $N$ and $M$ not all quantum numbers can be chosen. Therefore, only valid quantum numbers are included in these pictures.

![Figure 3.1.: Example of a distribution of quantum numbers (filled circles) and two holes (empty circles).](image)

3.1. Classification for the XXX model

The classification for the XXX model is the best understood of the three regimes. Completeness of the Bethe equations was already showed in Bethe’s first paper [2].

3.1.1. Number of real solutions

The Bethe equations in the XXX case (2.51) are:

\[
\frac{2\pi}{N} I_j = 2 \arctan(2\lambda_j) - \frac{1}{N} \sum_{l=1}^{M} 2 \arctan(\lambda_j - \lambda_l).
\]

For real rapidities we can find an upper bound $I_{\text{max}}$ on the quantum numbers by sending one rapidity to infinity. The RHS of the Bethe equations become:

\[
\lim_{\lambda_j \to \infty} RHS = \pi - \pi \frac{M - 1}{N} = \frac{2\pi}{N} I_{\text{max}}.
\]
Classification of states

This gives \( \tilde{I}_{\text{max}} = (N - M + 1)/2 \). When \( N - M \) is even(odd), \( \tilde{I}_{\text{max}} \) is a half odd(even) integer, so we can define \( I_{\text{max}} = (N - M - 1)/2 \) such that states with \( |I_j| \leq I_{\text{max}} \) yield finite real rapidities. In our analysis we tacitly assumed \( \lambda_j > \lambda_k \) iff \( I_j > I_k \forall j, k \). However, this is not necessarily the case and the value we found for \( I_{\text{max}} \) is actually a lower bound for \( I_{\text{max}} \). If we substract the \( k \)-th Bethe equation from the \( j \)-th:

\[
\frac{2\pi}{N} (I_j - I_k) = 2(\arctan(2\lambda_j) - \arctan(2\lambda_k)) - \frac{1}{N} \sum_{l=1}^{M} 2(\arctan(\lambda_j - \lambda_l) - \arctan(\lambda_k - \lambda_l)) \tag{3.2}
\]

we see that the slope of the RHS may become negative for \( \lambda_j > \lambda_k \), Bethe pointed this out already [2]. An exact analysis for \( M = 2 \) was done by Essler et al. [22]. They found that there exist extra real solutions with coinciding quantum numbers, for system sizes larger than \( N_{\text{crit}} = 21.86 \).

Having found \( I_j \leq I_{\text{max}} \) and assuming that the quantum numbers should be noncoinciding we can count the total number of vacancies for the quantum numbers. In case of odd \( M \) we have: \( 2I_{\text{max}} + 1 \). The extra one is added to take \( I_j = 0 \) into account. For even \( M \) we have: \( 2(I_{\text{max}} + \frac{1}{2}) \), where \( \frac{1}{2} \) is added since the \( I_j \) are half odd integers. In both cases we have: \( 2I_{\text{max}} + 1 \), resulting in a total number of states:

\[
\binom{N - M}{M} \tag{3.3}
\]

This is indeed less than the total number of required solutions. The missing solutions should have coinciding quantum number of should be complex. For \( M = N/2 \) there is only one real solution, according to this classification. In chapter 4 we show that this is the ground state.

3.1.2. Number of string solutions

In case of finite magnetization, we can use the string hypothesis and the Bethe-Takahashi equations (2.80)

\[
\frac{2\pi}{N} I^n_\alpha = \theta_n(\lambda^n_\alpha) - \frac{1}{N} \sum_{(m,\beta)\neq(n,\alpha)} \Theta_{nm}(\lambda^n_\alpha - \lambda^m_\beta). \tag{3.4}
\]

In a similar way as we did for finite real rapidities, we now have:

\[
|I^n_j| < \frac{1}{2} \left( N - \frac{1}{2\pi} \sum_{(m,\beta)\neq(n,\alpha)} \Theta_{nm}(\infty) \right) < \frac{1}{2} \left( N - \sum_{m=1}^{M} t_{nm} M_m + (2n - 1) \right), \quad t_{nm} = 2\min(n, m) - \delta_{nm}. \tag{3.4}
\]

The summation over \( m \) in the first step is represented by the factor \( M_m \) in the second line. Using the definition of \( \Theta_{nm}(\lambda) \) it is easy to convince oneself that \( \Theta_{nm}(\infty) = t_{nm} \). The term \( (2n - 1) \) makes up for the fact the summation now runs over all \( m \). This maximum turns out to be too high. For the case of real rapidities only one term \( \theta_2 \) was sent to infinity. For an \( n \)-string, it is less clear how to take the limit to infinity because now \( 2n - 1 \) terms are
3.2 Classification for XXZ gapped

simultaneously sent to infinity. Although no proof is known, Faddeev and Takhtadjan [28] argued that the correct bound should be:

\[ |I^*_j| \leq I_{\text{max}}^n = \frac{1}{2} \left( N - 1 - \sum_{m=1}^{M} t_{nm} M_m \right), \] (3.5)

which can be verified by an explicit calculation using a computer. Takahashi [20] proved that the total number of string states is \( \binom{N}{M} - \binom{N}{M-1} \).

3.1.3. Completeness of states

Since the XXX model has an SU(2)-symmetry only the highest-weight states are obtained by the Bethe-equations. The other states at \( S_{\text{tot}} = S - 1, S - 2 \ldots - S \) can be obtained by applying the lowering operator: \( S^-_{\text{tot}} \). This can be done by sending one or more rapidities to infinity. Recalling that:

\[ k(\lambda_j) = \pi - 2 \arctan(\lambda_j), \] (3.6)

we see that \( k(\infty) = 0 \), hence the wavefunction: (2.33) reduces to a wavefunction for \( M - 1 \) down spins. We should check that \( M - 1 \) finite rapidities and one infinite rapidity satisfies the Bethe equation for \( M - 1 \) rapidities:

\[ 2 \arctan(2\lambda_j) = \frac{2\pi}{N} I_j + \frac{1}{N} \sum_{i=1}^{M-1} 2 \arctan(\lambda_j - \lambda_i) - \frac{\pi}{N}. \] (3.7)

The term \(-\frac{\pi}{N}\) should be absorbed into the quantum numbers \( \tilde{I}_j = I_j - 1/2 \), because going from even(odd) \( M \) to odd(even) \( M - 1 \), the quantum numbers should also change from odd(even) to even(odd). The total number of states for a given magnetization is:

\[ \sum_{m=0}^{M} \binom{N}{m} - \binom{N}{m-1} = \binom{N}{M} \] (3.8)

and the total number of states obtained after a summation over all \( M \):

\[ \sum_{M=0}^{N} \binom{N}{M} = 2^N, \] (3.9)

which coincides with the dimension of the Hilbert space. Thus, we have found a complete set. Although the string hypothesis is not generally true, it is believed that the non-string solutions should be interpreted as strongly deviated strings and the classification still holds.

3.2. Classification for XXZ gapped

In case of the XXX regime we could completely determine the RHS of the Bethe equations by sending one rapidity to infinity. In the XXZ gapped case, the real parts of the rapidities lie in the interval \((-\pi/2, \pi/2]\). Sending one rapidity to \( \pi/2 \) does not determine the RHS of the Bethe equations. Previously, no classification of states was known in the literature. The author (see also [29]), introduces a method for counting the number of states for a given configuration by explicitly making use of the symmetry \( \lambda + \pi \equiv \lambda \). Proving completeness remains an open question.
3.2.1. Real rapidities

Recall the Bethe equations for the gapped XXZ chain:

\[
\left( \frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)} \right)^N = \prod_{k \neq j}^{M} \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k - i\eta)}. \tag{3.10}
\]

Taking the logarithm gives:

\[
2\pi \frac{I_j}{N} = 2 \arctan \left( \frac{\tan \lambda_j}{\tanh \eta/2} \right) + 2\pi \left[ \frac{\lambda_j}{\pi} + \frac{1}{2} \right] - \frac{1}{N} \sum_{l=1}^{M} 2 \arctan \left( \frac{\tan(\lambda_j - \lambda_l)}{\tanh \eta} \right) + 2\pi \left[ \frac{\lambda_j - \lambda_l}{\pi} + \frac{1}{2} \right]. \tag{3.11}
\]

The RHS of (3.11) is in most cases monotonic in \( \lambda_j \), although there might be exceptions. For example, the case of \( M = 2 \) where both rapidities lie in the vicinity of \( \pm \pi/2 \). However, we will only focus on the solutions with: \( \lambda_j < \lambda_k \) iff \( I_j < I_k \), \( \forall j,k \). We also assume that the quantum numbers should be noncoinciding. In order to have \( \lambda_M - \lambda_1 < 1 \) we must have a bound on \( I_M - I_1 \). Let \( \lambda_M = \lambda_1 + \pi \). The difference between (3.11) for \( \lambda_M \) and \( \lambda_1 \) is:

\[
2\pi \frac{(I_M - I_1)}{N} = 2\pi - 2\pi \sum_{l=1}^{M} \left[ \frac{\lambda_M - \lambda_l}{\pi} + \frac{1}{2} \right] - \frac{1}{N} \sum_{l=1}^{M} 2 \arctan \left( \frac{\tan(\lambda_j - \lambda_l)}{\tanh \eta} \right) + 2\pi \left[ \frac{\lambda_M - \lambda_l}{\pi} + \frac{1}{2} \right] = 2\pi \left( 1 - \frac{M}{N} \right). \tag{3.12}
\]

Therefore: \( \lambda_M - \lambda_1 < 1 \) iff \( I_M - I_1 < N - M \). Sets of quantum numbers satisfying this condition are:

\[
A_i = \left\{ I_j \right\} \begin{array}{c}
- N - M - 1 \\
\leq \frac{1}{2}
\end{array} + i \leq \frac{N - M - 1}{2} + i \right\}, \tag{3.13}
\]

which is the set defined on the interval of width \( N - M \) right-shifted by \( i \). We are looking for all transformations: \( S : \{ (\lambda_j, I_j) \} \rightarrow \{ (\tilde{\lambda}_j, \tilde{I}_j) \} \) that leave (3.11) invariant. Shifting one of the rapidities, \( \lambda_1 \rightarrow \lambda_1 + \pi \), while the other rapidities remain unchanged, leaves (3.10) invariant. In (3.11) the periodicity in \( \lambda \) is removed, so the quantum numbers should make up for this deficiency and must change like:

\[
(\tilde{\lambda}_j, \tilde{I}_j) = (\lambda_{j+1}, I_{j+1}+1) \quad j = 1 \ldots M-1,
(\tilde{\lambda}_M, \tilde{I}_M) = (\lambda_1 + \pi, I_1 + N - M + 1). \tag{3.14}
\]

Two explicit examples for \( N = 20 \), \( M = 9 \), of sets of \( I_j \) that are related through \( S \) are:

\{ -6, -5, -4, -3, -1, 0, 1, 2, 4 \} \approx \{ -4, -3, -2, 0, 1, 2, 3, 5, 6 \},
\{ -6, -4, -3, -1, 0, 1, 2, 4, 5 \} \approx \{ -3, -2, 0, 1, 2, 3, 5, 6 \}.

In the first example we have on the LHS a set in \( A_{-1} \) which is equivalent to a set in \( A_1 \). The LHS in the second example does not have the proper width, and is equivalent to a set with degenerate quantum numbers on the RHS.

We see that \( \tilde{\lambda}_j < \lambda_k \) iff \( \tilde{I}_j < \tilde{I}_k, \forall j,k \). \( \tilde{I}_M - \tilde{I}_1 < N - M \). \( S \) together with its inverse are the only two transformations satisfying these properties. If we had sent \( \lambda_j \rightarrow \lambda_j + \pi \) with \( j > 1 \), then \( \tilde{I}_1 = I_1 + 1 \) and \( \tilde{I}_M = I_J + N - M + 1 \). This is not a proper set since: \( \tilde{I}_M - \tilde{I}_1 = I_J - I_1 + N - M > N - M \).

As \( \tilde{I}_1 - I_1 \geq 2 \) and \( \tilde{I}_M > \frac{N-M-1}{2} + i \), we have: \( S((A_i \cup A_{i+1})/(A_{i+2} \cup A_{i+3})) = (A_{i+2} \cup A_{i+3})/(A_i \cup A_{i+1}) \). Hence, we have the equivalences \( A_i \cup A_{i+1} \sim A_{i+2n} \cup A_{i+1+2n} \). The total
number of states with real rapidities is the sum of the number of states in \( A_i \) and \( A_{i+1} \) minus the number of states in the overlap \( A_i \cap A_{i+1} \):

\[
2 \left( \frac{N-M}{M} \right) - \left( \frac{N-M-1}{M} \right) = \frac{N}{N-M} \left( \frac{N-M}{M} \right).
\]  (3.15)

This number significantly differs from the XXX case. In the next chapter we will discuss this in more detail. For example, if we again consider the case \( M = N/2 \) we now find two real solutions. These will turn out to be the ground state and the quasi-degenerate ground state.

**Remarks**

- In order to have: \( \lambda_j \in (-\pi/2, \pi/2] \) the quantum numbers must be taken from the set \( A_i \) such that \( \text{abs}(\sum_{j=1}^{M} I_j) \) is minimal. If there are two minimal choices, the set for which the sum is positive must be chosen.

- \( S(\{(\lambda_j, I_j)\}) \) is only valid if \( I_1 \leq -(N/2-M-1) \) in order to have all the \( \tilde{I}_j \) in the interval: \( \{-N/2 + 1, \ldots, N/2\} \).

### 3.2.2. String rapidities

String solutions should satisfy the Bethe-Takahashi equations. Similar to the case for real rapidities, we can find a bound on: \( I^n_{M_n} - I^n_1 \) by setting \( \lambda^n_{M_n} = \lambda^n_1 + \pi \).

\[
\frac{2\pi}{N}(I^n_{M_n} - I^n_1) = 2\pi - \frac{2\pi}{N} \sum_{(m,\beta)} \Theta_{nm}(\lambda^n_{M_n} - \lambda^n_{\beta}) - \Theta_{nm}(\lambda^n_1 - \lambda^n_\beta) = 2\pi - \frac{2\pi}{N} \sum_{m} t_{nm} M_m \quad (3.16)
\]

with: \( t_{nm} \equiv 2\text{min}(n, m) - \delta_{nm} \). Therefore: \( \lambda^n_{M_n} - \lambda^n_1 \leq \pi \) iff \( I^n_{M_n} - I^n_1 \leq N - \sum_{m} t_{nm} M_m \). Sets of quantum numbers satisfying this condition are:

\[
A^n_i = \left\{ \{I^n_j\} \mid \|I^n_j - i\| \leq (N - \sum_m t_{nm} M_m - 1)/2 \right\}. \quad (3.17)
\]

For every set \( A^n_i \) we have a transformation \( S^n_i : \{\{\lambda^n_j, I^n_j\}\} \to \{\{\tilde{\lambda}^n_j, \tilde{I}^n_j\}\} \) with:

\[
(\tilde{\lambda}^n_{M_n}, \tilde{I}^n_{M_n}) = (\lambda^n_1 + \pi, I^n_1 + (N - \sum_{m} t_{nm} M_m + (2n-1)))
\]

\[
(\tilde{\lambda}^n_j, \tilde{I}^n_j) = (\lambda^n_{M_n+1}, I^n_{M_n+1} + (2n-1)) \quad j = 1 \ldots M_n - 1
\]

\[
(\tilde{\lambda}^m_j, \tilde{I}^m_j) = (\lambda^m_j, \bar{I}^m_j + t_{nm}) \quad m \neq n, j = 1 \ldots M_m. \quad (3.18)
\]

In the case of real rapidities we had only \( S^1 \), so it was straightforward to find the minimal set of quantum numbers. Now having \( n \) transformations \( S^n \), we not only have to investigate the action of these transformations separately but also all possible products of transformations. This makes it difficult to obtain a general result using this approach. However, individual cases can be studied.
3.2.3. A single 2-string

For the case of \( N/2 - 2 \) real rapidities and one 2-string we have: \( A_1^1 = \{ \{ I_j^1 \} \} \mid I_j^1 - i \mid \leq (N - M - 1)/2 \) and \( A_1^2 = i \). These states will turn out to be two-spinon excitations in the next chapter. Shifting one of the real rapidities by \( \pi \) gives \( S^1 \):

\[
(\lambda_{M_1}^1, I_{M_1}^1) = (\lambda_1^1 + \pi, I_1^1 + (N - M + 1))
\]

\[
(\lambda_j^2, I_j^2) = (\lambda_{j+1}^2, I_{j+1}^2 + 1)
\]

\[
(\lambda_1^2, I_1^2) = (\lambda_1^2, I_1^2 + 2)
\]

Similarly, shifting the string rapidity gives \( S^2 \):

\[
(\lambda_1^2, I_1^2) = (\lambda_2^2, I_2^2 + 4)
\]

\[
(\lambda_j^1, I_j^1) = (\lambda_1^1, I_1^1 + 2)
\]

First we assume that the quantum number of the string \( I_1^2 \), can take all possible values. Using \( S^1 \) we can then reduce the set of real rapidities to \( A_0^1 \cup A_1^1 \equiv A_1^1 \). Since \( S^2 \) is an \( A_1^1 \) it has no effect on the real rapidities, we can use \( S^2 \) to show that: \( A_0^2 \cup A_1^2 \cup A_2^2 \cup A_3^2 \equiv A_2^2 \).

What is left to investigate is whether there are products of \( S^1 \) and \( S^2 \) that leave the selected sets invariant. If these products exist the sets can be further reduced. Since \( S^1 \) and \( S^2 \) commute, we only have to consider \( S^1(S^2)^{-1} \). If \( I_2^2 \in A_0^2 \cup A_1^2 \) then after applying \( S^1(S^2)^{-1} \) we have \( I_2^2 \in A_0^1 \cup A_1^1 \). If we apply \( S^1(S^2)^{-1} \) it is clear that \( I_1^2 \in A_1^1 \). The condition \( I_1^2 \) gives a bound \( I_1^2 \) for \( I_1^2 \). So we get: \( I_2^2 + N - M + 1 = (M - 1)/4 \) this gives \( I_2^2 = -(M - 1)/2 \). Hence, all states with \( I_2^2 \in A_2^2 \cup A_3^2 \) and \( I_1^2 \leq I_2^2 \) should not be considered.

Now we have determined the minimal set of quantum numbers, we can count the number of unique states. For every \( I_2^2 \) the number of configurations for the real rapidities is:

\[
2 \left( \frac{N/2}{N/2 - 2} \right) \cdot \left( \frac{N/2 - 1}{N/2 - 2} \right) = \frac{1}{4} (N - 2)^2.
\]

The number of double states due to the symmetry of \( S^1(S^2)^{-1} \) in case of \( I_1^1 \in A_2^2 \cup A_3^2 \) is:

\[
2 \left( \frac{N/2 - 1}{N/2 - 3} \right) = \frac{1}{4} (N - 2)(N - 4),
\]

so the total number of states is: \( (N - 2)^2 - \frac{1}{2}(N - 2)(N - 4) = \frac{N}{2}(N - 2) \).

3.2.4. Other string configurations

Having studied the case of a single 2-string in detail, we can now guess how to deal with other cases. First use \( S^1 \) to find the minimal set \( A_1^1 \), while ignoring the other strings. Secondly, use \( S^2 \) to find \( A_2^1 \), again ignoring the higher strings. Having found \( A_1^1 \cup A_2^1 \) we should use \( S^1(S^2)^{-1} \) to remove possible degenerate states. In general use \( S^n \) to find \( A^n \) and then use all possible products of \( S^m \) with \( m \leq n \) to reduce \( \cup_{n=1}^{n} A^n \).
4. Two-spinon excitations

The most interesting excitations are those just above the ground state, since these excitations are those which carry the most correlation weight. One of the characteristics of the XXZ model is that the excitations near the ground state, called spinons, can be described by only a few parameters; these excitations can be interpreted as quantum solitons.

4.1. The ground state

For fixed magnetization the lowest energy state with $M$ down spins, for all $\Delta > 0$, is represented by the following quantum numbers:

$$\{I_j\} = \{- (M - 1)/2, -(M - 1)/2 + 1, \ldots, (M - 1)/2\}. \quad (4.1)$$

This was proved by Yang and Yang [30]. In zero magnetic field, the lowest energy states with $M$ or $N - M$ down spins yield the same energy. Furthermore, lowering $M$ increases the energy because of the minus sign in front of the Hamiltonian (2.3), hence we have an antiferromagnetic ground state ($M = N/2$). This is in correspondence with the following theorem due to Lieb and Mattis [31]:

**Theorem 4.1.** For interacting electrons in one dimension subjected to an arbitrary periodic potential: if $S > S'$ then $E(S) > E(S')$ where $S = \langle S_{tot}^z \rangle$. Hence, electrons in one dimension do not exhibit a finite magnetization in the ground state.

For $\Delta > 1$ there is a slightly degenerate ground state with all the quantum numbers shifted to the right:

$$\{I'_j\} = \{- (M - 3)/2, -(M - 5)/2, \ldots, (M + 1)/2\}. \quad (4.2)$$

Of course, shifting all quantum numbers to the left yields the same result. The difference between the energy of the quasi-degenerate ground state and the true ground state goes as $E_\pi - E_0 = e^{-a(\Delta)N + b(\Delta)}/N$. In fig. 4.1 the difference $E_\pi - E_0$ is plotted for several values of $\Delta$. In the Ising limit ($\Delta \to \infty$) we have an exact degenerate ground state, the (anti)-symmetric sum $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle \pm |\downarrow\uparrow\downarrow\uparrow\ldots\rangle$ of the two Néel phases.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th>$a$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.2</td>
<td>0.00275</td>
<td>1.32787</td>
</tr>
<tr>
<td>2</td>
<td>0.08222</td>
<td>1.39819</td>
</tr>
<tr>
<td>4</td>
<td>0.32652</td>
<td>1.88917</td>
</tr>
<tr>
<td>8</td>
<td>0.64315</td>
<td>2.54274</td>
</tr>
</tbody>
</table>

Table 4.1.: Fit parameters $a$ and $b$ for the fits of the difference $E_0 - E_\pi$. 

