Dynamics of Heisenberg spin chains

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This thesis is based on the following papers:

- Jean-Sébastien Caux and Rob Hagemans
  *The 4-spinon dynamical structure factor of the Heisenberg chain*

- Rodrigo G. Pereira, Jesko Sirker, Jean-Sébastien Caux, Rob Hagemans, Jean Michel Maillet, Steven R. White, Ian Affleck
  *The dynamical spin structure factor for the anisotropic spin-1/2 Heisenberg chain*

- Rob Hagemans, Jean-Sébastien Caux, Jean Michel Maillet
  *How to calculate correlation functions of Heisenberg chains*
  in: *Lectures on the physics of highly correlated electron systems X*
  eds. A. Avella, F. Mancini, pp. 245
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- Jean-Sébastien Caux, Rob Hagemans, Jean Michel Maillet
  *Computation of dynamical correlation functions of Heisenberg chains: the gapless anisotropic regime*

Another paper resulting from my PhD research is

- Rob Hagemans, Jean-Sébastien Caux, Ute Löw
  *Gapped anisotropic spin chains in a field*
But here was a rare opportunity for stupidity even more flagrant and glorious.

— Neal Stephenson, Quicksilver

HOBBS: What’s the point of attaching a number to everything you do?
CALVIN: If your numbers go up, it means you’re having more fun.

— Bill Watterson, Calvin and Hobbes
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1.

Introduction

...but thou, whence intrudest thou into my realm of lineland?

— Edwin A. Abbott, *Flatland: a romance of many dimensions*

1.1 The physics of strongly-correlated systems

One of the most fruitful strategies in science is reduction: a complex problem can often be split up into sub-problems, each of which, when isolated, poses a smaller challenge. In physics, in particular, we like to describe systems in terms of constituent particles. The underlying assumption in such an approach is that interactions between those particles are small or, at the very least, do not change the character of the system in a substantial way. This way of thinking underlies many of the most successful theories in many-body physics, such as perturbation theory, mean-field theory, and Fermi liquid theory. One can build up a large system out of many particles, and the constituent particles can still be identified with the excitations of the system. Indeed, it is what we usually think of then we say a system ‘consists’ of certain particles.

A strongly-correlated system, by definition [1], is a system in which this picture is no longer valid. Such systems have properties and structures which cannot be traced back to their constituent parts in a simple way and which sometimes even tend to be independent [2] of their precise, microscopic details—a realisation that led to well-known aphorisms such as *the whole is more than the sum of its parts* [3] and *more is different* [4]. Important examples of such strongly-correlated systems are high-temperature superconductors and quantum Hall systems. Naturally, such systems that defy generically successful approaches attract the interest of a theorist, who always hopes to encounter something that is fundamentally different.
1.2 Physics in one dimension

The easiest way to increase the strength of interactions in a theoretical system is to restrict its number of dimensions: intuitively, the idea is that the less possibility particles have to bypass each other, the more they will behave as a collective. One-dimensional physical systems therefore behave in a way that is radically different from how higher-dimensional systems behave, even if they are built on the same principles. The resulting breakdown of usual theoretical approaches is alleviated by the fact that one-dimensional systems have a lot of mathematical structure that is absent (or at least unknown) in higher-dimensional systems. This makes completely different approaches possible; it has also led to the development of intriguing mathematics. A nice overview of the physics of one-dimensional quantum systems and the methods used to study them is given by Giamarchi’s book [5].

1.3 Spin chains and lattice models

Quantum systems are often studied on a lattice: either as an approximation to make a continuous system computationally manageable, or because the system in question truly has a lattice nature. Much interest in lattice models derives from the tight-binding approximation, which intends to describe electrons in a crystal by approximating the orbitals of electrons around a nucleus as unmovable points: the lattice sites. The simplest model of this class, in which the electrons are noninteracting, is hence known as the tight-binding model; it can be used to derive the band structure of conducting solids. It can be improved by adding the effects of electrostatic repulsion between electrons, leading to the Hubbard model. In insulators, the main excitations are those of the configuration of electron spins; they are described by spin lattice models, in one dimension also called spin chains. These models are used to address questions on magnetic order and magnetic excitations of solids. Due to their relative simplicity and physical relevance, such models have been considered since the very beginning of quantum mechanics.

1.3.1 Magnetic order

In ferromagnets, the spins of electrons tend to be aligned; the combined effect is a macroscopic magnetic moment that can be present even in the absence of an external field. Antiferromagnetism is more subtle: as the coupling between the spins favours antiparallel alignment, the total magnetic moment is zero. While ferromagnetism has been known since classical times, the discovery of antiferromagnetism is much more recent, due to the fact that it is less immediately noticeable.

In classical physics, it is quite obvious what state an antiferromagnet on a cubic lattice should be in: every pair of neighbours aligns in antiparallel direction, separating the lattice into two sublattices (usually denoted A and B) with spins in opposite directions. Thus, this ground state (called the Néel state) breaks isotropy
and shows a long-range order that is as dramatic as that of a ferromagnet. It would be natural to suppose that the quantum model also exhibits long-range antiferromagnetic order. However, this turns out to be a much much more complicated problem than that of ferromagnetism; it can be discussed in the context of the Heisenberg model.

1.3.2 The Heisenberg model

The Heisenberg model [6] of a ferromagnet was one of the first models of magnetism to be proposed in quantum mechanics, which Heisenberg presented in 1928, only three years after the development of the framework of quantum mechanics itself. It is introduced as a model for the ferromagnetic interaction in a crystal (although, as we will see, it is also applicable to antiferromagnetic interactions). The atoms in the crystal are taken as immovable cores, and the only interaction taken into account is the exchange interaction of the spins of adjacent valence electrons. All but the nearest neighbours are considered to be so far away as to have no effect on a given site. This model has since become known as the spin-$\frac{1}{2}$ isotropic Heisenberg model or the XXX model; it is perhaps the simplest non-trivial model of quantum mechanics and it is therefore quite surprising how much is still unknown about its behaviour. Its Hamiltonian is given by

$$H_{XXX} := J \sum_j S_j \cdot S_{j+1} .$$

where $S_j = (S_j^x, S_j^y, S_j^z)$ is the spin operator on the atom labelled by $j$ and the sum runs over nearest neighbours only. Here the spin operators can be given in terms of Pauli operators as $S := \frac{1}{2} \sigma$. In dimensions higher than one, the notation $j, j + 1$ is understood to refer to all adjacent pairs.

In one dimension, this model was solved (i.e. its spectrum was found) by Hans Bethe in his landmark paper [7]. His method of solution forms the basis for the study of the dynamics of the one-dimensional Heisenberg model presented in this thesis.

1.3.3 The XXZ model

The Heisenberg model was extended by Kasteleijn [8], by introducing an anisotropy $\Delta$ in the interaction

$$H_{XXZ} := \sum_{j=1}^{N} J \left[ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta(S_j^z S_{j+1}^z - \frac{1}{4}) \right] - hS_j^z .$$

The additive constants are chosen such that, if the coupling $J$ and the anisotropy $\Delta$ are positive, the model is antiferromagnetic. The anisotropic (or XXZ) model was subsequently solved by Orbach [9], applying a method analogous to Bethe’s [7] way of solving the isotropic model. In the limit $\Delta \to \infty$, the model becomes
Chapter 1. Introduction

equivalent to the Ising model \[10, 11\]; the model with $\Delta = 0$ is known as the XY
model \[12\]—or more precisely, its isotropic limit, the XX0 model.

Using spin raising and lowering operators defined as $S^\pm := S^x \pm iS^y$, we rewrite

$$H_{XXZ} = \sum_{j=1}^{N} J \left[ \frac{1}{2} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \Delta (S_j^z S_{j+1}^z - \frac{1}{4}) \right] - h S_j^z . \quad (1.3)$$

Going back to the question of magnetic order, one thing that can be immediately noted is that although the ferromagnetic ground state is an eigenstate of the Heisenberg XXX and XXZ models, the Néel state is not. Antiferromagnetic ordering can nonetheless be studied by considering correlation functions: it will show up as a long-range correlation, as spins separated by a large number of sites are still expected to be aligned or anti-aligned depending on the parity of the number of sites separating them. This is indeed the situation in dimensions higher than one: the model shows long-range order and has gapless Goldstone excitations. In one dimension, however, such an order cannot exist, as was proven by Mermin and Wagner \[13\]: the corrections to the ordered approximate ground state diverge. Nevertheless, the one-dimensional spin-$\frac{1}{2}$ Heisenberg model is gapless for $|\Delta| \leq 1$, as is known through the Bethe ansatz; although it does not show real long-range order, its correlation functions decay only algebraically. This gaplessness and algebraic decay shows that in fact the model is critical throughout this region.

A generalisation of Heisenberg’s model considers spins larger than $\frac{1}{2}$ on each site. Here, a surprising effect shows up: as shown by Haldane \[14, 15\], for all half-integer spins the Heisenberg model is gapless, but Heisenberg models of integer spin are gapped (see also \[16\]).

1.3.4 The Hubbard model

The tight-binding model can be improved by taking the repulsion between electrons into account. Since the electrons have spin $\frac{1}{2}$, two of them can occupy a single site, and the repulsion between these leads to an extra energy cost for this configuration, which the Hubbard model \[17, 18\] takes into account. This model correctly describes the Mott transition \[19, 20\] and is thought to be an accurate description of the electronic structure of many materials. In two dimensions, in particular, the Hubbard model describes the electrons on the copper-oxide planes of high-temperature superconductivity; understanding it is therefore thought to be the key to explaining this still elusive phenomenon.

The Hubbard model is given by

$$H_{\text{Hubbard}} := -t \sum_{\sigma} \sum_{j} \left[ c_{j+1,\sigma} c_{j,\sigma} + c_{j+1,\sigma} \dagger c_{j,\sigma} \right] + U \sum_{j} n_{j\uparrow} n_{j\downarrow} . \quad (1.4)$$

Since the electrostatic repulsion is strong, $U$ is generally a high energy. The one-dimensional model was solved by a (more complicated) form of the Bethe ansatz
by Lieb and Wu [21], who thereby showed that in one dimension, it only features a
Mott transition at zero temperature, where the transition takes place immediately
at \( U_c = 0 \).

At half-filling, each site is occupied by a single electron. Hopping to an adjacent
site now comes only at an energy cost \( U \). The main interaction between the elec-
trons is due to the second-order process where an electron hops to a neighbour site
and back. As shown by Anderson [22] this leads to an effective coupling between
the spins of the neighbouring electrons, which takes the form of the antiferromag-
netic Heisenberg interaction with \( J = 2t^2/U \). Thus, at half filling, the low-energy
excitations of the Hubbard model (1.4) are described by the (isotropic) Heisenberg
model (1.1).

### 1.3.5 Fractionalisation of charge

Thus, the Hubbard model demonstrates one unusual effect seen in one-dimensional
systems that has captured physicists' interests: the separation of spin and charge
excitations in one-dimensional electrons. The electron as a particle has both spin \( \frac{1}{2} \)
and a charge \( e \), and higher-dimensional electron systems likewise show excitations
that are electron-like in the sense that they have the same charge and spin. In a one-
dimensional system of electrons, however, excitations take the form of an uncharged
spin and a spinless charge. This is one example of the phenomenon I hinted at
earlier: although the system is made of electrons, its simplest manifestations are
not electrons or bound states of electrons; rather, they are 'parts' of electrons
which are inseparable in the free particle. To say that the electron consists of these
separate parts would, however, be pretty much meaningless. In a spin chain, a
similar effect arises: the chain is made of spins-\( \frac{1}{2} \), and it is simple to visualise one
of the spins flipping over, creating a magnon of spin 1. Indeed, this is the elementary
excitation in a ferromagnet where all spins in the ground state are aligned. In an
antiferromagnet, however, it turns out that the elementary excitation is a spin-\( \frac{1}{2} \)
excitation known as a spinon.

### 1.4 Experimental realisations of spin chains

Space, of course, is known to be three-dimensional. The question is therefore jus-
tified whether low-dimensional systems are not just theorist’s toys. This may in
fact have been the case when such models were first developed. In the mean-
time, however, the peculiar properties predicted for such systems (of which I men-
tioned criticality and quasi-long-range order, the Mott transition, the Haldane gap,
spin–charge separation, and the breakdown of Fermi liquid theory) have inspired
experimentalists and materials scientists to try and construct compounds which
display the characteristics of one-dimensional systems. For instance, spin chains
are realised in strongly anisotropic insulators; the idea being that the magnetic
excitations in perpendicular directions have very different energy scales, so that
excitations in one direction completely dominate the signal while those in other
dimensions are drowned out by thermal noise. Such materials are called quasi-one-
dimensional. Examples of other one-dimensional systems constructed experimen-
tally are quantum wires, nanotubes and quantum Hall edge states. The existence
of these materials and their experimental study has created renewed demand for a
detailed theoretical description of their properties.

1.4.1 Neutron scattering

In a theory thesis such as this, description of experiments is necessarily concise
and will not do justice to the challenges and delights of the experiments involved.
That said, let me give a rough sketch of neutron scattering, which is one of the
foremost methods to study the magnetic structure of solid-state systems experi-
mentally. Their electric neutrality allows neutrons to fully penetrate a compound
and reveal its inner structure. Neutrons couple to a solid-state system in two ways:
first, by colliding with the nuclei in the lattice, creating and absorbing phonons;
and second, by dipole–dipole interaction with the spins of unpaired electrons. Both
effects are of similar strength; to obtain information about the magnetic structure,
they need to be separated in some way, in general through knowledge of the struc-
ture of the system obtained by other means. In antiferromagnets, with which we
will be concerned, this task is made easier because the elementary cell of the mag-
netic structure (the two sublattices) is twice that of the atomic structure. Some
introductions into the theory of neutron scattering are [23, 24, 25].

In the context of this thesis, especially relevant are experiments on one-dimensional
Heisenberg chain materials; examples of these are KCuF$_3$, a nearly perfect isotropic
Heisenberg chain [26, 27, 28, 29, 30], copper pyrazine dinitrate [31], and SrCuO$_2$
[32], all examples of XXX chains. A realisation of the XXZ chain is given by
CsCoCl$_4$, with anisotropy $\Delta \approx 0.25$ [33].

1.4.2 Dynamical structure factor

The cross section for magnetic scattering by nuclear spins is proportional to [34]

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \frac{k'}{k_0} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{k}_\alpha \hat{k}_\beta) S^{\alpha\beta}(q, \omega)$$  (1.5)

where $k_0$ is the wave vector of the incoming neutron and the scattering vector
$q := k' - k_0$ is the change of the neutron’s wave vector brought about by scattering
with the spins. The change of energy is given by $\omega$. $S^{\alpha\beta}(q, \omega)$ is the (magnetic)
dynamical structure factor

$$S^{a\bar{a}}(q, \omega) := \frac{1}{N}\sum_{j,j'} e^{iq(j-j')} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S^a_j(t) S^\bar{a}_{j'}(0) \rangle_c ,$$  (1.6)
where the subscript $c$ indicates the connected correlator $\langle S^a S^{\bar{a}} \rangle_c := \langle S^a S^{\bar{a}} \rangle - \langle S^a \rangle \langle S^{\bar{a}} \rangle$. In these expressions, the pair $(a, \bar{a})$ is one of $(z, z)$, $(+, -)$, or $(-, +)$. In an experiment with unpolarised neutrons, one measures the structure factor of the scalar product $\mathbf{S} \cdot \mathbf{S}$; polarised neutrons access the components separately. Thus, the momentum exchange gives information about the spatial magnetic structure of the system; in an inelastic neutron scattering experiment, which moreover measures the energy transferred by the neutron to the sample, knowledge of the spin dynamics in the sample is obtained. In part, the structure factor merits its theoretical popularity through this connection with experiment; conversely, neutron scattering is a popular method partly because it is able to measure this simple but revealing theoretical quantity.

### 1.4.3 Inelastic neutron scattering setup

In an inelastic neutron scattering experiment, neutrons are obtained from a source, which is either a reactor or an accelerator. In both cases, the neutrons’ energy initially is too high to be useful to determine anything on the length scales interesting in condensed matter physics, so that they need to be slowed down. This is done by bringing them into thermal equilibrium with a moderator, a liquid kept at a known temperature, with whose atoms the neutron collides. The temperature of the moderator thus determines the energy distribution of the ‘thermal’ neutrons leaving it.

An accelerator produces pulsed neutron beams essentially by firing protons at high energy into a target made of heavy neutron-rich nuclei, which as a consequence fall apart, emitting neutrons. This setup is known as a spallation source. It emits neutrons in well-defined pulses, which allows to determine the energy of a neutron by measuring its time of flight. This is done through the use of choppers, basically fast-rotating discs which only let neutrons pass at a certain window of time after the emission of the pulse. Since they are placed some distance from the moderator, this selects a window of energy for the neutrons, which can be further narrowed down by other choppers. The neutrons, whose energy is now known to a desired resolution, subsequently scatter on the sample. Detectors are placed around the sample, so that it is possible to record the angle at which the neutron is scattered, from which the scattering vector $\mathbf{q}$ can be deduced, as well as the time of flight between the chopper and the detector, which determines the energy of the scattered neutron and hence the energy transfer $\omega$.

Inelastic neutron scattering experiments can also be done with a reactor source. In a reactor, neutrons are produced by nuclear fission, which goes on continuously—so that one cannot use the time of flight to determine their energy. Instead, neutrons of a specific energy are selected by scattering the neutron at a given angle on a crystal whose properties are well known (this is known as a monochromator). By changing the angle, neutrons of different energy can be obtained. After scattering, another monochromator is needed to select the energy of the outgoing neutron. A disadvantage of such a triple-angle spectrometer is that it only measures a small section of $(k, \omega)$ space at a time.
1.5 Mathematical physics of 1D models

The study of one-dimensional systems has led to many interesting developments in mathematical physics. Of those, two are especially relevant to this thesis: the theory of integrability and conformal field theory.

1.5.1 Integrable models

The theory of integrable models is a direct outcome of the study of one-dimensional magnetism; indeed, the Heisenberg model [6] we study in this thesis is the bedrock of that field. Bethe [7] solved this model by explicitly constructing its eigensystem. His method, nowadays known as the Bethe ansatz, turned out to be applicable to a range of quantum mechanical and statistical physics models. Mathematically, it turns out to have a rich structure, which started to unfold after Baxter [35] made the connection between the Hamiltonian of the Heisenberg model and vertex models of classical statistical physics.

The importance of the Bethe ansatz lies in the fact that its results are mathematically exact. Its limitation is, however, that these exact results can be very hard to obtain and, when obtained, to evaluate. Thus, a picture arises where a model has been ‘exactly solved’, but the solution is inaccessible. For real-world problems, of course, an accessible solution would be preferable. Specifically, the problem of extracting the dynamical properties of a model from the Bethe ansatz, such as the dynamical structure factor needed to describe neutron scattering, is notoriously hard.

*Extracting the dynamics of the Heisenberg model from the Bethe ansatz, and getting results that are applicable to real experiments, is the central theme of this thesis.*

A lot of good books have been written on the subject of integrable models and the Bethe ansatz (e.g. [36] [37] [38]). Many of the original research papers have been collected in Mattis’s book [39].

1.5.2 Conformal field theory

Another very powerful tool for one-dimensional quantum systems is conformal field theory [40], an extensive theoretical framework, ultimately based on the observation that all holomorphic mappings from the complex plane onto itself are locally conformal, i.e. they preserve the angle between two intersecting curves. Since systems with one space and one time dimension are naturally described by the complex plane, this theory is a very powerful tool in treating one-dimensional quantum systems. Among many other things, it gives expressions for the asymptotic structure of dynamical correlation functions. Conformal field theory plays a pivotal role in string theory; this connection makes spin chains also a topic of some interest in that field (see e.g. [41]).

Conformal field theory often turns out to be complementary to the Bethe ansatz in the sense that the Bethe ansatz can address what conformal field theory cannot,
and vice versa. Thus, field theory alleviates another limitation of the Bethe ansatz approach, viz. that it is only applicable to a rather limited set of models. If both methods are used together, results from the Bethe ansatz may be extended to more general models.

1.6 Outline of this thesis

In the next chapter, based on Bethe’s famous article, I will give an introduction to the coordinate Bethe ansatz for the XXZ and XXX chains, and derive the Bethe equations. This will also serve to introduce conventions and notations to be used throughout the thesis. Chapter 3 then addresses many subtleties of finding solutions to the Bethe equations, in particular the structure of complex solutions. In this chapter, I outline a numerical method that succeeds in finding the largest class of those solutions, in finite chains, to machine precision. In chapter 4, I discuss a method of calculating the dynamical structure factor from the solutions of Bethe’s equations on a finite chain, which is then applied to several experimentally relevant cases. Chapter 5 changes the focus to the infinite chain; here, I give results for the dynamical structure factor in the thermodynamic limit. Chapter 6 is devoted to the connection between the results of the previous chapters and the field theory approach to the same problems. Finally, I draw general conclusions and discuss possible directions for future research.
2. Eigenstates of the Heisenberg model

In this chapter, we will recall Bethe’s [7] solution of the isotropic Heisenberg model (generalised by Orbach [9] for the anisotropic case) and along the way fix the conventions and notations we will use throughout this thesis. Good discussions of this material can be found in the books by Gaudin [36], Korepin et al. [38], and Takahashi [37].

2.1 Hilbert space basis

The Heisenberg Hamiltonian (1.3) conserves the spin component in the $z$ direction. Therefore, the Hilbert space it acts on separates into disjunct subspaces with different expectation values of the magnetisation. We will specify the subspace by the number of spins pointing downward,

$$ M := N/2 - \left\langle \sum_{j=1}^{N} S_j^z \right\rangle. $$

Two of the eigenstates are readily recognised: one for $M = 0$ and one for $M = N$. The former, with all spins up, is defined to be the reference state:

$$ |0\rangle := \bigotimes_{j=1}^{N} |\uparrow\rangle_j. $$
Chapter 2. Eigenstates of the Heisenberg model

The constant term in the Hamiltonian (1.3) is chosen in such a way that the reference state has energy eigenvalue zero at zero field; the ground state therefore has a negative energy. With this choice of reference state, the Bethe ansatz approach that we will introduce shortly only allows to consider \( M \leq N/2 \). If we wish to consider a state with more down spins, we must start from the \( M = N \) reference state and follow an analogous procedure. However, the properties of such states can easily be inferred from those we shall consider here, by symmetry considerations.

Starting from the reference state, we can construct a basis of the full Hilbert space \( \mathcal{H} := \bigotimes_{j=1}^{N} \mathbb{C}^2 \) by flipping spins over. We will denote a state by giving the positions of the down spins:

\[
|j_1, j_2, \ldots, j_M\rangle := S^{-}_{j_1} S^{-}_{j_2} \cdots S^{-}_{j_M} |0\rangle .
\]

Whenever we write such a sequence of positions, we will give them in ascending order, so that every state in the Hilbert space has a unique notation. A wave function can then be defined as

\[
|\chi_M\rangle := \sum_{\{j\}} \chi_M(j_1, \ldots, j_M) |j_1, \ldots, j_M\rangle .
\]

Given these definitions, it is natural to think of a down spin as a particle and an up spin as an empty site.

### 2.2 The Bethe ansatz

We closely follow Bethe’s original paper [7] in constructing the eigenstates of (1.3). The magnetic field \( h \) only changes the energies of the eigenstates by an amount \( hM \), but does not alter the states themselves. We will therefore set \( h = 0 \); it is easy to re-introduce at the end.

#### 2.2.1 Schrödinger equation

Consider the Hamiltonian (1.3). As the hopping term \( \frac{1}{2}(S^+_j S^-_{j+1} + S^-_j S^+_{j+1}) \) can only move a particle to the left or right insofar as that site is unoccupied, and the \( S^z S^z - \frac{1}{4} \) term is only nonzero where two spins point in opposite direction, Schrödinger’s equation acts on the state given by a wave function \( \chi_M \) as

\[
\begin{align*}
(E/J) |\chi_M\rangle &= \sum_{\{j\}} \chi_M(j_1, \ldots, j_M) \left[ -\frac{1}{2} \Delta W(j_1, \ldots, j_M) |\{j\}\rangle ight. \\
&+ \frac{1}{2} \sum_{\alpha=1}^{M} (1 - \delta_{j_\alpha+1,j_\alpha}) |\ldots, j_\alpha + 1, \ldots\rangle + (1 - \delta_{j_\alpha-1,j_\alpha}) |\ldots, j_\alpha - 1, \ldots\rangle 
\end{align*}
\]

where \( W(\{j\}) \) counts the number of links along which the spins point in opposite directions.
The inner product with $\langle \{l\} |$ gives an equation for the wave function,
\[
\frac{(E/J)}{2} \chi_M(l_1, \ldots, l_M) = -\frac{1}{2} \Delta W(l_1, \ldots, l_M) \chi_M(l_1, \ldots, l_M)
\]
\[
+ \frac{1}{2} \sum_{\alpha=1}^{M} [1 - \delta_{l_{\alpha-1}, l_{\alpha-1}}] \chi_M(\ldots, l_\alpha - 1, \ldots) + [1 - \delta_{l_{\alpha+1}, l_{\alpha+1}}] \chi_M(\ldots, l_\alpha + 1, \ldots)
\]

**Single particle**

To get a feeling for the equation, we will start trying to solve it for a single particle, and later generalise. For a single particle, we simply have $W = 2$ and thus
\[
\left(\frac{E_1}{J}\right) \chi_1(j_1) = \frac{1}{2} \chi_1(j_1 + 1) + \frac{1}{2} \chi_1(j_1 - 1) - \Delta \chi_1(j_1),
\]
which is readily solved by the plane wave $\chi_{1k_1}(j_1) = e^{ik_1j_1}$ and we see that
\[
E_1/J = \cos k_1 - \Delta.
\]

**Isolated particles**

Now consider putting in $M$ particles, but making sure that they are all separated by at least one empty site. Then, we still have $W = 2M$ so that the Schrödinger equation becomes
\[
\left(\frac{E_M}{J}\right) \chi_M(j_1 \ldots j_M) = -\Delta M \chi_M(j_1 \ldots j_M)
\]
\[
+ \frac{1}{2} \sum_{\alpha=1}^{M} [\chi_M(\ldots, j_\alpha - 1, \ldots) + \chi_M(\ldots, j_\alpha + 1, \ldots)].
\]

In analogy to the single-particle case, we can solve this equation by assuming a product of plane waves,
\[
\chi_{1k_1 \ldots k_M}(j_1 \ldots j_M) = e^{i \sum_\alpha k_\alpha j_\alpha},
\]
and see that the energy is the sum of the single-particle energies,
\[
E_M = J \sum_\alpha [\cos k_\alpha - \Delta].
\]

**Single pair of neighbours**

Now consider what happens when we move two of the $M$ particles right next to each other. The system now satisfies
\[
\left(\frac{E_M}{J}\right) \chi_M(j_1 \ldots j_\beta, j_\beta + 1 \ldots j_M) = -\Delta (M - 1) \chi_M(j_1 \ldots j_\beta, j_\beta + 1 \ldots j_M)
\]
\[
+ \frac{1}{2} \sum_{\alpha \not\in \{\beta, \beta + 1\}} [\chi_M(\ldots, j_\alpha - 1, \ldots) + \chi_M(\ldots, j_\alpha + 1, \ldots)]
\]
\[
+ \frac{1}{2} [\chi_M(\ldots, j_\beta - 1, j_\beta + 1, \ldots) + \chi_M(\ldots, j_\beta, j_\beta + 2, \ldots)].
\]
In other words, on top of the terms as in (2.9) produced by the $M - 2$ isolated particles the couple of neighbouring particles contribute a term

$$-\Delta \chi_M(\ldots j_\beta, j_\beta + 1\ldots) + \frac{1}{2} \left[ \chi_M(\ldots j_\beta - 1, j_\beta + 1\ldots) + \chi_M(\ldots j_\beta, j_\beta + 2\ldots) \right].$$

(2.13)

Now the trouble begins. If, in the Schrödinger equation, we were to try a product of plane waves for the wave function, this would give us

$$0 = e^{i \sum \alpha k_\alpha j_\alpha} \left[ \frac{E}{J} + \Delta - \frac{1}{2} \left( e^{-ik_\beta} - e^{ik_{\beta + 1}} \right) - \sum_{\alpha \not\in \{\beta, \beta + 1\}} \left( \cos k_\alpha - \Delta \right) \right].$$

(2.14)

Clearly, this does not work: the eigenvalue cannot depend on $\beta$. Should we, however, add another plane wave, with $\beta, \beta + 1$ interchanged, we would again get the eigenvalue (2.11).

### 2.2.2 Bethe’s wave function ansatz

Thinking along these lines, but noting that the Schrödinger equation must be satisfied for every possible choice of the neighbour pair’s position, we try a sum over all permutations:

$$\chi_{k1\ldots kM}^{BA}(j_1\ldots j_M) = \sum_P (-1)^{|P|} A_P e^{i \sum \alpha k_P \alpha j_\alpha},$$

(2.15)

in which $|P|$ denotes the parity of the permutation. At this point, putting this sign in front is an arbitrary choice—it could have been absorbed by the prefactor $A_P$—but this choice will turn out to be convenient later.

The wave function ansatz$^1$ (2.15) is called Bethe’s ansatz; it is the key to solving the Heisenberg model. Introducing this ansatz into the Schrödinger equation,

$$0 = \sum_P (-1)^{|P|} A_P e^{i \sum \alpha k_P \alpha j_\alpha} \left[ \frac{E}{J} - \sum_{\alpha = 1}^M \left( \cos k_\alpha - \Delta \right) \right.$$

$$\left. - \sum_{\gamma \text{ pairs}} \left( \Delta - \frac{1}{2} \left( e^{ik_P \gamma} + e^{-ik_P (\gamma + 1)} \right) \right) \right].$$

(2.16)

As the term on the lower line must not depend on the number or location of pairs, it ought to be equal to zero for each neighbour pair.

$$\sum_P (-1)^{|P|} A_P e^{i \sum \alpha k_P \alpha j_\alpha} \left[ \Delta - \frac{1}{2} \left( e^{ik_P \gamma} + e^{-ik_P (\gamma + 1)} \right) \right] = 0.$$

(2.17)

$^1$being a german Noun, Ansatz is often capitalised; however I argue that it is sufficiently common in scientific Usage to be considered an established Loan-Word in this Context.
2.2. The Bethe ansatz

The equation (2.17) determines $A_P$ in the following way. Suppose there is a pair $j_\gamma + 1 = j_{\gamma + 1}$. Consider two permutations, $\mathcal{P}$ and $\mathcal{Q}$, such that they only differ by exchanging the momenta associated to these two neighbours:

$$Q = \mathcal{P}\gamma, \mathcal{P}(\gamma+1)\mathcal{P}.$$  
(2.18)

By definition, these permutations have different parity and therefore, a different sign associated to them. Comparing the terms in the sum associated to these permutations, we see that they equal

$$e^{i\sum_{\alpha \in \{\gamma, \gamma+1\}} k_{\mathcal{P}_\alpha} j_\alpha} \left\{ A_P e^{ik_{\mathcal{P}_\gamma} j_\gamma + ik_{\mathcal{P}(\gamma+1)} j_{\gamma+1}} \left[ (\Delta - \frac{1}{2}(e^{ik_{\mathcal{P}_\gamma}} + e^{-ik_{\mathcal{P}(\gamma+1)}})) \right] 
- A_Q e^{ik_{\mathcal{Q}_\gamma} j_\gamma + ik_{\mathcal{Q}(\gamma+1)} j_{\gamma+1}} \left[ (\Delta - \frac{1}{2}(e^{ik_{\mathcal{Q}_\gamma}} + e^{-ik_{\mathcal{Q}(\gamma+1)}})) \right] \right\}. \quad (2.19)$$

As $Q\gamma = \mathcal{P}(\gamma+1)$ and vice versa, these terms cancel if

$$A_P = A_Q e^{i\Phi(k_{\mathcal{P}_\gamma}, k_{\mathcal{P}(\gamma+1)})}, \quad (2.20)$$

where the exchange phase $\Phi(k, k')$ is defined by

$$e^{i\Phi(k, k')} := \frac{2\Delta e^{ik} - e^{ik+i'k'} - 1}{2\Delta e^{ik'} - e^{ik+i'k'} - 1}. \quad (2.21)$$

For the following it is important to note that this exchange phase is antisymmetric

$$\Phi(k, k') = -\Phi(k', k). \quad (2.22)$$

Equation (2.20) can be used to construct a closed expression for $A_P$. To do so, we use that every permutation can be written as a sequence of transpositions, in such a way that every step in the sequence exchanges only the momenta corresponding to two subsequent particles,

$$\mathcal{P} = \cdots \mathcal{P}^{(3)} \mathcal{P}^{(2)} \mathcal{P}^{(1)}(\gamma_2), \mathcal{P}^{(2)} \mathcal{P}^{(1)}(\gamma_2+1) \mathcal{P}^{(2)} \mathcal{P}^{(1)}(\gamma_2), \mathcal{P}^{(1)}(\gamma_2+1) \mathcal{P}^{(1)}(\gamma_2), \mathcal{P}^{(1)}(\gamma_1+1) \mathcal{P}^{(1)}(\gamma_1) \mathcal{P}^{(1)}(\gamma_1), \mathcal{P}^{(1)}(\gamma_1+1) \mathcal{P}^{(1)}(\gamma_1) \mathcal{P}^{(1)}(\gamma_1+1), \quad (2.23)$$

where the indices $(n)$ that denotes the position of the transposition in the sequence is also used to identify it, e.g. $\mathcal{P}^{(1)} := \mathcal{P}_{\gamma_1}, \gamma_{1+1}$.

Now the relative phase of $\mathcal{P}$ and the identity permutation must be the product of the exchange phases associated with each neighbour transposition in the sequence, since for every one of those transpositions we can construct a set of positions $j_1 < j_2 < \cdots < j_M$ such that the particles whose momenta are exchanged are actually adjacent. In other words, for every transposition in the sequence there is at least one configuration of particles such that equation (2.20) must hold, so it is required to hold for all transpositions in the sequence.

Since the transpositions exchange only subsequent particles and therefore leave the order of the other particles as it was, and since the exchange phase shift $\Phi$ is antisymmetric, this requirement is satisfied by

$$A_{\mathcal{P}}(\{k\}) = e^{\frac{i}{2} \sum_{\alpha < \beta} \Phi(k_{\mathcal{P}_\alpha}, k_{\mathcal{P}_\beta})}. \quad (2.24)$$

This solves the Schrödinger equation in the bulk of the system.
2.2.3 Bethe wave function

Written out in full, the (non-normalised) wave function reads
\[ \chi^{BA}_k(\{ j \}) = \sum_P (-1)^P e^{\frac{i}{2} \sum_{\alpha<\beta} \Phi(k_P, k_P)} e^{i \sum_{\alpha} k_P j_{\alpha}}, \]  
(2.25)
and the energy is
\[ E_k = J \sum_{\alpha} [\cos k_{\alpha} - \Delta] - h \left( \frac{N}{2} - M \right), \]  
(2.26)
where we have re-introduced the magnetic field \( h \).

2.2.4 Pauli principle

One thing we can immediately note is the following. If two of the momentum parameters are the same, \( k_{\alpha} = k_{\beta} \) for \( \alpha \neq \beta \), we can pair up every term with another, where the only difference between the two terms is a permutation in which the two equal parameters are exchanged. This means that the permutations have a different sign and therefore these terms cancel. Since all terms cancel, the wave function is identically zero. Such a wave function is not admissible and as a consequence, all particles must have different momentum parameters. In an analogy with fermions, this is called the Pauli exclusion principle.

2.3 The Bethe equations

Let us now turn our attention to the periodicity of the chain, given by the identification \( \mathbb{C}^2_j \equiv \mathbb{C}^2_{j+N} \) where \( \mathbb{C}^2_j \) is the Hilbert space for the \( j \)th site. On a closed chain with \( N \) sites, the wave function must satisfy the periodic boundary conditions
\[ \chi(1, j_2, j_3 \ldots j_M) = \chi(j_2, j_3 \ldots j_M, N + 1). \]  
(2.27)
Imposing these conditions on the Bethe wave function (2.15),
\[ \sum_P (-1)^{[P]} A_P e^{i \sum_{\alpha \neq 1} k_P j_{\alpha}} = \sum_P (-1)^{[P]} A_P e^{ik_P N} e^{i \sum_{\alpha \neq 1} k_P j_{\alpha}}. \]  
(2.28)
To make the terms on the left-hand side match those on the right, we have to move the momentum associated to particle number 1 at site 1 all the way across the chain, until it is associated to particle number \( M + 1 \equiv 1 \) at site \( N + 1 \equiv 1 \). Along the way we pass \( M - 1 \) other particles and pick up exchange phases for each of them. In other words, we consider \( P P_1 P_{M-1} \ldots P_1 P_3 P_1 P_2 P \) on the left-hand side vs. \( P \) on the right-hand side
\[ \sum_P (-1)^{M-1+[P]} A_{P P_1 P_M \ldots P_1 P_3 P_1 P_2 P} e^{i \sum_{\alpha \neq 1} k_P j_{\alpha}} \]  
(2.29)
so that, for all permutations $\mathcal{P}$,

$$ A_{\mathcal{P}} e^{ik_{\mathcal{P}M}N} = (-1)^{M-1} A_{\mathcal{P}_{P_1 \times \cdots \times P_3 \times p_1 \times p_2 \times \mathcal{P}}} $$

$$ e^{ik_{\mathcal{P}M}N} = (-1)^{M-1} e^{i \sum_{\alpha \neq 1} \Phi(k_{P_1}, k_{P_2})} \tag{2.30} $$

These equations should be valid for all permutations $P$, and therefore we have

$$ e^{ik_{\alpha}N} = (-1)^{M-1} e^{i \sum_{\alpha \neq 0} \Phi(k_{\alpha}, k_{\beta})} . \tag{2.31} $$

Taking the logarithm of these equations,

$$ k_{\alpha} = \pi + 2\pi \left( J_{\alpha} + \sum_{\beta \neq \alpha} \Phi(k_{\alpha}, k_{\beta}) \right) \mod 2\pi . \tag{2.32} $$

where we have the freedom to introduce a Bethe quantum number $J_{\alpha}$ as a consequence of the multiple-valuedness of the logarithm. The arbitrary extra term $\pi$ will turn out to be convenient in a short while. Note that we have absorbed $\log \left[ (-1)^{M-1} \right]$ into $J_{\alpha}$; as a consequence, for $M$ even, $J_{\alpha}$ is a half-integer, whereas for $M$ odd it is an integer. For every value of the quantum number $J_{\alpha} \mod N$, this defines a separate equation. In the following, we will always choose $-N/2 < J_{\alpha} \leq N/2$.

The set of equations (2.31) or, alternatively, equations (2.32) are known as Bethe’s equations.

Because of the antisymmetry of $\Phi$, an equation for the momentum of the system immediately follows by summing over all logarithmic Bethe equations.

$$ q := \sum_{\alpha} k_{\alpha} = \pi M + \frac{2\pi}{N} \sum_{\alpha} J_{\alpha} \mod 2\pi \tag{2.33} $$

### 2.4 Parametrisation

Written out in full, the Bethe equations read

$$ e^{ik_{\alpha}N} = \prod_{\alpha \neq \beta} \left[ -\frac{2\Delta e^{ik_{\alpha} - e^{ik_{\alpha}+ik_{\beta}}} - 1}{2\Delta e^{ik_{\beta} - e^{ik_{\alpha}+ik_{\beta}}} - 1} \right] . \tag{2.34} $$

Now we will introduce a reparametrisation, due to Orbach [9], that will turn out to be very convenient. The reparametrisation will be different for the three physically different classes of values of the anisotropy $\Delta$: the gapless anisotropic case $|\Delta| < 1$, the gapped anisotropic antiferromagnetic case $\Delta > 1$, and the isotropic antiferromagnetic case $\Delta = 1$. First we consider the gapless anisotropic case, from which we derive the parametrisation for the other cases.
Gapless anisotropic model

Since $|\Delta| < 1$, we can define $0 < \zeta < \pi$ such that

$$\Delta = \cos \zeta$$

(2.35)

Furthermore, we define the rapidity $\lambda$, such that

$$e^{ik} = \frac{\sinh(\lambda - i\zeta/2)}{\sinh(\lambda + i\zeta/2)}$$

(2.36)

In terms of the rapidity, the exchange phase becomes

$$e^{i\Phi(k,k')} = \frac{2\Delta e^{ik_\alpha} - e^{ik_\alpha + ik_\beta} - 1}{2\Delta e^{ik_\alpha} - e^{ik_\alpha + ik_\beta} - 1} = \frac{\sinh(\lambda - \lambda' - i\zeta)}{\sinh(\lambda - \lambda' + i\zeta)} = e^{i\Phi(\lambda - \lambda')}$$

(2.37)

$$\Phi(\lambda - \lambda') = 2 \arctan \frac{\tanh(\lambda - \lambda')}{\tan \zeta} \pmod{2\pi}$$

(2.38)

and we see that the exchange phase has become a function of the difference of rapidities.

This brings the Bethe equations to the form

$$\left[ \frac{\sinh(\lambda_\alpha - i\zeta/2)}{\sinh(\lambda_\alpha + i\zeta/2)} \right]^N = \prod_{\beta \neq \alpha} \frac{\sinh(\lambda_\alpha - \lambda_\beta - i\zeta)}{\sinh(\lambda_\alpha - \lambda_\beta + i\zeta)}$$

(2.39)

And the reason for the earlier term $\pi$ in the definition of the quantum numbers becomes clear as we get the Bethe equations in the form we will most often use,

$$\arctan \frac{\tanh \lambda_\alpha}{\tan \zeta/2} = \pi J_\alpha + \frac{1}{N} \sum_{\beta \neq \alpha} \arctan \frac{\tanh(\lambda_\alpha - \lambda_\beta)}{\tan \zeta} \pmod{\pi}.$$  \hspace{1cm} (2.40)

To a single rapidity we can associate the momentum

$$k_\alpha = -i \log \left[ \frac{\sinh(\lambda_\alpha - i\zeta/2)}{\sinh(\lambda_\alpha + i\zeta/2)} \right] = \pi + 2 \arctan \frac{\tanh \lambda_\alpha}{\tan \zeta/2} \pmod{2\pi}$$

(2.41)

and the energy

$$E_\alpha = J \left[ \cos k_\alpha - \Delta \right] + h = -J \frac{\sin^2 \zeta}{\cosh 2\lambda_\alpha - \cos \zeta} + h.$$  \hspace{1cm} (2.42)

Gapped anisotropic antiferromagnet

The expressions for the other antiferromagnetic cases can be derived analogously. For the case $\Delta > 1$, we can define $\zeta \in \mathbb{R}$ such that

$$\Delta = \cosh \zeta$$

(2.43)
so that we may put $\zeta_{|\Delta|<1} = i\zeta_{|\Delta|>1}$ in the equations for the gapless case to derive those for the gapped case. For the rapidity we take $\lambda_{|\Delta|>1} = i\lambda_{|\Delta|<1}$.

The expressions in the gapped case are all periodic in the rapidity $\lambda$ with period $\pi$. To remove this periodicity and make the quantum numbers well-defined, we use

$$\text{atan} \tan \frac{\lambda}{\tanh n\zeta/2} \rightarrow \text{atan} \tan \frac{\lambda}{\tanh n\zeta/2} + \pi \left\lfloor \frac{\lambda}{\pi} + \frac{1}{2} \right\rfloor . \quad (2.44)$$

**Isotropic antiferromagnet**

The parameters for the isotropic case can be found by taking the limit from the anisotropic case, using

$$\lambda_{\Delta=1} := \lim_{\zeta \to 0} \lambda_{|\Delta|<1}/\zeta \quad (2.45)$$

(or, equivalently, by taking a limit from the gapped case).