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Two-spinon excitations

Figure 4.1.: The difference $E_\pi - E_0$ is plotted for $\Delta = 1.2, 2, 4$ and 8. The dots are data obtained from a computer calculation. The fitted curves go like $e^{-aN+b}/N$, where $N$ is the number of sites.

4.2. Quasi-particle excitations: spinons

Starting with the ground state $M = N/2$ we can build two types of excitations:

- Flipping one down spin back to a up spin: $M = N/2 - 1$, the spin of this state is 1.
- Introducing one 2-string: $M_1 = N/2 - 2$, $M_2 = 1$, the spin of this state is 0.

Since the classifications in the $\Delta = 1$ case and the $\Delta > 1$ case are different, we will study the excitations separately. But we will come to the same conclusion in both cases.

4.2.1. XXX

If case of $M = N/2$ down spins, (3.3) gives exactly one state with real rapidities: the ground state. This shows that the ground state is indeed nondegenerate.

Spin flip: $M=N/2-1$

When $M = N/2 - 1$, $I_{max} = (N - M - 1)/2 = N/4$. Therefore, the number of vacancies for the quantum numbers is $2I_{max} + 1 = N/2 + 1$, this two more than the number of $I_j$. An excitation can be parametrized by two holes in the distribution of $I_j$. This can be visualized as fig. 4.2. The number of states according to (3.3) is: $\binom{N/2 + 1}{N/2} = (N/2 + 1)(N/4)$. This reparametrization in terms of holes will turn out to be very convenient. Instead of having $M - 1$ parameters, we only need the positions of the two holes to describe the complete state.
4.2 Quasi-particle excitations: spinons

A single 2-string: \( M_1 = N/2 - 2, M_2 = 1 \)

In case of a single 2-string: \( M_1 = N/2 - 2, M_2 = 1 \), we have \( I_{\text{max}}^1 = \frac{1}{2} \left( \frac{N}{2} - 1 \right) \) and \( I_{\text{max}}^2 = 0 \). For the real rapidities we have \( N/2 \) vacancies, which is two more than the number of real rapidities. The 2-string can only have \( I_2 = 0 \). Since there is no freedom in the choice for \( I_2 \), we can again parametrize the state with two holes in the distribution of the real rapidities.

Spinons

The holes in this context are called spinons, which are the quasi-particles of our system. Starting with the ground state, we can build excited states by ‘adding’ spinons, this can be done by either removing down spins or by increasing the number of strings. Spinons always come in pairs. For real rapidities the number of spinons is: \( N_{\text{sp}} = 2I_{\text{max}} + 1 - M = N - 2M \), since \( N \) is even \( N_{\text{sp}} \) is also even. For string solutions we have: \( I_{\text{max}}^n = \frac{1}{2} \left( N - 1 - 2 \sum_{j<n} jM_j \right) \) so \( N_{\text{sp}}^n = N - 2 \sum_{j<n} jM_j - 2(n-1)M_n - 2 \sum_{j>n} nM_j \), hence \( N_{\text{sp}}^n \) is always even. This is in accordance with [32].

The contribution of states with more than two spinons is negligible in most case.

4.2.2. XXZ \( \Delta > 1 \)

The \( \Delta > 1 \) case is a bit more complicated. Using (3.15) we see that for \( M = N/2 \) real rapidities there are two states, namely: the ground state \( \{ I_j \} = \{ -(M-1)/2, -(M-1)/2 + 1, \ldots, (M-1)/2 \} \), also called the set \( A_0 \), and the quasi-degenerate ground state: \( \{ -(M - 1)/2 + 1, -(M-1)/2 + 2, \ldots, (M+1)/2 \} \), which is the set \( A_1 \).

Spin flip: \( M=N/2-1 \)

In case of \( M = N/2 - 1 \) and using the notation (3.13), we have two sets of quantum numbers \( A_0 \) and \( A_1 \). Both sets leave room for two holes, so we can interpret the states in \( A_0 \) as two-spinon excitations on the ground state. The states in \( A_1 \) are the two-spinon excitations on the almost degenerate ground state with momentum \( P = \pi \). The number of states with real rapidities is: \( \left( \frac{N}{2} + 1 \right) \frac{N}{2} - \frac{N}{2} = \frac{N^2}{2} \), and the two-spinon spectrum for \( N = 100 \) is plotted in: 4.3. The plots were generated using the computer implementation discussed in appendix C.

We can also argue the other way around and ask which sets produce the complete two-spinon excitations on the ground state and which ones on the quasi-degenerate one. In case of the true ground state, the complete spectrum is generated by \( A_0 \). The case for the quasi-degenerate ground state is more subtle. Instead of \( A_1 \), one might also choose \( A_{-1} \) to form a complete spectrum together with \( A_0 \). However, the sets \( A_{-1} \) and \( A_1 \) are not equivalent, or to be more precise: \( (A_{-1} \cup A_1)/(A_{-1} \cap A_1) = (A_{-1} \cap A_0) \cup (A_0 \cap A_1) \). Hence, the complete two-spinon spectrum on the quasi-degenerate ground state is generated by \( A_{-1} \cup A_1 \).
Two-spinon excitations

Figure 4.3.: Two-spinon energy spectrum for \( N = 100, M = 49 \) and \( \Delta = 4 \). Top left: excitations on the true ground state (\( A_0 \)). Top right: excitations on the quasi degenerate ground state (\( A_1 \)). Bottom left: the overlap \( A_0 \cap A_1 \). It looks like there are states missing near \( q = \pi \). Because the set \( A_1 \) is not completely symmetric around \( q = \pi \) these missing states lie only \( A_0 \). Bottom right: complete two-spinon spectrum.
4.3 Soliton excitations: intuitive picture

The limit $\Delta \to 1$

The number of two-spinon states in the $\Delta = 1$ case and the $\Delta > 1$ case are distinct, namely $N_4 (N_2 + 1)$ and $N^2$, respectively. However, in the limit $\Delta \to 1$ these numbers should coincide. The $N_4 (N_2 - 1)$ states in the set $A_1/(A_0 \cap A_1)$ contain one rapidity equal to $\pi/2$, which corresponds to an infinite rapidity in the isotropic parametrizations. These are the states obtained by applying the lowering operator in the isotropic case, due to the $SU(2)$ symmetry. Since this $SU(2)$ symmetry is not present in the $\Delta > 1$ case, the limit $\Delta \to 1$ is well understood.

A single 2-string: $M_1 = N/2 - 2, M_2 = 1$

In case of $M_1 = N/2 - 2, M_2 = 1$ we have the following sets of quantum numbers: $A_4^1 = \{ \{I_j\}||I_j - i| \leq (N - M - 1)/2 \}$ and $A_4^2 = i$. So for the real rapidities we have room for two spinons, which was also the case for $M = N/2 - 1$ real rapidities. The possible sets are $A^1 = A_0^1 \cup A_1^1$ and $A^2 = A_2^1 \cup A_0^2 \cup A_1^2 \cup A_2^2$. This might seem confusing, but, since these sets cannot be used simultaneously, the number of spinons is still two. In turns out that it can be divided into two sets $A^1$ together with $A_2^1$ and $A_1^1$ and the other set: $A^1$ with $A_0^2$ and $A_2^2$. Here, the former are interpreted as the excitations on the ground state, while the quantum numbers in the second set belong to the excitations on the quasi-degenerate ground state.

4.3. Soliton excitations: intuitive picture

In order to understand what the two-spinon excitations look like, it is useful to picture the ground state of the Ising antiferromagnet, i.e. sending $\Delta \to \infty$. In this case the degenerate ground states are the two Néel phases: all neighboring spins are anti-parallel.

In case of an excitation with $S_{\text{tot}}^z = 1$, this can be considered as flipping one down spin into an up spin, see fig. 4.4. Between sites with parallel spins we have a domain wall (a transition from one Néel phase into the other), in this context usually called a kink. We see that at these kinks there is a local magnetization. The other type of excitation is for $S_{\text{tot}}^z = 0$ by adding one 2-string, see fig. 4.5. Again we have two kinks.

In case of finite $\Delta$ this picture of two-spinon excitations is more or less retained. In this case the ground state is much more complicated, but locally it still looks like one of the Néel phases. Instead of a kink at a well defined location, the kink decays exponentially. These kinks behave like quantum solitons, which means:

1. they are localized objects
2. they are of permanent form
3. when solitons interact with each other, they emerge from the collision unchanged, apart from a possible phase shift.
Two-spinon excitations

Figure 4.4.: We start with an antiferromagnetic Néel phase (top picture). Then we flip the fifth spin from the left, so $\Delta S_{tot}^z = 1$ (middle picture). There is some local magnetization in the form of solitons. In the bottom picture the solitons move away from each other.

Figure 4.5.: Again we start with an antiferromagnetic Néel phase (top picture). In the middle picture the fifth and sixth spin are interchanged, so $\Delta S_{tot}^z = 0$. In the bottom picture the solitons move away from each other.
5. Thermodynamic limit

Instead of working on a finite lattice we can also study the XXZ model in the thermodynamic limit: \( N \to \infty \) while keeping \( M/N \) fixed and for zero magnetic field. The advantage of working in the thermodynamic limit is that the ground state energy and the two-spinon spectra can be obtained by solving a single integral equation instead of \( M \) coupled equations. We will study both the \( \Delta = 1 \) as the \( \Delta > 1 \) case and compare them.

5.1. Thermodynamic limit: general case

In the thermodynamic limit: \( N \to \infty \) while keeping \( M/N \) fixed, the distribution of rapidities becomes a continuous function:

\[
\rho(\lambda) = \lim_{N \to \infty} \frac{1}{N} \sum_{l=1}^{M} \delta(\lambda - \lambda_l) \quad (5.1)
\]

and the summation of rapidities is replaced by an integral: \( \frac{1}{N} \sum_{l} \to \int_{-B}^{B} d\lambda' \rho(\lambda') \). The Bethe equations (A.2) in the thermodynamic limit become in terms of \( \theta_n(\lambda) \) defined as in (2.4.4):

\[
\theta_1(\lambda) - \int_{-B}^{B} d\lambda' \theta_2(\lambda - \lambda') \rho(\lambda') = 2\pi X(\lambda). \quad (5.2)
\]

When \( \lambda_j \) is a solution of the Bethe equations, \( X(\lambda_j) = I_j/N \) is the corresponding quantum number, see also fig. 5.1. The integration region \( B \) depends on the magnetic field and the parametrization chosen for the rapidities. Taking the derivative with respect to \( \lambda \) of (5.2), and using the notation \( a_n(\lambda) \equiv \frac{1}{2\pi} \frac{d\theta_n(\lambda)}{d\lambda} \) yields:

\[
a_1(\lambda) - \int_{-B}^{B} d\lambda' a_2(\lambda - \lambda') \rho(\lambda') = \rho(\lambda) + \rho_h(\lambda). \quad (5.3)
\]

The density \( \rho_h(\lambda) \) is the density of the holes and is defined as: \( \rho_h(X(\lambda)) = 1 - \rho(X(\lambda)) \). We can write the density as function of \( \lambda \): \( \rho(\lambda) = \rho(X(\lambda))dX(\lambda)/d\lambda \) and \( \rho_h(\lambda) = \rho_h(X(\lambda))dX(\lambda)/d\lambda \). So we get:

\[
\frac{dX(\lambda)}{d\lambda} = \rho(\lambda) + \rho_h(\lambda). \quad (5.4)
\]

The total energy in the thermodynamic limit becomes:

\[
E = -\pi J \sum_{l=1}^{M} a_n(\lambda_l) \varphi(i\eta) = -NJ\pi \varphi(i\eta) \int_{-B}^{B} d\lambda a_1(\lambda) \rho(\lambda) \quad (5.5)
\]

and the total momentum:

\[
P = \pi M - \frac{2\pi}{N} \sum_{j=1}^{M} I_j = 2\pi \int_{-\infty}^{\infty} d\lambda N \left( X(\lambda) + \frac{1}{N} \sum_{j}^{\#holes} \Theta(X(\lambda) - I_j/N) \right). \quad (5.6)
\]
The strategy is now clear: we should solve the integral equation (5.3) for \( \rho(\lambda) \) from which we can compute the energy spectrum using (5.5). In case of zero field the integration region \( B \) goes over the whole interval. For \( |\Delta| \leq 1 \) the rapidities are defined in the interval \( \lambda \in (-\infty, \infty) \). This allows us to Fourier transform both sides of (5.3). The Fourier transform of \( \rho(\lambda) \) together with its inverse are:

\[
\rho(\omega) = \int_{-\infty}^{\infty} d\lambda e^{-i\omega\lambda} \rho(\lambda) \quad \rho(\lambda) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega\lambda} \rho(\omega). \tag{5.7}
\]

In case of zero field the Bethe equations (5.3) can be written as a convolution:

\[
a_1(\lambda) - (a_2 * \rho)(\lambda) = \rho(\lambda) + \rho_h(\lambda). \tag{5.8}
\]

**Theorem 5.1.** Let \( (f * g)(\lambda) = \int_{-\infty}^{\infty} d\lambda' f(\lambda - \lambda') g(\lambda') \) be the convolution of \( f(\lambda) \) and \( g(\lambda) \). Then the Fourier transform of the convolution factorizes as: \( (f * g)(\omega) = f(\omega)g(\omega) \).

**Proof.**

\[
f * g(\lambda) = \int_{-\infty}^{\infty} d\lambda' f(\lambda - \lambda') g(\lambda') = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega(\lambda - \lambda')} f(\omega)g(\omega') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega\lambda} f(\omega)g(\omega) \tag{5.9}
\]

Fourier transforming both sides of the equation gives:

\[
(f * g)(\omega) = f(\omega)g(\omega). \tag{5.10}
\]

Using the convolution theorem, equation (5.3) transforms into:

\[
a_1(\omega) = a_2(\omega)\rho(\omega) + \rho(\omega) + \rho_h(\omega), \tag{5.11}
\]

so instead of solving (5.3), we now have to solve the much easier equation (5.11). We will solve this equation for the ground state and in case of two-spinon excitations.
5.2 Thermodynamic limit: isotropic case

5.2. Thermodynamic limit: isotropic case

In order to solve (5.11) we need the Fourier transform of $a_n(\lambda)$:

$$a_n(\omega) = \int_{-\infty}^{\infty} d\lambda e^{i\omega\lambda} \frac{1}{2\pi X^2 + n^2/4} = \frac{1}{2\pi} \frac{2\pi in}{in} e^{-|\omega|n/2} = e^{-|\omega|n/2}. \quad (5.12)$$

The integral was performed using contour integration. The function $a_n(\lambda)$ has two poles at: $\pm in/2$. When $\omega$ is positive we can close the contour in the UHP. Next, we will calculate the ground state energy and the two-spinon spectrum.

5.2.1. The ground state at zero field

Because the system is antiferromagnetic the number of down spins for the ground state at zero field is: $M = N/2$. From chapter four we know that in the ground state all rapidities $\lambda_j$ are real and that the corresponding quantum numbers $I_j$ fill up all available quantum numbers. So in the limit $N \to \infty$ the integration region $B \to \infty$ spans whole the space. Since there are no holes in the distribution of the quantum numbers we have: $\rho_h(\lambda) = 0$. Therefore, the Fourier transform of the Bethe equations (5.11), become:

$$a_1(\omega) = \rho(\omega)(1 + a_2(\omega)).$$

If we plug $a_n(\omega)$ into this equation we get a solution for $\rho(\omega)$:

$$\rho(\omega) = \frac{e^{-|\omega|/2}}{1 + e^{-|\omega|}} = \frac{1}{2\cosh(\omega/2)}. \quad (5.13)$$

The density $\rho(\lambda)$ can now be found by taking the inverse Fourier transformation of $\rho(\omega)$:

$$\rho(\lambda) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-\omega\lambda} \rho(\omega) = \frac{2}{4\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\cosh(\omega)} e^{-i\omega\lambda}. \quad (5.14)$$

This integral can be performed using contour integration. The function $1/\cosh(\omega)$ has poles in the complex plane at $\omega = i\pi(n + 1/2)$ with $n \in \mathbb{Z}$. The corresponding residues are:

$$\frac{d}{d\omega} \cosh(\omega) \bigg|_{i\pi(n+1/2)} = \sinh(i\pi(n + 1/2)) = i(-1)^{n-1}.$$

For $\lambda < 0$ we can close the contour in the UHP resulting in:

$$\rho(\lambda < 0) = \sum_{n=0}^{\infty} (-i)(-1)^n e^{-2|\lambda|\pi(n+1/2)} = \frac{e^{-|\lambda|\pi/2}}{1 + e^{-|\lambda|2\pi}}.$$

When $\lambda > 0$ we can close the contour in the LHP and get the same result, hence:

$$\rho(\lambda) = \frac{1}{\cosh(\pi\lambda)}. \quad (5.15)$$
Thermodynamic limit

Now we have found the \( \rho(\lambda) \) we can calculate the ground state energy:

\[
E = -NJ\pi \int_{-\infty}^{\infty} \frac{a_1(\lambda) \rho(\lambda)}{2\pi} \, d\lambda = -NJ\pi \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-|\omega|/2}}{2 \cosh \omega/2} \rho(\omega) = -J \int_{-\infty}^{\infty} \frac{d\omega}{2} \frac{e^{-|\omega|}}{1 + e^{-|\omega|}} \, d\omega
\]

\[
= - NJ \pi \int_{-\infty}^{\infty} \frac{d\omega}{2} \frac{e^{-|\omega|}}{1 + e^{-|\omega|}} \ln(1 + e^{-\omega})
\]

\[
= - NJ \ln 2.
\]

(5.16)

This result was first obtained by Hulthén [33]. For the total momentum we find:

\[
P = \pi M - 2\pi N \sum_{j=1}^{M} I_j = \pi M \mod 2\pi.
\]

(5.17)

5.2.2. Two-spinon excitations

The most important excitation is if we turn one down spin into an up spin, so \( M = N/2 - 1 \). In section 4.2.1 we showed that in case of only real rapidities there is room for two spinons. These spinons are holes in the distribution \( X \) labeled by \( I_{h1} \) and \( I_{h2} \):

\[
X \rightarrow X + \frac{1}{N} \Theta \left( X - \frac{I_{h1}}{N} \right) + \frac{1}{N} \Theta \left( X - \frac{I_{h2}}{N} \right).
\]

(5.18)

If we take the derivative we see that \( \rho_h(\lambda) \) in case of a two-spinon excitation is:

\[
\rho_h(\lambda) = \frac{1}{N} \delta(\lambda - \lambda_{h1}) + \frac{1}{N} \delta(\lambda - \lambda_{h2}),
\]

(5.19)

so we can parametrize a two-spinon excitation by \( \lambda_{h1} \) and \( \lambda_{h2} \) instead of \( I_{h1} \) and \( I_{h2} \). The Fourier transformed Bethe equations (5.11) in case of two-spinon excitations are:

\[
a_1(\omega) = \rho(\omega)(1 + a_2(\omega)) + \frac{e^{i\omega \lambda_{h1}}}{N} + \frac{e^{i\omega \lambda_{h2}}}{N}. \]

(5.20)

We can solve this equation for \( \rho(\omega) \):

\[
\rho(\omega) = (1 + a_2(\omega))^{-1} a_1(\omega) - (1 + a_2(\omega))^{-1} \frac{1}{N} \left( e^{i\omega \lambda_{h1}^b} + e^{i\omega \lambda_{h2}^b} \right)
\]

\[
= \rho_{GS}(\omega) - \frac{1}{N} \rho_{sp}(\omega) \left( e^{i\omega \lambda_{h1}^b} + e^{i\omega \lambda_{h2}^b} \right)
\]

(5.21)

\[
\rho_{GS}(\omega) = \frac{1}{2 \cosh \omega/2} \quad \rho_{sp}(\omega) = \frac{1}{1 + e^{-|\omega|}}.
\]

Taking the inverse Fourier transformation of \( \rho(\omega) \), we get:

\[
\rho(\lambda) = \rho_{GS}(\lambda) - \frac{1}{N} \rho_{sp}(\lambda - \lambda_{h1}^b) - \frac{1}{N} \rho_{sp}(\lambda - \lambda_{h2}^b).
\]

(5.22)

A closed form of \( \rho_{sp}(\lambda) \) is not known. However, by truncating the Fourier sum we are still able to obtain an accurate plot for \( \rho(\lambda) \) in case of two spinons. A typical density function

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5.2 Thermodynamic limit: isotropic case

\[ \rho(k) \], which is now a function of momentum \( k \) rather than a rapidity \( \lambda \), in case of a two-spinon excitation looks like fig. 5.2. The energy of such a two-spinon excitation is:

\[
\epsilon(\lambda_1^h, \lambda_2^h) = -NJ\pi \int_{-\infty}^{\infty} d\lambda a_1(\lambda) (\rho(\lambda) - \rho_{GS}(\lambda)) = \epsilon_{sp}(\lambda_1^h) + \epsilon_{sp}(\lambda_2^h)
\]  

(5.23)

where \( \epsilon_{sp}(\lambda^h) \) is the energy of a spinon, which is defined as:

\[
\epsilon_{sp}(\lambda^h) = J\pi \int_{-\infty}^{\infty} d\lambda a_1(\lambda) \rho_{sp}(\lambda - \lambda^h) = J\pi \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} a_1(\omega) \rho_{sp}(\omega) e^{-i\omega\lambda^h} = \frac{J\pi}{2\cosh(\pi\lambda^h)}.
\]  

(5.24)

The total momentum of a two-spinon excitations is:

\[
P = \pi M - 2\pi \sum_{j=1}^{M} I_j = 2\pi \int_{-\infty}^{\infty} d\lambda N \left( X(\lambda) + \frac{1}{N} \theta(X(\lambda) - \frac{I_1^h}{N}) + \frac{1}{N} \theta(X(\lambda) - \frac{I_2^h}{N}) \right) \rho(\lambda).
\]  

(5.25)

We can compare this with the ground state momentum, to obtain the momenta of the two spinons:

\[
\Delta P = 2\pi \int_{-\infty}^{\infty} d\lambda \left( \theta(X(\lambda) - \frac{I_1^h}{N}) + \theta(X(\lambda) - \frac{I_2^h}{N}) \right) \rho(\lambda)
\]

\[
= 2\pi \int_{\lambda_1^h}^{\infty} d\lambda \rho(\lambda) + 2\pi \int_{\lambda_2^h}^{\infty} d\lambda \rho(\lambda)
\]

\[
\equiv k_{sp}(\lambda_1^h) + k_{sp}(\lambda_2^h).
\]  

(5.26)
Since $\rho(\lambda) = \rho_{GS}(\lambda) - \frac{1}{N^2} \rho_{sp}(\lambda - \lambda_1^h) - \frac{1}{N^2} \rho_{sp}(\lambda - \lambda_2^h)$, it is safe to neglect the contribution from $\rho_{sp}$ in the thermodynamic limit. The momentum of a spinon is therefore:

$$k_{sp}(\lambda^h) = 2\pi \int_{\lambda^h}^{\infty} d\lambda \rho_{GS}(\lambda) = 2\pi \int_{\lambda^h}^{\infty} d\lambda \frac{e^{-\pi \lambda^h}}{1 + e^{-2\pi \lambda^h}}$$

$$= -2 \int_0^e \frac{dx}{1 + x^2} = -2 \arctan(e^{-\pi \lambda^h})$$

$$= -\frac{\pi}{2} + \arctan(\sinh(\pi \lambda^h)). \quad (5.27)$$

Since $\lambda \in (-\infty, \infty)$, we have: $k_{sp}(\lambda^h) \in [-\pi, 0]$. The dispersion relation in terms of $k$ is:

$$\epsilon_{sp}(k_{sp}) = \frac{J\pi}{2} |\sin k_{sp}|. \quad (5.28)$$

By letting $k_1^h$ and $k_2^h$ run over the interval $[0, \pi]$ we can plot the complete two spinon spectrum as function of total momenta using equations (5.23) and (5.27), see fig. 5.3. The lowest band can be obtained by setting either $k_1^h$ or $k_2^h$ to zero and is called the des Cloizeaux-Pearson mode [34].