**General expressions**

The expressions for the three cases of the antiferromagnetic Heisenberg chain can be summarised as follows. We define functions $\theta_n(\lambda), \phi_n(\lambda)$ (see table 2.1) such that the momentum associated to a rapidity $\lambda$ reads

$$k = \pi + \theta_1(\lambda) \mod 2\pi \quad e^{ik_j} = \frac{\phi_1(\lambda)}{\phi_1(\lambda)} , \quad (2.46)$$

and its energy contribution

$$E = -2J |\phi_2(0)| \pi a_1(\lambda) + h , \quad (2.47)$$

where

$$a_n^\nu(\lambda) := \frac{1}{2\pi} \partial_\lambda \theta_n^\nu(\lambda) . \quad (2.48)$$

The derivative in the energy formula (2.47), which comes a bit out of the blue here (but can be checked in each case separately), actually emerges naturally in the context of the algebraic Bethe ansatz (see chapter 4).

The Bethe equations are written

$$\left[ \frac{\phi_{-1}(\lambda_\alpha)}{\phi_{+1}(\lambda_\alpha)} \right]^N = \prod_{\beta \neq \alpha} \frac{\phi_{-2}(\lambda_\alpha - \lambda_\beta)}{\phi_{+2}(\lambda_\alpha - \lambda_\beta)} \quad (2.49)$$

In the logarithmic form, we choose the branch of the logarithm such that

$$\theta_1(\lambda_\alpha) = 2\pi J_\alpha N + \frac{1}{N} \sum_{\beta} \theta_2(\lambda_\alpha - \lambda_\beta) \mod 2\pi , \quad (2.50)$$

All definitions are conveniently summarised in table 2.1. For later convenience, the functions in this table are defined in a slightly more general way than is currently needed.
Table 2.1: An overview of the definitions of $\phi$, $\theta$, and $a$ for various regions of the anisotropy parameter. If the parity $v$ is left out, it defaults to $v = 1$; we also sometimes write $\phi_{\pm}$ for $\phi_{\pm 1}$ and likewise for $\theta$ and $a$.

2.5 Real roots

The Bethe equations are easiest to solve when their roots lie on the real axis. Indeed, a number of important solutions, such as the ground state, have this structure.

2.5.1 The ground state

Consider a subspace with fixed number of particles. It was proven by Yang and Yang [42] that the state with lowest energy in a subspace with a given number $M$ of down spins is found by setting the quantum numbers to

$$\{I\} = \{-\frac{(M - 1)}{2}, -\frac{(M - 1)}{2} + 1, \ldots, \frac{(M - 1)}{2}\} \quad (2.51)$$

In zero magnetic field, the energy can not rise as we add particles; consequently, the ground state is the above state for the maximum number of particles that is allowed, $M = N/2$. Then, the total spin of the state is zero, in accordance with the Lieb-Mattis theorem [43]. The rapidities of the subspace ground states are all finite real numbers.

2.5.2 Total spin and infinite rapidities in the isotropic chain

The Hamiltonian of the XXX chain commutes with the total spin operator, so that they can be simultaneously diagonalised. Indeed, the Bethe ansatz wave functions for the isotropic model, which are constructed as eigenstates of total spin in the $z$ direction $S^z_{\text{tot}}$ (which equals $\sqrt{NS^z_0}$ if we define the lattice Fourier transform as in 4.2), form multiplets of well-defined total spin. Given a highest-weight state $\langle S_{\text{tot}} \rangle = \langle S^z_{\text{tot}} \rangle$, one can construct the other states in the multiplet by repeatedly applying the total spin-down operators $S^-_0$, which is equivalent to the $k = 0$ magnon creation operator.
2.6. Complex roots

From equation (2.46) it follows that the rapidity of such magnons is $\lambda = \infty$, and such an infinite rapidity contributes only a shift of $\pi$ to the logarithmic Bethe equations (2.50), equivalent to a shift of the quantum numbers by $\frac{1}{2}$. Thus the rapidities of lower-weight solutions are exactly the same as for the highest-weight solution, supplemented by a number of formally infinite rapidities. The energy of the states in the multiplet only differs by the splitting due to the magnetic field. Thus, for the isotropic chain, it is sufficient to find only the highest-weight solutions in a given $M$ subspace, reducing the number of solutions to be found from $\binom{N}{M}$ to $\binom{N}{M} - \binom{N}{M-1}$.

The quantum numbers for infinite rapidities can be easily found from the Bethe equations,

$$J_\infty = \frac{N + 1 - M}{2} \quad (2.52)$$

where it is assumed that all roots are real. Since larger quantum numbers correspond to larger rapidities, this implies that finite all-real solutions must have distinct quantum numbers strictly below this bound. The number of such solutions equals

$$\binom{2J_\infty + 1}{M} = \binom{N - M + 2}{M} \quad (2.53)$$

which is much lower than the required number. The remaining solutions must therefore either have equal quantum numbers or not lie on the real axis, or both. In chapter 3 we show that this is indeed the case. Although infinite solutions do not exist for the XXZ chain, we can derive a similar bound analogously.

### 2.6 Complex roots

We have shown that the roots of the Bethe equations (2.50), in general, lie in the complex plane. In this section we will explore the structure of root configurations.

#### 2.6.1 Pairs

It is easily seen that, if the set $\{\lambda\}$ is a solution to the Bethe equations, so is $\{\lambda^*\}$. A stronger statement was proven by Vladimirov [44], viz. that all solutions of the Bethe equations are self-conjugate, i.e. $\{\lambda\} = \{\lambda^*\}$. As a consequence, complex roots of the Bethe equations always come in pairs of conjugate roots, $\{\lambda_+, \lambda_-\}$ where $\text{Im} \lambda_+ > 0$ and $\lambda_- := \lambda^*_+$. Note that in the XXZ case, due to the periodicity mod $i\pi$ in the definition of the rapidity, a rapidity with $\text{Im} \lambda = \pi/2$ is to be considered conjugate to itself.

For the quantum numbers $\{I_+, I_-\}$ associated to the two roots, we find the following. Subtracting the Bethe equation associated to $\lambda_-$ from that of $\lambda_+$, we find
\[
\pi \frac{J_+ - J_-}{N} = \frac{\tanh \lambda}{\tan \zeta/2} - \frac{\tanh \lambda^*}{\tan \zeta/2} \\
- \frac{1}{N} \left[ \frac{\tanh(\lambda - \lambda^*)}{\tan \zeta} - \frac{\tanh(\lambda^* - \lambda)}{\tan \zeta} \right] \\
- \frac{1}{N} \sum_{k} \frac{\tanh(\lambda - \lambda_k)}{\tan \zeta} - \frac{\tanh(\lambda^* - \lambda_k)}{\tan \zeta} \pmod{\pi}. 
\]

As the inverse tangent has a branch cut, such that \( \tan \frac{\zeta}{2} = (\tan \zeta) \pm \pi \) if \( z \in \{ -i, \infty \} \) and \( \tan \frac{\zeta}{2} = (\tan \zeta)^* \) elsewhere, and we work modulo \( \pi \), the real part of the equation becomes

\[
J_- - J_+ = \begin{cases} 
0 & \text{if } 0 < \text{Im} \lambda_+ < \frac{\zeta}{2} \pmod{\pi} \\
1 & \text{if } \frac{\zeta}{2} < \text{Im} \lambda_+ < \frac{\pi}{2} \pmod{\pi} 
\end{cases}
\]

In other words, there are two kinds of pairs: narrow pairs (also called close pairs), which are separated in the imaginary direction by less than \( i\zeta \), and whose quantum numbers are equal; and wide pairs, which are separated by more than \( i\zeta \) and whose quantum numbers differ by one, where the higher quantum number is associated to the root in the negative half-plane. This distinction is found in e.g. Destri and Löwenstein [45] and Babelon et al. [46]. If \( \text{Im} \lambda_+ = \frac{\zeta}{2} \), the Bethe equations become singular; we will study this important limit in more detail in the following sections.

The above derivation for quantum numbers is valid only when the real part of the root is not exactly zero. If it is, \( \lambda_+ = -\lambda_- \) and we find

\[
J_- - J_+ = \frac{2N}{\pi} \text{Im} \frac{\tanh \text{Im} \lambda_+}{\tan \zeta/2} \\
= \begin{cases} 
0 & \text{if } 0 < \text{Im} \lambda_+ < \frac{\zeta}{2} \pmod{\pi} \\
N & \text{if } \frac{\zeta}{2} < \text{Im} \lambda_+ < \frac{\pi}{2} \pmod{\pi} 
\end{cases}
\]

In particular, both for zero and nonzero imaginary part, it should be noted that (narrow-pair) solutions exist with repeated quantum numbers. This makes the counting of allowed states much more complicated. This problem is addressed by a conjecture that, among other things, introduces a new type of quantum number which is strictly non-repeating.

### 2.6.2 The string hypothesis

In this section we discuss a highly influential conjecture, first formulated by Bethe in his original article [7] and further developed by Takahashi [47, 48], as to the structure of complex solutions of the Bethe equations: the string hypothesis. It
states that, for large system size $N$, complex roots will be grouped in strings$^2$ of $n$ roots, such that

$$
\lambda_{j\alpha} = \lambda_{\alpha} + \frac{i\zeta}{2} (n_j + 1 - 2a) + \frac{i\pi}{4} (1 - v_j) + i\delta_{j\alpha}
$$

(2.57)

where the deviations $\delta_{j\alpha}$ are exponentially suppressed with system size, i.e. $|\delta| = O\left(e^{-\text{(const)}N}\right)$. In this equation, $n_j$ is the length of the string of type $j$, and $v_j = \pm 1$ is called its parity. The real parameter $\lambda_{j\alpha}$ is called the string centre and, together with the string type $j$, uniquely determines the $n_j$ roots, up to deviations.

The reason to conjecture this is as follows. For large $N$, if the imaginary part of $\lambda$ is nonzero, the left-hand side of the Bethe equations goes to either zero or infinity,

$$
N^{-1/2} \left| \frac{\phi_{v-1}(\lambda)}{\phi_{v0}^{\prime}(\lambda)} \right|^N = O\left(e^{-Nv\text{sign Im }\lambda\text{sign }\zeta} \right).
$$

(2.58)

It is natural to assume that this is accompanied, on the right-hand side, by a (single) scattering phase factor diverging exponentially—which is exactly what happens if we insert a string of roots as defined above: for instance, for a 2-string, as $\delta = O\left(e^{-\text{(const)}N}\right)$, we get a factor

$$
\left| \frac{\phi_{v0}^{\prime}(i\zeta + i\delta/2)}{\phi_{v0}^{\prime}(\delta/2)} \right|^{\text{sign Im }\lambda} = O\left(e^{-Nv\text{sign Im }\lambda\text{sign }\zeta} \right).
$$

(2.59)

This assumption has been proven [49] to hold in the presence of a magnetic field, where the number of down spins is much smaller than the chain length.

### 2.6.3 Allowed string lengths

Constraints as to which string lengths are allowed were found by Takahashi and Suzuki [48]. A discussion can also be found in Takahashi’s book [37]. Hida [50] and Fowler and Zotos [51] give proofs of these constraints based on the condition of normalisablity of the wave function. However, they can also be derived directly as a consequence of the assumption underlying the string hypothesis, viz. that the vanishing or divergence of the left-hand side of the Bethe equations with large $N$ is compensated by a single factor on the right-hand side. This avoids the reference to a normalisability condition and the problems that come with it on a finite chain, where all wave functions are normalisable.

The conditions can be derived as follows. Start from a string’s bottom root, $\lambda_{\alpha n_j}$. The Bethe equation associated to it reads

$$
\left[ \frac{\phi_{v0}^{\prime}(\lambda - i\zeta n/2)}{\phi_{v0}^{\prime}(\lambda + i\zeta (2 - n)/2)} \right]^N = P_{\text{other}} \frac{\phi_{v0}^{\prime}(-2i\zeta)}{\phi_{v0}^{\prime}(i\delta_n - i\delta_{n-1})} \frac{\phi_{v0}^{\prime}(-3i\zeta)}{\phi_{v0}^{\prime}(-i\zeta)} \cdots \frac{\phi_{v0}^{\prime}(-ni\zeta)}{\phi_{v0}^{\prime}(-(n-2)i\zeta)},
$$

(2.60)

$^2$von Bethe selber als Wellenkomplex bezeichnet.
where all $\delta$s are assumed to be small and $P_{\text{other}}$ denotes the scattering of the root with roots outside of the string, which is a finite number. Therefore, the right-hand side is large; so should the left-hand side be, so that we conclude
\[
\left| \frac{\phi_v^\nu(\lambda - i\zeta n/2)}{\phi_v^\nu(\lambda + i\zeta(2 - n)/2)} \right| > 1 .
\] (2.61)

For the second root from the bottom, the Bethe equation reads
\[
\left[ \frac{\phi_v^\nu(\lambda + i\zeta(2 - n)/2)}{\phi_v^\nu(\lambda + i\zeta(4 - n)/2)} \right]^{N} = P_{\text{other}} \frac{\phi_v^\nu(i\delta_{n-1} - i\delta_n)}{\phi_v^\nu(2i\zeta)} \frac{\phi_v^\nu(-2i\zeta)}{\phi_v^\nu(i\delta_{n-1} - i\delta_{n-2})} \frac{\phi_v^\nu(-3i\zeta)}{\phi_v^\nu(-i\zeta)} \cdots \frac{\phi_v^\nu(-(n - 1)i\zeta)}{\phi_v^\nu(-(n - 3)i\zeta)} .
\] (2.62)

Now there is a vanishing factor in the numerator as well, and we don’t know the ratio between the two vanishing factors. However, the factor in the numerator equals that in the denominator of the bottom equation; multiplying the equations gives
\[
\left[ \frac{\phi_v^\nu(\lambda - i\zeta n/2)}{\phi_v^\nu(\lambda + i\zeta(2 - n)/2)} \right]^{N} = -P_{\text{other}}^2 \frac{\phi_v^\nu(-2i\zeta)}{\phi_v^\nu(i\delta_{n-1} - i\delta_{n-2})} \left[ \frac{\phi_v^\nu(-3i\zeta)}{\phi_v^\nu(-i\zeta)} \right]^2 \cdots \left[ \frac{\phi_v^\nu(-(n - 1)i\zeta)}{\phi_v^\nu(-(n - 3)i\zeta)} \right]^2 \frac{\phi_v^\nu(-ni\zeta)}{\phi_v^\nu(-(n - 2)i\zeta)}
\] (2.63)

and we may conclude
\[
\left| \frac{\phi_v^\nu(\lambda - i\zeta n/2)}{\phi_v^\nu(\lambda + i\zeta(2 - n)/2)} \right| > 1 .
\] (2.64)

This reasoning can be continued along the string and leads to the conditions
\[
\prod_{b=a}^{n} \left| \frac{\phi_v^\nu[\lambda + i\frac{n}{2}(n-2b+2)]}{\phi_v^\nu[\lambda + i\frac{n}{2}(n-2b)]} \right| < 1 \quad 1 < a \leq n .
\] (2.65)

For $\Delta \geq 1$, these conditions are always satisfied; all string lengths are allowed (Also, in this case, there are no parities $v$). For $-1 < \Delta < 1$, however, the situation is more involved:
\[
1 > \prod_{b=a}^{n} \left| \frac{\sinh[\lambda + i(n-2b+2)\zeta/2 + i(1-v)\pi/4]}{\sinh[\lambda + i(n-2b)\zeta/2 + i(1-v)\pi/4]} \right| \quad \text{(2.66)}
\]
\[
= \left| \frac{\sinh[\lambda + i(n-2a+2)\zeta/2 + i(1-v)\pi/4]}{\sinh[\lambda - i\zeta/2 + i(1-v)\pi/4]} \right| \quad = \sqrt{\frac{\cosh 2\lambda - v \cos[(n - 2a + 2)\zeta]}{\cosh 2\lambda - v \cos n\zeta}} .
\]

The requirement can thus be written as
\[
v \sin(a-1)\zeta \sin(n-a+1)\zeta \geq 0 \quad 1 < a \leq n ,
\] (2.67)
2.6. Complex roots

or, equivalently,

\[ [a \zeta / \pi] + [(n - a) \zeta / \pi] = (1 - v)/2 \pmod 2 \quad 1 \leq a \leq n - 1, \quad (2.68) \]

where the floor function \([x]\) denotes the highest integer that is less than or equal to \(x\). Note that equation (2.67) is always satisfied for \(n = 1, v = \pm 1\) and \(n = 2, v = 1\). We proceed to find the other solutions of the equation.

Since \(\zeta < \pi\), the equation for \(a = 1\) can also be written as an equation for the parity in terms of the string length,

\[ [(n - 1) \zeta / \pi] = (1 - v)/2 \pmod 2 \quad (2.69) \]

so that we may also write an equation for the string length only,

\[ [a \zeta / \pi] + [(n - a) \zeta / \pi] = [(n - 1) \zeta / \pi] \quad 1 \leq a \leq n - 1. \quad (2.70) \]

Summing over all \(a\), we finally get the expression conjectured by Takahasi and Suzuki [48]

\[ 2 \sum_{j=1}^{n-1} [j \zeta / \pi] = (n - 1) [(n - 1) \zeta / \pi]. \quad (2.71) \]

In order to find a solution, let us follow Takahashi and Suzuki and express \(\zeta / \pi\) as a continued fraction,

\[ \frac{\zeta}{\pi} =: \frac{1}{\nu_1 + \frac{1}{\nu_2 + \cdots}}. \quad (2.72) \]

For rational \(\zeta / \pi\), where the continuous fraction terminates after some number \(l\) of quotients, there is an ambiguity in this definition; to eliminate it, we require the final partial quotient \(\nu_l \geq 2\).

The algorithm for finding the partial quotients \(\nu_i\)—invert, subtract integer part, repeat—yields the recurrence relation

\[ p_0 = \pi / \zeta , \quad p_1 = 1 , \quad p_i = p_{i-2} - p_{i-1} \nu_{i-1} ; \quad \nu_i = [p_{i-1} / p_i]. \quad (2.73) \]

The *convergents* give successive approximations to the continued fraction:

\[ \frac{\zeta}{\pi} < \frac{1}{\nu_1} =: f_1 , \quad \frac{\zeta}{\pi} > \frac{1}{\nu_1 + \frac{1}{\nu_2}} =: f_2 , \quad \frac{\zeta}{\pi} < \frac{1}{\nu_1 + \frac{1}{\nu_2 + \frac{1}{\nu_3}}} =: f_3 , \quad \cdots \quad (2.74) \]

The convergents are given by the lowest terms fraction \(x_i / y_i\) where the numerators and denominators are found from the recurrence relation

\[ x_0 = 0 , \quad x_1 = 1 , \quad x_2 = \nu_2 , \quad x_i = x_{i-2} + \nu_i x_{i-1} \]

\[ y_0 = 1 , \quad y_1 = \nu_1 , \quad y_2 = \nu_1 \nu_2 + 1 , \quad y_i = y_{i-2} + \nu_i y_{i-1}. \quad (2.75) \]
It can be shown that the allowed string lengths and parities (apart from the two at \( n = 1, \nu = \pm 1, \) which we have already found) are given by

\[
\begin{align*}
n_j &= y_{i-1} + (j - m_i)y_i \\
v_j &= (-1)^{(n_j - 1)\zeta/\pi}
\end{align*}
\]

(2.76)

where \( i \) is chosen such that \( m_i < j \leq m_{i+1} \),\(^3\) and \( m \) is defined by \( m_0 = 0 \) and

\[
m_i = \sum_{k} \nu_k .
\]

(2.77)

The number of possible string types is \( N_s = m_1 + 1 \) for rational \( \zeta/\pi \) with \( l \) partial convergents, and infinity for irrational \( \zeta/\pi \). In practice, of course, we will consider only a finite set of string types.

### 2.6.4 Bethe–Takahashi equations

In the presence of bound states, factors \( \delta/\delta \) appear in the Bethe equations, which become indeterminate as \( \delta \to 0 \). These factors, however, can be cancelled by taking a product of the Bethe equations for all roots constituting a string. First consider the left-hand side of the Bethe equations. A product of the \( n \) equations corresponding to the roots in an \( n \)-string has on the left

\[
\frac{\phi_n^\nu(\lambda)}{\phi_n^\nu(\lambda)} \cdot \frac{\phi_{n-2}^\nu(\lambda)}{\phi_{n-2}^\nu(\lambda)} \cdots \frac{\phi_{n-4}^\nu(\lambda)}{\phi_{n-4}^\nu(\lambda)} = \frac{\phi_n^\nu(\lambda)}{\phi_n^\nu(\lambda)} ,
\]

(2.78)

with \( \phi_n^\nu(\lambda) \) as defined in table (2.1).

The right-hand side is more involved, since there is an extra product. First consider the equation for a single root. If there is an \( m \)-string present, the product on the right-hand side involves

\[
\frac{\phi_{m-1}^\nu(\lambda)}{\phi_{m}^\nu(\lambda)} \cdot \frac{\phi_{m-3}^\nu(\lambda)}{\phi_{m}^\nu(\lambda)} \cdots \frac{\phi_{m-1}^\nu(\lambda)}{\phi_{m}^\nu(\lambda)} = \frac{\phi_{m-1}^\nu(\lambda)}{\phi_{m}^\nu(\lambda)} \cdot \frac{\phi_{m+1}^\nu(\lambda)}{\phi_{m}^\nu(\lambda)}
\]

(2.79)

In fact, this relation also holds when \( m = 1 \). After we’ve consolidated the equations in this way, let’s now consider the product over \( n \) equations.

\[
\begin{align*}
\frac{\phi_{m+n-2}^\nu(\lambda)}{\phi_{m+n}^\nu(\lambda)} \cdot \frac{\phi_{m+n-4}^\nu(\lambda)}{\phi_{m+n-2}^\nu(\lambda)} \cdots \frac{\phi_{m+n-2}^\nu(\lambda)}{\phi_{m+n}^\nu(\lambda)} & \cdot \frac{\phi_{m+n-4}^\nu(\lambda)}{\phi_{m+n-2}^\nu(\lambda)} \cdots \frac{\phi_{m+n+2}^\nu(\lambda)}{\phi_{m+n}^\nu(\lambda)} \\
= \frac{\phi_{m+n-2}^\nu(\lambda)}{\phi_{m+n-2}^\nu(\lambda)} \cdot \frac{\phi_{m+n-4}^\nu(\lambda)}{\phi_{m+n-4}^\nu(\lambda)} & \cdot \frac{\phi_{m+n-2}^\nu(\lambda)}{\phi_{m+n-2}^\nu(\lambda)} \cdots \frac{\phi_{m+n+2}^\nu(\lambda)}{\phi_{m+n+2}^\nu(\lambda)}
\end{align*}
\]

(2.80)

\(^3\)Note that Takahashi [48, 37] chooses the bounds as \( m_i \leq j < m_{i+1} \). Due to (2.75), our current choice produces the same string lengths and parities, but has the advantage that the strings produced are ordered by length. Furthermore, no zero-length strings are produced.
2.6. Complex roots

If \( n > m \), we have \( m - n = -|m - n| \) and the product cancels between

\[
\left[ \frac{\phi_v^{m-n}-2(\lambda)}{\phi_v^{m-n}+2(\lambda)} \right]^2 \left[ \frac{\phi_v^{m-n}-4(\lambda)}{\phi_v^{m-n}+4(\lambda)} \right]^2 \cdots \left[ \frac{\phi_v^{m-n}+2(\lambda)}{\phi_v^{m-n}-2(\lambda)} \right]^2 = 1 \quad (2.81)
\]

so that on the right-hand side we are left with

\[
\phi_v^{m-n} \phi_v^{m+n} \left[ \frac{\phi_v^{m-n}-2(\lambda)}{\phi_v^{m-n}+2(\lambda)} \right]^2 \left[ \frac{\phi_v^{m+n}-4(\lambda)}{\phi_v^{m+n}+4(\lambda)} \right]^2 \cdots \left[ \frac{\phi_v^{m-n}+2(\lambda)}{\phi_v^{m+n}-2(\lambda)} \right]^2 .
\]

(2.82)

Obviously, the first factor in the product is also unity if \( m = n \).

Taking the logarithm leads to what is known as the Bethe–Takahashi equations,

\[
N \theta_v^{n_j}(\lambda_j^j) - \sum_{k=1}^{N_s} \sum_{\alpha=1}^{M_j} \Theta_{jk}(\lambda_\alpha^j - \lambda_\beta^k) = 2 \pi I_j^j ,
\]

(2.83)

with

\[
\Theta_{jk}(\lambda) = (1 - \delta_{n_j n_k}) \theta_v^{n_j n_k}(\lambda) + 2 \theta_v^{n_j n_k}(\lambda) + \cdots + 2 \theta_v^{n_j n_k}(\lambda) + \theta_v^{n_j n_k}(\lambda)
\]

(2.84)

These equations give the string centres \( \lambda_j^j \) in terms of a new set of quantum numbers \( I_j^j \). As we took the logarithm leading to the Bethe–Takahashi equations (2.83), we have made a specific choice for their definition; to find the relation with the Bethe quantum numbers \( J_\alpha^j \) defined earlier we have to be careful about the way we take the limit \( \delta \to 0 \). This will be done in chapter 3.

\( M_j \) is the number of strings of type \( j \). The \( I_j^j \) are integer for odd \( M_j \) and half-integer for even \( M_j \). Note that the \( M_j \) must satisfy \( \sum_{k=1}^{N_s} n_k M_k = M \).

2.6.5 Energy and momentum of bound states

The energy associated to a string of length \( n \) and parity \( v \) is

\[
E = -J[-i\phi_2(0)]\pi a_v^v(\lambda) + hn
\]

(2.85)

and its momentum equals

\[
k = \pi + \theta_v^v(\lambda) \pmod{2\pi} ,
\]

(2.86)

so that the total momentum of a state is

\[
q = \pi \sum_j \delta_{\nu_j,1} M_j + \frac{2\pi}{N} \sum_j I_j^j \pmod{2\pi} .
\]

(2.87)
2.6.6 Strings, pairs, and quartets

Notwithstanding the fact that most of the literature involves it in one way or another, the string hypothesis is known to be not rigorously valid. Working from the thermodynamic limit of the XXZ model, Babelon et al. [46] and Woynarovich [52] show that roots of the Bethe equations form configurations of two-strings, wide pairs, and quartets, which are pairs of two-strings shifted in the imaginary direction. Though not normalisable in the large-$N$ limit unless they approach string configurations, such configurations would be possible in finite chains. Vladimirov [53] showed that, in the $M = 2$ subspace, there exist complex pairs which deviate as $\lambda_{\pm} = N \pm i\sqrt{N}$ with large $N$. An exact analysis of the solutions in the $M = 2$ sector of the isotropic model by Essler et al. [54] (confirmed for the anisotropic model in [55, 56]) shows that from $N = 21.86$ sites onward pairs of extra real solutions appear where the string hypothesis predicts two-strings. These solutions fit into the string picture insofar as the number of extra real solutions agrees with the number of missing two-strings; they can therefore be construed as arising from narrow two-strings that deviated too far. This agrees with the observation that the quantum numbers $J$ for the two extra real roots are equal. In chapter 3 we will attempt to shed more light on the string hypothesis, trying to explicitly solve for its deviations.

2.7 Classification of states

One of the great advantages of the string hypothesis is that it leads to the correct number of states in the Hilbert space, and thereby provides a classification of those states.

2.7.1 Quantum number bounds

It has been proposed [7, 47, 57, 58] that in the isotropic Heisenberg model, the Bethe–Takahashi quantum numbers of lowest-weight states should be non-coinciding and bounded by

$$|I_\alpha| < I_\infty := \frac{1}{2} \left[ N + 1 - \sum_{k \geq 1} M_k (2 \min(n_j, n_k) - \delta_{j,k}) \right]$$  \quad \text{for } \Delta = 1 \quad (2.88)$$

$$|I^1| < \frac{1}{2\pi} \left| N \theta_j(\infty) - \sum_{k \geq 1} M_k \Theta_{j,k}(\infty) \right|$$  \quad \text{for } |\Delta| < 1 \quad (2.89)$$

where $M_k$ is the number of strings of type $k$, which form restricted partitions such that $\sum_{j \geq 1} n_j M_j = M$. Note that the inequality is strict; in the isotropic case, it is chosen such that only finite rapidities (corresponding to highest-weight states) are generated. In the absence of higher strings, infinite rapidities correspond to the quantum number $J_\infty = I_\infty^1$. 36
Bethe argued, and Takahashi showed, that for the isotropic chain this way one constructs exactly \( \binom{N}{M} - \binom{N}{M-1} \) unique sets of quantum numbers for \( M \) down spins, or exactly the number of highest-weight states. As the Bethe–Takahashi equations have at least one solution for each set \( \{I\} \), if every one of them corresponds to a valid eigenstate of the system, it follows that each solution must be unique and the solutions form a complete set. Thus one can classify the full Hilbert space according to string content. For short chains, we can in fact show that this classification works by solving the Bethe ansatz equations numerically for all states (see appendix A). For the anisotropic chain, it has also been shown (by a much more complicated analytical analysis) that the string hypothesis leads to the correct number of states [59].

A rationale for deriving (2.88) would be to let the rapidity \( \lambda_j^{\alpha} \to \infty \) and consider what happens to the Bethe–Takahashi equations. This leads indeed to the correct maximum value for the quantum numbers of real roots. For higher strings, however, this gives a value that is too high,

\[
I_j^\alpha < \tilde{I}_\infty := \frac{1}{2} \left[ N + 2n_j - 1 - \sum_{k \geq 1} M_k (2 \min(n_j, n_k) - \delta_{j,k}) \right].
\] (2.90)

To know where the correct lower value comes from, we have to study what happens to the outermost \( n_j \)-string. We will make some remarks about this in chapter 3, but the picture remains not completely clear and some more study will be needed to find the correct reason for the bound (2.88).

### 2.7.2 Particle–hole excitations

As the Bethe–Takahashi quantum numbers are assumed to be non-coinciding, the number of quantum number positions (either occupied or vacant) in the \( j \)th string sector is \( 2I_j^\infty + 1 \). The number of vacancies then equals

\[
V_n := 2I_j^\infty + 1 - M_j = N - 2M + 2 \sum_{k > j} (k - j)M_k
\] (2.91)

In the XXX model, at zero field, we see that the quantum number bounds (2.88) leave place for no more than one state with finite real rapidities, viz. the ground state (2.51). To create room for excitations, we have to either let rapidities go to infinity, or create bound states. This always creates an even number of holes, which can then be put anywhere in the ground state interval. These holes correspond to the spinons found in the thermodynamic limit (see chapter 5) and are the quasi-particle excitations of the system. Schematically, in an \( N = 16, M = 8 \) state, the lowest spinon excitation created by letting a rapidity go to infinity looks like

\[
\begin{array}{ccccccc}
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\downarrow & & & & & & \\
\circ & \bullet & \bullet & \bullet & \bullet & \bullet & \circ
\end{array}
\]
Note that if we create an infinite rapidity or a string of odd length, the quantum numbers change from integers to half integers or vice versa, as the parity of the number of real rapidities changes. This guarantees that spinons are always created in even numbers.

At finite field, a number of \( N - 2M \) vacancies is present in the ground state, so that there is no such fundamental difference between the ground state and low-lying excitations: there is a class of excitations with the same number of vacancies as the ground state. These can be constructed by taking the ground state quantum numbers and moving one of the two outermost particles to a position further outward. Schematically, in an \( N = 16, M = 6 \) state,

\[
\begin{array}{c}
\circ \circ \cdots \circ \circ \circ \circ \\
\circ \circ \circ \circ \circ \circ \circ \circ \circ \\
\end{array}
\]

Thus a fermion-like picture arises: the low-lying excitations in a nonzero-field model take the form of particle–hole excitations over a Fermi sea; the lowest excitations are those where the particles and holes are close to the Fermi level. These particles and holes have been coined ‘psinons’ and ‘antipsinons’ in the literature [60, 61], but this confusing\(^4\) terminology is somewhat unhelpful. As is seen in the thermodynamic limit (see chapter 5) at zero field, spinons (corresponding to holes in the picture above) can be seen as particles with a well-defined dispersion relation. The particle-hole picture just introduced is slightly different; here, the particles and holes are mainly a bookkeeping device used to scan through all states in a convenient manner.

For the anisotropic model, we can use a similar scheme, with the exception that in this case no infinite rapidities arise as the model is no longer symmetric under rotations. Instead, extra vacancies arise because the \( I_\infty \) is higher, and there is an extra sector for one-strings with negative parity. At zero field, however, the particles still fill all available positions, and particles of another stringtype must be created to make holes; one can therefore extend the spinon picture from the isotropic chain to anisotropic chains.

### 2.7.3 Enumerating states

Now we can scan through all states by moving particles and holes from their ground-state position. To keep track of the states we are scanning through, it is convenient to denote them using Young tableaux [62].

For clarity, let us first discuss only states with real rapidities. We separate the available positions into two sectors: the hole sector \( s_0 \), consisting of the positions that are occupied in the ground state, and the particle sector \( s_1 \). To each sector we associate a Young diagram. The empty diagram corresponds to the configuration of lowest energy: in the hole sector, all holes (if any) as far outward as possible; in the particle sector, all particles (if any) as far inward as possible. The number

\(^4\)I often mistype ‘psi’ for ‘spi’
2.7. Classification of states

Figure 2.1: An example of counting in the isotropic chain at zero field in a base with \( N = 12, M_1 = 6, M_2 = 3 \), in base \((0,0,3)\). Sector numbers are indicated. The lower line represents real roots, the upper line 2-strings. Note that sector \( s_2 \) leaves no space for excitations; the first excitation would be obtained by moving a particle from position \( s_0 : 0 \) to position \( s_1 : 0 \).

of boxes in the first column is the number of positions the outermost particle (innermost hole) is moved from its ground position, the second column represents the same for the second outermost particle, and so on. We number the positions in alternating fashion; thus, positions with even numbers are located to the left of the centre whereas positions with odd numbers are located to the right. In this way, when moving a particle outward, we go consecutively through pairs of states which differ only by moving a particle from the left to the right at the same distance of the centre. This numbering scheme is illustrated in figure 2.1. The width of the diagram is therefore less than or equal to the total number of positions in the sector minus the number of filled ones; the height is less than or equal to the number of particles in the sector.

We can include bound states simply by writing an extra Young tableau \( j \) for each string type \( j \). Here, the empty diagram corresponds to the configuration with all particles in the centre of the sector, the first row corresponds to the displacement of the outermost particle, etcetera.

The enumeration of the Young diagrams is such that, if the maximum width is \( w_{\text{max}} \) and the height of the \( c \)th column is \( h_c \), the ordinal of a diagram is given by

\[
\text{id}(\{h\}) := \sum_{c=1}^{w_{\text{max}}} \left( w_{\text{max}} - c + h_c \right) \left( w_{\text{max}} - c + 1 \right)
\] (2.92)

This means that we order the states in the sector such that we first let the first particle go outward as far as possible, then start again at the beginning but move a second particle by one, etcetera. In total there are \( n_j = \left( w_{\text{max}}' - h_j' \right)^{h_{\text{max}}'} \) possible diagrams. For example, in figure 2.2, we show the excitation given by \( \otimes \).

Combining the Young diagram ordinals for each sector, we can associate an ordinal to every state,

\[
\text{id}(\{h^0\}, \{h^1\}, \ldots) = \sum_{s \geq 0} \text{id}_s \prod_{j=0}^{s} n_j
\] (2.93)
Using this recipe we can uniquely identify a Bethe–Takahashi state by its ordinal (ID number) and the number of particles in each sector (this set of numbers we call its base; a similar concept was used in [63]).

The ordering is such that matrix elements of local spin operators with respect to the ground state by and large decreases with increasing ID number, as we will discuss in chapter 4.
3.

Bethe roots in the complex plane

The Bethe equations may present an exact solution to the eigenvalue problem of the Heisenberg chain, to get actual results, it is still necessary to solve them. Since they are a set of coupled nonlinear equations, an analytical solution in terms of simple functions is out of the question; the way forward is by numerical solution. In general, Bethe equations with real rapidities lend themselves well to solution by iteration. The simplest and standard approach is to invert the kinematic phase term, e.g., in the XXZ model, the iteration prescription

\[ \lambda'_\alpha = \text{atanh} \left[ \tan(\zeta/2) \tan \left( \pi J_\alpha \frac{1}{N} + \sum_{\beta=1}^{M} \frac{\tanh(\lambda_\alpha - \lambda_\beta)}{\tan \zeta} \right) \right] \]  

(3.1)

does the trick. In a relatively small number of steps the equations can be solved to machine precision.

Unfortunately, for many calculations on the finite chain, real solutions alone are not enough. Since Bethe’s original article [7] it has been known that there are not enough real solutions to fill the Hilbert space; complex solutions must exist. These complex solutions, which represent bound states of magnons, can play an important role. This is, for instance, the case in an approximation of the dynamical correlation functions such as we will discuss in chapter 4. Restricting oneself to real solutions, in that case, unnecessarily restricts the accuracy of the calculation rather severely.

It is therefore necessary to find the complex roots of the Bethe equations. Due to the branch cuts of the inverse tangent, solving the Bethe equations directly in the complex plane is much harder than finding real-valued solutions. A method such as Newton–Raphson (see e.g. [64]), while in principle suitable for finding complex roots, requires the construction and computation of the determinant of a large
matrix; moreover, it is only successful in this case if the initial guess is very close
to the actual solution, and can therefore only be used to refine a solution already
found by other means. This problem was noted in, for instance, [65] in the context
of the spin-1 Heisenberg model.

This problem is avoided in the Bethe–Takahashi approach, where all rapidities are
real. However, the solutions in that approach are only approximately correct. For
high values of the magnetic field, hence low number of down spins, this approx-
imation is expected to get more accurate with increasing chain length; however,
the chain length accessible to numerics is limited and we would also like to address
magnetic fields close to zero. On numerically attainable lengths of a few hundred
sites, the deviations from Bethe–Takahashi solutions turn out to be still significant.

Here we are presented with a paradox that is common, but sometimes overlooked,
in ‘exact’ methods: though we have an exact expression, it is not useful until we find
a way of evaluating it, of getting the numbers out within the available calculation
time and memory. While the exact solution presents a genuine step forward, it is
not yet the final answer to the problem.

In this chapter we will address the problem of finding complex solutions to the
Bethe equations for the isotropic Heisenberg chain. Our strategy is first to solve
the Bethe–Takahashi equations and then to use that solution as an initial guess
to solve the full Bethe equations. In this way we are able to find a large class of
solutions in the complex plane to high precision.

The first section of this chapter deals with estimating the degree of accuracy of a
given Bethe–Takahashi solution and addresses all isotropy cases of the antiferro-
magnetic chain; the remaining sections, in which the method for finding a complex
solution is outlined, address the isotropic chain only. The method, with some more
work, may well be extendible to anisotropic chains; this, however, has not yet been
attempted.

### 3.1 First-order deviations

To check whether the approximation $\delta \to 0$ is justified, once we have found a
solution to the Bethe-Takahashi equations we can explicitly check whether or not
it is a solution of the original Bethe equations (2.31) to sufficient accuracy, by
estimating $\delta$ to first order.

Let us parametrise the deviations as follows. For the roots in an $n$-string,

$$
\lambda_a = \lambda + i \frac{\zeta}{2} (n + 1 - 2a) + i \frac{\pi}{4} (1 - v) + d_a 
$$

where $d_a := i \delta_a + \epsilon_a$. The string is fixed to its centre as

$$
\delta_{(n+1)/2} = \epsilon_{(n+1)/2} = 0 \quad \text{for } n \text{ odd}
$$

$$
\epsilon_{n/2} = 0 \quad \text{for } n \text{ even}
$$

(3.3)
3.1. First-order deviations

Furthermore, as the roots are grouped in pairs of conjugates, 

\[ d_{n-a} = d_a^* \quad (3.4) \]

In the Bethe equation for a given root, the scattering phase features a product over the other roots of the string,

\[ R_a := \prod_{b \neq a}^{b \neq a+1} \frac{\phi_2(b-a+1)(d_a - d_b)}{\phi_2(b-a-1)(d_a - d_b)} \quad (3.5) \]

To lowest order in \( d \), for \( a \neq 1, n \),

\[ R_a \approx - \frac{d_a - d_{a-1}}{d_a - d_{a+1}} \prod_{b \neq a}^{b \neq a-1} \frac{\phi_2(b-a+1)}{\phi_2(b-a-1)} \frac{\phi_2(n-a+1)}{\phi_2(n-a)} \frac{\phi_2(n-a-1)}{\phi_2(n-a-2)} \quad (3.6) \]

where we write \( \phi_a := \phi_a(0) \) for compactness.

For \( a = 1 \) or \( a = n \),

\[ R_1 \approx - \frac{\phi_{2n} \phi_2(n-1)}{(d_1 - d_2) \phi_1} \quad R_n \approx - \frac{(d_n - d_{n-1}) \phi_1}{\phi_{2n} \phi_2(1-n)} \quad (3.7) \]

Thus, starting from \( a = 1 \), we can successively construct the differences

\[ d_{a+1} - d_a = - \frac{\phi_{2n} \phi_2(n-1)}{\phi_{2a}} \left[ \prod_{b=1}^{a} K_b \right] \left[ \prod_{b=1}^{a-1} \frac{\phi_2(n-b)}{\phi_2 b} \right]^2 \quad (3.8) \]

where \( K_a \) is given by the other factors in the Bethe equation,

\[ K_a := \left[ \frac{\phi_{n+2-2a}(\lambda)}{\phi_{n-2a}(\lambda)} \right]^{-N(k\beta) \neq (j\alpha)} \prod_{k\beta}^{(k\beta) \neq (j\alpha)} \left[ \frac{\phi_{n+3-2a}(\lambda - \lambda_k^{k\beta})}{\phi_{n-2a}(\lambda - \lambda_k^{k\beta})} \right] ; \quad (3.9) \]

the product is understood to run over all complex roots not belonging to the same string.

For odd \( n \), we can use \( d_{(n+1)/2} = 0 \) and sum over the differences to get

\[ d_b = - \sum_{a=b}^{(n-1)/2} \frac{\phi_{2a} \phi_2(n-a)}{\phi_{2a}} \left( n - 1 \right)^2 \prod_{c=1}^{a} K_c \quad \text{for } b \leq (n-1)/2 \quad , \quad (3.10) \]

where we have introduced a generalised binomial coefficient

\[ \prod_{c=1}^{a-1} \frac{\phi_2(n-c)}{\phi_2 c} =: \binom{n-1}{a-1}_\phi \quad . \quad (3.11) \]
For even \( n \), we have \( \text{Re} d_{n/2} = 0 \) and therefore \( d_{n/2} = -d_{n/2+1} \). We now have, for \( b \leq n/2 - 1 \),

\[
d_b = \frac{1}{2} \left[ \phi_{2n} \left( \frac{n-1}{n/2-1} \right)^2 \prod_{c=1}^{n/2} K_c \right] - \sum_{a=b}^{n/2-1} \left[ \frac{\phi_{2n} \phi_{2(n-a)}}{\phi_{2a}} \left( \frac{n-1}{a-1} \right)^2 \prod_{c=1}^{a} K_c \right].
\]

(3.12)

The behaviour of \( K_a \) for large \( N \) and \( \lambda \) depends on the order in which we take the limits. In particular, let us consider the limit for large \( \lambda \), i.e. a string centre far away from the origin, while the other rapidities remain small. Then, \( \lim_{\lambda \to \infty} K_a = 1 \) and, for odd \( n \),

\[
\lim_{\lambda \to \infty} d_b = -\sum_{a=b}^{n-1/2} \frac{\phi_{2n} \phi_{2(n-a)}}{\phi_{2a}} \left( \frac{n-1}{a-1} \right)^2
\]

(3.13)

Note that this number is of order unity and independent of the chain length \( N \).