### 5.3. Thermodynamic limit: XXZ gapped case

The thermodynamic limit for the XXZ model was first studied by des Cloizeaux and Gaudin [35]. In the XXZ gapped case the rapidities lie in the periodic interval $[-\pi/2, \pi/2]$. The corresponding Fourier transforms are:

$$\rho(n) = \int_{-\pi/2}^{\pi/2} d\lambda e^{-i2n\lambda} \rho(\lambda) \quad \rho(\lambda) = \frac{1}{\pi} \sum_{n=-\infty}^{\infty} e^{i2n\lambda} \rho(n). \quad (5.29)$$
5.3 Thermodynamic limit: XXZ gapped case

Using these Fourier transformations we can derive the Fourier transformed Bethe equations, analogous to (5.11):

\[ a_1(n) = \rho(n)a_2(n) + \rho(n) + \rho_h(n), \]  

where \( a_m(n) \) is the Fourier transform of \( a_m(\lambda) \):

\[ a_m(n) = \int_{-\pi/2}^{\pi/2} d\lambda e^{-i2n\lambda} a_m(\lambda) = \int_{-\pi/2}^{\pi/2} d\lambda e^{-i2n\lambda} \frac{\sinh mn\eta}{\pi \cosh mn\eta - \cos 2\lambda} \]

\[ = \frac{1}{2\pi} \sinh mn\eta \int_{-\pi}^{\pi} \frac{1}{\cosh mn\eta - \cos \theta} d\theta. \]  

(5.31)

It is useful to make the substitution \( z = e^{-\text{sign}(n)\theta} \) so that: \( \cos \theta = (z + \frac{1}{z})/2 \). The variable \( z \) runs once around the unit circle \( |z| = 1 \).

\[ a_m(n) = \frac{1}{2\pi i} \sinh mn\eta \oint_{|z|=1} z^{\lfloor n \rfloor} \frac{1}{\cosh mn\eta - (z + \frac{1}{z})/2} \frac{dz}{z} \]

\[ = \frac{1}{2\pi i} \sinh mn\eta \oint_{|z|=1} z^{\lfloor n \rfloor} \frac{-2}{(z - e^{-mn\eta})(z - e^{mn\eta})} dz \]

(5.32)

In the last step we used the fact that the integrand has two poles in the complex plane: \( z_{\pm} = e^{\pm mn\eta} \). Only \( z_- \) with residue \( 2 \sinh mn\eta \) lies within the unit circle.

If we want to calculate the ground state energy and the two-spinon excitations we will encounter some integrals over the interval \((-\pi/2, \pi/2)\). These integrals turn out to be elliptic functions which we will introduce briefly below.

A Short Introduction to Elliptic Functions

An elliptic integral of the first kind is defined as:

\[ F(\phi, u) \equiv \int_{0}^{\phi} d\theta \frac{1}{\sqrt{1 - u^2 \sin^2 \theta}}. \]  

(5.33)

with \( u^2 < 1 \). The parameter \( u \) is called the modulus, \( u^2 = 1 - u^2 \) is called the complementary modulus. When this elliptic function is integrated over the completed interval (from 0 to \( \pi/2 \)) it is called a complete elliptic integral of the first kind:

\[ K = F(\pi/2, u) \]

\[ K' = F(\pi/2, u') \]  

(5.34)

One can also define the inverse of the elliptic integral of the first kind, called the Jacobi elliptic function:

\[ \text{dn}(F|u) = \sqrt{1 - u^2 \sin^2 \phi}, \]  

(5.35)

which has a useful expansion:

\[ \text{dn}(F|u) = \frac{\pi}{2K} + \frac{2\pi}{K} \sum_{n=1}^{\infty} \frac{q^n}{1 + q^{2n}} \cos 2nv \]  

(5.36)

with: \( q = e^{-\pi K'/K} \) and \( v = \pi F/(2K) \).
5.3.1. The ground state at $h = 0$

Similar as for the isotropic case the quantum all quantum number $I_j$ are filled (see section 4.1). Therefore, the integration boundary $B = \pi/2$ and the $\rho_h(\lambda) = 0$. Hence, the Fourier transformed Bethe equations (5.30) reduces to:

$$a_1(n) = \rho_{GS}(n)(1 + a_2(n)).$$

(5.37)

If we plug $a_m(n)$ into this equation we find the solution for $\rho_{GS}(n)$:

$$\rho_{GS}(n) = \frac{e^{-|n|\eta}}{1 + e^{-2|n|\eta}} = \frac{1}{2\cosh n\eta}.$$  

(5.38)

We can find $\rho(\lambda)$ by taking the inverse Fourier transform of $\rho(n)$:

$$\rho_{GS}(\lambda) = \frac{1}{\pi} \sum_{n=-\infty}^{\infty} e^{i2n\lambda} \rho_{GS}(n).$$

(5.39)

Next, we want to express $\rho_{GS}(\lambda)$ in a closed form. Since $\rho_{GS}(n)$ is an even function in $n$ we can forget about the $i\sin n\lambda$ term and write $\rho_{GS}(\lambda)$ in terms of the Jacobi elliptic function (5.36):

$$\rho_{GS}(\lambda) = \frac{1}{\pi} \sum_{n=-\infty}^{\infty} \cos 2n\lambda \frac{e^{-|n|\eta}}{1 + e^{-2|n|\eta}} = \frac{1}{2} \sum_{n=1}^{\infty} \cos 2n\lambda \frac{q^n}{1 + q^{2n}}$$

$$= \frac{K}{\pi^2} \text{dn}(K2\lambda/\pi|u)$$

(5.40)

with $\eta = \pi K'/K$ which determines $u$ and $2\lambda = \pi F/K$. The function $\rho_{GS}(\lambda)$ is plotted in fig. 5.4 for various values of $\Delta$.

Now that we have found $\rho_{GS}(n)$, we can calculate the ground state energy:

$$E = -JN \sinh(\eta) \pi \int_{-\infty}^{\infty} d\lambda a_1(\lambda) \rho(\lambda)$$

$$= -JN \sinh(\eta) \sum_{n=-\infty}^{\infty} \frac{1}{e^{2|n|\eta} + 1}.$$  

(5.41)

This result was first obtained by Walker [36]. If we take the limit $\eta \to 0$ (or equivalently $\Delta \to 1$), we can replace the sum over $n$ by an integral and it reduces to the energy of the isotropic case, as it should.

5.3.2. Two-spinon excitations

Similar to the XXX case, there are two holes in the distribution of $I_j$ for $M = N/2 - 1$ and in case of real rapidities. Therefore, analogous to the XXX case, $\rho_h(\lambda)$ is:

$$\rho_h(\lambda) = \frac{1}{N} \delta(\lambda - \lambda_1^h) + \frac{1}{N} \delta(\lambda - \lambda_2^h).$$

(5.42)

The Fourier transformed Bethe equations (5.30) for $\Delta > 1$ in case of a two-spinon excitation are:

$$a_1(n) = \rho(n)(1 + a_2(n)) + \frac{1}{N} e^{in\lambda_1^h} + \frac{1}{N} e^{in\lambda_2^h}.$$  

(5.43)
5.3 Thermodynamic limit: XXZ gapped case

We can solve this equation for $\rho(n)$ using (5.32):

$$\rho(n) = \rho_{GS}(n) - \frac{1}{N} \rho_{sp}(n) \left( e^{in\lambda_1^h} + e^{in\lambda_2^h} \right)$$

(5.44)

$$\rho_{GS}(n) = \frac{1}{2 \cosh n\eta} \quad \rho_{sp} = \frac{1}{1 + e^{-2|n|}}.$$  

(5.45)

The energy of a two-spinon excitation is calculated using (5.5):

$$\epsilon(\lambda_1^h, \lambda_2^h) = -NJ \varphi(i\eta)\pi \int_{-\pi/2}^{\pi/2} d\lambda a_1(\lambda)(\rho(\lambda) - \rho_{sp})$$

$$= \epsilon_{sp}(\lambda_1^h) + \epsilon_{sp}(\lambda_2^h)$$

(5.46)

where the spinon energies are defined as:

$$\epsilon_{sp}(\lambda^h) = J \sinh(\eta) \pi \int_{-\pi/2}^{\pi/2} d\lambda a_1(\lambda) \rho_{sp} = J \sinh(\eta) \sum_{n=-\infty}^{\infty} a_1(n) \rho_{sp}(n) e^{-in\lambda^h}$$

$$= J \sinh(\eta) \sum_{n=-\infty}^{\infty} \frac{e^{-|n|\eta}}{1 + e^{-2|n|\eta}} \cos 2n\lambda^h = J\pi \sinh(\eta) \rho_{GS}(\lambda^h)$$

$$= J \frac{1}{\pi} \sinh(\eta) K(u) \text{dn}(K2\lambda^h/\pi|u).$$

(5.47)
The modulus $u$ is determined by $\eta = \pi K'/K$. The momentum of the two spinons is calculated in a way similar to the XXX case:

$$\Delta P = 2\pi \int_{-\infty}^{\infty} d\lambda \left( \theta(X(\lambda) - \frac{r_1^h}{N}) + \theta(X(\lambda) - \frac{r_2^h}{N}) \right) \rho(\lambda)$$

$$= 2\pi \int_{\lambda_1^h}^{\infty} d\lambda \rho(\lambda) + 2\pi \int_{\lambda_2^h}^{\infty} d\lambda \rho(\lambda)$$

$$\equiv k_{sp}(\lambda_1^h) + k_{sp}(\lambda_2^h)$$ \hspace{1cm} (5.48)

where the momentum of a spinon is defined as:

$$k_{sp}(\lambda^h) = 2\pi \int_{\lambda_0^h}^{\pi/2} \rho_{GS}(\lambda) d\lambda$$

$$= -\arcsin sn\left(2\lambda K/\pi, u\right)_{\lambda_0^h}^{\pi/2}$$

$$= -\frac{\pi}{2} + \arcsin sn(2\lambda^h K/\pi, u).$$ \hspace{1cm} (5.49)

We used: $\int \text{dn}(F|u) dF = \arcsin sn(F|u)$ with: $sn(F|u) = \sqrt{1 - u^2} \text{dn}^2(F|u)$. Again, we have: $k_{sp} \in [-\pi, 0]$. So, finally, we have:

$$\Delta E = \frac{JK(u) \sinh \eta}{\pi} \left( \sqrt{1 - u^2} \cos^2 k_1 + \sqrt{1 - u^2} \cos^2 k_2 \right)$$

$$\Delta P = k_1 + k_2.$$ \hspace{1cm} (5.50)

The two-spinon spectrum at zero field is shown in fig. 5.5. The analog of the des Cloizeaux-Pearson mode is the plotted (thick line) but in this case for the $k$ near zero or $2\pi$ it is not the lowest mode. We see that there is energy gap between the ground state and the two-spinon spectrum, something which is not apparent for $|\Delta| \leq 1$. Another difference is that the spectrum near $k = \pi$ is now quadratic instead of linear as in the $|\Delta| \leq 1$ case.

The energy gap which is the difference between the ground state and the lowest energy point of the two energy spectrum (5.50), is at $k_1 = k_2 = 0$,

$$E_{gap} = \frac{2JK(u')u' \sinh \eta}{\eta}.$$ \hspace{1cm} (5.51)

In the limit $\Delta \to \infty$ we can show that the energy gap grows linear in $\Delta$: $E_{gap}(\Delta)/J \approx \Delta - 2$. The energy gap together with its large $\Delta$ approximation are plotted in fig. 5.6. The fact that a gap appears for $\Delta > 1$ is not a big surprise, because for large $\Delta$ the Ising part of the XXZ Hamiltonian becomes dominant. In the Ising limit the ground state is one of the two Néel phases, and excitations are made by reversing one spin.
5.3 Thermodynamic limit: XXZ gapped case

Figure 5.5.: The two-spinon spectrum for $\Delta = 1.2, 2, 4, 8$. All spectra are plotted at the same scale. One can clearly see that when $\Delta \to 1$ the spectrum of the XXX is approached.
Figure 5.6.: The energy gap of a two-spinon $\Delta S_{\text{tot}}^1 = 1$ is plotted as function of $\Delta$, together with the large $\Delta$ approximation (linear line)
6. Algebraic Bethe Ansatz

In chapters two to five, we derived the Bethe equations and obtained the two-spinon spectrum. The next logical step is to compute expectation values of physical observables such as correlation functions. Unfortunately, we cannot continue to use the Bethe wavefunctions as they were formulated in chapter two. First of all, the wavefunctions are not normalized. Secondly, in order to compute scalar expectation values of operators we need to know how an operator acts on an eigenvector. The solution of these problems is to reformulate the Bethe wavefunctions in a second quantized notation. That is, we want to write a wavefunction in terms of operators $B(\lambda)$ acting on a pseudo-vacuum $|0\rangle$ (for example a state with all spins up), that create a downspin with rapidity $\lambda$. So instead of working with complicated wavefunctions, we can use commutation relations between the various operators to calculate the desired quantities.

6.1. Introduction to integrability

6.1.1. Classical integrability

Consider a classical Hamiltonian $H(q,p)$ which describes the motion of $N$ point particles in terms of canonical momenta $p = (p_1, \ldots, p_N)$ and position variables $q = (q_1, \ldots, q_N)$. The equations of motion are:

$$
\dot{p} = -\frac{\partial H(q,p)}{\partial q}, \quad \dot{q} = \frac{\partial H(q,p)}{\partial p}.
$$

(6.1)

We want to find $N$ constants of motion $I_j(q,p)$ ($H$ is one of them). So we should have:

$$
\frac{dI_j}{dt} = \{I_j, H\} = 0,
$$

(6.2)

where $\{.,.\}$ denotes the Poisson bracket. Now, suppose the $I_j$ are in involution:

$$
\{I_j, I_k\} = 0 \quad \forall j, k
$$

(6.3)

Then Liouville’s theorem states that a canonical transformation can be constructed in terms of action-angle variables: $(q,p) \rightarrow (\Theta, I)$. Where $\Theta = (\Theta_1, \ldots, \Theta_N)$ are cyclic coordinates defined on an $N$–dimensional torus, and $I = (I_1, \ldots, I_N)$ are the constants of motion. The new Hamiltonian $\tilde{H}(I)$ is now only a function of $I$. Then the equations of motion are simply:

$$
\frac{dI}{dt} = -\frac{\partial \tilde{H}(I)}{\partial \Theta} = 0,
\frac{d\Theta}{dt} = \frac{\partial \tilde{H}(I)}{\partial I} = \Omega(I) = \text{constant}.
$$

(6.4)

We call a system integrable if all $N$ $I_j$ are constants of motion.
6.1.2. Quantum integrability

If we now turn to a quantum theory, the Poisson bracket is replaced by a commutator. A system is called quantum integrable if all quantum operators $I_j$ commute:

$$[I_j, I_k] = 0.$$

(6.5)

However, there is no analogous Liouville’s theorem which would explain how to obtain the spectrum and eigenfunctions of $H$ just from the commutation relations, as was the case in the classical theory. We need some additional information, unlike the classical case to know a system is integrable does not mean that the eigenfunctions can be found.

6.2. The general algebraic Bethe Ansatz

The Algebraic Bethe Ansatz, also known as the Quantum Inverse Scattering Method, is the quantum mechanical adaptation of the classical inverse scattering method used to solve non-linear classical wave equations that have solitons as solutions. The Algebraic Bethe Ansatz was developed by the Leningrad school [37, 38], see also the book [39].

The idea is to introduce the concept of an integrable model, without specifying what this model should be. From the integrability condition we derive the Yang-Baxter algebra. Next, we should search for representation of the Yang-Baxter algebra from which we will rederive the XXZ model. In the algebraic formulation we can construct eigenfunctions of the Hamiltonian by letting raising operators, which create a down spin with rapidity $\lambda$, act on a pseudo vacuum, and rederive the Bethe equations.

6.2.1. Integrable model

We start with a quantum Hilbert space $\mathcal{H}$ and assume there is a complete set of operators $\{I_n\}$ in $\mathcal{H}$ that are in involution, that is:

$$[I_n, I_l] = 0 \quad \forall n, l$$

(6.6)

A model that satisfies this condition is called integrable. What these operators are is not defined up to this point, but they will correspond to conserved quantities such as the Hamiltonian $H$. Since the set $\{I_n\}$ may be infinite, it is wise to generate all $I_n$ at once. This is done by introducing a transfer matrix $T(\lambda)$, which is a function of a spectral parameter $\lambda \in \mathbb{C}$:

$$\ln T(\lambda) = \sum_{n=0}^{\infty} I_n(\lambda - \xi)^n \quad I_n = \frac{1}{n!} \frac{d^n}{d\lambda^n} \ln T(\lambda) \bigg|_{\lambda = \xi},$$

(6.7)

where $\xi$ is some parameter which we will specify later. The reason to take the logarithm of $T(\lambda)$ is to assure the theory is local (we will explain this later). Since all $I_n$ are in involution, the transfer matrix $T(\lambda)$ should obey the commutation relation:

$$[T(\lambda), T(\mu)] = 0.$$

(6.8)

In order to construct an integrable model we have to find such a $T(\lambda)$. However, it is not straightforward to find solutions of these conditions. It is convenient to introduce the monodromy matrix $T(\lambda)$:

$$T(\lambda) = \text{Tr}_0 T(\lambda).$$

(6.9)
6.2 The general algebraic Bethe Ansatz

The trace is taken over an auxiliary space \( V_0 \); \( T \) therefore acts in \( V_0 \otimes \mathcal{H} \). Condition (6.9) is fulfilled when:

\[
[\text{Tr}_0 T(\lambda), \text{Tr}_0 T(\mu)] = 0. \tag{6.10}
\]

It is useful to put the trace outside the commutator, using the properties of the tensor product (see (B.4)):

\[
[\text{Tr}_0 T(\lambda), \text{Tr}_0 T(\mu)] = \text{Tr}_0 T(\lambda)\text{Tr}_0 T(\mu) - \text{Tr}_0 T(\mu)\text{Tr}_0 T(\lambda) = \text{Tr}_{V_0 \otimes V_0} (T(\lambda) \otimes T(\mu) - T(\mu) \otimes T(\lambda)).
\]

Consider a tensor product of two auxiliary spaces and define:

\[
T_1(\lambda) = T(\lambda) \otimes 1_0, \quad T_2(\lambda) = 1_0 \otimes T(\lambda). \tag{6.11}
\]

Then \( T_{1,2} \) act in \( V_0 \otimes V_0 \otimes \mathcal{H} \). Note that \( T_1 T_2 = (T(\lambda) \otimes 1_0)(1_0 \otimes T(\mu)) = T(\lambda) \otimes T(\mu) \). Then (6.11) becomes:

\[
\text{Tr}_{V_0 \otimes V_0} [T_1(\lambda), T_2(\mu)] = 0, \tag{6.12}
\]

which is equivalent with:

\[
\text{Tr}(T_1T_2) = \text{Tr}(T_2T_1). \tag{6.13}
\]

Since the trace is invariant under cyclic permutations in \( V_0 \otimes V_0 \), this equation is satisfied if the \( T_1 \) and \( T_2 \) are **intertwined**. That is, they obey the following relation:

\[
R(\lambda, \mu)T_1(\lambda)T_2(\mu)R^{-1}(\lambda, \mu) = T_2(\mu)T_1(\lambda)
\]

\[
R(\lambda, \mu)T_1(\lambda)T_2(\mu) = T_2(\mu)T_1(\lambda)R(\lambda, \mu), \tag{6.14}
\]

where the \( R \)–**matrix** is defined in \( V_0 \otimes V_0 \). So instead of looking for \( T(\lambda) \) which commutes with itself for every \( \lambda \), we now ‘only’ have to search for a nontrivial representation of the intertwining relation with a corresponding \( R \)–**matrix**.