This order of limits is relevant for instance when we consider the limit to large \( N \) at a fixed magnetisation density \( M/N \), as in that case the number of rapidities grows with \( N \). Then, assuming a constant rapidity density, strings on the periphery will always be strongly deviated.

Shortly we will give equations to calculate the deviations exactly, thereby allowing to solve the Bethe equation on finite chains without assuming the string hypothesis to be strictly valid. However, the present equations have the advantage that they are directly given in terms of the rapidities found using the string hypothesis: no extra sets of coupled nonlinear equations need to be solved. In this way they provide a valuable check on solutions found using the string hypothesis.

### 3.2 Exact deviations for the isotropic chain

If it has been established that the string hypothesis does not hold for a given Bethe state, we need to find the deviations exactly. To do so, we rewrite the Bethe equations. The Bethe–Takahashi equations are given by a product over the Bethe equations associated to all roots in a string. This leaves a number of independent equations unused. These equations are degenerate in the limit \( \delta \to 0 \); however, when rewritten, they can be used as an iterative prescription for the exact deviations. In such an iteration, we take the solution of the Bethe–Takahashi equation as the initial guess.

We derive these equations in the following sections, starting from the two- and three-string case and then generalising to the \( n \)-string case.

#### 3.2.1 Deviated two-strings

The Bethe–Takahashi equations (2.83) are found from the sum of the logarithmic Bethe equations, absorbing all contributions from branch cut crossings in the
3.2. Exact deviations for the isotropic chain

Bethe–Takahashi quantum numbers. To find their relation with the Bethe quantum numbers, let us carefully redo the derivation. We concentrate on the isotropic chain.

Deviated two-strings are parametrised as \( \lambda_{\alpha \pm}^{(2)} := \lambda_{\alpha}^{(2)} \pm i(1 + 2\delta_{\alpha}^{(2)})/2 \) where \( \lambda_{\alpha}^{(2)} \) and \( \delta_{\alpha}^{(2)} \) are real numbers. Assuming all \(|\delta_{\alpha}| < 1/2\), the sum of the (log-) Bethe equations for \( \lambda_{\alpha \pm}^{(2)} \) equals,

\[
\begin{align*}
\sum_{k=1}^{N} \left[ \tan \left( \frac{\lambda - \lambda_{\beta}^{(2)} \delta + 3/2}{\delta + 3/2} \right) + \tan \left( \frac{\lambda - \lambda_{\beta}^{(2)} \delta - 3/2}{-\delta + 3/2} \right) \right] + \tan \left( \frac{\lambda - \lambda_{\beta}^{(2)} \delta + 3/2}{\delta - 3/2} \right) + \tan \left( \frac{\lambda - \lambda_{\beta}^{(2)} \delta - 3/2}{-\delta - 3/2} \right) + \pi \text{sign}(\lambda - \lambda_{\beta}^{(2)}) \Theta(\delta - \delta_{\beta}^{(2)})
\end{align*}
\]

(3.14)

where, for legibility, we dropped the indices \( \alpha \) and \( \beta \) and we have added primes to the \( \lambda \)s in the left-hand side to stress that these represent the next value in the iteration, to be determined from the values on the right-hand side. Taking the limit for all \( \delta \to 0 \) and comparing with the Bethe–Takahashi equations, we conclude for the relation between the quantum numbers

\[
I_{\alpha}^{(2)} = \Theta(\delta) + 2J^{+} - \frac{N}{2} + \frac{1}{2} \sum_{\beta} \text{sign}(I_{\alpha}^{(2)} - I_{\beta}^{(2)}) \quad (\text{mod } N)
\]

(3.15)

taking this equation modulo 2, we see that the criterion for a two-string with quantum number \( I_{\alpha}^{(2)} \) to be wide is

\[
\Theta(\delta) = I_{\alpha}^{(2)} + \frac{N}{2} - M + 1 - \frac{1}{2} \sum_{\beta} \text{sign}(I_{\alpha}^{(2)} - I_{\beta}^{(2)}) \quad (\text{mod } 2).
\]

(3.16)

The sum of the Bethe equations gives the equation for the string centres; therefore, we must look at the difference of the Bethe equations to find the deviations. The imaginary part of this equation can be written

\[
\left[ 1 + \delta' \right]^{2} = \left[ \frac{(1 + \delta)^{2} + \lambda^{2}}{\delta^{2} + \lambda^{2}} \right]^{N} \prod_{\beta} \frac{(\delta - 1/2)^{2} + (\lambda - \lambda_{\beta}^{(2)})^{2}}{\delta + 3/2 + (\lambda - \lambda_{\beta}^{(2)})^{2}} \times \prod_{\beta} \frac{(\delta + \delta_{\beta}^{(2)})^{2} + (\lambda - \lambda_{\beta}^{(2)})^{2}}{2 + (\delta + \delta_{\beta}^{(2)})^{2} + (\lambda - \lambda_{\beta}^{(2)})^{2}}
\]

(3.17)
Together, equations (3.14), (3.17), and (3.16) determine the rapidity $\lambda^{(2)}_\alpha$ and deviation $\delta^{(2)}_\alpha$. It is of importance to note that the right-hand side of this equation is not strongly dependent on $\delta^{(2)}_\alpha$, as long as $\delta^{(2)}_\alpha$ is small compared to $\lambda^{(2)}_\alpha$, so that an iterative approach to solving these coupled equations is expected to converge rapidly.

### 3.2.2 Deviated three-strings

Let us consider the equations for the deviation of a three-string in the presence of other strings of length not more than 2, which is enough to illustrate the general idea. In the presence of longer strings, terms will have to be added to these expressions but as these become quite unwieldy we defer this derivation to the treatment of the general case in the next section.

Parametrising the three-string as

\[
\lambda^{(3)}_{\alpha \pm} = \lambda^{(3)}_\alpha + \epsilon^{(3)}_\alpha \pm i(1 + \delta^{(3)}_\alpha)
\]

and again assuming $|\delta^{(3)}_\alpha| < 1/2$, we consider the sum over all three Bethe equations,

\[
\text{atan} \frac{2(\lambda' + \epsilon)}{3 + 2\delta} - \text{atan} \frac{2(\lambda' + \epsilon)}{1 + 2\delta} + \pi \text{sign}(\lambda' + \epsilon) = \mod \pi
\]

\[
\frac{\pi}{N} (J^- + J^0 + J^+) + \frac{1}{N} \sum_{\beta} \text{atan}(\lambda - \lambda^k_{\beta}) + \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{3 + 2\delta} + \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\delta}
\]

\[
+ \pi \Theta(\delta) \text{sign}(\lambda + \epsilon - \lambda^k_{\beta})
\]

\[
+ \frac{1}{N} \sum_{\beta} \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\frac{3}{2} + \delta^k_{\beta}} + \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\frac{1}{2} - \delta^k_{\beta}} + \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\frac{5}{2} + \delta + \delta^k_{\beta}}
\]

\[
- \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\frac{1}{2} + \delta + \delta^k_{\beta}} + \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\frac{3}{2} + \delta - \delta^k_{\beta}} + \text{atan} \frac{\lambda + \epsilon - \lambda^k_{\beta}}{\frac{1}{2} - \delta - \delta^k_{\beta}}
\]

\[
+ \pi \text{sign}(\lambda - \lambda^k_{\beta} + \epsilon - \epsilon^k_{\beta}) [\Theta(\frac{1}{2} + \delta + \delta^k_{\beta}) + \Theta(-\frac{1}{2} + \delta - \delta^k_{\beta})]
\]

Taking its limit for $\delta, \epsilon \rightarrow 0$, and comparing to the Bethe–Takahashi equations, we find

\[
J^- + J^0 + J^+ = I^{(3)} - \frac{1}{2} \sum_{\beta} \text{sign}(\lambda - \lambda^k_{\beta}) - \sum_{\beta} \text{sign}(\lambda - \lambda^k_{\beta}) \mod N.
\]

The real part of the difference between the + and − logarithmic Bethe equations yields $J_+ - J_- = -1$. This leaves $J_0$ as of yet undetermined, but it turns out to be unnecessary to know this quantum number to be able to solve the equations.
The imaginary part of the difference between the + and − equations gives, when exponentiated,

$$\delta^2 + \epsilon^2 = r^2 := [(2 + \delta)^2 + \epsilon^2] \left[\frac{3 + 2\delta}{1 + 2\delta}\right]^2 \left[\frac{(1 + 2\delta)^2 + 4(\lambda + \epsilon)^2}{(3 + 2\delta)^2 + 4(\lambda + \epsilon)^2}\right]^N \times \prod_{\beta} \frac{(2 + \delta)^2 + (\lambda + \epsilon - \lambda_\beta^k)^2}{\delta^2 + (\lambda + \epsilon - \lambda_\beta^k)^2} \times \prod_{\beta} \frac{(\frac{5}{2} + \delta + \delta_\beta^k)^2 + (\lambda + \epsilon - \lambda_\beta^k)^2}{(\frac{1}{2} + \delta + \delta_\beta^k)^2 + (\lambda + \epsilon - \lambda_\beta^k)^2}$$

(3.21)

The other independent equation is the Bethe equation for \(\lambda^0\). However, for later generalisation it is more convenient to consider the sum of the + and − equations,

$$-\tan \epsilon/\delta + \pi \Theta(\delta) \operatorname{sign} \epsilon = \theta$$

(3.22)

$$:= -\tan \frac{\epsilon}{2 + \delta} - \pi (J^+ + J^-) + N \left[\tan \frac{2(\lambda + \epsilon)}{3 + 2\delta} - \tan \frac{2(\lambda + \epsilon)}{1 + 2\delta}\right]$$

$$- \sum_{\beta} \tan \frac{\lambda + \epsilon - \lambda_\beta^k}{2 + \delta} - \tan \frac{\lambda + \epsilon - \lambda_\beta^k}{\delta} + \pi \operatorname{sign}(\lambda + \epsilon - \lambda_\beta^k) \Theta(\delta)$$

$$- \sum_{\beta} \tan \frac{\frac{5}{2} + \delta + \delta_\beta^k}{\delta_\beta^k} - \tan \frac{\frac{1}{2} + \delta + \delta_\beta^k}{\delta_\beta^k} + \pi \operatorname{sign}(\lambda + \epsilon - \lambda_\beta^k) \Theta(\frac{1}{2} + \delta + \delta_\beta^k)$$

$$+ \tan \frac{\lambda + \epsilon - \lambda_\beta^k}{\frac{5}{2} + \delta - \delta_\beta^k} - \tan \frac{\lambda + \epsilon - \lambda_\beta^k}{\frac{1}{2} - \delta + \delta_\beta^k} + \pi \operatorname{sign}(\lambda + \epsilon - \lambda_\beta^k) \Theta(-\frac{1}{2} + \delta - \delta_\beta^k)$$

Both equations are written such that the terms on the right-hand side do not strongly depend on \(\epsilon\) and \(\delta\). Now we can simply iterate

$$\delta' = - |r| \cos \theta \quad \epsilon' = |r| \sin \theta$$

(3.23)

### 3.2.3 Deviated \(n\)-strings

Now that we know how to solve two- and three-strings, we are ready to generalise our approach to strings of any length. Consider a generic string of type \(j\),

$$\lambda_{\alpha}^j = \lambda_{\alpha}^b + \epsilon_{\alpha a}^j + \frac{i}{2}(n_j + 1 - 2a) + i \delta_{\alpha a}^j$$

(3.24)

where the deviations \(\delta\) and \(\epsilon\) are real and satisfy \(\delta_a = -\delta_{n+1-a}\), \(\epsilon_a = \epsilon_{n+1-a}\). Furthermore, for even \(n\), \(\epsilon_{n/2} = 0\); for odd \(n\), \(\epsilon_{[n/2]+1} = \delta_{[n/2]+1} = 0\).
Argument of deviations

First we consider the sum of Bethe equations for two conjugate roots. We use the relation

\[ \text{atan}(a + ib) + \text{atan}(a - ib) = \xi(a, 1 + b) + \xi(a, 1 - b) \],

where we defined

\[ \xi(\epsilon, \delta) := \text{atan} \frac{\epsilon}{\delta} + \pi \text{sign} \epsilon \Theta(-\delta) \].

This is in fact an argument of \( i\epsilon - \delta \), such that \( \xi(0, \delta) = 0 \) and

\[-\pi < \xi(\epsilon, \delta) \leq -\pi/2 \quad \text{for} \quad \epsilon < 0, \delta \geq 0 \]
\[-\pi/2 \leq \xi(\epsilon, \delta) < 0 \quad \text{for} \quad \epsilon < 0, \delta \leq 0 \]
\[0 < \xi(\epsilon, \delta) \leq \pi/2 \quad \text{for} \quad \epsilon > 0, \delta \leq 0 \]
\[\pi/2 \leq \xi(\epsilon, \delta) < \pi \quad \text{for} \quad \epsilon > 0, \delta \geq 0 \] (3.27)

Another likeable feature of \( \xi(\epsilon, \delta) \) is that, unlike the inverse tangent, it is continuous in \( \delta = 0 \). Therefore the value for zero deviations is well-defined and we need not keep track of the sign of \( \delta \) in the limit.

The sum equation reads

\[ \pi (J_{\alpha,a}^j + J_{\alpha,n+1-a}^j) = \theta_{\text{kin}}^a - \theta_{\text{other}}^a - \theta_{\text{self}}^a \quad (\text{mod} \ N\pi) \],

where

\[ \theta_{\text{kin}}^a := N [\xi(2(\lambda + \epsilon_a), n_j + 2 - 2a + 2\delta_a) + \xi(2(\lambda + \epsilon_a), -n_j + 2a - 2\delta_{aa})] \]

\[ (k, \beta) \neq (j, \alpha) \]

\[ \theta_{\text{other}}^a := \sum_{k, \beta} \sum_{1 \leq b \leq n_k} \xi (\lambda - \lambda(k) + \epsilon_a - \epsilon_{k\beta}, 1 + (n_j - n_k)/2 - (a - b) + (\delta_a - \delta_{k\beta})) \]
\[ + \xi (\lambda - \lambda(k) + \epsilon_a - \epsilon_{k\beta}, 1 - (n_j - n_k)/2 + (a - b) - (\delta_a - \delta_{k\beta})) \]

\[ \theta_{\text{self}}^a := \sum_{b=1}^{n_j} \xi (\epsilon_a - \epsilon_b, 1 - (a - b) + (\delta_a - \delta_b) + \xi (\epsilon_a - \epsilon_b, 1 + (a - b) - (\delta_a - \delta_b)) \]

Indices \( j^\alpha \) are suppressed to reduce the strain on the eye.

Assuming \(|\delta| < 1/2\), many of the sign terms become independent of \( \delta \). Singling out the terms for which this is not the case, we write the self-scattering term as

\[ \theta_{\text{self}}^a = \xi (\epsilon_a - \epsilon_{a-1}, \delta_a - \delta_{a-1}) + \xi (\epsilon_a - \epsilon_{a+1}, -\delta_a + \delta_{a+1}) \]
\[ + \text{atan} \frac{\epsilon_a - \epsilon_{a-1}}{2 - \delta_a + \delta_{a-1}} + \text{atan} \frac{\epsilon_a - \epsilon_{a+1}}{2 + \delta_a - \delta_{a+1}} \]
\[ + \sum_{1 \leq b \leq a - 2} \text{atan} \frac{\epsilon_a - \epsilon_b}{1 - (a - b) + (\delta_a - \delta_b)} + \text{atan} \frac{\epsilon_a - \epsilon_b}{1 + (a - b) - (\delta_a - \delta_b)} \]
\[ + \pi \text{sign}(\epsilon_a - \epsilon_b) \]
where it should be kept in mind that the terms which involve \( a - 1 \) must be left out for \( a = 1 \), as must terms with \( a + 1 \) for \( a = n \).

Taking the equation modulo \( 2\pi \), we can now write

\[
\xi(\epsilon_1 - \epsilon_2, -\delta_1 + \delta_2) = \theta_1 \quad (\text{mod 2}\pi)
\]

\[
\xi(\epsilon_a - \epsilon_{a-1}, \delta_a - \delta_{a-1}) + \xi(\epsilon_a - \epsilon_{a+1}, -\delta_a + \delta_{a+1}) = \theta_a \quad (\text{mod 2}\pi) \quad \text{for } 1 < a < n
\]

\[
\xi(\epsilon_n - \epsilon_{n-1}, \delta_n - \delta_{n-1}) = \theta_n \quad (\text{mod 2}\pi)
\]

where \( \theta_a \) is defined as all remaining terms in the above expressions. We use that

\[
J_a + J_{n+1-a} = 2J_a + 1 = M \quad (\text{mod 2}) \quad \text{if } a \neq n/2 \ ;
\]

if \( a = n/2 \) we need to use a criterion such as (3.16) to find out whether the pair is wide or close.

Noting that \( \xi(\epsilon, \delta) + \xi(-\epsilon, \delta) = 0 \), we can sum the above equations to

\[
\xi(\epsilon_a - \epsilon_{a+1}, -\delta_a + \delta_{a+1}) = \sum_{b=1}^{a} \theta_b \quad (\text{mod 2}\pi) .
\]

Applying the inverse function of \( \xi \) (the tangent, using (3.27) to determine signs) on both sides, we determine \( \epsilon_a - \epsilon_{a+1} \) and \( \delta_a - \delta_{a+1} \) up to a common prefactor.

**Norm of deviations**

To find the latter, we must consider the difference between the Bethe equations. Writing this as

\[
1 = r_{\text{kin}}^2 r_{\text{self}}^{-2} r_{\text{other}}^{-2} ,
\]

with

\[
r_{\text{kin}}^2 := \left[ \frac{(\lambda + \epsilon_a)^2 + (n/2 - a - \delta_a)^2}{(\lambda + \epsilon_a)^2 + (n/2 - a + 1 + \delta_a)^2} \right]^N
\]

\[
r_{\text{other}}^{(k,\beta)\neq(j,a)} := \prod_{k,\beta} \prod_{1 \leq b \leq n_k} \left[ \frac{(\lambda - \lambda_{\beta}^k + \epsilon_a - \epsilon_{\beta b}^k)^2 + (-1 + \frac{n_j-n_k}{2} - a + b + \delta_a - \delta_{\beta b})^2}{(\lambda - \lambda_{\beta}^k + \epsilon_a - \epsilon_{\beta b}^k)^2 + (1 + \frac{n_j-n_k}{2} - a + b + \delta_a - \delta_{\beta b})^2} \right] \]

\[
r_{\text{self}}^2 := \prod_{1 \leq b \leq n_j} \left[ \frac{(\epsilon_a - \epsilon_b)^2 + (-1 - a + b + \delta_a - \delta_b)^2}{(\epsilon_a - \epsilon_b)^2 + (1 - a + b + \delta_a - \delta_b)^2} \right] .
\]

Writing the self-scattering as

\[
r_{\text{self}}^2 = \left[ \frac{(\epsilon_a - \epsilon_{a+1})^2 + (\delta_a - \delta_{a+1})^2}{(\epsilon_a - \epsilon_{a-1})^2 + (\delta_a - \delta_{a-1})^2} \right] \left[ \frac{(\epsilon_a - \epsilon_{a-1})^2 + (-2 + \delta_a - \delta_{a-1})^2}{(\epsilon_a - \epsilon_{a+1})^2 + (2 + \delta_a - \delta_{a+1})^2} \right] \times
\]

\[
\times \prod_{1 \leq b \leq n} \frac{(\epsilon_a - \epsilon_b)^2 + (-1 - a + b + \delta_a - \delta_b)^2}{(\epsilon_a - \epsilon_b)^2 + (1 - a + b + \delta_a - \delta_b)^2} ,
\]

(3.34)
(where we again must leave out the $a-1$ factor for $a = 1$, as well as the $a+1$ factor if $a = n$), so that we can write, in similar fashion as before,

$$
(\epsilon_1 - \epsilon_2)^2 + (\delta_1 - \delta_2)^2 = r_1^2
$$

$$
\frac{(\epsilon_a - \epsilon_{a+1})^2 + (\delta_a - \delta_{a+1})^2}{(\epsilon_a - \epsilon_{a-1})^2 + (\delta_a - \delta_{a-1})^2} = r_a^2
$$

$$(\epsilon_n - \epsilon_{n-1})^2 + (\delta_n - \delta_{n-1})^2 = r_n^{-2},
$$

and we may multiply these equations out to get the norm we sought,

$$(\epsilon_a - \epsilon_{a+1})^2 + (\delta_a - \delta_{a+1})^2 = \prod_{b=1}^{a} r_b^2. \quad (3.35)$$

Equations (3.35) and (3.31) completely determine $\epsilon_a - \epsilon_{a+1}$ and $\delta_a - \delta_{a+1}$. For odd $n$, this sequence ends at $a = \lfloor n/2 \rfloor$, where $\epsilon_{a+1} = \delta_{a+1} = 0$. For even $n$, the endpoint is at $n/2$, where $\epsilon_a = \epsilon_{a+1} = 0$ and $\delta_a = -\delta_{a+1}$. In both cases this allows us to find $\epsilon$ and $\delta$ themselves at the endpoint, after which all other deviations are found by summing the differences.

For odd $n$, therefore, the deviations are found by the iterative prescription

$$
\delta'_a = -\sum_{b=a}^{\lfloor n/2 \rfloor} \cos \left( \sum_{c=1}^{b} \theta_c \right) \prod_{c=1}^{b} |r_c| \quad (3.36)
$$

$$
\epsilon'_a = \sum_{b=a}^{\lfloor n/2 \rfloor} \sin \left( \sum_{c=1}^{b} \theta_c \right) \prod_{c=1}^{b} |r_c| \quad (3.37)
$$

For even $n$, the value $\theta_{n/2}$ cannot be determined as above; we must decide the width of the middle pair $\sigma := \text{sign} \, \delta_{n/2}$ on the basis of a criterion such as (3.16), which we shall derive shortly. Here, the deviations are found from

$$
\delta'_a = \frac{1}{2} \sigma \prod_{c=1}^{n/2} |r_c| - \sum_{b=a}^{n/2-1} \cos \left( \sum_{c=1}^{b} \theta_c \right) \prod_{c=1}^{b} |r_c| \quad (3.38)
$$

$$
\epsilon'_a = \sum_{b=a}^{n/2-1} \sin \left( \sum_{c=1}^{b} \theta_c \right) \prod_{c=1}^{b} |r_c| \quad (3.39)
$$

**Rapidities**

In an iterative procedure, we also need an equation for the rapidities in terms of themselves and the deviations. This is found from the total sum of the string Bethe equations, which becomes the Bethe–Takahashi equation for the string in the limit where the deviations vanish. Annoyingly, we need to pay attention to all branch
3.2. Exact deviations for the isotropic chain

cut terms to make the correct connection with the Bethe–Takahashi equation. The self-scattering terms all cancel, so that the total sum reads

\[ \pi \sum_{a=1}^{n} J_{\alpha,a}^j = \frac{1}{2} \sum_{a=1}^{n} \theta^{a}_{\text{kin}} - \theta^{a}_{\text{other}} . \]  

(3.40)

The kinematic phases add up to

\[ \frac{1}{2} \sum_{a=1}^{n} \theta^{a}_{\text{kin}} = N \left[ \xi(2\lambda + 2\epsilon_1, n + 2\delta_1) + [\text{if } n \text{ even}] \xi(2\lambda, -2\delta_{n/2}) \right] 
+ \sum_{a=1}^{[(n-1)/2]} \xi(2\lambda + 2\epsilon_{a+1}, n - 2a + 2\delta_{a+1}) + \xi(2\lambda + 2\epsilon_a, -n + 2a - 2\delta_a) \]  

(3.41)

For the scattering phases, writing

\[ \xi^{\pm}_{ab} := \xi(\lambda^j_{\alpha} - \lambda^k_{\beta} + \epsilon_{\alpha a}^j - \epsilon_{\beta b}^k, 1 \pm [(n_j - n_k)/2 + b - a + \delta^j_{\alpha a} - \delta^k_{\beta b}]) \]  

(3.42)

and using

\[ \sum_{b=1}^{n_k} \xi^+_{ab} + \xi^-_{ab} = \xi^-_{a1} + \xi^-_{a2} + \xi^+_{a,n-1} + \xi^+_{a,n} + \sum_{b=1}^{n_k-2} \xi^+_{ab} + \xi^-_{a,b+2} , \]  

(3.43)

we can group terms together as

\[ \frac{1}{2} \sum_{a=1}^{n_j} \theta^{a}_{\text{other}} = \sum_{k\neq j} \sum_{a=1}^{n_j} \frac{1}{2} \left[ \xi^-_{a1} + \xi^-_{a2} + \xi^+_{a,n-1} + \xi^+_{a,n} + \sum_{b=1}^{n_k-2} \xi^+_{ab} + \xi^-_{a,b+2} \right] . \]  

(3.44)

The iterative prescription is then

\[ \xi(2\lambda' + 2\epsilon_1, n + 2\delta_1) + [\text{if } n \text{ even}] \xi(2\lambda', -2\delta_{n/2}) \]  

\[ = \frac{2\pi}{N} \sum_{a=1}^{n} J_{\alpha,a}^j + \frac{1}{N} \sum_{a=1}^{n} \theta^{a}_{\text{other}} \]  

\[ - \sum_{a=1}^{[(n-1)/2]} \xi(2\lambda + 2\epsilon_{a+1}, n - 2a + 2\delta_{a+1}) + \xi(2\lambda + 2\epsilon_a, -n + 2a - 2\delta_a) . \]  

These equations take the place of the Bethe–Takahashi equations when solving for a deviated string. However, to make the connection with those, we need to establish a relationship between the various quantum numbers used. This we can do by taking the limit as \( \delta, \epsilon \to 0. \)
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Using \(\xi(\epsilon, \delta) + \xi(\epsilon, -\delta) = \pi \text{ sign } \epsilon\) and \(\xi(\epsilon, 0) = (\pi/2) \text{ sign } \epsilon\), and taking the equation modulo \(N\pi\), the kinetic phase goes to

\[
\lim_{\epsilon \to 0} \frac{1}{2} \sum_{a=1}^{n} \theta_{\text{kin}}^a = N \left[ \text{atan} \frac{2\lambda}{n} + \frac{n-1}{2} \pi \text{ sign } \lambda \right] \pmod{N\pi}.
\] (3.46)

For the scattering phase, we use

\[
\lim_{\epsilon \to 0} \frac{1}{2} \sum_{a=1}^{n_j} \sum_{b=1}^{n_k-2} \xi_{ab}^+ + \xi_{a,b+2}^- = \frac{n_j(n_k-2)}{2} \pi \text{ sign}(\lambda_\alpha^j - \lambda_\beta^k)
\] (3.47)

and

\[
\lim_{\epsilon \to 0} \frac{1}{2} \left[ \xi_{1,2}^+ + \xi_{1,n_k}^- + \xi_{n_j,1}^+ + \xi_{n_j,n_k-1}^+ + \sum_{a=1}^{n_j-1} \left( \xi_{a,1}^- + \xi_{a+1,2}^- + \xi_{a,n_k-1}^+ + \xi_{a+1,n_k}^+ \right) \right]
\]

\[= \xi(2(\lambda_\alpha^j - \lambda_\beta^k), n_j - n_k) + \xi(2(\lambda_\alpha^j - \lambda_\beta^k), n_j + n_k)
\]

\[+ (n_j - n_k) \text{Theta}(n_j - n_k) \pi \text{ sign}(\lambda_\alpha^j - \lambda_\beta^k) + 2 \sum_{c=|n_j - n_k|+2}^{n_j+n_k-2} \xi(2(\lambda_\alpha^j - \lambda_\beta^k), c)
\]

\[= (1 - \delta_{n_j,n_k}) \text{atan} \frac{2(\lambda_\alpha^j - \lambda_\beta^k)}{|n_k - n_j|} + \text{atan} \frac{2(\lambda_\alpha^j - \lambda_\beta^k)}{n_k + n_j}
\]

\[+ \left[ (n_j - n_k) \text{Theta}(n_j - n_k) + \frac{1}{2} \delta_{n_j,n_k} \right] \pi \text{ sign}(\lambda_\alpha^j - \lambda_\beta^k)
\]

\[+ 2 \sum_{c=|n_k - n_j|+2}^{n_j+n_k-2} \text{atan} \frac{2(\lambda_\alpha^j - \lambda_\beta^k)}{c}
\] (3.48)

where the \(\Theta\) term derives from the cancellation of terms between \(n_k - n_j\) and \(n_j - n_k\), which occurs if \(n_j > n_k\). The last equality follows because all remaining terms have positive values for the second argument of \(\xi\).

Observing that \(n_j(n_k - 2) + (n_j - n_k) \text{Theta}(n_j - n_k) = n_jn_k/2 - \min(n_j, n_k)\), we may conclude that the relation between Bethe and Bethe–Takahashi quantum numbers is, modulo \(N\),

\[
\sum_{a=1}^{n_j} J_{\alpha, a}^j = J_{\alpha}^j + N \frac{n_j - 1}{2}
\] (3.49)

\[
- \sum_{k, \beta \neq (j, \alpha)} \text{sign}(\lambda_\alpha^j - \lambda_\beta^k) \left\{ \frac{n_jn_k}{2} - \min(n_j, n_k) + \frac{1}{2} \delta_{j,k} \right\}.
\]

This expression sheds some light on the quantum number bounds: comparing (2.88) to the above expression (3.49), we see that, for a string with the highest allowed
Quantum number $I_\alpha^j = I_{\infty}^j - 1,$
\[
\sum_{a=1}^{n_j} J_{\alpha}^j = n_j \left[-1 + \frac{1}{2} (N - M + n_j) \right] = \sum_{a=1}^{n_j} \left[\frac{1}{2} (N - M - 1) + (a - 1) \right] \quad \text{(mod } N),
\]
(3.50)
as long as its rapidity is higher than all others. This expression suggests that the quantum numbers of such strings form a series of consecutive (half-)integers.

**Width of innermost pair**

We can use expression (3.49) to determine the width of the innermost pair of an even string. By taking it modulo 2, we find
\[
\Theta(\delta_{n/2}) = \frac{1}{2} \left[ 2I_\alpha^j + N(n_j - 1) - n_j(M + 1) - n_j - 2 \right. \\
\left. - \sum_{(k,\beta) \neq (j,\alpha)} \text{sign}(\lambda_\alpha^j - \lambda_\beta^k) \{n_jn_k - 2 \min(n_j, n_k) + \delta_{j,k}\} \right] \quad \text{(mod } 2),
\]
(3.51)
so that with $\sigma = 2\Theta(\delta_{n/2}) - 1$ we have found the last ingredient needed to find the deviations of even strings by equation (3.38).

### 3.3 Singular states in the isotropic chain

If the Bethe–Takahashi quantum numbers are distributed symmetrically around zero, then so are the rapidities. Such symmetric states merit special attention. The simplest example is the ground state, which has already been discussed. In the presence of bound states, the situation becomes more complicated. As we will discuss in this section, it turns out that there are two classes of symmetric states: those with only odd strings, and those which include even strings. Whereas the solution of the former class involves a subtlety but no real issues, the latter class is fundamentally different. Again, we concentrate on the isotropic chain, although a similar issue exists in the XXZ chain.

#### 3.3.1 Multiple symmetric odd strings

In a symmetric state with more than one odd string at the origin, the solution of the Bethe–Takahashi equations is not a valid state: since there are two or more roots present at the origin, the exclusion principle is violated. However, if we take the deviations into account, this problem does not arise: the two roots that coincide in the limit are actually nonzero and each other’s opposites.

As an example, we will show the solution for the simplest case where this problem arises: the symmetric state with one three-string and one real root at the origin,
$I^{(3)} = 0$ and $I^{(1)} = 0$. Defining the rapidities $\lambda_{\pm i} = \pm (i + \delta)$, $\lambda_{-0} = -\lambda_{+0} > 0$, we find from the difference of Bethe equations that $J_{+i} = -J_{-i} = (N - 1)/2$ (where also $J_{-i} = J_{+i} + 1 \pmod{N}$). The quantum numbers for the real roots in the complex must be half-integer, opposite, and as small as possible, leading to $J_{\pm 0} = \pm 1/2$.

The fixed points of the iterative equations for the deviations as given in section 3, however, are repulsive in this case; therefore we need to either use another method (such as Newton–Raphson) or rewrite the iterative equations. An easy prescription that works is to take the sum of the equations for the positive-real and positive-imaginary root, which gives

$$\lambda' + i(1 + \delta') = \tan \left[ \frac{N - 1}{2} \left( \atan 2\lambda + i \atanh(2 + 2\delta) \right) - \frac{\theta_{\text{other}}}{2} \right],$$  \hspace{1cm} (3.52)

where, in the presence of other roots,

$$\theta_{\text{other}} := \sum_{\beta} \atan (\lambda - \lambda_{\beta}) + \atan (i + i\delta - \lambda_{\beta}).$$  \hspace{1cm} (3.53)

The full solution has no coinciding roots and the wave functions are regular Bethe wave functions. The roots do, however, tend to grow very close as the chain length increases, leading to numerical problems: at more than 40 sites machine precision is too low to find an acceptable result (see figure 3.1). However, for smaller chains it is already clear that the values are exponentially decreasing. For large $N$, inserting the assumption $\lambda \ll 1$, $\delta \ll 1$ in the Bethe equation, and noting that by symmetry of the set $\{\lambda_{\beta}\}$, the contribution of the other roots is the real number $0 < F < 1$ given by

$$F = \prod_{\beta} \frac{|\lambda_{\beta}|}{\sqrt{\lambda_{\beta}^2 + 1/4}},$$  \hspace{1cm} (3.54)

we get

$$\lambda = \sqrt{\frac{12}{F}} \cdot 3^{-N/2} \quad \delta = \frac{24(N - 1)}{F} \cdot 3^{-N} e^{-i\Phi},$$  \hspace{1cm} (3.55)

proving that the opposite real roots are exponentially close to each other, but can be pushed a finite distance apart in the presence of a macroscopic number of down spins (i.e. at low magnetic fields).

In this approximation, the reduced Bethe equations that must be satisfied by the remaining roots are

$$N \atan 2\lambda_j - 2 \atan \lambda_j - \atan \lambda_j/2 = \pi(J_j + \frac{1}{2}) + \sum_{k=1}^{M-4} \atan (\lambda_j - \lambda_k) \pmod{\pi},$$  \hspace{1cm} (3.56)
3.3. Singular states in the isotropic chain

Figure 3.1: Comparison of the values \( \lambda \) (squares), \( \delta \) (circles), in the absence of other roots, calculated by iteration of equation (3.52) and by the large-\( N \) approximation (3.55) (lines). The plot is limited to those values for which the iteration procedure remains within machine precision. It is seen that even for short chains, the large-\( N \) approximation yields very good results.

if we order the rapidities such that the last four are the set \( \{\pm 0, \pm i\} \). The energy associated to the four roots \( \{\pm 0, \pm i\} \) equals, for large \( N \),

\[
E_{\{\pm 0, \pm i\}} = -\frac{8}{3} .
\] (3.57)

3.3.2 Singular state at \( M = 2 \)

Solving the latter class of states is more involved, due to the presence of roots at the points \( \pm i/2 \). At this point, the Bethe equations are singular; moreover, the singularity in the kinetic phase is stronger than in the usual case for a string, \( O(e^{\mp N \log \delta}) \) instead of \( O(e^{\pm N}) \). This would suggest that this divergence cannot be countered in the usual way by the divergence in the scattering phase. Yet, if we carefully consider the way in which we take the limit \( \lambda_{\pm} \to \pm i/2 \), we shall see that we get a bona fide solution of the Bethe equations.

Note that the problem of singular states also arises in the XXZ model at ‘root of unity’ values for the anisotropy parameter, as was shown by Fabricius and McCoy [66, 67]: indeed, the exact complete \( N \)-strings of those articles correspond to the singular strings discussed here.

It was noted in [54] that, in the \( M = 2 \) sector, the wave function corresponding to the roots \( \pm i/2 \) is

\[
\chi_{\pm i/2}(j_1, j_2) = (-1)^{j_1} \delta_{j_1+1,j_2} + (-1)^{j_2} \delta_{j_1+N,j_2+1} .
\] (3.58)

Here we have made the periodicity of the chain explicit. This is only an eigenstate on \( \Delta = 1 \) chains with an even number of sites. We shall see that if we take the limit \( \lambda_{\pm} \to \pm i/2 \) along the path prescribed by the Bethe equations, we recover the wave function (3.58).
Consider $\lambda_{\pm} := \epsilon \pm i(1 + 2\delta)/2$. We will take the limit $\epsilon \to 0$, $\delta \to 0$. As of yet, the signs of $\delta$ and $\epsilon$ are unspecified. To first order, the kinetic phase satisfies

$$e^{ik_+} = e^{iRek_+}e^{-Imk_+} = \delta - i\epsilon,$$  \hfill (3.59)

so that $e^{-Imk_+} = \sqrt{\delta^2 + \epsilon^2}$, $e^{iRek_+} = \sqrt{\frac{\delta - i\epsilon}{\delta + i\epsilon}}$. The scattering phase has

$$\tan\Phi(k_+, k_-)/2 = i(1 - 2e^{i\Phi(k_+, k_-)}) = \lambda_+ - \lambda_- = i(1 + 2\delta);$$  \hfill (3.60)

thus $e^{i\Phi} = -\delta$. Looking at the Bethe equations we now see

$$e^{ik_+N} = -e^{i\Phi(k_+, k_-)} \Rightarrow (\delta - i\epsilon)^N = \delta.$$  \hfill (3.61)

so that we must have $|\epsilon| \gg |\delta|$; from which we deduct

$$(-i)^Ne^N = \delta \quad e^{-Imk_+} = |\epsilon| \quad e^{iRek_+} = i$$  \hfill (3.62)

We see that, for $\epsilon$ and $\delta$ both to be real, we need $N$ even. Furthermore,

$$\text{sign } \delta = (-1)^{N/2}$$  \hfill (3.63)

Let us turn our attention to the wave function. We write $\chi(\pm i/2)(j_1, j_2) = \chi^+_{\text{sign } \delta} - \chi^-_{\text{sign } \delta}$ where, for later convenience, we have defined

$$\chi^+_{\alpha}(j_1, j_2) := \lim_{\delta \to 0} \frac{|\epsilon| = (a\delta)^{1/N}}{\delta} e^{ik_+ j_1 + ik_- j_2 e^{i\Phi/2}}$$  \hfill (3.64)

$$\chi^-_{\alpha}(j_1, j_2) := \lim_{\delta \to 0} \frac{|\epsilon| = (a\delta)^{1/N}}{\delta} e^{ik_+ j_1 + ik_- j_2 e^{-i\Phi/2}}.$$  \hfill (3.65)

Inserting the first-order values just found

$$\chi^+_{\alpha}(j_1, j_2) = e^{iRek(j_1 + j_2)} e^{i\Phi/2} = i^{j_1 + j_2} (a\delta)^{\pm(j_1 - j_2)/N} (-\delta)^{\pm 1/2}$$

so that

$$\chi^+_{\alpha}(j_1, j_2) = -(a\delta)^{1/N} \delta^{-1/2} \left[a^{-1}(-1)^{N/2 + j_2} \delta_{j_1 + N, j_2 + 1} + O(\delta)\right]$$  \hfill (3.66)

$$\chi^-_{\alpha}(j_1, j_2) = -(a\delta)^{1/N} \delta^{-1/2} \left[(-1)^{j_1} \delta_{j_1 + 1, j_2} + O(\delta)\right]$$  \hfill (3.67)

and we see that the prefactor, though divergent, is independent of position and therefore the wave function $\chi^+_{\text{sign } \delta} - \chi^-_{\text{sign } \delta}$ is normalisable. Due to (3.63), it has the correct periodicity; we recover (3.58).

We did not have so specify the sign of $\epsilon$ in this derivation; it turns out that we can choose whether to approach the limit from the left or from the right half-plane.
Quantum numbers

We find the values of the quantum numbers when we consider the sum of the Bethe equations, viz.

\[ \pi(J_+ + J_-) = \lim_{\delta \to 0} N[\tan(2\epsilon + i(1 + 2\delta)) + \tan(2\epsilon - i(1 + 2\delta))] \]

\[ = N \text{sign}\epsilon \text{sign}\delta \lim_{\delta \to 0} \tan|\delta|^{-1+1/N} = N\pi/2 \quad (\text{mod} N\pi) , \quad (3.68) \]

so that the Bethe quantum numbers for the singular state at \( M = 2 \) are the half-integers

\[ J_+ = \frac{1}{4}[\pm N - (2 - N \text{ mod } 4)] \quad J_- = \frac{1}{4}[\pm N + (2 - N \text{ mod } 4)] \quad (3.69) \]

in agreement with (3.63). The sign of these quantum numbers is not uniquely determined: it equals the sign of \( \epsilon \) we chose in the limiting procedure.

Naturally, the Bethe–Takahashi quantum number corresponding to a single two-string at the origin is \( I^{(2)} = 0 \).

### 3.3.3 Singular states at \( M = 3 \)

For \( M = 3 \), one singular state is already known: the \( M = 2 \) state we just found, with an extra rapidity at infinity (i.e., quasimomentum at zero). However, another choice for the quasimomentum that respects the lattice inversion symmetry is \( k_3 = \pi \text{ (mod } 2\pi) \) (i.e., \( \lambda_3 = 0 \)). Let us use \( \lambda_\pm = \epsilon \pm i(1 + 2\delta)/2 \) and \( |\epsilon| \gg |\delta| \) again.

The Bethe equation for \( J_+ \) yields

\[ \left[ \frac{\epsilon + i\delta}{\epsilon + i(1 + \delta)} \right]^N = -e^{i\Phi_{13}} \left[ \frac{\delta}{1 + \delta} \right] \quad (3.70) \]

As \( \lambda_3 \to 0, \lambda_+ \to i/2 \), we have \( e^{i\Phi_{13}} = e^{-i\Phi_{23}} = 1/3 \), so that, to first order, \( (-i\epsilon)^N = -\delta e^{i(\Phi_{13} - \Phi_{23})}/2 \), and it turns out that we have to set \( \text{sign}\delta = (-1)^{1+N/2} \).

Given this limiting procedure, we can now write the wave function as

\[ \chi(j_1, j_2, j_3) \propto \left[ \chi_a^+(j_1, j_2) - \chi_a^-(j_1, j_2) \right] e^{ik_3j_3} e^{i(\Phi_{13} + \Phi_{23})/2} \]

\[ + \left[ \chi_a^+(j_2, j_3) - \chi_a^-(j_2, j_3) \right] e^{ik_3j_1} e^{-i(\Phi_{13} + \Phi_{23})/2} \]

\[ + \left[ \chi_a^+(j_1, j_3) e^{i(\Phi_{13} - \Phi_{23})/2} - \chi_a^-(j_1, j_3) e^{-i(\Phi_{13} - \Phi_{23})/2} \right] e^{ik_3j_2} , \quad (3.71) \]

where \( a = (-1)^{1+N/2} e^{i(\Phi_{13} - \Phi_{23})/2} \).