### 6.2.2. Yang-Baxter equation

In general we could have a product of \( n \) \( T_i \). And an \( R_{ij} \)–**matrix** relates the \( i \)-th auxiliary with the \( j \)-th one. In case of a product of three monodromy matrices: \( T(\lambda) \otimes T(\mu) \otimes T(\nu) \) can be transformed into \( T(\nu) \otimes T(\mu) \otimes T(\lambda) \) in two different ways. Therefore, we need an additional consistency relation on \( R \). Using the intertwining relation, there are two different ways of transforming: \( T(\lambda) \otimes T(\mu) \otimes T(\nu) \) into \( T(\nu) \otimes T(\mu) \otimes T(\lambda) \). First it is useful to rewrite the tensor product as:

\[
T(\lambda) \otimes T(\mu) \otimes T(\nu) = T_1 T_2 T_3,
\]

\[
T_1 = T(\lambda) \otimes 1 \otimes 1,
\]

\[
T_2 = 1 \otimes T(\mu) \otimes 1,
\]

\[
T_3 = 1 \otimes 1 \otimes T(\nu).
\]

The two possible ways of transforming \( T_1 T_2 T_3 \) into \( T_3 T_2 T_1 \) are:

\[
T_1 T_2 T_3 = R_{12}^{-1} T_2 T_3 R_{12} = R_{12}^{-1} R_{13}^{-1} T_3 T_1 R_{13} R_{12} = R_{12}^{-1} R_{13}^{-1} R_{23}^{-1} T_3 T_1 R_{12} R_{23} R_{13} R_{12},
\]

\[
T_1 T_2 T_3 = R_{23}^{-1} T_1 T_3 R_{23} = R_{23}^{-1} R_{13}^{-1} T_3 T_1 R_{13} R_{23} = R_{23}^{-1} R_{13}^{-1} R_{12}^{-1} T_3 T_1 R_{12} R_{13} R_{23},
\]

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where we used: \([R_{ij}, T_k] = 0\) for \(i \neq j \neq k\) since they act in different subspaces of \(V_0 \otimes V_0 \otimes V_0\). Comparing these two equations and reinserting the spectral parameters gives the famous Yang-Baxter equation, see also fig. 6.1:

\[
R_{23}(\mu, \nu) R_{13}(\lambda, \nu) R_{12}(\lambda, \mu) = R_{12}(\lambda, \mu) R_{13}(\lambda, \nu) R_{23}(\mu, \nu). \tag{6.15}
\]

A product of \(n\) \(T\) monodromy matrices will not give any new relation. We can use the fact that: \([R_{ij}, R_{kl}] = 0\) for \(i \neq j \neq k \neq l\) and reorder all the R-matrices so that we end up with a product of Yang-Baxter equations.

\[
\begin{array}{c}
\text{Figure 6.1.: A graphical presentation of the Yang-Baxter equation.}
\end{array}
\]

### 6.3. The Algebraic Bethe Ansatz for the XXZ model

The Hilbert space of the XXZ model is constructed as the product of \(N\) Hilbert spaces \(\mathcal{H}_i\) defined on every site of the spin chain:

\[
\mathcal{H} = \bigotimes_{i=1}^{N} \mathcal{H}_i. \tag{6.16}
\]

The monodromy matrix \(T(\lambda)\) can be expressed as a product of \(N\) so called \(L\)-operators defined in \(V_0 \otimes \mathcal{H}_i\):

\[
T(\lambda) = L_N(\lambda, \xi_N)L_{N-1}(\lambda, \xi_{N-1}) \ldots L_1(\lambda, \xi_1). \tag{6.17}
\]

The \(\xi_i\) are inhomogeneity parameters, when all \(\xi_i\) are equal we have a homogeneous system. We choose the auxiliary space \(V_0\) isomorphic to \(\mathcal{H}_i\). Following [37] we take:

\[
L_j(\lambda, \xi_j) = R_{0j}(\lambda, \xi_j). \tag{6.18}
\]

It is easy to see that this choice for the \(L\) –operators satisfies the intertwining relation (6.14):

\[
R_{0102}(\lambda, \mu) T_1(\lambda) T_2(\mu) = R_{01}(\lambda, \mu) (R_{01N}(\lambda, \xi_N) \ldots R_{011}(\lambda, \xi_1)) (R_{02N}(\mu, \xi_N) \ldots R_{021}(\mu, \xi_1))
\]

\[
= (R_{02N}(\mu, \xi_N) \ldots R_{021}(\mu, \xi_1)) (R_{01N}(\lambda, \xi_N) \ldots R_{011}(\lambda, \xi_1)) R_{0102}(\lambda, \mu),
\]
6.3 The Algebraic Bethe Ansatz for the XXZ model

where $0_i$ denotes the indices of the auxiliary space and $j$ are the indices of the Hilbert space. In the last step we used the Yang-Baxter equation (6.15).

For a spin–1/2 chain (which has an SU(2) on each site) we take $\mathcal{H}_i$ isomorphic to $\mathbb{C}^2$. An $R$–matrix which obeys the Yang-Baxter equation is [37]:

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda, \mu) & c(\lambda, \mu) & 0 \\ 0 & c(\lambda, \mu) & b(\lambda, \mu) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

(6.19)

where:

$$b(\lambda, \mu) = \frac{\varphi(\lambda - \mu)}{\varphi(\lambda - \mu + \eta)}, \quad c(\lambda, \mu) = \frac{\varphi(\eta)}{\varphi(\lambda - \mu + \eta)}$$

(6.20)

$$\varphi(\lambda) = \begin{cases} \lambda & \text{XXX} \quad \eta = i \\ \sinh(\lambda) & \text{XXZ} \quad |\Delta| = \cos \eta < 1 \\ \sin(\lambda) & \text{XXZ} \quad |\Delta| = \cosh \eta > 1 \end{cases}$$

(6.21)

Next, we should show that the monodromy matrix together with its corresponding $R$–matrix indeed leads to the XXZ model via the trace identities.

6.3.1. The XXX case

Writing the $R$–matrix in the parametrization of the XXX case a putting all $\xi_j = i/2$, the $L$–operator takes the form:

$$L_j(\lambda, i/2) = R_{0j}(\lambda - i/2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{\lambda - i/2}{\lambda + i/2} & \frac{i}{\lambda + i/2} & 0 \\ 0 & \frac{\lambda + i/2}{\lambda - i/2} & \frac{\lambda - i/2}{\lambda + i/2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \frac{\lambda - i/2}{\lambda + i/2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \frac{i}{\lambda + i/2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \frac{1}{\lambda + i/2} \{ (\lambda - i/2) \mathbf{1}_{0j} + iP_{0j} \}. \quad (6.22)$$

The matrix $P_{0j}$ is called the permutation matrix, which interchanges the auxiliary space with the $j$–th quantum space. In general, $P_{jk}$ interchanges the $j$–th and $k$–th space like: $P_{jk}(V_j \otimes V_k) = (V_k \otimes V_j)$ and satisfies the relations:

$$P_{0j} P_{0k} P_{0j} = P_{jk}$$

$$P_{0j}^2 = \mathbf{1}_{0j}. \quad (6.23)$$

Now that we have a representation of the $L$–operator, we can construct the monodromy matrix:

$$T(\lambda) = (\lambda + i/2)^{-N} \{ (\lambda - i/2) \mathbf{1} + iP \}_{0N} \cdots \{ (\lambda - i/2) \mathbf{1} + iP \}_{01}. \quad (6.24)$$

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A useful quantity is the transfer matrix, $T(\lambda) = \text{Tr} \psi_0 T(\lambda)$, evaluated at $\lambda = i/2$:

$$
T(i/2) = \text{Tr}_0 T(i/2) = \text{Tr}_0 \{P_0 N \ldots P_{01}\}
$$

$$
= \text{Tr}_0 \{P_{0N} \ldots P_{03} P_{01} P_{01} P_{02}\}
$$

$$
= \text{Tr}_0 \{P_{0N} \ldots P_{03} P_{01} P_{12}\}
$$

$$
= \text{Tr}_0 \{P_{01}\} P_{1N} \ldots P_{13} P_{12}
$$

$$
= P_{1N} \ldots P_{12}
$$

$$
\equiv U. \quad (6.25)
$$

Since it is quite complicated to take the trace of $N$ operators, we inserted $N-1$ times the identity operator $P_2^0 = 1_{01}$ to shift $P_{01}$ from the far right to the left using (6.23). We thus end up with only one operator in the auxiliary space. The operator $U$ is called the cyclic shift operator. If we apply $U$ $n$ times on a operator $A_{j,k}$ defined in the $j$–th and $k$–th space:

$$
A_{j,k} U^n = U^n A_{j-n,k-n}. \quad (6.26)
$$

**Integrals of motion**

We can obtain the integrals of motion by calculating the Taylor coefficients of the transfer matrix (6.7). The first integral of motion is the zero-th coefficient:

$$
I_0 = \ln T(i/2) \equiv iP, \quad (6.27)
$$

where $P$ is defined by $U = e^{iP}$. Since $U^N = 1$ we can interpret $P$ as the momentum operator, see also section 2.1.2. For the second integral of motion we need to calculate the derivative of the transfer matrix:

$$
I_1 = \frac{d}{d\lambda} \ln T(\lambda) \bigg|_{i/2}. \quad (6.28)
$$

First, we compute the derivative of the $L$–operator:

$$
\frac{d}{d\lambda} L_j(\lambda, i/2) \bigg|_{i/2} = -i (1_{0j} - P_{0j}).
$$

Recalling that $T(\lambda) = \text{Tr} \psi_0 T(\lambda)$, we write the monodromy matrix in the form of (6.24):

$$
i \frac{d}{d\lambda} T(\lambda) \bigg|_{i/2} = \text{Tr}_0 \{[1 - P]_{0N} P_{0N-1} \ldots P_{01} + P_{0N} [1 - P]_{0N-1} P_{0N-2} \ldots P_{01} + P_{0N} P_{0N-1} [1 - P]_{0N-2} \ldots P_{01} + \ldots\}
$$

$$
= \text{Tr}_0 \{P_{01} [1 - P]_{1N} P_{1N-1} \ldots P_{12}\} + \text{Tr}_0 \{P_{0N} [1 - P]_{N-1N} P_{N-1N-2} \ldots P_{N-1N}\}
$$

$$
+ \text{Tr}_0 \{P_{0N-1} [1 - P]_{N-1N-2} P_{N-1N-3} \ldots P_{N-1N}\}
$$

$$
= [1 - P]_{1N} P_{1N-1} P_{1N-2} \ldots P_{12} + \text{cyclic permutations}
$$

$$
= [P - 1]_{1N} P_{1N-1} P_{1N-2} \ldots P_{12} + \text{cyclic permutations}. \quad (6.29)
$$
6.3 The Algebraic Bethe Ansatz for the XXZ model

Again, we shifted $P_{01}$ to the left in order to be able to take the trace. Taking the derivative of $\ln T(\lambda)$ yields:

$$
\left. i \frac{d}{d\lambda} T(\lambda) \right|_{i/2} = \left[ P - 1 \right]_{1N} + \left[ P - 1 \right]_{NN-1} + \ldots
$$

$$
= \sum_{j=1}^{N} [P_{j+1j} - 1_{j+1j}].
$$

(6.30)

Hopefully, we can identify this with a known quantity. Since it relates the $j$–th site with the $j + 1$–th site, we expected it to be the Hamiltonian. The Heisenberg interaction between a spin at the $j$–th site and the $j + 1$–th site is terms of Pauli matrices $\sigma^a_j$ is:

$$
\sum_{a \in \{x, y, z\}} \sigma^a_j \otimes \sigma^a_{j+1} = \left( \begin{array}{cccc}
1 & 0 & 0 & 1 - 1 \\
0 & -1 & 1 + 1 & 0 \\
0 & 1 + 1 & -1 & 0 \\
1 - 1 & 0 & 0 & 1
\end{array} \right) = 2P_{jj+1} - 1_{jj+1}.
$$

This enables us to express $I_1$ in terms of Pauli matrices:

$$
i \left. \frac{d}{d\lambda} \ln T(\lambda) \right|_{i/2} = \sum_{a \in \{x, y, z\}} \sum_{j=1}^{N} \frac{1}{2} (\sigma^a_j \sigma^a_{j+1} - 1).
$$

(6.31)

Hence, it follows that the second integral of motion $I_1$ is related to the Hamiltonian by what is called the trace identity:

$$
H_{XXX} = \sum_{j=1}^{N} \vec{S}_j \cdot \vec{S}_{j+1} - \frac{1}{4} = i \frac{d}{d\lambda} \ln T(\lambda) \bigg|_{i/2}.
$$

(6.32)

We could also compute $I_j$ for $j > 1$, but these integrals of motions do not necessarily have a clear physical interpretation. For our purposes, the momentum operator and the Hamiltonian are sufficient. So the monodromy matrix we constructed indeed corresponds to the XXX model.

6.3.2. XXZ $|\Delta| > 1$ case

For the case $|\Delta| > 1$ the $L$–operator takes the form:

$$
L_j(\lambda, \ieta/2) = R_{0j}(\lambda - \ieta/2) = \left( \begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & \frac{\sin(\lambda-\ieta/2)}{\sin(\ieta)} & \frac{0}{\sin(\ieta)} & 0 \\
0 & \frac{\sin(\lambda+\ieta/2)}{\sin(\ieta)} & \frac{\sin(\lambda+\ieta/2)}{\sin(\ieta)} & 0 \\
0 & 0 & 0 & 1
\end{array} \right)
$$

$$
= \frac{1}{\sin(\lambda + \ieta/2)} \left\{ c_1 1_{0j} + c_P P_{0j} + c_z \sigma^z_0 \otimes \sigma^z_j \right\}
$$

(6.33)

with coefficients:

$$
c_1 = \frac{1}{2} (\sin(\lambda + \ieta/2) + \sin(\lambda - \ieta/2) - \sin(i\eta))
$$

$$
c_P = \sin(i\eta)
$$

$$
c_z = \frac{1}{2} (\sin(\lambda + \ieta/2) - \sin(\lambda - \ieta/2) - \sin(i\eta)).
$$

(6.34)
Algebraic Bethe Ansatz

Similar to the XXX case we have \( L_j(i\eta/2, i\eta/2) = P_{0j} \), so we can write the monodromy matrix as:

\[
T(\lambda) = \sin(\lambda + i\eta/2)^{-N} \{ c_1 \mathbf{1} + c_P P + \sigma^z \otimes \sigma^z \}_{0N} \ldots \{ c_1 \mathbf{1} + c_P P + \sigma^z \otimes \sigma^z \}_{01}.
\] (6.35)

Analogous to the XXX case we have:

\[
T(i\eta/2) = \text{Tr}_0 T(i\eta/2) = \text{Tr}_0 \{ P_{0N} \ldots P_{01} \} = P_{1N} \ldots P_{13} P_{12} \equiv U.
\] (6.36)

Integrals of motion

The first integral of motion is the same momentum operator as in the XXX case:

\[
I_0 = \ln T(i/2) = iP.
\] (6.37)

The second integral of motion,

\[
I_1 = \frac{d}{d\lambda} \ln T(\lambda) \bigg|_{i\eta/2},
\] (6.38)

is a little bit more complicated. The derivative of the \( L \)–operator is:

\[
\frac{d}{d\lambda} L_j(\lambda, i\eta/2) \bigg|_{i\eta/2} = \frac{1}{\sin i\eta} \{ c'_1 \mathbf{1} + c'_P P + c_z \sigma^z \otimes \sigma^z \}_{0j}.
\] (6.39)

with coefficients:

\[
c'_1 = \cos (i\eta/2)^2
\]
\[
c'_P = -\cos(i\eta)
\]
\[
c'_z = -\sin (i\eta/2)^2,
\] (6.40)

so the derivative of the transfer matrix is:

\[
\sin(i\eta) \frac{d}{d\lambda} T(\lambda) \bigg|_{i\eta/2} = \left[ c'_1 \mathbf{1} + c'_P P + c'_z \sigma^z \otimes \sigma^z \right]_{1N} P_{1N-1} P_{1N-2} \ldots P_{12} + \text{cyclic permutations} = \left[ c'_1 P + c'_P \mathbf{1} + c'_z \sigma^z \otimes \sigma^z P \right]_{1N} P_{1N} P_{1N-1} \ldots P_{12} + \text{cyclic permutations}
\] (6.41)

and in logarithmic form:

\[
\sin(i\eta) \frac{d}{d\lambda} \ln T(\lambda) \bigg|_{i\eta/2} = \sum_{j=1}^{N} \left[ c'_1 P + c'_P \mathbf{1} + c'_z \sigma^z \otimes \sigma^z P \right]_{jj+1} = \sum_{j=1}^{N} \frac{1}{2} \left( \sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \cos(i\eta) \sigma^z_j \sigma^z_{j+1} - \cos(i\eta) \mathbf{1} \right).
\] (6.42)

Identifying: \( \cos(i\eta) \equiv \Delta \), we finally have the trace identity for the XXZ model:

\[
H_{XXZ} = \sum_{j=1}^{N} S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \Delta(S^z_j S^z_{j+1} - \frac{1}{4}) = \sin(i\eta) \frac{1}{2} \frac{d}{d\lambda} \ln T(\lambda) \bigg|_{i\eta/2},
\] (6.43)

so the \( T \) matrix we constructed indeed corresponds to the XXZ model. Next, we want to use this new representation of the XXZ model to construct wavefunctions in an algebraic way.
6.4 The inverse problem

We want to find the eigenstates and eigenvalues of $P$ and $H$. It is sufficient to construct the eigenstates of the transfer matrix since it commutes both with $P$ and $H$. The corresponding eigenvalues can be found through the relations between the transfer matrix and the operators $P$ and $H$. If we represent the monodromy matrix in auxiliary space:

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix},$$  \hspace{1cm} (6.44)

we can identify the operators $A, B, C, D$ as non-local operators defined in $\mathcal{H}$. $B$ and $C$ will turn out to be raising and lowering operators, respectively. If we plug this monodromy matrix into (6.14), we get 16 quadratic commutation relations:

$$[A(\lambda), A(\mu)] = [B(\lambda), B(\mu)] = [C(\lambda), C(\mu)] = [D(\lambda), D(\mu)] = 0$$  \hspace{1cm} (6.45a)

$$[A(\lambda), D(\mu)] = \frac{c(\lambda - \mu)}{b(\lambda - \mu)} \{ C(\mu)B(\lambda) - C(\lambda)B(\mu) \}$$  \hspace{1cm} (6.45b)

$$[B(\lambda), C(\mu)] = \frac{c(\lambda - \mu)}{b(\lambda - \mu)} \{ D(\mu)A(\lambda) - D(\lambda)A(\mu) \}$$  \hspace{1cm} (6.45c)

$$[D(\lambda), A(\mu)] = \frac{c(\lambda - \mu)}{b(\lambda - \mu)} \{ B(\mu)C(\lambda) - B(\lambda)C(\mu) \}$$  \hspace{1cm} (6.45d)

$$[C(\lambda), B(\mu)] = \frac{c(\lambda - \mu)}{b(\lambda - \mu)} \{ A(\mu)D(\lambda) - A(\lambda)D(\mu) \}$$  \hspace{1cm} (6.45e)

$$A(\lambda)B(\lambda) = \frac{1}{b(\lambda - \mu)} B(\lambda)A(\mu) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} B(\mu)A(\lambda)$$  \hspace{1cm} (6.45f)

$$B(\mu)A(\lambda) = \frac{1}{b(\lambda - \mu)} A(\lambda)B(\mu) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} A(\mu)B(\lambda)$$  \hspace{1cm} (6.45g)

$$A(\lambda)C(\mu) = \frac{1}{b(\lambda - \mu)} C(\mu)A(\lambda) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} C(\lambda)A(\mu)$$  \hspace{1cm} (6.45h)

$$C(\lambda)A(\mu) = \frac{1}{b(\lambda - \mu)} A(\mu)C(\lambda) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} A(\lambda)C(\mu)$$  \hspace{1cm} (6.45i)

$$B(\lambda)D(\mu) = \frac{1}{b(\lambda - \mu)} D(\mu)B(\lambda) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} D(\lambda)B(\mu)$$  \hspace{1cm} (6.45j)

$$D(\lambda)B(\mu) = \frac{1}{b(\lambda - \mu)} B(\mu)D(\lambda) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} B(\lambda)D(\mu)$$  \hspace{1cm} (6.45k)

$$D(\mu)C(\lambda) = \frac{1}{b(\lambda - \mu)} C(\lambda)D(\mu) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} C(\mu)D(\lambda)$$  \hspace{1cm} (6.45l)

$$C(\mu)D(\lambda) = \frac{1}{b(\lambda - \mu)} D(\lambda)C(\mu) - \frac{c(\lambda - \mu)}{b(\lambda - \mu)} D(\mu)C(\lambda)$$  \hspace{1cm} (6.45m)

Pseudovacuum

To construct eigenstates of the transfer matrix $T(\lambda)$, there should exist a pseudovacuum $|0\rangle$ (highest-weight state), which must satisfy the following requirements:

$$A(\lambda)|0\rangle = a(\lambda)|0\rangle \hspace{1cm} D(\lambda)|0\rangle = d(\lambda)|0\rangle$$

$$C(\lambda)|0\rangle = 0 \hspace{1cm} (|0\rangle B(\lambda)|0\rangle = 0.$$

(6.46)

The existence of a pseudovacuum is a nontrivial thing; for example, the transfer matrix for the XYZ model can be constructed, but a pseudovacuum does not exist.