Because the \( js \) are ordered, \( \chi^+ \) is zero unless its arguments are \( j_1 \) and \( j_M \), and \( \chi^- \) vanishes in that case only. Using \( e^{ik_3} = -1 \) and the values from equations (3.66), (3.67), with the common prefactors divided out,

\[ \chi_a^+(j_1, j_2) = (-1)^{j_1-j_2} \delta_{j_2+1,j_1} \]

\[ \chi_a^-(j_1, j_2) = -e^{-i(\Phi_{13} - \Phi_{23})/2} (-1)^{j_2} \delta_{j_2+N,j_1+1} , \quad (3.72) \]
we find that the wave function equals

\[ \chi(\pm i/2,0)(j_1, j_2, j_3) \]

\[ \propto (\pm 1)^{j_3} \chi_1(j_1, j_2) + (\pm 1)^{j_1} \chi_1(j_2, j_3) + (\pm 1)^{j_2} \chi_1(j_1, j_3) \]

\[ \propto (\pm 1)^{j_3+j_1} \delta_{j_1+1, j_2} + (\pm 1)^{j_1+j_2} \delta_{j_2+1, j_3} + (\pm 1)^{j_2+j_1} \delta_{j_1+N, j_3+1} , \]

Note that this wave function can be formed by simply creating a down spin of momentum \( \pi \) on top of the \( M = 2 \) singular state.

The Bethe quantum numbers are

\[ J_+ = \frac{1}{4}[\pm N - (N \mod 4)] \quad J_0 = 0 \quad J_- = \frac{1}{4}[\pm N + (N \mod 4)] \]

(3.74)

The Bethe–Takahashi quantum numbers are

\[ I^{(1)} = 0 \quad I^{(2)} = 0 . \]

(3.75)

### 3.3.4 Singular states at \( M = 4 \)

Consider \( M = 4 \) and \( \lambda_\pm := \epsilon \pm i(1+2\delta) \). Apart from the solutions we just found, extended with the appropriate number of infinite rapidities, we can find a few more.

Note that for finite nonzero lambda, by symmetry, \( \lambda_3 = -\lambda_4 =: \lambda \). The Bethe equation for \( \lambda_+ \) now gives

\[ \delta = (-1)^{N/2} e^{-i(\Phi_{13} + \Phi_{14})} e^N . \]

(3.76)

By symmetry, \( \Phi_{13} + \Phi_{14} = -\Phi_{23} - \Phi_{24} =: \Phi/2 \) and wave function can be written

\[ \chi(j_1, j_2, j_3, j_4) = \]

\[ \chi_{-1}^{1/2, e^{i\Phi}}(j_1, j_2) \left[ e^{i(k(j_3-j_4))} e^{i\Phi_{34}/2} - e^{i(k(j_4-j_3))} e^{-i\Phi_{34}/2} \right] + e^{i\Phi} \chi_{-1}^{1/2, e^{i\Phi}}(j_1, j_4) \left[ e^{i(k(j_2-j_3))} e^{i\Phi_{34}/2} - e^{i(k(j_3-j_2))} e^{-i\Phi_{34}/2} \right] + \chi_{-1}^{1/2, e^{i\Phi}}(j_3, j_4) \left[ e^{i(k(j_1-j_2))} e^{i\Phi_{34}/2} - e^{i(k(j_2-j_1))} e^{-i\Phi_{34}/2} \right] + \chi_{-1}^{1/2, e^{i\Phi}}(j_2, j_3) \left[ e^{i(k(j_1-j_4))} e^{i\Phi_{34}/2} e^{i\Theta} - e^{i(k(j_4-j_1))} e^{-i\Phi_{34}/2} e^{-i\Theta} \right] \]

where an extra phase factor has to be introduced for the terms in which the sites associated to \( \lambda_3, \lambda_4 \) surround the sites associated to the string,

\[ \Theta := \frac{1}{2}(\Phi_{13} + \Phi_{23} - \Phi_{14} - \Phi_{24}) = 2 \atan \frac{2}{3} \lambda + 2 \atan 2 \lambda . \]

(3.78)

The Bethe equation for \( \lambda \) can be reduced, using symmetry and the values \( \lambda_\pm = \pm i/2 \), to

\[ (N - 2) \atan 2 \lambda - \atan \frac{2}{3} \lambda = \pi J_3 . \]

(3.79)
For $J_3 < (N - 3)/2$, the solutions of (3.79) are real and the Bethe–Takahashi quantum numbers are $I^{(2)} = 0$ and $I^{(1)}_2 = -I^{(1)}_1 = J_3$. For $J_3 = (N - 2)/2$, $\lambda$ is imaginary; this configuration can be identified as a deviated four-string with $I^{(4)} = 0$.

The Bethe quantum numbers associated with $\lambda_\pm$ are the same as in the $M = 2$ cases.

### 3.3.5 Singular states at general $M$

We will now generalise the approach of the last sections. Again, we only consider highest-weight states. Consider a configuration of $M$ roots, two of which form a singular two-string, $\lambda^\pm := \epsilon \pm i \frac{1}{2}(1 - 2\delta)$. The other roots must be distributed symmetrically; the total momentum is $\pi$ for even $M$, and $0$ for odd $M$. For ease of notation, let the number of non-singular nonzero roots be $\tilde{M} := M - 2 - (M \mod 2)$; we’ll indicate the particle at $k_0 = \pi$ with the index $0$, and the two singular roots with $\pm$. The set is ordered $+, -, 0, 1 \ldots \tilde{M}$, such that we always have $k_a = -k_{\tilde{M}-a+1}$ for $a > 0$.

The Bethe equation for $\lambda^+$ gives

$$\delta = e^N(-1)^{N/2}(-1)^M \prod_{\beta=0}^{\tilde{M}} e^{-i\Phi_{1\beta}},$$

(3.80)

where $\Phi_{10}$ is understood to be zero if $M$ even.

Consider the Bethe wave function (2.25). There will be one nonzero term with $\chi^+:$ the one involving $\chi^+ (j_1, j_M)$. This term has a nontrivial scattering with the singular string, equal to $e^{-i(\sum_{\beta=0}^{M} \phi_{+,\beta} - \phi_{-,\beta})}$; again, this cancels against the factor that arises taking the limit as above.

Another nontrivial scattering phase occurs when the sites $j_p, j_{p+1} = j_p + 1$ are surrounded by a pair of sites associated with opposite momenta, yielding a phase

$$\Theta_\beta := \Phi(k_+, k_{\beta}) + \Phi(k_-, k_{\beta}) - \Phi(k_+, -k_{\beta}) - \Phi(k_-, -k_{\beta})$$

$$= -2[\Phi(k_+, |k_{\beta}|) + \Phi(k_-, |k_{\beta}|)],$$

(3.81)

for $b \leq \tilde{M}/2$.

Moreover, only such permutations need be retained in the sum as make it possible for the sites involved in the singular complex to be adjacent. With these considerations, the Bethe wave function becomes

$$\chi_{\pm i/2,k}(\{j\}) \propto \sum_{\mathcal{P}} (-1)^{|\mathcal{P}|} \left[ (-1)^{j_{1+\mathcal{P}(+)} \delta_{\mathcal{P}(-), 1+\mathcal{P}(+) \delta_{j_{\mathcal{P}(+)+1}, j_{1+\mathcal{P}(+)}}}ight.$$

$$+ (-1)^{j_{1+\mathcal{P}(+)} \delta_{1+\mathcal{P}(-), M+\mathcal{P}(+) \delta_{j_{\mathcal{P}(+)+1}, N, j_{1+\mathcal{P}(+)}}}} \times$$

$$\times e^{i \sum_{n=0}^{\tilde{M}} [k_n j_{\mathcal{P}(n) + \frac{1}{2} \sum_{0 \leq m \leq \tilde{M}} \Phi_{mn}]]} \times e^{i \sum_{n=1}^{\tilde{M}/2} \Phi(k_+, |k_n|) + \Phi(k_-, |k_n|) [1 + \text{sign}(\mathcal{P}(+) - \mathcal{P}(n)) \text{sign}(\mathcal{P}(\tilde{M}-n+1) - \mathcal{P}(n))]}.$$ 

(3.82)
Note that, for convenience, the permutations $\mathcal{P}$ are the inverse of those in the earlier expression for the Bethe wave function (2.25). The permutation $\mathcal{P}$ is understood to be a map from $\{+, -, 0, 1 \ldots \tilde{M}\}$ to $\{1 \ldots M\}$.

We can make this expression slightly less ugly by splitting up the permutation $\mathcal{P}$ such that $\mathcal{P} = \mathcal{P}_+ a \mathcal{P}_- (a + 1) \mathcal{Q}_a$ where the permutation $\mathcal{Q}_a$ maps $\{0, 1 \ldots \tilde{M}\}$ to $\{1 \ldots a - 1, a + 2 \ldots M\}$. Note that $[\mathcal{Q}_a] = [\mathcal{P}]$; this separation is possible because the Kronecker symbols in the sum select only those permutations that map $+, -$ onto the neighbours $a, a + 1$. Thus, the general Bethe wave function in the presence of a singular string reads

$$\chi_{\pm i/2,\{k\}}(\{j\}) \propto \sum_{a} \left[ (1)_{\mathcal{Q}_a} \sum_{n=1}^{\tilde{M}} \left[ k_n j_n + \frac{1}{2} \sum_{0 \leq m \leq \tilde{M}} \mathcal{Q}_m \mathcal{Q}_n \Phi_{mn} \right] \times \sum_{\mathcal{Q}_a} (-1)^{\mathcal{Q}_a} e^{i \sum_{n=1}^{\tilde{M}} (k_n j_n + \frac{1}{2} \sum_{0 \leq m \leq \tilde{M}} \mathcal{Q}_m \mathcal{Q}_n \Phi_{mn})} \times e^{\frac{2}{3} \sum_{n=1}^{\tilde{M}} [\Phi(k_+,|k_n|) + \Phi(k_-,|k_n|)][1 - \text{sign}(a - \mathcal{Q}_n) \text{sign}(a - \mathcal{Q}(\tilde{M} - n + 1))]} \right] .$$

The reduced Bethe equations that must be satisfied by the remaining roots are

$$(N - 1) \tan 2\lambda_j - \tan \frac{2}{3} \lambda_j = \pi j_{+} + \sum_{k=1}^{\tilde{M}} \tan(\lambda_j - \lambda_k) \pmod{\pi} .$$

The Bethe quantum numbers $J_+, J_-$ are those of the $M = 2$ case (for $M$ even) or the $M = 3$ case (for $M$ odd).

### 3.3.6 Energy of singular pair

In computing the energy contribution of the singular pair $\pm i/2$ we have to be careful to take the correct limit (3.80) arising from the Bethe equations. In this limit, the imaginary deviation is negligible compared to the real deviation, so that we may set $\lambda_{\pm} = \epsilon \pm i/2$. The energy contribution of the singular pair is then always

$$E_{\{i/2, -i/2\}} = -1 .$$

### 3.3.7 Validity of singular states

It has been argued by Siddharthan [68] (on the basis of numerically calculated energies) and Noh et al. [69] (by symmetry considerations) that singular states such as we just discussed, though they are solutions to the Bethe equations, do not (or not always) represent eigenstates of the Heisenberg model. However, we have shown above that they are valid solutions; moreover, we have checked the solutions of states found in this way against complete diagonalisation at $N = 6$ and $N = 8$, and find perfect agreement.
3.4. Completeness of solutions for short chains

In appendix A, full solutions are presented for chains of length $N = 8$ and $N = 10$. Complete solutions up to $N = 6$ can be found in the literature (see e.g. [70]). From $N = 12$ onwards, not all allowed four-string quantum numbers lead to solutions using the methods of this chapter; we will now analyse the number of states for which this is the case.

3.4.1 Missing solutions

An interesting question is the fate of string-like solutions with increasing chain length $N$. Only four the two-magnon sector $M = 2$ the analytic solution is known; from $N = 22$ onward narrow two-strings ‘collapse’ and form pairs of roots on the real line, as described in [54]. The number of missing solutions equals

$$n_{\text{missing}}^{(M=2)} = \left\lfloor \frac{\sqrt{N}}{\pi} - \frac{1}{2} \right\rfloor. \quad (3.86)$$
Chapter 3. Bethe roots in the complex plane

The method described in this chapter can shed some light on this question, as we can try and find all solutions of the Bethe equations for a given number of magnons with increasing chain length. The number of missing solutions then gives an upper bound to the number of non-string solutions. For \( M = 3 \), this is shown in figures 3.2. The number of missing solutions turns out to follow a rule much like equation (3.86), namely

\[
 n^{(M=3)}_{\text{missing}} = 2(N - 2) \left( \frac{\sqrt{N - 1}}{\pi} - \frac{1}{2} \right).
\]

(3.87)

The situation for \( M = 4 \) is shown in figure 3.3. Here a fit for the number of missing solutions is

\[
 n^{(M=4)}_{\text{missing}} = (N - 2)(N - 3) \left( \frac{\sqrt{N - 4}}{\pi} - \frac{1}{2} \right).
\]

(3.88)

Note that, especially around the jumps in the graphs, the number of solutions found is rather sensitive to the degree of convergency required in iteration. This effect may shift the jumps a bit to the left and right; however, the number of solutions remains on the \( O(N\sqrt{N}) \) and \( O(N^2\sqrt{N}) \) curves above.

Finally, in figure 3.4 we show the number of missing solutions in a single log-log graph for \( M \) between 2 and 7. It is clear that at every \( M \), the number of missing solutions grows as \( O(N^{M-2}\sqrt{N}) \) and exhibits jumps on or very close to the locations dictated by the \( M = 2 \) rule (3.86). These numbers fit in a picture where the collapse of narrow pairs—either only from two-strings or, presumably, from higher strings as well—is the only aberration from the string hypothesis, if one allows for deviations in the strings themselves. Of course, it would be desirable to have a method to solve for the collapsed pairs as well, so that this statement can be checked. Since the number of higher strings is much lower than that of two-strings, a collapse of higher strings would not make a big difference in these graphs.
3.5 Scaling of deviations

Figure 3.4: Log-log plot of number of missing solutions at \( M \in \{2 \ldots 7\} \).

This also shows that, at least at the small numbers of magnons and chain lengths considered here, the method we describe captures the vast majority of solutions of the Bethe equations: the number of highest-weight solutions is \( n_{\text{total}} = \binom{N}{M} - \binom{N}{M-1} = O\left(\frac{2^M}{M!}\right) \) so that the fraction of missing solutions scales as

\[
\frac{n_{\text{missing}}^{(M)}}{n_{\text{total}}} = O\left(\frac{N^{-3/2}}{M!}\right). \tag{3.89}
\]

3.5 Scaling of deviations

The string hypothesis states that deviations should decrease with increasing chain length as \( O(e^{-cN}) \) for some constant \( c \). In figure 3.5 the average deviation of string solutions is shown, where the average is taken over all solutions (including real roots) and the magnitude of deviation for a single string is given by

\[
d := \sum_{a=1}^{n_j} \delta_a^2 + \epsilon_a^2. \tag{3.90}
\]

Remarkably, the curves for all values of \( M \) collapse onto that of \( M = 2 \), if the average deviations are divided by \( \sum_{l=1}^{n_j} l \). Another noteworthy observation is that, although the decrease is stronger than algebraic, it is weaker than exponential. It would be interesting to split the average deviation out by string length.

3.6 Discussion

In the above chapter we have discussed a method that finds a large class of solutions of the Bethe equations in the complex plane, by calculating deviations to the string-hypothesis solution. For fixed \( M \) at increasing \( N \), the fraction of solutions that
cannot be found decreases algebraically with the number of sites and factorially with the number of magnons. The behaviour of the number of missing solutions suggests that collapsing narrow pairs are the only source of failure of the string picture in this regime. The average deviation of the string hypothesis is found to decrease with $N$, but not exponentially.

If the number of magnons becomes macroscopic, it is to be expected that the method, since it builds on the string hypothesis, should fail more often.

In this chapter, we have also shown that singular states exist whenever a symmetric configuration includes an even string at the origin, leading to a singularity in the Bethe equations. These states are generalisations of the $M = 2$ singular state that had been known for a long time. We also show that, in contrast to what is claimed in the literature, these states can be seen as solutions to the Bethe equations, as long as the limit is taken in the correct way. In the next chapter we will also show that all states in this class have zero form factors for local spin operators, and can therefore be ignored in the calculation of correlation functions of local quantities.

Another class of special solutions arises when a symmetric configuration includes two odd-length strings at the origin. This leads to solutions with two roots that are exponentially close to each other as $N$ becomes large, without violating the exclusion principle. Form factors for these states are nonzero, but hard to calculate due to the exponential degeneracy. What happens when more than two odd-length strings coincide is still unclear.
4.

Dynamical correlations in finite chains

One of the problems of the Bethe ansatz has always been that it could not be used to calculate the dynamics of a system. While, as we have seen, the Bethe ansatz easily yields the energy levels of a system, calculation of dynamical quantities requires information about matrix elements of operators. Although the expression for the wave function of a Bethe state is known (2.25), constructing it, thereby enabling us to calculate these matrix elements, requires a number of operations of order $M!$ and is therefore not feasible for any but the lowest numbers of magnons.

To make progress in this direction, much more analytical work is needed. In the framework of the algebraic Bethe ansatz, extremely useful exact expressions were derived for the norm [71, 72] and scalar product [73] of different Bethe states; much later, finally, a manageable expression for matrix elements of local spin operators (known as form factors) was found [74, 75]. These expressions, written below, are given in terms of determinants of matrices whose entries are given in terms of the rapidities for the state.

In this chapter, we will show how these expressions allow us to calculate extremely accurate approximations of the structure factor of finite (isotropic as well as anisotropic) Heisenberg chains\(^1\). In chapter 5 we shall discuss an approach to the structure factor in the thermodynamic limit for zero field.

4.1 Form factors

By inserting a complete set of eigenstates, the structure factor can be expressed as a sum over squares of matrix elements of spin operators with respect to the

\(^{1}\)This work was done in collaboration [76] with Jean-Sébastien Caux and Jean Michel Maillet.
Chapter 4. Dynamical correlations in finite chains

$M$-particle ground state $|G_M\rangle$ and these eigenstates,

$$S_{\text{conn}}^{\alpha\bar{\alpha}} = 2\pi \sum_{\alpha \neq G_M} \left| \langle G_M | S_q^\alpha | \alpha \rangle \right|^2 \delta(\omega - \omega_\alpha) .$$

(4.1)

Here, the lattice Fourier transformed versions of the spin operators are defined as

$$S_q^\alpha := \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{iqj} S_j^\alpha ,$$

(4.2)

which means, in particular, that the total spin in z direction is $S_z^{\text{tot}} = \sqrt{N}S_0^z$ and accordingly, the average spin $S_{\text{av}}^z = S_0^z/\sqrt{N}$. The ground state itself is excluded from the sum as we calculate the connected correlator. For transverse form factors this is immaterial, as all intermediate states must be in a subspace with a number of magnons that is different from the ground state.

The matrix elements that appear in the above sum (4.1) are known as form factors.

In this chapter we will discuss the longitudinal form factor $F_z^\prime$ and the transverse form factors $F_{\pm}$, defined by

$$F_q^\pm(\{\mu\}, \{\lambda\}) := \langle \{\mu\} | S_q^z | \{\lambda\} \rangle = [F_q^- (\{\lambda\}, \{\mu\})]^*$$

for normalised states $|\mu\rangle$, $|\lambda\rangle$.

Note that for the form factors to be non-zero $\alpha$ must be in the right subspace: for the $S_z$ form factor, with equal number $M$ of down spins as the ground state; for $S^-$, the space with $(M - 1)$ down spins (where $M$ is the number of down spins in the left state $\{\mu\}$). The rest of the Hilbert space can be excluded from the sum.

4.2 The algebraic Bethe ansatz

The expressions for form factors are derived by Kitanine et al. [74] in the context of the algebraic Bethe ansatz, a more abstract (and more powerful) mathematical formulation of the structure behind the Bethe ansatz. This method was developed by the Leningrad school [77, 78, 79] and also goes by the name of quantum inverse scattering method. It was applied to the Heisenberg model in [80, 81]. Good discussions of the method are found in [38, 58, 82, 83].

The central object in the algebraic Bethe ansatz is the $R$-matrix, which (for the antiferromagnetic Heisenberg model) can be seen as an operator acting on the tensor product of two spin-$\frac{1}{2}$ spaces. It is given by

$$[R(\lambda)]_{\alpha\beta\gamma\delta} := \frac{1 + b(\lambda)}{2} \delta_{\alpha\beta} \delta_{\gamma\delta} + \frac{1 - b(\lambda)}{2} \sigma_{\alpha\beta}^x \sigma_{\gamma\delta}^x + \frac{c(\lambda)}{2} \left[ \sigma_{\alpha\beta}^y \sigma_{\gamma\delta}^y + \sigma_{\alpha\beta}^z \sigma_{\gamma\delta}^z \right] ,$$

(4.6)
where $\sigma^a$ are the Pauli matrices, $\sigma^\pm := \frac{1}{2}(\sigma^x \pm i \sigma^y)$, and

$$b(\lambda) := \frac{\phi(\lambda)}{\phi(\lambda + i \zeta)}, \quad c(\lambda) := \frac{\phi(i \zeta)}{\phi(\lambda + i \zeta)}.$$  \hspace{1cm} (4.7)

From the $R$ matrix we construct an object known by such names as the Lax matrix, the local transition matrix, or simply the $L$-matrix, by identifying one of the spin-$\frac{1}{2}$ spaces with the Hilbert space associated to a site of the chain. We get the following $2 \times 2$ matrix whose elements are spin-$\frac{1}{2}$ operators operating on the $j$th site of the chain,

$$[L_j(\lambda, \xi_j)]_{\alpha\beta} := R(\lambda - \xi_j)_{\alpha\beta}$$

$$= \frac{1 + b(\lambda - \xi_j)}{2} \delta_{\alpha\beta} I_j + [1 - b(\lambda - \xi_j)] \sigma^z_{\alpha\beta} S^z_j + c(\lambda - \xi_j) \left[ \sigma^y_{\alpha\beta} S^y_j + \sigma^x_{\alpha\beta} S^x_j \right],$$  \hspace{1cm} (4.8)

where $\xi_j$ is an arbitrary parameter associated to the $j$th site; it is known as an inhomogeneity and is inserted to be able to address local observables. To get the homogeneous chain we consider, we set all $\xi_j \rightarrow i\zeta/2$ at the end of the calculation.