6.4.1. Eigenstates

Theorem 6.1. $|\Psi_M\rangle = \prod_{i=1}^{M} B(\lambda_i)|0\rangle$ is an eigenstate of the transfer matrix $T$ iff the $\lambda_j$ satisfy the Bethe equations.
Recall, from the definition of the transfer matrix that: $T(\lambda) = A(\lambda) + D(\lambda)$. So we should use the commutation relations to compute:

\[
A(\mu) \prod_{j=1}^{M} B(\lambda_j)|0\rangle = A \prod_{j=1}^{M} B(\lambda_j)|0\rangle + \sum_{n=1}^{M} \Lambda_n B(\mu) \prod_{j \neq n}^{M} B(\lambda_j)|0\rangle \tag{6.47}
\]

\[
D(\mu) \prod_{j=1}^{M} B(\lambda_j)|0\rangle = \tilde{A} \prod_{j=1}^{M} B(\lambda_j)|0\rangle + \sum_{n=1}^{M} \Lambda_n B(\mu) \prod_{j \neq n}^{M} B(\lambda_j)|0\rangle \tag{6.48}
\]

with the following coefficients:

\[
\Lambda = a(\mu) \prod_{j=1}^{M} \frac{1}{b(\lambda_j - \mu)}; \quad \Lambda_n = -a(\lambda_n) \frac{c(\lambda_n - \mu)}{b(\lambda_n - \mu)} \prod_{j \neq n}^{M} \frac{1}{b(\lambda_j - \lambda_n)} \tag{6.49}
\]

\[
\tilde{\Lambda} = d(\mu) \prod_{j=1}^{M} \frac{1}{b(\mu - \lambda_j)}; \quad \tilde{\Lambda}_n = -d(\lambda_n) \frac{c(\mu - \lambda_n)}{b(\mu - \lambda_n)} \prod_{j \neq n}^{M} \frac{1}{b(\lambda_n - \lambda_j)}. \tag{6.50}
\]

**Proof.** The commutation relation (6.45f) allows us to pull the operator $A(\mu)$ from the left to right. The first term of (6.45f) corresponds to preserving the arguments of the operators, and the second corresponds to an exchange of the arguments. To compute $\Lambda$ we can only use the first term of (6.45f), otherwise a $B(\mu)$ will appear and never vanish. So the second term will never contribute to $\Lambda$. After interchanging $A(\mu) \ M$ times and using: $A(\mu)|0\rangle = a(\mu)|0\rangle$, we obtain $\Lambda$. For computing $\Lambda_n$, we use the fact that:

\[
|\Psi_M(\{\lambda_j\})\rangle = B(\lambda_n) \prod_{j \neq n}^{M} B(\lambda_j)|0\rangle.
\]

For the first step we use the second term of (6.45g), such that $B(\mu)$ will appear:

\[
-\frac{c(\lambda_n - \mu)}{b(\lambda_n - \mu)} B(\mu) A(\lambda_n) \prod_{j \neq n}^{M} B(\lambda_j)|0\rangle. \tag{6.51}
\]

If we now apply the first term of (6.45g) $M - 1$ times, we get $\Lambda_n$. Of course, it is possible to apply the second term more than once, but then we will not get a contribution to $\Lambda_n$. Since it is always possible to put $B(\lambda_n)$ in front, we can calculate the other $\Lambda_n$ in the same way. The coefficients $\tilde{\Lambda}$ and $\tilde{\Lambda}_n$ can be obtained in a similar way. \qed

$|\Psi_N\rangle$ is eigenfunction of $T(\lambda) = A(\lambda) + D(\lambda)$ iff $\Lambda_n + \tilde{\Lambda}_n = 0$. This requirement leads to the Bethe equations:

\[
\frac{a(\lambda_n)}{d(\lambda_n)} \prod_{j \neq n}^{M} b(\lambda_n - \lambda_j) \frac{b(\lambda_n)}{b(\lambda_j - \lambda_n)} = 1. \tag{6.52}
\]

The vacuum eigenvalues $a(\lambda)$ and $d(\lambda)$ of the monodromy matrix are:

\[
a(\lambda) = \prod_{j=1}^{N} a_j(\lambda), \quad d(\lambda) = \prod_{j=1}^{N} d_j(\lambda), \tag{6.53}
\]

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6.4 The inverse problem

where \( a_j(\lambda), d_j(\lambda) \) are vacuum eigenvalues of: \( L_j(\lambda, \xi_j) = R_{0j}(\lambda - \xi_j) \). The eigenvalues of the R-matrix (6.19) corresponding to the eigenvectors \((1,0,0,0)\) and \((0,0,1,0)\) are:

\[
a(\lambda) = 1, \quad d(\lambda) = \prod_{j=1}^{N} b(\lambda, \xi_j). \quad (6.54)
\]

Combining (6.52) with (6.20) leads to the Bethe equations we found in chapter 2. The eigenvalue \( \tau(\mu, \{\lambda_j\}) \) of the transfer matrix is:

\[
\tau(\mu, \{\lambda_j\}) = \Lambda(\mu) + \tilde{\Lambda}(\mu) = a(\mu) \prod_{j=1}^{M} \frac{1}{b(\lambda_j - \mu)} + d(\mu) \prod_{j=1}^{M} \frac{1}{b(\mu - \lambda_j)} \quad (6.55)
\]

with the \( \{\lambda_j\} \) satisfying the Bethe equations.

**Eigenvalues of \( P \) and \( H \)**

Now we have found the eigenvalues \( \tau(\mu, \{\lambda\}) \) of the transfer matrix for a state \( |\Psi_M{\lambda}\rangle \) we can compute the eigenvalues of \( P \) and \( H \) using (6.37) and (6.43):

\[
P = -i \ln \tau(i\eta/2, \{\lambda_j\}) = -i \sum_{l=1}^{M} \ln(b^{-1}(\lambda_j, i\eta/2)) \quad (6.56)
\]

\[
E = \varphi(i\eta) \left. \frac{1}{2} \frac{d}{d\lambda} \ln \tau(\mu, \{\lambda_j\}) \right|_{\mu=i\eta/2} = \varphi(i\eta) \frac{1}{2} \sum_{l=1}^{M} \left. \frac{d}{d\lambda} \ln b^{-1}(\lambda_j, \mu) \right|_{\mu=i\eta/2} = -\pi \varphi(i\eta) \sum_{l=1}^{M} a_1(\lambda_l), \quad (6.57)
\]

where we used \( d(i\eta/2) = 0 \). These expressions for \( P \) and \( E \) corresponds with what we found in chapter two.

6.4.2. Quantum inverse problem

So far, we have reformulated the XXZ model in an algebraic way in terms of non-local operators \( A(\lambda), B(\lambda), C(\lambda), D(\lambda) \). Using the commutation relations we obtained the Bethe equations and expressions for the total energy and total momentum. If we now want to relate a local operator, for example a spin-flip at the j-th site: \( S^+_j \), we should express these operators in terms of \( A(\lambda), B(\lambda), C(\lambda), D(\lambda) \). In general this is a very nontrivial procedure, but fortunately Maillet [40] found an inverse mapping.

A clever trick to obtain this inverse mapping is to consider the monodromy matrix at \( \lambda = \xi \). In this case we can write the monodromy matrix as permutation operator times the shift operator (6.36):

\[
T(\xi) = P_{01} U. \quad (6.58)
\]

In auxiliary space, this looks like:
\[
\begin{pmatrix}
A(\xi) & B(\xi) \\
C(\xi) & D(\xi)
\end{pmatrix} = \left(\frac{1+\sigma_j^+}{\sigma_1^+} \quad \frac{\sigma_j^-}{1-\sigma_1^-} \right) U.
\] (6.59)

Solving this for all four matrix entries gives:

\[
\begin{align*}
A(\xi) + D(\xi) &= U, \\
A(\xi) - D(\xi) &= \sigma_1^+ U, \\
B(\xi) &= \sigma_1^- U, \\
C(\xi) &= \sigma_1^+ U.
\end{align*}
\] (6.60)

To obtain similar equations for the local operators acting on the other sites, we use the translation operator: \( \sigma_j^z = U^{j-1} \sigma_1^z U^{1-j} \) together with \( U^N = 1 \)

\[
\begin{align*}
\sigma_j^z &= [A(\xi) + D(\xi)]^{j-1} (A(\xi) - D(\xi))[A(\xi) + D(\xi)]^{N-j}, \\
\sigma_j^+ &= [A(\xi) + D(\xi)]^{j-1} B(\xi)[A(\xi) + D(\xi)]^{N-j}, \\
\sigma_j^- &= [A(\xi) + D(\xi)]^{j-1} C(\xi)[A(\xi) + D(\xi)]^{N-j}.
\end{align*}
\] (6.61)

This concludes the mapping between the local and non-local operators, namely all local operators were represented in terms of \( A(\lambda), B(\lambda), C(\lambda), D(\lambda) \). What is left is to use the algebra of these operators to compute all desired quantities.

### 6.5. Scalar products: Slavnov’s theorem

One of the goals, for introducing the Algebraic Bethe Ansatz was to normalize the wavefunctions in a clever way. Before we turn to this problem, we will first consider a very important result by Slavnov [41] which concerns the scalar product of states constructed by the action of \( B(\lambda) \) on the vacuum. The scalar product is defined by:

\[
\tilde{S}_M = \langle 0 | \prod_{j=1}^{M} C(\mu_j) \prod_{j=1}^{M} B(\lambda_j) | 0 \rangle,
\] (6.62)

where \( C(\lambda) = C(\lambda)/d(\lambda) \) and \( B(\lambda) = B(\lambda)/d(\lambda) \). The scalar product is in general a function of \( 4M \) independent variables \( \tilde{S}_M(\{\mu_j\}, \{\lambda_j\}, \{r_j^C\}, \{r_j^B\}) \) where:

\[
\begin{align*}
r_j^B &= \frac{a(\lambda_j)}{d(\lambda_j)}, \\
r_j^C &= \frac{a(\mu_j)}{d(\mu_j)}.
\end{align*}
\] (6.63)

The scalar product has poles for \( \mu_k = \lambda_j \):

\[
\tilde{S}_M(\{\mu\}, \{\lambda\}, \{r_j^C\}, \{r_j^B\}) |_{\lambda_m - \mu_M} = \frac{c(\mu_M - \lambda_m)}{b(\mu_M - \lambda_m)} (r_m^C - r_m^B) \prod_{j \neq M} \frac{1}{b(\mu_M - \mu_j)} \prod_{j \neq m} \frac{1}{b(\lambda_m - \lambda_j)}
\]

\[
\tilde{S}_{M-1}(\{\mu\} \cup \{\lambda\}) |_{\lambda_j \neq \mu_M, \lambda_n \neq \mu_m, \lambda_j \neq \mu_j} + \text{finite terms}. \] (6.64)
6.5 Scalar products: Slavnov’s theorem

First, we put \( C(\mu_M) \) and \( \mathbb{B}(\lambda_m) \) right next to each other using (6.45a). Then we apply (6.45c) once. The first term now has a pole coming from the factor \( \frac{c(\mu_M - \lambda_m)}{b(\mu_M - \lambda_m)} \). Shifting \( C(\mu_M) \) to the right in the second term using (6.45e) repeatedly, we get \( M - 1 \) finite factors: \( \frac{c(\mu_M - \lambda_j)}{b(\mu_M - \lambda_j)} \) when \( \mu_M \neq \lambda_j \) for all \( j \neq m \). So the second term is finite. The next step is to shift \( A \) to the left and \( D \) to the right using (6.45i) and (6.45k), respectively. Now the scalar product \( \hat{S}_{M-1} \) is a function of \( \tilde{r} \), which are:

\[
\begin{align*}
\tilde{r}_j^B &= r_j b(\lambda_j - \lambda_m) / b(\lambda_m - \lambda_j) \\
\tilde{r}_j^C &= r_j b(\mu_j - \lambda_m) / b(\lambda_m - \mu_j).
\end{align*}
\]

(6.65)

A special case of the scalar product is when the vector \( \prod_{j=1}^{M} \mathbb{B}(\lambda_j) |0 \) is an eigenstate of the Hamiltonian. In that case \( \lambda \) and \( r(\lambda) \) are not independent anymore since the \( \lambda_j \) should satisfy the Bethe equations which are a function of \( r_j^B \):

\[
r(\lambda_j) \prod_{l \neq j} b(\lambda_j, \lambda_l) / b(\lambda_l, \lambda_j) = 1.
\]

(6.66)

In this case we can explicitly compute the scalar product due to the following theorem:

**Theorem 6.2.** Let \( \{ \lambda_j \} \) be a solution of the Bethe equations (6.5) and \( \{ \mu_j \} \) be an arbitrary set. Then the scalar product can be written as:

\[
\mathbb{S}_M(\{ \mu_j \}, \{ \lambda_j \}) = \frac{\det H(\{ \mu_j \}, \{ \lambda_j \})}{\prod_{j > k} \phi(\mu_k - \mu_j) \prod_{j < k} \phi(\lambda_k - \lambda_j)}
\]

(6.67)

where the matrix elements of the \( M \times M \) matrix \( H_{ab} \) are:

\[
H_{ab} = \frac{\phi(i\eta)}{\phi(\lambda_a - \mu_b)} \left( r(\mu_b) \prod_{l \neq a} \phi(\lambda_l - \mu_b + i\eta) - \prod_{l \neq a} \phi(\lambda_l - \mu_b - i\eta) \right).
\]

(6.68)

**Proof.** The proof goes by induction. For \( M = 1 \) we can calculate the scalar product explicitly by means of the commutation relations:

\[
\langle 0 | C(\mu) \mathbb{B}(\lambda) | 0 \rangle = \mathbb{S}_1 = \frac{\phi(i\eta)}{\phi(\lambda - \mu)}.
\]

(6.69)

The next step is to prove that (6.67) obeys the residue formula (6.64). Let \( \mathbb{S}_{M-1} = \hat{\mathbb{S}}_{M-1} \). We consider \( \mathbb{S}_{M-1} \) as an analytic function of \( \mu_M \) with simple poles at the points \( \mu_M = \lambda_j \). Next, consider: \( \mu_N \to \lambda_m \). Writing the denominator of (6.67) like \( G_M = \prod_{j > k} \phi(\mu_k - \mu_j) \prod_{j < k} \phi(\lambda_k - \lambda_j) \), the denominator becomes:

\[
G_M = G_{M-1} \prod_{j < M} \phi(\mu_j - \mu_M) \prod_{j < m} \phi(\lambda_m - \lambda_j) \prod_{k > m} \phi(\lambda_k - \lambda)
\]

\[
= G_{M-1} \prod_{j \neq M} \phi(\mu_j - \mu_M) (-1)^{M-m} \prod_{j \neq m} \phi(\lambda_m - \lambda_j),
\]

(6.70)
and the determinant:
\[ \det M \mathbf{H} = \frac{\varphi(i \eta)}{\varphi(\lambda_m - \mu_M)} \left( r(\mu_M) \prod_{l \neq a} \varphi(\lambda_l - \mu_M + i \eta) - \prod_{l \neq a} \varphi(\lambda_l - \mu_M - i \eta) \right) \det H. \]  
(6.71)

Combining (6.70) and (6.71) gives:
\[ S_M(\{ \mu_j \}, \{ \lambda_j \})|_{\mu_M \rightarrow \lambda_m} = \frac{C(\mu_M - \lambda_m)}{b(\mu_M - \lambda_m)} \left( \prod_{j \neq M} b(\mu_M - \mu_j) \prod_{j \neq \lambda, a} 1 \right) \det H. \]  
(6.72)

Next, we want to show that \( S_M(\{ \mu_j \}, \{ \lambda_j \}) = \mathcal{S}_M(\{ \mu_j \}, \{ \lambda_j \}) \), hence the finite terms in (6.64) vanish. Using (6.64) we see that the difference \( D = \mathcal{S}_M(\{ \mu_j \}, \{ \lambda_j \}) - S_M(\{ \mu_j \}, \{ \lambda_j \}) \) as a function of \( \mu_M \) is bounded in the complex plane. According to Liouville’s theorem (see (B.1)) a bounded function is a constant. The finite terms in (6.64) vanish when \( \mu_M \rightarrow \infty \) (or in the XXZ case with \( |\Delta| > 1 \) when \( \mu_M \rightarrow \pi/2 \)). So the difference \( D \) vanishes in the entire complex plane. \( \square \)

A much more useful quantity is the scalar product defined in terms of \( B(\lambda), C(\mu) \) operators instead of \( \mathbb{B}(\lambda), C(\mu) \). Making this replacement in (6.67) gives:
\[ S_M(\{ \mu_j \}, \{ \lambda_j \}) = \left( \prod_{j=1}^{M} C(\lambda_j) \prod_{j=1}^{M} B(\lambda_j) \right) 0 = \frac{\det H'(\{ \mu_j \}, \{ \lambda_j \})}{\prod_{j<k} \varphi(\lambda_k - \lambda_j)}, \]  
(6.73)

where is \( H' \) is now a different matrix:
\[ H'_{ab} = \frac{\varphi(i \eta)}{\varphi(\lambda_a - \mu_b)} \left( a(\mu_b) \prod_{l \neq a} \varphi(\lambda_l - \mu_b + i \eta) - d(\mu_b) \prod_{l \neq a} \varphi(\lambda_l - \mu_b - i \eta) \right). \]  
(6.74)

We can write this in terms of the eigenvalues of the transfer matrix \( \tau(\mu, \{ \lambda \}) = a(\mu) \prod_{j=1}^{M} b^{-1}(\lambda_j, \mu) + d(\mu) \prod_{j=1}^{M} b^{-1}(\mu, \lambda_j) \):
\[ S_M(\{ \mu \}, \{ \lambda \}) = \frac{\prod_{j=1}^{M} \varphi(\mu_j - \lambda_k)}{\prod_{j<k} \varphi(\mu_j - \mu_k) \prod_{j>k} \varphi(\lambda_j - \lambda_k) \det T(\{ \mu \}, \{ \lambda \})}, \]  
(6.75)

where \( T_{ab} = \frac{\partial}{\partial \lambda_a} \tau(\mu_b, \{ \lambda \}) \). We can verify this by explicitly taking the derivative:
\[ T_{ab} = \frac{\partial}{\partial \lambda_a} \tau(\mu_b, \{ \lambda \}) \]
\[ = a(\mu_b) \prod_{j=1}^{M} b^{-1}(\lambda_j, \mu_b) \left( b(\lambda_j, \mu_b) \frac{\partial}{\partial \lambda_b} b(\lambda_j, \mu_b) \right) + d(\mu_b) \prod_{j=1}^{M} b^{-1}(\mu_b, \lambda_j) \left( b(\mu_b, \lambda_j) \frac{\partial}{\partial \lambda_b} b(\mu_b, \lambda_j) \right) \]
\[ = \prod_{j=1}^{M} \frac{1}{\varphi(\mu_b - \lambda_j)} \varphi(i \eta) \left( a(\mu_b) \prod_{l \neq a} \varphi(\mu_l - \lambda_b + i \eta) - d(\mu_b) \prod_{l \neq a} \varphi(\mu_l - \lambda_b - i \eta) \right) \]
\[ = \prod_{j=1}^{M} \frac{1}{\varphi(\mu_b - \lambda_j)} H'_{ab}. \]  
(6.76)
6.6 Form factors

We could take \( \{\mu_j\} \) as a solution of the Bethe equations, instead of \( \{\lambda_j\} \). A similar calculation gives:

\[
S_M(\{\mu_j\}, \{\lambda_j\}) = S_M(\{\lambda_j\}, \{\mu_j\}).
\]  

(6.77)

The expression for the scalar product can also be proved by means of quantum algebras [40].

6.5.1. Norm of eigenstates: Gaudin’s formula

The norm of an eigenstate can be calculated by taking the limit \( \mu_j \to \lambda_j \) in (6.73):

\[
N_M = \langle 0 | \prod_{j=1}^M C(\lambda_j) \prod_{k=1}^M B(\lambda_k) | 0 \rangle
= S(\{\mu_j\}, \{\lambda_j\})|_{\{\mu_j\} \to \{\lambda_j\}}.
\]  

(6.78)

We should carefully take the limit by:

\[
\mu_j = \lambda_j + \epsilon, \quad \epsilon \to 0.
\]

Taylor expanding \( r(\mu) \) around \( \epsilon \) gives:

\[
r(\mu) = r(\lambda) + (\mu - \lambda) \frac{\partial}{\partial \mu} r(\mu) \bigg|_{\mu \to \lambda}
= r(\lambda) \left( 1 + \epsilon \frac{\partial}{\partial \mu} \ln r(\mu) \right)_{\mu \to \lambda}.
\]  

(6.79)

If we plug this into (6.67) we get:

\[
N_M = \varphi(i\eta)^M \prod_{j \neq k} \frac{\varphi(\lambda_j - \lambda_k + i\eta)}{\varphi(\lambda_j - \lambda_k)} \det \Phi(\{\lambda_j\})
\]  

(6.80)

with the entries of the determinant being:

\[
\Phi_{ab} = -\frac{\partial}{\partial \lambda_b} \ln \left( \frac{a(\lambda_a)}{d(\lambda_a)} \prod_{l \neq a}^M b(\lambda_l, \lambda_a) \right).
\]  

(6.81)

We could also define the norm in terms of \( B(\lambda) \) and \( C(\lambda) \) operators. Using the Bethe equations it follows that \( \prod_{j=1}^M d(\lambda_j) = 1 \), hence we get an equivalent expression:

\[
N_M(\{\lambda_j\}) = \langle 0 | \prod_{j=1}^M C(\lambda_j) \prod_{k=1}^M B(\lambda_k) | 0 \rangle = N_M(\{\lambda_j\}).
\]  

(6.82)

The determinant expression for the norm of the eigenstates is usually called the Gaudin norm, since he was the first who conjectured it. Korepin [42] was the first who proved Gaudin’s conjecture using a more cumbersome approach than the one discussed here.

6.6. Form factors

For the calculation of correlation functions we make use of an expression for the expectation value of local spin-operators, known as form factors. Using the inverse mapping of the local spin-operators into non-local operators of the Algebraic Bethe Ansatz we obtain a determinant expression both for the transverse form factor as for the longitudinal one.
6.6.1. Transverse form factor

The transverse form factor is a spin-flip in the transverse direction:

\[ F_j^- (\{\mu\}_{M+1}, \{\lambda\}_M) = \langle 0 \prod_{k=1}^{M+1} C(\mu_k) \sigma_j^- \prod_{l=1}^{M} B(\lambda_l)|0 \rangle. \quad (6.83) \]

The set \( \{\mu\}_{M+1} \) is a solution of the Bethe equations for the case \( M = N/2 + 1 \), whereas \( \{\lambda\}_M \) is a solution for the case \( M = N/2 \). Recalling from the \( \sigma_j^- \) operator in terms of non-local operators:

\[ \sigma_j^- = [A(\xi) + D(\xi)]^{j-1} B(\xi)[A(\xi) + D(\xi)]^{N-j}. \]

The action of \( A(\xi_j) + D(\xi_j) \) is easily computed, since it is the transfer matrix evaluated at \( \xi_j \):

\[
(A(\xi_j) + D(\xi_j)) \prod_{l=1}^{M} B(\lambda_l)|0 \rangle = \left( a(\xi_j) \prod_{k=1}^{M} \frac{1}{b(\lambda_k - \xi_j)} + d(\xi_j) \prod_{k=1}^{M} \frac{1}{b(\xi_j - \lambda_k)} \right) \prod_{l=1}^{M} B(\lambda_l)|0 \rangle = \prod_{k=1}^{M} b^{-1}(\lambda_k, \xi_j) \prod_{l=1}^{M} B(\lambda_l)|0 \rangle. \quad (6.84)
\]

We used \( a(\lambda) = 1 \) and \( d(\xi) = 0 \). After working through all the factors of \( A(\xi_j) + D(\xi_j) \) we are left with a scalar product between an eigenstate in terms of \( \{\mu\}_{M+1} \) and a state \( \{\xi_j, \{\lambda\}_M\} \) which is not an eigenstate, hence we should use Slavnov’s result for the scalar product (6.73):

\[
F_j^- (\{\mu\}_{M+1}, \{\lambda\}_M) = \left( \prod_{l=1}^{M+1} \prod_{k=1}^{j-1} b^{-1}(\mu_l, \xi_k) \right) \times \left( \prod_{l=1}^{M+1} \prod_{k=j+1}^{N} b^{-1}(\lambda_l, \xi_k) \right) \prod_{l=1}^{M+1} C(\mu_k) B(\xi_j) \prod_{j=1}^{M} B(\lambda_l)|0 \rangle \]

\[
= \frac{\phi_{j-1}(\{\lambda\}) \phi_{j-1}(\{\mu\}) S_{M+1}(\{\mu\}_{M+1}, \{\xi_j, \{\lambda\}_M\})}{\phi_{j-1}(\{\lambda\}) \phi_{j-1}(\{\mu\}) S_{M+1}(\{\mu\}_{M+1}, \{\xi_j, \{\lambda\}_M\})} \det H(\{\mu\}, \{\lambda\}) \]

\[
= \frac{\phi_{j-1}(\{\mu\}) \prod_{l=1}^{M+1} \varphi(\mu_l - \xi_j + i\eta) \prod_{l=m}^{M+1} \varphi(\mu_l - \lambda_m) \prod_{l=m}^{M+1} \varphi(\lambda_l - \lambda_m)}{\phi_{j-1}(\{\lambda\}) \prod_{l=1}^{M+1} \varphi(\lambda_l - \xi_j + i\eta) \prod_{l=m}^{M+1} \varphi(\mu_l - \lambda_m) \prod_{l=m}^{M+1} \varphi(\lambda_l - \lambda_m)}, \quad (6.85)
\]

in which we have defined:

\[ \phi_j = (\{\lambda\}) = \prod_{l=1}^{j} \prod_{k=1}^{M} b^{-1}(\lambda_k, \xi_j) \quad (6.86) \]

and used the fact that \( \phi_N(\{\lambda\}) = 1 \), as can be seen from the Bethe equations. The entries of the matrix \( H^- \) are the same for the one in \( H \) except for the last column which is simplified because \( \lambda_{M+1} = \xi_j \):

\[
H^-_{ab} = \frac{\varphi(i\eta)}{\varphi(\mu_a - \lambda_b)} \left( a(\lambda_b) \prod_{l=1}^{M+1} \varphi(\mu_l - \lambda_b + i\eta) - d(\lambda_b) \prod_{l=1}^{M+1} \varphi(\mu_l - \lambda_b - i\eta) \right) \quad b < M + 1
\]

\[
H^-_{aM+1} = \frac{\varphi(i\eta)}{\varphi(\mu_a - \xi_j + i\eta) \varphi(\mu_a - \xi_j)}.
\]
6.6.2. Longitudinal form factor

The longitudinal form factor is defined as:

\[ F^z_j (\{ \mu \}_M, \{ \lambda \}_M) = \langle 0 | \prod_{k=1}^{M} C(\mu_k) \sigma_j^z \prod_{l=1}^{M} B(\lambda_l) | 0 \rangle. \]  

(6.88)

The expression for the \( \sigma_j^z \) in terms of non-local operators is:

\[ \sigma_j^z = [A(\xi) + D(\xi)]^{j-1} (A(\xi) - D(\xi))[A(\xi) + D(\xi)]^{N-j}. \]

The presence of the factor \( A(\xi_j) - D(\xi_j) \) makes the computation of the form factor more complicated than the transverse one. Using the fact that \( (A(\xi_j) + D(\xi_j))^N = U^N = 1 \) we can rewrite \( \sigma_j^z \) as:

\[ \sigma_j^z = 2 \prod_{k=1}^{j-1} (A(\xi_k) + D(\xi_k)) A(\xi_j) \prod_{k=1+j}^{N} (A(\xi_k) + D(\xi_k)) - 1. \]  

(6.89)

The operator \( A(\xi_j) \) acts on an eigenstate as (6.47):

\[ A(\xi_j) \prod_{l=1}^{M} B(\lambda_l) | 0 \rangle = \prod_{l=1}^{M} b^{-1}(\lambda_l - \xi_j) \prod_{l=1}^{M} B(\lambda_l) | 0 \rangle - \sum_{n=1}^{M} c(\lambda_n - \xi_j) \prod_{j \neq n}^{M} b^{-1}(\lambda_j - \lambda_n) B(\xi_j) \prod_{l \neq n}^{M} B(\lambda_l) | 0 \rangle. \]  

(6.90)

Since we are looking for form factors with \( \{ \mu_l \} \neq \{ \lambda_l \} \), we can use the fact that different Bethe eigenstates are orthogonal\(^1\) to drop the first term in (6.90). This results in:

\[ F^z_j = -2 \phi_{j-1}(\{ \mu \}) \phi_{j+1-N}(\{ \lambda \}) \sum_{n=1}^{M} \frac{c(\lambda_n - \xi_j)}{b(\lambda_n - \xi_j)} \prod_{j \neq n}^{M} b^{-1}(\lambda_j - \lambda_n) \langle 0 | \prod_{k=1}^{M} C(\mu_k) B(\xi_j) \prod_{l \neq n}^{M} B(\lambda_l) | 0 \rangle. \]  

(6.91)

Now we have a summation of scalar products between the eigenstates \( \{ \mu_l \}_M \) and the state \( \{ \lambda_l \} \) with \( \lambda_n \to \xi_j \). Using Slavnov’s formula:

\[ \langle 0 | \prod_{k=1}^{M} C(\mu_k) B(\xi_j) \prod_{l \neq n}^{M} B(\lambda_l) | 0 \rangle = \frac{\text{det} H(\{ \mu \}, \{ \lambda \})}{\prod_{l>l_m} \varphi(\mu_l - \mu_m) \prod_{l=m} \varphi(\lambda_l - \lambda_m)} \frac{\lambda_n \rightarrow \xi_j}{\prod_{l>l_m} \varphi(\mu_l - \mu_m) \prod_{l=m} \varphi(\lambda_l - \lambda_m)} \right. \]  

(6.92)

\[ \left. = \frac{\text{det} \hat{H}^{\lambda}}{\prod_{l>l_m} \varphi(\mu_l - \mu_m) \prod_{l<m} \varphi(\lambda_l - \lambda_m) \prod_{l \neq n} \varphi(\lambda_l - \xi_j)} \right. \]  

\[ \frac{1}{\phi_{j-1}(\{ \lambda \})} \sum_{l=1}^{M} \frac{\varphi(\lambda_l - \lambda_n + \eta)}{\prod_{l>l_m} \varphi(\mu_l - \mu_m) \prod_{l<m} \varphi(\lambda_l - \lambda_m)} \]  

The longitudinal form factor becomes:

\[ F^z_j = -2 \phi_{j-1}(\{ \mu \}) \prod_{l=1}^{M} \frac{1}{\varphi(\lambda_l - \xi_j + \eta)} \sum_{n=1}^{M} \prod_{l=1}^{M} \varphi(\lambda_l - \lambda_n + \eta) \frac{\text{det} \hat{H}^{\lambda}}{\prod_{l>l_m} \varphi(\mu_l - \mu_m) \prod_{l<m} \varphi(\lambda_l - \lambda_m)}. \]  

(6.93)

\(^1\)For \( \{ \mu_l \} = \{ \lambda_l \} \) the form factor can be calculated using the spin algebra.
Algebraic Bethe Ansatz

We can bring the factor $-2 \prod_{l=1}^{M} \varphi(\lambda_l - \lambda_n + \eta)$ into the determinant by multiplying it with the $n$-th column of the matrix $H_n$. Similarly, we can extract a factor $\prod_{l=1}^{M} \varphi(\mu_l - \xi_j + \eta)$ from the $n$-th column, to get the result:

$$F^z_j = \frac{\phi_{j-1}({\mu})}{\phi_{j-1}({\lambda})} \prod_{l=1}^{M} \varphi(\mu_l - \xi_j + \eta) \sum_{n=1}^{M} \frac{\det H^n}{\prod_{l>m} \varphi(\mu_l - \mu_m) \prod_{l<m} \varphi(\lambda_l - \lambda_m)}$$  \hspace{1cm} (6.94)

$$H_{ab}^n = H_{ab} \hspace{0.5cm} b \neq a$$

$$H_{an}^n = -2P_{an}$$  \hspace{1cm} (6.95)

$$P_{ab} = \varphi(\eta) \frac{\prod_{l=1}^{M} \varphi(\lambda_l - \lambda_b + \eta)}{\varphi(\mu_a - \xi_j + \eta) \varphi(\mu_a - \xi_j)}$$  \hspace{1cm} (6.96)

Since $P_{ab}$ is a rank one matrix (all the columns/rows are multiples of each other), we can use the following. If $A$ is an arbitrary $n \times n$ matrix and $B$ a rank one $n \times n$ matrix the determinant of the sum $A + B$ is:

$$\det(A + B) = \det(A) + \sum_{j=1}^{n} \det(A^j),$$  \hspace{1cm} (6.97)

where

$$A^j_{ab} = A_{ab} \hspace{0.5cm} b \neq j$$

$$A^j_{aj} = B_{aj}$$  \hspace{1cm} (6.98)

Using this formula, and the fact that $\det(P) = 0$:

$$F^z_j = \frac{\phi_{j-1}({\mu})}{\phi_{j-1}({\lambda})} \prod_{l=1}^{M} \varphi(\mu_l - \xi_j + \eta) \frac{\det(H - 2P)}{\prod_{l>m} \varphi(\mu_l - \mu_m) \prod_{l<m} \varphi(\lambda_l - \lambda_m)}$$

With this result, the Algebraic Bethe Ansatz brought us precisely what we hoped for: an expression for the norm and both form factors which are the key ingredients for calculating correlation functions.

6.7. Reduced determinants

The Bethe equations in case of string solutions are ill defined. In order to solve this problem, we introduced the Bethe-Takahashi equations. The Gaudin norm and the form factors, which were derived in this chapter, also become ill defined in case of string solutions. Therefore, we should regularize these expressions by hand. To see where the problem occurs, we study the Gaudin norm in case of a single 2-string. Recall the definition of the Gaudin norm(6.80):

$$N_M = \varphi(i\eta)^M \prod_{j \neq k} \frac{\varphi(\lambda_j - \lambda_k + i\eta)}{\varphi(\lambda_j - \lambda_k)} \det \Phi({\lambda_j})$$  \hspace{1cm} (6.100)
6.7 Reduced determinants

and the entries of the Gaudin matrix in explicit form are:

\[
\Phi_{ab} = \delta_{ab} \left( N \frac{-i \sinh(\eta)}{\sin(\lambda_a)^2 + \sinh(\eta/2)^2} - \sum_{k=1}^{M} \frac{-i \sinh(\eta)}{\sin(\lambda_a - \lambda_k)^2 + \sinh(\eta/2)^2} \right) \\
+ (1 - \delta_{ab}) \frac{-i \sinh(\eta)}{\sin^2(\lambda_a - \lambda_b) + \sin^2(\eta)} \\
= \delta_{ab} \left( N \frac{-i \sinh(\eta)}{\sin(\lambda_a + i\eta/2) \sin(\lambda_a - i\eta/2)} - \sum_{k=1}^{M} \frac{-i \sinh(\eta)}{\sin(\lambda_a - \lambda_k + i\eta) \sin(\lambda_a - \lambda_k - i\eta)} \right) \\
+ (1 - \delta_{ab}) \frac{-i \sinh(\eta)}{\sin(\lambda_a - \lambda_b + i\eta) + \sin(\lambda_a - \lambda_b - i\eta)}. \\
\]

(6.101)

Consider one 2-string: \( \lambda_a^2 = \lambda^2 + i\eta(2 + 1 - 2a)/2 + i\delta^2 a \). Let the first two rapidities in the determinant be the 2-string. We will show that \( \Phi_{11}, \Phi_{12}, \Phi_{21} \) and \( \Phi_{22} \) will be divergent. So we examine them in detail:

\[
\Phi_{11} = i \delta_{12} - i \coth(2\eta) - \frac{iN \sinh(\eta)}{\sin(\lambda^2 + i\eta) \sin(\lambda^2)} + \sum_{k=3}^{M} \frac{i \sinh(2\eta)}{\sin(\lambda^2 - \lambda_k + i\eta/2) \sin(\lambda^2 - \lambda_k - i\eta/2)} \\
= \Phi_{12} = \Phi_{21} = \frac{-i \sinh(2\eta)}{\sin(2\eta + i\delta_{12}) \sin(i\delta_{12})} = \frac{-i \sinh(2\eta)}{\sin(2\eta + i\delta_{12}) \sin(i\delta_{12})} = -1 + i \coth(2\eta) + O(\delta) \quad (6.102)
\]

\[
\Phi_{22} = i \delta_{12} - i \coth(2\eta) - \frac{iN \sinh(\eta)}{\sin(\lambda^2 + i\eta) \sin(\lambda^2 - i\eta)} + \sum_{k=3}^{M} \frac{i \sinh(2\eta)}{\sin(\lambda^2 - \lambda_k + i\eta/2) \sin(\lambda^2 - \lambda_k - i\eta/2)}. \\
\]

(6.103)

We want to extract the deviations \( \delta_{12} \) from the determinant. This can be done by row- and column manipulations.

\[
\det\Phi = \begin{vmatrix} \frac{i}{\delta_{12}} + \Phi_{11} & \frac{-i}{\delta_{12}} + \Phi_{12} & \Phi_{13} & \ldots \\
\frac{-i}{\delta_{12}} + \Phi_{12} & \frac{i}{\delta_{12}} + \Phi_{12} & \Phi_{23} & \ldots \\
\Phi_{13} & \Phi_{23} & \Phi_{33} \\
\vdots & \vdots & \ddots & \ddots \\
\end{vmatrix}_{M \times M} \\
= \begin{vmatrix} \frac{i}{\delta_{12}} + \Phi_{11} & \Phi_{11} + \Phi_{12} & \Phi_{11} + 2\Phi_{12} + \Phi_{22} & \Phi_{13} + \Phi_{23} \\
\Phi_{11} + \Phi_{12} & \Phi_{11} + \Phi_{12} & \Phi_{13} + \Phi_{23} \\
\Phi_{13} & \Phi_{13} + \Phi_{23} & \Phi_{33} \\
\vdots & \vdots & \ddots & \ddots \\
\end{vmatrix}_{M \times M} \\
= \begin{vmatrix} \Phi_{11} + 2\Phi_{12} + \Phi_{22} & \Phi_{13} + \Phi_{23} & \ldots \\
\Phi_{13} + \Phi_{23} & \Phi_{33} \\
\vdots & \ddots & \ddots \\
\end{vmatrix}_{M-1 \times M-1} + O(\delta^0) \\
= \frac{i}{\delta_{12}} \det \Phi^{(r)} + O(\delta^0). \\
\]

(6.105)
In the first step we added the first column to the second. The next step was to add the first row to the second row. The final step was to explicitly reduce the determinant to a sum over $M - 1 \times M - 1$ determinants and keep only the leading term. The reduced matrix $\Phi^{(r)}$ is now an $M - 1 \times M - 1$ matrix. The factor $1/\delta^{12}$ cancels against another term in the expression for the Gaudin norm, namely:

$$\frac{\varphi(\lambda_2^2 - \lambda_1^2 + i\eta)}{\varphi(\lambda_2^2 - \lambda_1^2)} \approx \frac{i\delta^{12}\varphi(i2\eta)}{\varphi(i\eta)\varphi(-i\eta)}. \quad (6.106)$$

So the complete expression of the Gaudin norm is now independent of the string deviation $\delta^{12}$:

$$N_M = \varphi(i\eta)^{M-2}\varphi(2i\eta) \prod_{j \neq k, 1 \neq 2} \frac{\varphi(\lambda_j - \lambda_k + i\eta)}{\varphi(\lambda_j - \lambda_k)} \det \Phi^{(r)}(\{\lambda_j\}). \quad (6.107)$$

We can generalize this result to an arbitrary string solution. Focusing on the determinant in the Gaudin norm, it can be written in terms of the reduced determinant:

$$\det \Phi(\{\lambda\}) = \prod_j M_j \prod_{\alpha=1}^{n_j-1} \prod_{a=1}^{\delta_{n_j,a}^{\alpha}} (\delta_{\alpha,\alpha}^{\alpha,a} - \delta_{\alpha,\alpha}^{\alpha,a+1})^{-1} \det \Phi^{(r)} \quad (6.108)$$

and the reduced Gaudin matrix is:

$$\Phi^{(r)}_{(j,\alpha)(k,\beta)} = \delta_{jk}\delta_{\alpha,\beta} \left( N \frac{d}{d\lambda_{\alpha,j}} \Theta_{j}(\lambda_{\alpha,j}) - \sum_{(l,\gamma) \neq (j,\alpha)} \frac{d}{d\lambda_{\alpha,l}} \Theta_{jl}(\lambda_{\alpha,l} - \lambda_{\gamma,l}) \right)$$

$$+ \left( 1 - \delta_{jk}\delta_{\alpha,\beta} \right) \frac{d}{d\lambda_{\alpha}} \Theta_{jk}(\lambda_{\alpha,j} - \lambda_{\beta,j}). \quad (6.109)$$

The expressions for $H_{ab}$, $H_{-ab}$ and $P_{ab}$ contain similar divergences, which can be dealt with in a similar (although much more cumbersome) way[43].

While we have not used these expressions in this thesis, they would be indispensable for further applications, for example calculating the longitudinal form factors.
7. Correlation functions

In this chapter we will answer the theme question of this thesis: what are the dynamics of the XXZ model. We will do this by computing the dynamical correlation function in terms of the form factors obtained in chapter six.

When an experimentalist wants to study a system, he or she usually perturbs the system by means of an external probe (this can be done by means of X-rays, magnetic field, a beam of neutrons, etc.) and measures the response of the system. Up until now we only looked at the unperturbed Hamiltonian of the XXZ model. However, if we want to make a connection with experiments, we should consider a perturbed Hamiltonian. We will do this by means of linear response theory, which gives us the dynamical structure factor. Calculating the DSF is the central goal of this thesis.

7.1. Linear response theory

We consider a system in equilibrium, subject to an external perturbation that may be time dependent:

\[ H_{\text{tot}} = H_0 + H_{\text{ext}}. \]  

(7.1)

We assume that the external perturbation couples linearly to an observable \( \hat{A} \).

\[ H_{\text{ext}} = \sum_{j=1}^{N} \hat{A}_j F_j(t) \]  

(7.2)

Here \( F_j(t) \) is called a generalized force causing the perturbation. Suppose we measure the response of another observable \( \hat{B} \). Using the Heisenberg picture: \( \hat{B}_j(t) = \hat{U}_0^{-1}(t) \hat{B}_j \hat{U}_0(t) \), where \( \hat{U}_0 \) is the time evolution operator of the unperturbed Hamiltonian, we can define the response as:

\[ \langle \delta \hat{B}_j(t) \rangle \equiv \langle B_j(t) \rangle_{H_{\text{tot}}} - \langle B_j(t) \rangle_{H_0} = \langle \hat{U}_F^{-1}(t) \hat{B}_j(t) \hat{U}_F \rangle_{H_0}, \]  

(7.3)

where \( \hat{U}_F(t) = \hat{U}_0^{-1}(t) \hat{U}(t) \) with \( \hat{U} \) the evolution operator of the full Hamiltonian. The operator \( \hat{U}_F \) obeys the differential equation:

\[ \frac{d}{dt} \hat{U}_F(t) = -i H_{\text{ext}} \hat{U}_F(t) = -i \sum_{j'} F_{j'}(t) \hat{A}_{j'} \hat{U}_F(t). \]  

(7.4)

Integrating both sides and using that \( \hat{U}_F(t \to -\infty) \to 1 \) we get:

\[ \hat{U}_F(t) = \exp \left(-i \sum_{j'} \int_{-\infty}^{t} dt' F_{j'}(t') \hat{A}_{j'}(t') \right) = 1 - i \sum_{j'} \int_{-\infty}^{t} dt' F_{j'}(t') \hat{A}_{j'}(t') + O(F^2). \]  

(7.5)
Correlation functions

Substituting this into (7.3) yields
\[
\langle \delta \hat{B}_j(t) \rangle = -i \sum_{j'} \int_{-\infty}^{\infty} dt' \theta(t - t') F_{jj'}(t') \left\langle \left[ \hat{B}_j(t), \hat{A}_{j'}(t') \right] \right\rangle = \sum_{j'} \int_{-\infty}^{\infty} dt' D_{BA}(t - t')_{jj'} F_{jj'}(t'),
\] (7.6)
where \( D_{BA}(t, t')_{jj'} \) is the retarded Green’s function. If the unperturbed system is homogeneous in space and time, \( D_{AB}(t, t')_{jj'} \) can only be a function of \( t - t' \) and \( j - j' \), and the response term is a convolution. Using the convolution theorem, the Fourier transform is:

\[
\langle \delta B(q, \omega) \rangle = \chi_{AB}(q, \omega) F(q, \omega)
\] (7.7)
where \( \chi_{AB} \) is the generalized susceptibility:

\[
\chi(q, \omega) = \frac{1}{N} \sum_{j,j'} e^{-iq(j-j')} \int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t) \left\langle \hat{B}(t) \hat{A}(0) - \hat{A}(0) \hat{B}(t) \right\rangle.
\] (7.8)
We shifted \( t \) such that \( t' = 0 \). Using the integral representation of the Heaviside function:

\[
\theta(t) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' e^{i\omega' t} / (\omega' - i0^+)
\] (7.9)
and the fact that: \( \langle \hat{A}(0) \hat{B}(t) \rangle = \langle \hat{A}(0) \hat{B}(0) \rangle \). We can express the susceptibility as:

\[
\chi(q, \omega) = \frac{1}{N} \int_{-\infty}^{\infty} d\omega' S(q, \omega') - S(q, -\omega') / 2\pi (\omega - \omega' + i0^+),
\] (7.10)
where \( S(q, \omega) \) is the dynamical structure factor (DSF), which is defined as:

\[
S(q, \omega) = \frac{1}{N} \sum_{j,j'} e^{-iq(j-j')} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \hat{A}_j(t) \hat{B}_{j'}(0) \rangle,
\] (7.11)
which is the Fourier transform of the dynamical correlation function. In the next section we write the DSF in terms of the form factors we derived in chapter six.

7.2. The dynamical structure factor
A typical two-point function for an operator \( \mathcal{O}_j^\alpha(t) \), and its Hermitian conjugate \( \mathcal{O}_j^\beta(0) \), is:

\[
\langle \mathcal{O}_j^\alpha(t) \mathcal{O}_j^\beta(0) \rangle_{\beta},
\] (7.12)
in which \( \langle ... \rangle = \frac{1}{Z} \sum_{\lambda} e^{-\beta E_{\lambda}} \), where \( Z \) is the partition function. In case of the spin chain we have a longitudinal operator \( S_j^z \) and transverse operators: \( S_j^+, S_j^- \). So the DSF becomes:

\[
S^{a\bar{a}}(q, \omega) = \frac{1}{N} \sum_{j,j'=1}^N e^{-iq(j-j')} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S_j^a(t) S_{j'}^{\bar{a}}(0) \rangle_{\beta},
\] (7.13)
where \( a \in \{-, +, z\} \). We can express this in terms of form factors by introducing a summation over intermediate states:

\[
S^{a\bar{a}}(q, \omega) = \frac{1}{N} \sum_{j,j'=1}^N e^{-iq(j-j')} \int_{-\infty}^{\infty} dt \frac{e^{i\omega t}}{Z} \sum_{\lambda,\mu} \langle \lambda | S_j^a(t) | \mu \rangle \langle \mu | S_{j'}^{\bar{a}}(0) | \lambda \rangle e^{-\beta E_{\lambda}}.
\] (7.14)
7.3 Sum rules

To remove the $t-$dependence in the operators we switch to the Schrödinger picture:

$$\langle \lambda | O^a_j(t) | \mu \rangle = \langle \lambda | e^{iHt} O^a_j e^{-iHt} | \mu \rangle = e^{i(E_\lambda - E_\mu)t} \langle \lambda | O^a_j | \mu \rangle$$  \hspace{1cm} (7.15)$$

and using the Fourier transform of the form factors:

$$\frac{1}{\sqrt{N}} \sum_j e^{-ijqj} \langle \lambda | O^a_j | \mu \rangle = \langle \lambda | O^a_q | \mu \rangle.$$ \hspace{1cm} (7.16)$$

Using this and performing the $t$ integral gives the DSF in terms of Fourier transformed form factors:

$$S^{\alpha \bar{\alpha}}(q,\omega) = 2\pi \frac{1}{Z} \sum_{\lambda,\mu} |\langle GS | S^\alpha_j | \mu \rangle|^2 e^{-\beta E_\lambda} \delta(\omega - E_\mu + E_\lambda).$$ \hspace{1cm} (7.17)$$

At zero temperature the system is in the ground state and the DSF reduces to a single summation of form factors:

$$S^{\alpha \bar{\alpha}}(q,\omega) = 2\pi \sum_{\mu} |\langle GS | S^\alpha_q | \mu \rangle|^2 \delta(\omega - E_\mu + E_0).$$ \hspace{1cm} (7.18)$$

Now we can compute the DSF by summing of all form factors.

**DSF in zero field**

For zero field the system is rotational invariant around the $z-$axis. We therefore have: $S^{-+}(q,\omega) = S^{+-}(q,\omega) = 2S^{xx}(q,\omega) = 2S^{yy}(q,\omega)$.

### 7.3 Sum rules

An important property of the correlation function is that it obeys a number of sum rules. These rules will turn out to be an important check for numerical calculations. It is useful to write the spin operators in position space:

$$S^{\alpha \bar{\alpha}}(q,\omega) = \frac{1}{N} \sum_{j,j'} e^{i(q(j-j'))} \sum_{\mu} 2\pi \delta(\omega - E_\mu + E_0) \langle GS | S^\alpha_j | \mu \rangle \langle \mu | S^{\bar{\alpha}}_{j'} | GS \rangle.$$ \hspace{1cm} (7.19)$$

Integrating over all $\omega$ and summing of over all $q$:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} 2\pi \frac{1}{N} \sum_q S^{\alpha \bar{\alpha}}(q,\omega) = \frac{1}{N} \sum_{j,j'} N \delta_{j,j'} \sum_{\mu} \langle GS | S^\alpha_j | \mu \rangle \langle \mu | S^{\bar{\alpha}}_{j'} | GS \rangle = \frac{1}{N} \sum_j \langle GS | S^\alpha_j S^{\bar{\alpha}}_j | GS \rangle.$$ \hspace{1cm} (7.20)$$

The sum rules for the transverse and longitudinal correlation function now readily follow:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} 2\pi \frac{1}{N} \sum_q S^{-+}(q,\omega) = \frac{1}{N} \sum_j \langle GS | S^z_j S^z_j | GS \rangle = \frac{1}{N} \sum_j \langle GS | \frac{1}{2} - S^z_j | GS \rangle = \frac{1}{2} - \langle S^z \rangle = \frac{M}{N}.$$ \hspace{1cm} (7.21)$$

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} 2\pi \frac{1}{N} \sum_q S^{zz}(q,\omega) = \frac{1}{N} \sum_j \langle GS | S^z_j S^z_j | GS \rangle = \frac{1}{4}.$$ \hspace{1cm} (7.22)$$
7.3.1. First frequency moments

Another useful sum rule is called the first frequency moment\(^1\): it is the expectation value of the transferred energy \(\langle \omega \rangle\) at momentum \(q\):

\[
\langle \omega_{\text{at}} \rangle \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega S_{\text{at}}(q, \omega).
\] (7.23)

For the zero-temperature DSF (7.18), and in case of Hermitian operators, we can re-express this in a more useful form:

\[
\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega S_{\text{a}}(q, \omega) = \frac{1}{N} \sum_{j,j'} e^{ik(j-j')} \sum_{\mu} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} 2\pi \delta(\omega - E_\mu - E_0) \langle GS | S^q_{j} | \mu \rangle \langle \mu | S^q_{j'} | GS \rangle
\]

\[
= \frac{1}{N} \sum_{j,j'} e^{ik(j-j')} \sum_{\mu} (E_\mu - E_0) \langle GS | S^q_{j} | \mu \rangle \langle \mu | S^q_{j'} | GS \rangle
\]

\[
= \frac{1}{N} \sum_{j,j'} e^{ik(j-j')} (-1) \langle GS | [H, S^q_{j}] | \mu \rangle \langle \mu | S^q_{j'} | GS \rangle
\]

\[
= \frac{1}{2N} \sum_{j,j'} e^{ik(j-j')} (-1) \langle GS | [H, S^q_{j}] , S^q_{j'} | GS \rangle.
\] (7.24)

It is easy to check that (putting \(J\) temporarily to unity):

\[
[H, S^x_j] = -i S^y_{j-1} S^z_j - i S^z_{j-1} S^y_j + i \Delta S^z_{j-1} S^y_j + i \Delta S^y_{j-1} S^z_j.
\] (7.25)

When computing \([H, S^q_j], S^q_{j'}\) we need to consider three cases:

\[
[H, S^q_j], S^q_{j'} = S^q_{j-1} S^q_{j} + S^q_{j} S^q_{j+1} + \Delta S^q_{j-1} S^q_{j} + \Delta S^q_{j} S^q_{j+1}
\] (7.26a)

\[
[H, S^q_j], S^q_{j-1} = -e^{iq} \left( S^q_{j-1} S^q_{j} + \Delta S^q_{j-1} S^q_{j} \right)
\] (7.26b)

\[
[H, S^q_j], S^q_{j+1} = -e^{-iq} \left( S^q_{j-1} S^q_{j} + \Delta S^q_{j-1} S^q_{j} \right)
\] (7.26c)

If we take the sum over \(j'\) we get:

\[
\sum_{j,j'} [H, S^q_j], S^q_{j'} = 2 \sum_{j} (1 - \Delta \cos q) S^q_{j} S^q_{j+1} + (\Delta - \cos q) S^q_{j} S^q_{j-1}.
\] (7.27)

Similarly, we have:

\[
\sum_{j,j'} [H, S^q_j], S^q_{j'} = 2 \sum_{j} (1 - \Delta \cos q) S^q_{j} S^q_{j+1} + (\Delta - \cos q) S^q_{j} S^q_{j-1}
\] (7.28)

\[
\sum_{j,j'} [H, S^q_j], S^q_{j'} = 2 \sum_{j} (1 - \cos q) \left( S^q_{j} S^q_{j+1} + S^q_{j} S^q_{j-1} \right).
\] (7.29)

The first moment frequency in the transverse case is (after reinserting \(J\)):

\[
\langle \omega_{-} \rangle \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega 2S^{xx}(q, \omega) = -\frac{2J}{N} ((1 - \Delta \cos q) X^y + (\Delta - \cos q) X^z)
\] (7.30)

\(^1\)“First” refers to the power of \(\omega\), in general you have the n-th frequency moment \(\langle \omega^n \rangle\).
7.4 Transverse Dynamical Structure Factor (TDSF)

where \( X^a \equiv \sum_j \langle S_j^a S_{j+1}^a \rangle \), \( a = x, y, z \). Note that for \( \Delta = 1 \) the first frequency moment is identically zero for \( q = 0, 2\pi \). In the longitudinal case we have:

\[
\langle \omega_{zz} \rangle = -\frac{J}{N} (1 - \cos(q)) (X^x + X^y).
\]  

(7.31)

The \( X^a \) can be computed from the ground state energy \( E_0 \) and the anisotropy \( \Delta \) dependence. For the XXX model we use the rotational symmetry at zero field: \( X^a = \langle H \rangle_{GS}/3 = E_0/3 \) with \( a \in \{x, y, z\} \). In case of the XXZ model we can compute \( X^z \) using: \( X^z = \langle \frac{dH}{d\Delta} \rangle = \frac{dE_0(\Delta)}{d\Delta} \) and \( X^y = (\langle H \rangle - \Delta X^z)/2 = (E_0 - \Delta \frac{dE_0}{d\Delta})/2 \).

### 7.4. Transverse Dynamical Structure Factor (TDSF)

In order to compute the TDSF at zero temperature and zero field,

\[
S^{+}(q, \omega) = 2\pi \sum_{\mu} |\langle GS | S_q^- | \mu \rangle|^2 \delta(\omega - E_\mu + E_0),
\]  

(7.32)

we need to compute the Fourier transform of the form factors (6.85):

\[
|\langle \mu \rangle | S_q^- | \lambda \rangle \rangle|^2 = \frac{\sum_{j,j'} e^{-i\eta(j-j')} F_{j}^{-} F_{j'}^{-*}}{N(\{\mu\})N(\{\lambda\})}
\]  

(7.33)

with \( \{\mu_j\} \) the ground state. Recalling from chapter six the definition of the form factor (6.85):

\[
F_{j}^{-} (\{\mu\}_{M+1}, \{\lambda\}_M) = \frac{\phi_{j-1}(\{\mu\})}{\phi_{j-1}(\{\lambda\})} \prod_{l=1}^{M} \varphi(\lambda_l - \xi_j) \varphi(\lambda_l - \xi_j + \eta) \prod_{j<k} \varphi(\mu_j - \mu_k) \prod_{j>k} \varphi(\lambda_j - \lambda_k).
\]  

(7.34)

The only \( j \)-dependence comes from the factors \( \phi_j(\{\mu\}) \). We can express them in a more useful form, using the relation between the momentum operator and the transfer matrix: \( iP = \ln T(i\eta/2) \). We can relate the eigenvalues \( q \) of \( P \) to the eigenvalues of the transfer matrix:

\[
q_\mu = \frac{i}{N} \sum_{k=1}^{M} \frac{1}{\nu(\mu_k)}.
\]  

(7.35)

Hence, it follows that:

\[
\phi_j(\{\mu\}) = \prod_{l=1}^{M} \left( \frac{\varphi(\mu_l + i\eta/2)}{\varphi(\mu_l - i\eta/2)} \right)^j = e^{-i\eta q_j}.
\]  

(7.36)

This yields:

\[
|\langle \mu \rangle | S_q^- | \lambda \rangle \rangle|^2 = N \delta_{q,q(\lambda)-q(\mu)} |\varphi(i\eta)| \frac{\prod_{j=1}^{M} |\varphi(\mu_j - i\eta/2)|^2}{\prod_{j=1}^{M-1} |\varphi(\lambda_j - i\eta/2)|^2} \prod_{j>k}^{M} \left| \varphi^2(\mu_j - \mu_k) + \varphi^2(i\eta) \right|^{-1} \prod_{j>k}^{M-1} \left| \varphi^2(\lambda_j - \lambda_k) + \varphi^2(i\eta) \right|^{-1} \frac{\det H}{|\det \Phi(\{\mu\}) \det \Phi(\{\lambda\})|}.
\]  

(7.37)
Correlation functions

Similarly, one can compute the Fourier transform of the longitudinal form factor:

\[ |\langle \{\mu\}|S_z^2|\{\lambda\}\rangle|^2 = \frac{N}{4} \delta_{q,q(\lambda)-q(\mu)} \prod_{j=1}^{M} \frac{\varphi(\mu_j - i\eta/2)^2}{\varphi(\lambda_j - i\eta/2)^2} \prod_{j\neq k=1}^{M} \frac{|\varphi(\mu_j - \mu_k) + \varphi(\mu_j)|^{-1} |\varphi(\lambda_j - \lambda_k) + \varphi(\lambda_j)|^{-1} |\det H - 2P|^2}{|\det \Phi(\{\mu\})\det \Phi(\{\lambda\})|^2}. \]  

(7.38)

7.4.1. Results

We computed the TDSF (7.18) in case of two-spinon excitations. Since we should count every unique state only once, the classification presented in chapter three is very important. The form factors in (7.38) are not a continuous function of \(\omega\). Therefore, the delta-functions in (7.18) are replaced by Gaussian functions of width \(\epsilon \sim 1/N\): \(\delta_\epsilon(x) = (1/\sqrt{\pi\epsilon})e^{-x^2/\epsilon^2}\) and the integral is replaced by a sum:

\[
\int f(x)\delta(x) \to \sum_{x_i} \frac{f(x_i)}{\sqrt{\pi}} e^{-(x-x_i)^2/\epsilon^2}.
\]

There is no natural choice for the \(\epsilon\), however it should be larger than the minimal spacing between energy levels at fixed momentum. But fortunately, the DSF does not change significantly for various choices of the width of the Gaussians. The results for \(\Delta = 2, 4, 8, 16\) are plotted in fig. 7.1. In the limit \(\Delta \to 1\), the contribution of the two-spinon excitations of the quasi-degenerate ground state completely vanishes. While in the Ising limit \(\Delta \to \infty\) both sets of excitations have an equal contribution.

Since for \(\Delta > 1\) and large \(N\) the ground state becomes almost exactly degenerate, we should also take the quasi-degenerate ground state with momentum \(\pi\) into account. In fig. 7.2 the form factors are plotted both for excitations on the true ground state (-) and for the quasi-degenerate ground state (+). The lower curves are for momentum \(q = \pi/4\), both for the two sets – and +. The upper curves are for momentum \(q = 3\pi/4\). It is clear that form factors built on both ground states are equal up to \(1/N\) corrections. In the thermodynamic limit these should become equivalent.

Based on the work of Miwa and Jimbo, the TDSF at zero field can also be computed in the thermodynamic limit. Both methods are in excellent agreement; a detailed comparison can be found in [29]. In our results, there is a clear asymmetry around \(q = \pi/2\) which only vanishes when \(\Delta \to \infty\), see also fig. 7.2. This is in contradiction with the earlier result [44], where the same TDSF is calculated in the thermodynamic limit but with a symmetry around \(q = \pi/2\). A technical discussion of both approaches in the thermodynamic limit can be found in [29].

Sum rules

The number of states we used is only a very small fraction of the total number of states, namely:

\[
\frac{N}{N-M} \left( \frac{N-M}{M} \right) / \left( \frac{N}{M} \right). \]

(7.39)
7.4 Transverse Dynamical Structure Factor (TDSF)

Figure 7.1.: The transverse dynamical structure factor for $\Delta = 2, 4, 8, 16$ for $N = 200$ and zero field. The horizontal axis is the transferred momentum, the vertical axis is the transferred energy. The color indicates the weight of the DSF: red is maximum weight, blue is zero weight.
Figure 7.2.: The square of the form factor $F^-$ for two-spinon excitations over the true ground state (−) and over the quasi-degenerate ground state (+). The lower curves are for momentum $q = \pi/4$, both for the two sets − and +. The upper curves are for momentum $q = 3\pi/4$. In all cases $\Delta = 4$.

In case of $N = 200$ this fraction is: $1 \cdot 10^{-53}$, which is an extremely small number, so we should check the accuracy of our two-spinon results. By summing all form factors we can see how well it saturates to $1/2$, the value predicted by the sum rule (7.21):

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th>$N = 20$</th>
<th>$N = 100$</th>
<th>$N = 200$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>99.3681%</td>
<td>99.1154%</td>
<td>99.1153%</td>
</tr>
<tr>
<td>4</td>
<td>99.9497%</td>
<td>99.9496%</td>
<td>99.9496%</td>
</tr>
<tr>
<td>8</td>
<td>99.9969%</td>
<td>99.9969%</td>
<td>99.9969%</td>
</tr>
<tr>
<td>16</td>
<td>99.9998%</td>
<td>99.9998%</td>
<td>99.9998%</td>
</tr>
</tbody>
</table>

Table 7.1.: Saturation of the sum rule for different values of $\Delta$ and $N$.

It is clear that the TDSF for $\Delta > 0$ at zero temperature and zero field are almost completely dominated by two-spinon excitations. Only in the limit $\Delta \to 1$ one can expect significant contributions from higher spinon excitations. From table 7.1 one can also see that the system size has almost no influence on the saturation.
8. Conclusions and Outlook

8.1. Conclusions

The goal of this thesis was to study the dynamics of the XXZ chain for $\Delta > 1$. More specifically, to study the dynamical structure factor (DSF), which is measured in neutron scattering experiments performed on spin chains.

The eigenstates, in terms of the momenta of the down spins, were obtained exactly by means of the Bethe Ansatz. Following from the periodic boundary conditions for our spin chain, we obtained the Bethe equations, which are a restriction for the momenta of the down spins. These equations are in general extremely hard to solve. By taking the logarithm of the Bethe equations, solutions can be parametrized in terms of quantum numbers. A classification in terms of these quantum numbers is needed, as some different sets of quantum numbers may result in the same state. In case of the XXX model, and the XXZ model for $|\Delta| < 1$, such a classification was already known for the case where the string hypothesis holds.

One of the difficulties that had to be overcome during my research was to come up with a classification scheme for the region where $\Delta > 1$. The approach used for $|\Delta| \leq 1$ could not be adopted in case of the gapped regime, as the rapidities now lie in a finite interval, and the Bethe equations are periodic in $\lambda$. By studying explicitly these invariances of the Bethe equations both in terms of rapidities and in terms of quantum numbers, a classification has been made for real two-spinon excitations.

An interesting observation is that for $\Delta > 1$ the ground state is quasi-degenerate, which is not the case for $|\Delta| < 1$. The ground state becomes exactly degenerate either in the limit $\Delta \rightarrow \infty$ or in the thermodynamic limit. As a result of these quasi-degenerate ground states there are now two sets of two-spinon excitations, built on one of both sets.

The quantum numbers following from our classification enable us to obtain the rapidities up to machine precision, by solving the Bethe equations numerically. This allows us to explicitly construct the ground state and the two-spinon excitations, bringing us in the position to compute the transverse dynamical structure factor (TDSF).

The algebraic Bethe ansatz, which is the second-quantized version of the Bethe ansatz in which spin operators and wavefunctions are treated in the same manner, allows us to compute form factors. These form factors are matrix elements of local spin operators between different states. A summation over Fourier transformed form factors will eventually result in the DSF.

The sum over all form factors is truncated up to two-spinon states. For the transverse case this means that all two-spinon excitations are real, and therefore can easily be computed. The TDSF was obtained for $N = 200$ at zero temperature and zero field.

A drawback of calculating the DSF for a finite lattice is the fact that the result is a set of discrete points instead of a continuous function. To solve this, we approximated the delta-functions as Gaussians with a certain width. Unfortunately, there is no natural choice of the width of these Gaussians. One can play with several choices for the width, or, even more advanced, let the width depend on the energy. But fortunately, the DSF does not change
Conclusions and Outlook

significantly for various choices of the width of the Gaussians. Nevertheless, it is desirable to eliminate this freedom as much as possible by taking a sufficiently large system.

Although the number of two-spinon excitations is an incredibly small fraction of the total number of states, they carry almost 100% of the weight of the TDSF, which can be shown using the sum rules. In order to study the size dependence of the saturation for the sum rules, these results were calculated for different system sizes. For all $N$ the result saturates extremely well. Only in the limit $\Delta \to 1$ one can expect significant contributions from higher spinon excitations.

These results show that the Bethe Ansatz approach used to tackle the problem of computing the DSF was an extremely efficient method for obtaining very accurate results.

8.2. Further steps

To understand the full dynamics of the gapped XXZ model many remains to be done. Below we will discuss the most important ones.

8.2.1. Longitudinal DSF

The longitudinal dynamical structure factor (LDSF) at zero temperature is given by:

$$S_{zz}(q, \omega) = 2\pi \sum_{\mu} |\langle GS|O_{q}^{z}|\mu\rangle|^2 \delta(\omega - E_{\mu} + E_{0}).$$  \hspace{1cm} (8.1)

Both the ground state and the two-spinon excitations $\{\mu\}$ have $M = N/2$ down spins. This means that the two-spinon excitations are now not only composed of real rapidities, but contain a pair of complex rapidities.

For several reasons, complex solutions are more difficult to work with. First of all, the solutions to the complex case are harder to find. When the complex pair is a slightly deviated 2-string, the Bethe-Takahashi equations can be used. However, if the complex pair is a strongly deviated 2-string, there is no known procedure to find them. Furthermore, the determinant expressions for the norm and the form factors become indeterminate, a problem which is solved by regularizing the expression of the determinant by hand.

8.2.2. Temperature effects

The temperature-dependent dynamical structure factor is given by:

$$S^{a\bar{a}}(q, \omega) = 2\pi \frac{1}{Z} \sum_{\lambda,\mu} |\langle \lambda|O_{q}^{a}|\mu\rangle|^2 e^{-\beta E_{\lambda}} \delta(\omega - E_{\mu} + E_{\lambda}).$$  \hspace{1cm} (8.2)

There is a double sum, over $\mu$ and $\lambda$, which makes the calculation difficult to do, since the number of form factors to be calculated is very large. The situation is best for the XXZ model for $\Delta > 1$, since it is gapped and could expect a fewer number of states are needed. However, for finite temperature we should at least compute in the order of $N^4$ form factors, which is a large number compared with the $N^2$ needed for zero temperature. This makes large systems sizes using the current approach intractable. Another problem is the computation of the partition function $Z$ which is quite non-trivial since the sum over Boltzmann factors cannot easily be truncated.
8.3 Other directions

8.2.3. Finite magnetic field

The method used in this thesis is easily generalized for a finite magnetic field in the z-direction. In this case the number of down spins is \( M < N/2 \). This breaks the symmetry in the \( x \) and \( y \)–direction, hence for the TDSF we should now calculate both \( S^{+}(q,\omega) \) and \( S^{-}(q,\omega) \).

8.2.4. Roots of the Bethe equations

As already pointed out a couple of times in this thesis, very little is known of the complex solutions, especially for the case \( \Delta > 1 \) at zero field. It is important that these solutions are found, as they are necessary for further applications. Another reason is that a complete set of solutions would be desirable. First of all, one could try to prove completeness. Secondly, having found all solutions and knowing what they look like might give a better insight in the Bethe Ansatz. The problem is that in the parametrization we used the Bethe equations are transcendental. A different representation of the Bethe Ansatz equations would be desirable. A promising method is to use Baxter’s \( TQ \) equation instead of the Bethe equations to obtain the Bethe roots.

8.2.5. Thermodynamic limit

Instead of working with a finite lattice one could also work in the thermodynamic limit. The advantage of this approach is that for example the two-spinon TDSF in the gapped regime can be obtained analytically. However, much remains to be done. It is not clear how the LDSF should be calculated or how magnetic fields should be incorporated. A close comparison between the finite lattice results and infinite lattice results may be helpful.

8.2.6. Comparison with experiments

The ultimate goal is an accurate comparison between theory and experiments. The most common experiment related to spin chains is inelastic neutron scattering. Until recently, all experiments performed on spin chains in the gapped regime used a beam of unpolarized neutrons, which means that the transverse correlation function cannot be measured separately. The longitudinal dynamical structure factor should therefore also be computed.\(^1\) Furthermore, inelastic neutron scattering experiments are necessarily performed at \( T > 0 \), since for \( T \to 0 \) the correlation between spins becomes such that the material cannot be modeled by a one-dimensional theory. It is therefore necessary to include finite-temperature effects.

8.3. Other directions

Instead of focusing on the dynamics of the XXZ model, one can also apply the Bethe Ansatz techniques for other purposes. First one could think of generalizations of the XXZ, such as a chain with open boundaries or higher spin chains, nonuniform field etc. Secondly, one can also apply the obtained techniques to other integrable systems like the one-dimensional Bose gas or the one-dimensional Hubbard model.

One can also study quantum quenches: a parameter in the system, for example an interaction coupling or external field, is suddenly changed. After such a quench the system

\(^1\)Although recent experiments make use of polarized neutron beams, there are no results yet known for the gapped spin chain.
Conclusions and Outlook

will in general not be in equilibrium. An experiment one can think of are one-dimensional Bose gases that are trapped. When one wants to measure the momentum distribution, one usually releases the interacting gas from the trap. Now a mapping should be made between the distribution of the free theory and the interacting gas.

One could treat a spin chain as a register of coupled qubits. An essential ingredient in quantum computation is entanglement of qubits. Although entanglement between two qubits is well-defined, it is not clear what the definition for more than two qubits should be. For this reason various measures of entanglement exist. These different measures are difficult to compare because usually they are computed for different systems. However, the Bethe Ansatz technique brings us in a good position to calculate and compare various measures since the results are exact.

The use of the Bethe Ansatz is not only restricted to condensed matter problems. In the field of high-energy physics a remarkable correspondence between a $\mathcal{N} = 4$ supersymmetric Yang-Mills theory and a integrable spin chain was recently discovered.

When Bethe introduced his Ansatz in 1931 it was merely used as a trick to solve one specific model: the one-dimensional Heisenberg spin chain. In these days this was ‘just’ a theoretical model. Many years later it was realized that the Bethe Ansatz is an extremely powerful tool which can be applied for various integrable models, most of which nowadays have experimental realizations. The influence of the algebraic Bethe Ansatz cannot easily be overemphasized: on the one hand the Yang-Baxter equation gave birth to a pure mathematical concept of quantum groups, while on the other hand it led to predictions for experiments.
A. Bethe Ansatz function definitions

A.1. Bethe equation

The Bethe equations for the XXZ model are:

\[
\left( \frac{\varphi(\lambda_j + i\eta/2)}{\varphi(\lambda_j - i\eta/2)} \right)^N = \prod_{k \neq j} \frac{\varphi(\lambda_j - \lambda_k + i\eta)}{\varphi(\lambda_j - \lambda_k - i\eta)} \tag{A.1}
\]

and in logarithmic form:

\[
\theta_1(\lambda_j) = \frac{\pi}{N} I_j + \frac{1}{N} \sum_{l=1}^{M} \theta_2(\lambda_j - \lambda_l). \tag{A.2}
\]

In case the string hypothesis holds we should use the Bethe-Takahashi equations:

\[
\theta_1(\lambda_j) = \frac{\pi}{N} I_j + \frac{1}{N} \sum_{l=1}^{M} \Theta_{mn}(\lambda_j - \lambda_l). \tag{A.3}
\]

\[
\Theta_{mn}(\lambda) \equiv \begin{cases} 
\theta_{|n-m|}(\lambda) + 2\theta_{|n-m|+2}(\lambda) + \ldots + 2\theta_{n+m} + \theta_{|n-m|} & n \neq m \\
2\theta_2(\lambda) + 2\theta_4(\lambda) + \ldots + 2\theta_{2n-2}(\lambda) + \theta_{n+m} & n = m 
\end{cases} \tag{A.4}
\]

The several parametrizations are:

<table>
<thead>
<tr>
<th>( \Delta )</th>
<th>XXX</th>
<th>XXZ gapless</th>
<th>XXZ gapped</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \varphi(\lambda) )</td>
<td>( \lambda )</td>
<td>( \sinh \lambda )</td>
<td>( \sinh \lambda )</td>
</tr>
<tr>
<td>( \theta_n(\lambda) )</td>
<td>( 2 \arctan \frac{2\lambda}{n} )</td>
<td>( \frac{1}{\pi} \frac{n}{4\lambda^2 + n^2} )</td>
<td>( \frac{1}{\pi} \frac{n}{\cosh 2\lambda - \cos n\eta} )</td>
</tr>
<tr>
<td>( \frac{d}{d\lambda} \theta_n(\lambda) )</td>
<td>( \frac{1}{\pi} )</td>
<td>( \frac{1}{\pi} )</td>
<td>( \frac{1}{\pi} )</td>
</tr>
</tbody>
</table>

A.2. Algebraic Bethe Ansatz

\[
a(\lambda) = 1 \tag{A.5}
\]

\[
b(\lambda, \mu) = \frac{\varphi(\lambda - \mu)}{\varphi(\lambda - \mu + i\eta)} \tag{A.6}
\]

\[
c(\lambda, \mu) = \frac{\varphi(i\eta)}{\varphi(\lambda - \mu + i\eta)} \tag{A.7}
\]

\[
d(\lambda) = \prod_{i=1}^{N} b(\lambda, \xi_i) \tag{A.8}
\]

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In the homogeneous limit: $\xi_i = \eta/2, i = 1 \ldots N$. The Bethe equations in terms of these functions are:

$$\frac{a(\lambda_n)}{d(\lambda_n)} \frac{M}{\prod_{j \neq n} b(\lambda_n - \lambda_j)} = 1. \quad (A.10)$$

The eigenvalue of the transfer matrix is:

$$\tau(\mu, \{\lambda_j\}) = a(\mu) \prod_{j=1}^{M} \frac{1}{b(\lambda_j - \mu)} + d(\mu) \prod_{j=1}^{M} \frac{1}{b(\mu - \lambda_j)}. \quad (A.11)$$

$$\phi_j(\{\lambda\}) = \prod_{l=1}^{M} \prod_{k=1}^{j} b^{-1}(\lambda_l, \xi_k) \quad (A.12)$$

When the set $\{\lambda_j\}$ is a solution of the Bethe equation it reduces to:

$$\phi_j(\{\lambda\}) = \exp(-i q_\lambda j) \quad (A.13)$$

with $q_\lambda$ the total momentum of the state. Another frequently used is expression is:

$$\frac{d}{d\lambda} d(\lambda) = Nd(\lambda) \frac{\phi(i\eta)}{\phi(\lambda + i\eta/2)\phi(\lambda - i\eta/2)}. \quad (A.14)$$
B. Useful functions

B.1. Spin operators

For spin−1/2 particles we can represent the spin operators in terms of Pauli matrices:

\[ S_a = \frac{\hbar}{2} \sigma_a \quad a \in \{x, y, z\}. \]  \hspace{1cm} (B.1)

We will put \( \hbar \) to unity, and the Pauli matrices are defined as:

\[ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \] \hspace{1cm} (B.2)

These obey the following relations:

\[ [\sigma_i, \sigma_j] = i2\epsilon_{ijk}\sigma_k \]
\[ \{\sigma_i, \sigma_j\} = 2\delta_{ij} \]
\[ \sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k. \] \hspace{1cm} (B.3)

B.2. Trigonometric and hyperbolic functions

\[ \sin(x + y) = \sin(x)\cos(y) + \cos(x)\sin(y) \] \hspace{1cm} (B.4)
\[ \cos(x + y) = \cos(x)\cos(y) - \sin(x)\sin(y) \] \hspace{1cm} (B.5)
\[ \sin(x - y) = \sin(x)\cos(y) - \cos(x)\sin(y) \] \hspace{1cm} (B.6)
\[ \cos(x - y) = \cos(x)\cos(y) + \sin(x)\sin(y) \] \hspace{1cm} (B.7)
\[ \cos(2\arctan x) = \frac{1 - x^2}{1 + x^2} \] \hspace{1cm} (B.8)
\[ \sin(ix) = i\sinh(x), \quad \cos(ix) = \cosh(x) \] \hspace{1cm} (B.9)
\[ \sinh^2 x/2 = \frac{1}{2}(\cosh x - 1) \] \hspace{1cm} (B.10)
\[ \cosh^2 x/2 = \frac{1}{2}(\cosh x + 1) \] \hspace{1cm} (B.11)
\[ \tanh^2 x/2 = \frac{\cosh x - 1}{\cosh x + 1} \] \hspace{1cm} (B.12)
\[ \sinh x/2 \cosh x/2 = \frac{1}{2} \sinh x \]
\[ \frac{\sin(x + iy)}{\sin(x - iy)} = \frac{\tan(x) + i\tanh(y)}{\tan(x) - i\tanh(y)} \] \hspace{1cm} (B.14)
B.3. Complex analysis

B.3.1. Logarithm of complex numbers

Let \( z = x + iy = re^{i\phi} \) with \( r = \sqrt{x^2 + y^2} \) and \( \phi = \arctan(y/x) \). Therefore:

\[
\ln z = \ln r + i\phi = \frac{1}{2} \ln(x^2 + y^2) + i \arctan(y/x). \tag{B.15}
\]

Similarly we have

\[
\arctan x = \frac{i}{2} (\ln(1 - ix) - \ln(1 + ix)). \tag{B.16}
\]

A useful relation which will use a couple of times:

\[
\ln \frac{x + iy}{x - iy} = 2i \arctan(y/x). \tag{B.17}
\]

B.3.2. Liouville’s theorem

Theorem B.1. Every analytic function \( f(z) \) for which there exists a positive number \( M \) such that \(|f(z)| \leq M \) for all \( z \) in the complex plane is constant.

Proof. Because \( f(z) \) is bounded we can represent it as a Laurent series around \( z_0 \):

\[
f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n \tag{B.18}
\]

where:

\[
a_n = \frac{f^{(n)}}{n!} = \frac{1}{2\pi i} \oint_{C_r} \frac{f(z)}{(z - z_0)^{n+1}} dz \tag{B.19}
\]

and \( C_r \) is a circle centered about \( z_0 \) of radius \( r > 0 \). We can estimate the coefficients:

\[
|a_n| \leq \frac{1}{2\pi} \oint_{C_r} \frac{|f(z)|}{|z - z_0|^{n+1}} \frac{M}{r^{n+1}} dr \leq \frac{M}{r^n}. \tag{B.20}
\]

Sending \( r \to \infty \) gives \( a_n = 0 \) for all \( n \geq 1 \) and sending \( r \to 0 \) gives \( a_n = 0 \) for all \( n \leq -1 \).

Hence \( f(z) = a_0 \). \( \square \)

B.4. Tensor products

Let \( A \) and \( B \) be two \( k \times k \) matrices with elements: \( A_{ij} \) and \( B_{kl} \). The upper index denotes the row, the lower one the column. The tensor product: \( A \otimes B \) is \( k^2 \times k^2 \) matrix with elements:

\[
(A \otimes B)^{ik} jl = A_{ij} B_{kl}. \tag{B.21}
\]

The elements of a tensor product are labeled by the block indices \( i, j \) (\( i \) is the number of the block row and \( j \) is the number of the block column) and by intrinsic indices \( k, l \) (\( k \) is the number of the row and \( l \) of the column).

Consider a product of tensor products \((A \otimes B)(C \otimes D)\). If the matrices \( B \) and \( C \) are \( c \)-numbers we can write it a a single tensor product:

\[
(A \otimes B)(C \otimes D) = AC \otimes BD. \tag{B.21}
\]
B.4 Tensor products

Proof:

\[(A \otimes B)_{ik}^{ij}(C \otimes D)_{lm}^{jl} = A_i^j B_k^l C_j^m D_l^m \]

\[(AC)_{i}^i(BD)_{m}^m = (AC \otimes BD)_{ik}^{ik}.\]

The trace of a tensor product reduces to a product of traces:

\[\text{Tr}(A \otimes B) = (A \otimes B)_{ij}^{ij} = A_i^i B_j^j = \text{Tr}A \text{ Tr}B.\]  

(B.22)

B.4.1. Permutation matrix

Let \(V_1 \otimes V_2 \ldots \otimes V_N\) be a \(d^N\)-dimensional vector space. We can interchange \(V_j\) with \(V_k\) by means of the permutation matrix \(P_{jk}\):

\[P_{jk}(V_j \otimes V_k) = (V_k \otimes V_j),\]  

(B.23)

with the property: \(P_{jk}^2 = 1\). When the \(V_j\) are a 2-dimensional space, the permutation matrix is represented by:

\[
P = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}.
\]  

(B.24)

B.4.2. Logarithm of a matrix

If an \((n \times n)\) matrix \(A\) is invertible, a logarithm can be defined:

\[\ln A = V^{-1} \ln A' V.\]  

(B.25)

\(A' = VAV^{-1}\) is the diagonal matrix of \(A\), its logarithm is defined as: \(\ln A' = \text{diag}(\ln \lambda_1, \ln \lambda_2, \ldots)\).
C. Computer implementation

An important step in this research was a computer implementation. In fig. C.1 the program is sketched. Since only standard numerical methods have been used, we will describe the program in words. All necessary algorithms can be found in [45]. The program can be divided into three blocks:

- construction of states (groundstate, two-spinon excitations)
- computation of two-spinon transverse form factors
- computation of the two-spinon TDSF

State constructor

All sets of quantum numbers \( \{I_j\} \) are generated for the groundstate and two-spinon excitations according to the classification introduced in chapter three. We solve the Bethe equations for a given set \( \{I_j\} \). As these equations are transcendental, the \( \lambda_j \) cannot be written in terms of the other rapidities. The best we can do is rewrite the Bethe equations and solve them iteratively:

\[
\lambda_j^{(n+1)} = \arctan \left[ \tan \left( \pi \frac{I_j}{N} + \frac{1}{N} \sum_{l=1}^{M} 2 \arctan \left( \frac{\tan(\lambda_j^{(n)} - \lambda_l^{(n)})}{\tanh(\eta)} \right) + \pi \left( \frac{\lambda_j^{(n)} - \lambda_l^{(n)}}{\pi} + \frac{1}{2} \right) \right] \tanh(\eta/2) \right].
\]  
(C.1)

From the set \( \{\lambda_j^{(n)}\} \) the set \( \{\lambda_j^{(n+1)}\} \) is computed. The initial set \( \{\lambda_j^{(0)}\} \) is chosen to be an ordered set in the interval \((-\pi/2, \pi/2)\). We proceed by iterating these equations for approximately 20 steps. Now the solutions are pretty close to what they should be and we can apply the Newton-Raphson method. We rewrite the Bethe equations as a vector equation and bring all terms to the LHS:

\[
F_i(\vec{\lambda}) = 0,
\]  
(C.2)

where \( \vec{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_M) \). We can Taylor expand this around \( \delta\vec{\lambda} \):

\[
F_i(\vec{\lambda} + \delta\vec{\lambda}) = F_i(\lambda) + \sum_{j=1}^{M} J_{ij} \delta \lambda_j + O(\delta\vec{\lambda}^2).
\]  
(C.3)

The Jacobian \( J_{ij} = \partial F_i / \partial \lambda_j \) is precisely the Gaudin matrix \( \Phi_{ij} \) (6.81). If we now put \( F_i(\vec{\lambda} + \delta\vec{\lambda}) = 0 \) and neglecting terms of order \( \delta\vec{\lambda}^2 \) we obtain a set of linear equations for the corrections \( \delta\vec{\lambda} \) that move each \( F_i \) closer to zero simultaneously, namely:

\[
\sum_{j=1}^{M} \Phi_{ij} \delta \lambda_j = -F_i.
\]  
(C.4)
This matrix equation can easily be solved by either Gauss elimination or by LU decomposition (see [45]). Then the new set of rapidities is:

\[ \lambda_j^{(n+1)} = \lambda_j^{(n)} + \delta \lambda_j. \]  

Solving the matrix equation (C.4) consumes considerably more computation time than by solving the Bethe equations iteratively. However, the Newton-Raphson method reduces the error quadratically per iteration. Experience teaches that after having approximately 10 Newton-Raphson steps, the absolute error for all \( \lambda_j \) is \( \epsilon < 10^{-15} \).

After computed the set of rapidities we can compute the total energy \( E \) and momentum \( q \) of a state by means of (2.60) and (2.61). The Gaudin norm \( G \) is computed using (6.80).

Now we can store a complete state, which consists of a set of rapidities together with the corresponding energy \( E \), momentum \( q \) and norm \( G \).

After calculating one state we return to the state generator, ready to construct a new state. Now, most sets of quantum numbers are very similar. So instead of choosing an arbitrary set for \( \{ \lambda_j^{(0)} \} \), the final result of the previous computation serves as an input. This speeds up the process a little. We repeat this procedure until all two-spinon states and the groundstate are calculated.

**Computation of form factors**

Now that we have the groundstate and the two-spinon spectrum we can compute the two-spinon form factors. For each step, a state \( \mu \) is retrieved from the database. The two-spinon form factor is computed by means of equation (7.37). However, there are some terms that exceed the computational limits. In order to solve this problem, we rewrite (7.37) as:

\[
\langle \{ \mu \} \vert S_{q}^{-} \vert \{ \lambda \} \rangle^2 = N \delta_{q,q(\lambda)-q(\mu)} \varphi(i \eta)^{4M-1} \prod_{j=1}^{M} |\varphi(\mu_j - i \eta/2)|^2 
\prod_{j>k=1}^{M} |\varphi^2(\mu_j - \mu_k)/\varphi^2(i \eta) + 1|^{-1} \prod_{j>k=1}^{M-1} |\varphi^2(\lambda_j - \lambda_k)/\varphi^2(i \eta) + 1|^{-1} 
\frac{|\det \tilde{H}^{-}|^2}{|\det \Phi(\{ \mu \}) \det \Phi(\{ \lambda \})|} 
\]

with: \( \tilde{H}_{ab} = H_{ab} / \varphi(i \eta)^{M} \). Now all intermediate results are in the order of unity. The results \( \{ F^{-}, E, q \} \) are then written to another database, with: \( E = E_{\mu} - E_0 \), \( q = q_{\mu} - q_{\lambda} \). This process is repeated until all required form factors are computed.

**TDSF**

To be able to make a plot, it is convenient to define an \( n_q \times n_E \) grid. As there are \( N \) values of \( q \), which are all equidistant, the obvious choice is \( n_q = N \). The spacing between the energy levels is not equidistant. The spacing between the grid lines in the \( E \)-direction should be of the order of the minimal spacing between the energy levels.

We can compute the TDSF for the grid by approximating the delta functions with Gaussians and calculate the weight of each form factor at each grid point. To obtain the plots in fig. 7.1 the grid was loaded into MATLAB, where the following settings were used: \( n_q = N \), \( n_E = 32 \times N \), and the width of the Gaussians \( \epsilon = 32/N \).

The sum rule is easily calculated by summing over all form factors squared.
Computer implementation

Figure C.1.: Sketch of computer implementation. A dashed line means that the process is repeated for different states.
Bibliography


Bibliography