The $2 \times 2$ space in which the $L$-matrix acts is called the auxiliary space $V_0$; the Hilbert space of the spin on site $j$ is called the quantum space $H_j$. To avoid confusion\(^2\) we write matrices in auxiliary space in tensor notation, labelled by the indices $\alpha\beta$ for which we use the summation convention, and operators in quantum space as operators. The commutation relations of the local transition matrix are generated by the $R$-matrix,

$$[R(\lambda - \mu)]_{\alpha\beta\gamma\delta}[L_j(\lambda)]_{\beta\sigma}[L_j(\mu)]_{\delta\rho} = [L_j(\mu)]_{\alpha\beta}[L_j(\lambda)]_{\gamma\delta}[R(\lambda - \mu)]_{\beta\sigma\delta\rho}. \hspace{1cm} (4.9)$$

The monodromy matrix $T(\lambda)$ is the matrix product in auxiliary space of the local transition matrices over all sites,

$$[T(\lambda)]_{\alpha\beta} = [L_N(\lambda, \xi_N)]_{\alpha\gamma_1}[L_{N-1}(\lambda, \xi_{N-1})]_{\gamma_1\gamma_2} \cdots [L_1(\lambda, \xi_1)]_{\gamma_{N-1}\beta} \hspace{1cm} (4.10)$$

where the inhomogeneity parameters have been suppressed on the left-hand side. This way, the monodromy matrix is a matrix of operators acting on the full Hilbert space of the spin chain. It derives its name from the fact that it is associated to a movement all around the chain.

**Creation and annihilation operators**

From the elements of the monodromy matrix we define operators $T =: \begin{pmatrix} A & B \\ C & D \end{pmatrix}$, or, equivalently,

$$[T(\lambda)]_{\alpha\beta} =: \frac{1}{2} \delta_{\alpha\beta} T(\lambda) + \sigma^z_{\alpha\beta} X^z(\lambda) + \sigma^+_{\alpha\beta} X^-(\lambda) + \sigma^-_{\alpha\beta} X^+(\lambda). \hspace{1cm} (4.11)$$

\(^2\)that is, mainly my own confusion.
where
\[
X^+(\lambda) \equiv C(\lambda) \quad X^-(\lambda) \equiv B(\lambda) \quad X^z(\lambda) \equiv \frac{A(\lambda) - D(\lambda)}{2}
\] (4.12)
and the trace of the monodromy matrix is the transfer matrix
\[
T(\lambda) \equiv A(\lambda) + D(\lambda) .
\] (4.13)

From the transfer matrix we can generate a series of commuting operators by taking logarithmic derivatives with respect to $\lambda$. The Hamiltonian and the momentum operator are among these operators, viz.
\[
H = -J\phi(i\zeta) \partial_\lambda \log T(\lambda)|_{\lambda=\xi_j \equiv i\zeta/2} + JhS_{\text{tot}}^z \quad (4.14)
\]
\[
K = -i \log(-i)^N T(\lambda = \xi_j \equiv i\zeta/2) \quad (4.15)
\]
where all inhomogeneities must be set to $i\zeta/2$.

Thus, each of the operators generated from the transfer matrix represents a conserved quantity of the Heisenberg model. The presence of such a full set of commuting operators can be taken as the definition of an integrable model.

Commutation relations of the monodromy matrix are again given by the $R$-matrix,
\[
[R(\lambda - \mu)]_{\alpha\beta\gamma\delta}[T(\lambda)]_{\beta\sigma}[T(\mu)]_{\delta\rho} = [T(\mu)]_{\alpha\beta}[T(\lambda)]_{\gamma\delta}[R(\lambda - \mu)]_{\beta\sigma\delta\rho} ,
\] (4.16)
which can be specified for its elements
\[
[T(\lambda), T(\mu)] = 0 \quad (4.17)
\]
\[
[B(\lambda), B(\mu)] = 0 \quad (4.18)
\]
\[
A(\lambda)B(\mu) = b^{-1}(\mu - \lambda) [B(\mu)A(\lambda) - c(\mu - \lambda)B(\lambda)A(\mu)] \quad (4.19)
\]
\[
D(\lambda)B(\mu) = b^{-1}(\lambda - \mu) [B(\mu)D(\lambda) - c(\lambda - \mu)B(\lambda)D(\mu)] \quad (4.20)
\]

Given the reference state $|0\rangle$, the operators thus defined act as
\[
A(\lambda) |0\rangle = a(\lambda) |0\rangle \quad D(\lambda) |0\rangle = d(\lambda) |0\rangle \quad C(\lambda) |0\rangle = 0 \quad (4.21)
\]
where $a(\lambda) = 1$ and $d(\lambda) = \prod_{i=1}^N b(\lambda - \xi_i)$. We will keep $a(\lambda)$ in many formulas to remain in touch with the algebraic Bethe ansatz literature.

Consequently, $C(\lambda)$ can be seen as an annihilation operator, which would suggest that $B(\lambda)$ is the corresponding creation operator; indeed, with a lot of work (see e.g. [79]), it follows from equations (4.17–4.21) that
\[
|\{\lambda\} := B(\lambda_1) \cdots B(\lambda_N) |0\rangle \quad (4.22)
\]
is an eigenstate of the transfer matrix $T(\mu)$ for all $\mu$, and consequently of the Hamiltonian and all other conserved quantities, if the $\{\lambda\}$ satisfy the Bethe equations
\[
\frac{d(\lambda_j)}{a(\lambda_j)} = \prod_{k \neq j} \frac{b(\lambda_k - \lambda_j)}{b(\lambda_j - \lambda_k)} \quad (4.23)
\]
The eigenvalue of the transfer matrix $T(\mu)$ with respect to the state $|\{\lambda\}\rangle$ is
\[
\tau(\mu, \{\lambda\}) = a(\mu) \prod_{j=1}^{M} b^{-1}(\lambda_j - \mu) + d(\mu) \prod_{j=1}^{M} b^{-1}(\mu - \lambda_j). \tag{4.24}
\]

Local spin operators

The expression for the creation and annihilation operators in terms of the local spin operators takes the form of an immense sum over products of operators on all sites of the chain. Expressing expectation values of a local spin operator between Bethe states therefore generates a combinatoric problem that has for a long time been intractable. However, it has been shown by Kitanine et al. [74] that, by expressing the monodromy matrix elements in a special basis found by Maillet and de Santos [84], the combinatoric problem can be greatly simplified, thus allowing the local spin operators on site $j$ to be represented in terms of the monodromy matrix elements.

A simpler derivation, also due to Maillet, uses the fact that $c(0) = 1$ and $b(0) = 0$, so that if one sets $\lambda = \xi_j$, the $L$-matrix becomes
\[
[L_j(\xi_j; \xi_j)]_{\alpha\beta} = R(0)_{\alpha\beta} = \frac{1}{2} \delta_{\alpha\beta} I_j + \sigma^z_{\alpha\beta} S^z_j + \sigma^+_{\alpha\beta} S^-_j + \sigma^-_{\alpha\beta} S^+_j =: [P_{0j}]_{\alpha\beta}, \tag{4.25}
\]
which is the permutation operator exchanging the quantum space of the $j$th spin with the auxiliary space. In the homogeneous case $\xi_j \equiv \xi$, then, the monodromy matrix becomes simply
\[
[T(\xi)]_{\alpha\beta} = [P_{0N}]_{\alpha\gamma_1}[P_{0,N-1}]_{\gamma_1\gamma_2} \cdots [P_{01}]_{\gamma_{N-1}\beta} = [P_{01}]_{\alpha\beta} U, \tag{4.26}
\]
where $U$ is the operator that cyclically shifts the whole chain by one site in positive direction. In terms of the operators $X^a$ defined earlier in equation (4.11),
\[
\frac{1}{2} \delta_{\alpha\beta} T(\xi) + \sigma^z_{\alpha\beta} X^z(\xi) + \sigma^+_{\alpha\beta} X^-(\xi) + \sigma^-_{\alpha\beta} X^+(\xi) \tag{4.27}
\]
\[
= \left[ \frac{1}{2} \delta_{\alpha\beta} I + \sigma^z_{\alpha\beta} S^z_1 + \sigma^+_{\alpha\beta} S^-_1 + \sigma^-_{\alpha\beta} S^+_1 \right] U,
\]
so that for site $j = 1$ we have $S^a = X^a(\xi) U^{-1}$ and $U = T(\xi)$. This result can be extended to the other sites, by applying the cyclic shift operator and noting that $U^N = I$, so that we find
\[
S^a_j = T(\xi)^{j-1} X^a(\xi) T(\xi)^{N-j}. \tag{4.28}
\]

Similarly, one can prove the inhomogeneous generalisation
\[
S^a_j = \left[ \prod_{l=1}^{j-1} T(\xi_l) \right] X^a(\xi_j) \left[ \prod_{l=j+1}^{N} T(\xi_l) \right] \tag{4.29}
\]
4.3 Scalar product and norm

Another very important result is Slavnov’s [73] formula for the scalar product (overlap) between a Bethe wave function given by the \(M\) rapidities \(\{\lambda\}\) and an arbitrary wave function given in terms of \(M\) rapidities \(\{\mu\}\),

\[
\langle \{\mu\} | \{\lambda\} \rangle = \frac{\det H(\{\lambda\}, \{\mu\})}{\prod_{j>k} \phi(\mu_k - \mu_j) \prod_{j<k} \phi(\lambda_k - \lambda_j)} .
\]

(4.30)

where the \(M \times M\) matrix \(H\) is given by

\[
H_{ab} = \frac{\phi(i\zeta)}{\phi(\lambda_a - \mu_b)} \left[ a(\mu_b) \prod_{j \neq a}^{1 \ldots M} \phi(\lambda_j - \mu_b + i\zeta) + d(\mu_b) \prod_{j \neq a}^{1 \ldots M} \phi(\lambda_j - \mu_b - i\zeta) \right] .
\]

(4.31)

Taking the limit \(\{\mu\} \to \{\lambda\}\) in this formula, one obtains Gaudin’s [71] formula (first proven by Korepin [72]) for the norm of the Bethe wave function,

\[
\| \{\lambda\} \| = |\det \Phi(\{\lambda\})| ,
\]

(4.32)

where the Gaudin matrix \(\Phi\) is the Jacobi matrix for the logarithmic Bethe equations,

\[
\Phi_{ab} := -\partial_{\lambda_b} \log \left[ \frac{a(\lambda_a)}{d(\lambda_a)} \prod_{k \neq a}^{1 \ldots M} \frac{b(\lambda_k - \lambda_a)}{b(\lambda_a - \lambda_k)} \right] \]

(4.33)

\[
= \delta_{a,b} \left[ N \partial_{\lambda_a} \theta_1(\lambda_a) - \sum_{k \neq a} \partial_{\lambda_a} \theta_2(\lambda_a - \lambda_k) \right] + (1 - \delta_{a,b}) \partial_{\lambda_a} \theta_2(\lambda_a - \lambda_b) .
\]

4.4 Determinant expressions for form factors

Using (4.29), we can now express the form factor \(F^-(4.4)\) on site \(l\) as

\[
F_l^z = \langle 0 \prod_{k=1}^{M} C(\mu_k) B(\xi_l) \prod_{k=1}^{M-1} B(\lambda_k) | 0 \rangle \left[ \prod_{j=1}^{l-1} \prod_{k=1}^{M} b^{-1}(\mu_k - \xi_j) \right] \left[ \prod_{j=l+1}^{N} \prod_{k=1}^{M} b^{-1}(\lambda_k - \xi_j) \right] ,
\]

(4.34)

where we have used the fact that Bethe states are eigenstates of the transfer matrix. The factor on the left is now a scalar product between a Bethe state \(\{\mu\}\) and a state with rapidities \(\xi_l, \{\lambda\}\). Using formula (4.30), the Bethe equations for the state \(\{\lambda\}\), and some manipulations with the determinant, we derive the formula for the lowering form factor at site \(l\),

\[
F_l^{-}(\{\mu\}, \{\lambda\}) = \left[ \prod_{j=1}^{l-1} \prod_{k=1}^{M} b^{-1}(\mu_k - \xi_j) \right] \left[ \prod_{j=1}^{l} \prod_{k=1}^{M} b(\lambda_k - \xi_j) \right] \frac{\det H^-(\{\mu\}, \{\lambda\})}{\prod_{j>k} \phi(\mu_k - \mu_j) \prod_{j<k} \phi(\lambda_k - \lambda_j)} ,
\]

(4.35)
4.5 Reduced determinants for string states

where the matrix $H^-$, explicitly given below, is very similar to the $H$ of Slavnov’s formula. The derivation for the longitudinal form factor is more complicated, but goes along the same lines [74].

For the numerical calculation of structure factors, an explicit expression for the square of the form factors in $k$-space is desirable. The transverse form factor squared can be expressed as

$$|F_q^2|^2 = \frac{1}{4}N\delta_{q,q_a-q_b} \rho_2(0) \left| \prod_{j=1}^M \phi^{-1}_1(\mu_j) \right|^2 \prod_{1 \leq j, k \leq M} \left| \phi_2(\mu_j - \mu_k) \right|^{-1} \times$$

$$\times \prod_{1 \leq j, k \leq M-1} \left| \phi_2(\lambda_j - \lambda_k) \right|^{-1} \left| \frac{\det [H^-(\{\mu\}, \{\lambda\})]}{||\{\mu\}|| ||\{\lambda\}||} \right|^2$$

and the longitudinal form factor squared as

$$|F_q^2|^2 = \frac{1}{4}N\delta_{q,q_a-q_b} \prod_{j=1}^M \left| \phi^{-1}_1(\mu_j) \right|^2 \prod_{1 \leq j, k \leq M} \left| \phi_2(\mu_j - \mu_k) \right|^{-1} \times$$

$$\times \prod_{1 \leq j, k \leq M} \left| \phi_2(\lambda_j - \lambda_k) \right|^{-1} \left| \frac{\det [H(\{\mu\}, \{\lambda\}) - 2P(\{\mu\}, \{\lambda\})]}{||\{\mu\}|| ||\{\lambda\}||} \right|^2 , \quad (4.37)$$

where the norm of the Bethe state is given by (4.32).

The matrices $H$, $H^-$, and $P$ are defined as

$$H_{ab} := \phi_0^{-1}(\mu_a - \lambda_b) \left[ \prod_{1 \leq j \leq M} \phi_{-2}(\mu_j - \lambda_b) - \left[ \phi_1(\lambda_b) \right] \prod_{1 \leq j \leq M} \phi_{-1}(\lambda_b) \phi_2(\mu_j - \lambda_b) \right]$$

$$P_{ab} := \phi_1^{-1}(\mu_a) \phi_1^{-1}(\mu_a) \prod_{k=1}^M \phi_{-2}(\lambda_k - \lambda_b)$$

$$H^-_{ab} := \begin{cases} H_{ab} & \text{if } b < M \\ \phi_1^{-1}(\mu_a) \phi_1^{-1}(\mu_a) & \text{if } b = M \end{cases} \quad (4.38)$$

$$H_{ab} := \phi_0^{-1}(\mu_a - \lambda_b) \left[ \prod_{1 \leq j \leq M} \phi_{-2}(\mu_j - \lambda_b) - \left[ \phi_1(\lambda_b) \right] \prod_{1 \leq j \leq M} \phi_{-1}(\lambda_b) \phi_2(\mu_j - \lambda_b) \right]$$

$$P_{ab} := \phi_1^{-1}(\mu_a) \phi_1^{-1}(\mu_a) \prod_{k=1}^M \phi_{-2}(\lambda_k - \lambda_b)$$

$$H^-_{ab} := \begin{cases} H_{ab} & \text{if } b < M \\ \phi_1^{-1}(\mu_a) \phi_1^{-1}(\mu_a) & \text{if } b = M \end{cases} \quad (4.39)$$

4.5 Reduced determinants for string states

The determinant expressions (4.37, 4.36) are problematic when the set of rapidities $\{\lambda\}$ contains string configurations. Both the product $\prod_{1 \leq j, k \leq M} \phi_2(\lambda_j - \lambda_k)\left|^{-1}$ and the norm contain singular factors. Moreover, the determinants of the matrices $H, H^-$ become ill-defined: the prefactor of the second term in (4.38) diverges, vanishes or becomes of the indeterminate form $\delta/\delta$, and columns of the matrix become equal to leading order. However, it turns out that all divergencies can be removed by carefully reorganising the determinants, leading to an expression in terms of reduced versions of the above matrices.
Gaudin matrix

Consider the Gaudin matrix (4.33) in the presence of an \( n \) string. The determinant equals

\[
\begin{vmatrix}
  d_1 - \sum_{k=2}^{M} o_{1k} & o_{12} & \cdots & o_{1n} \\
  o_{21} & d_2 - \sum_{k \neq 2}^{1\ldots M} o_{2k} & \cdots \\
  \vdots & \vdots & \ddots \\
  o_{n1} & \cdots & \cdots & d_n - \sum_{k=1}^{1\ldots M-1} o_{Mk}
\end{vmatrix}
\]

(4.41)

where, for notational convenience, we have reordered the matrix such that the block corresponding to the string under consideration appears in the upper left. Its elements are given by

\[
d_a = N \partial_{\lambda_a} \theta_1 (\lambda_a) \quad \quad o_{ab} = \partial_{\lambda_a} \theta_2 (\lambda_a - \lambda_b) .
\]

(4.42)

It is important to note that, for adjacent roots in a string, \( o_{a,a+1} = o_{a+1,1} = (\delta_{a+1} - \delta_a)^{-1} + O(1) \), whereas \( d \) and the other \( o \) remain finite. We will exploit this observation to reduce the matrix.

Adding the first \( n-1 \) rows in the matrix to the \( n \)th, and subsequently adding the first \( n-1 \) columns to the \( n \)th, the \( n \)th row and column become

\[
\Phi_{an} = \Phi_{na} = \begin{cases} 
  d_a - \sum_{k=n+1}^{M} o_{ka} & \text{for } a < n \\
  \sum_{k=1}^{n} \left[ d_k + \sum_{l=n+1}^{M} o_{kl} \right] & \text{for } a = n \\
  \sum_{k=1}^{n} o_{ka} & \text{for } a > n
\end{cases}
\]

(4.43)

The rest of the matrix \( \Phi \) remains unchanged. To leading order, the first \( n-1 \) rows and columns form the tridiagonal matrix

\[
\Phi^s_0 = \begin{pmatrix}
  -o_{12} & o_{12} & \cdots \\
  o_{21} & -o_{23} - o_{21} & \cdots \\
  \cdots & \cdots & \cdots \\
  o_{n-1,n-2} & -o_{n-1,n} - o_{n-1,n-2} & o_{n-2,n-1}
\end{pmatrix}
\]

(4.44)

Adding the first row of this matrix to the second, we see that the determinant satisfies \( \det \Phi^s_0 = -o_{12} \det \Phi^s_1 + O(1) \), where \( \Phi^s_1 \) is the string block with the first \( j \) rows and columns cut off. Repeating this process, we see that

\[
\det \Phi^s_0 = (-1)^{n-1} o_{12} o_{23} \cdots o_{n-1,n} = \prod_{a}^{1\ldots n-1} (\delta_{a+1} - \delta_a)^{-1}.
\]

(4.45)
4.5. Reduced determinants for string states

The matrix $\Phi$ is finite and can therefore be left out of consideration; what remains is the reduced Gaudin matrix

$$\Phi^r := \left( \begin{array}{c} \sum_{b}^{1...n} d_b - \sum_{c}^{n+1...M} o_{bc} & \sum_{b}^{1...n} o_{n+1,b} & \cdots & \sum_{b}^{1...n} o_{Mb} \\ \vdots \\ \sum_{b}^{1...n} o_{bM} \\ \end{array} \right). \quad (4.46)$$

Returning to string-index notation, we see that the $n_k$ rows and columns of the Gaudin matrix that correspond to a string of type $k$ are represented, in the reduced matrix, by a single row and column with elements as above, where the sums are given by

$$d_{\beta}^k := \sum_{b}^{1...n_k} d_{\beta b} = N \sum_{b}^{1...n_k} \partial_{\lambda_{\beta b}^k} \theta_1(\lambda_{\beta b}^k) = N \partial_{\lambda_{\beta}^k} \theta_n(\lambda_{\beta}^k), \quad (4.47)$$

keeping in mind that $\lambda_{\alpha a}^j = \lambda_{\alpha}^j + i(n_j + 1 - 2a)\zeta/2$, and

$$o_{\alpha \beta}^{jk} := \sum_{b}^{1...n_k} o_{\alpha \beta b} = \partial_{\lambda_{\alpha}^j} \sum_{b}^{1...n_k} \theta_2(\lambda_{\alpha a}^j - \lambda_{\beta b}^k) = \partial_{\lambda_{\alpha}^j} \Theta_{1k}(\lambda_{\alpha a}^j - \lambda_{\beta}^k), \quad (4.48)$$

in analogy to the derivation of the Bethe–Takahashi equations. If multiple strings are present, this procedure can be repeated for all of them; in this case, the terms of (4.48) sum to

$$\sum_{a}^{1...n_j} \partial_{\lambda_{\alpha a}^j} \Theta_{1k}(\lambda_{\alpha a}^j - \lambda_{\beta}^k) = \partial_{\lambda_{\alpha}^j} \Theta_{jk}(\lambda_{\alpha}^j - \lambda_{\beta}^k). \quad (4.49)$$

In general, the Gaudin determinant equals

$$\det \Phi = \det \Phi^r \prod_{j}^{M_j} \prod_{a=1}^{n_j-1} \prod_{a=1}^{n_j} (\delta_{\alpha a+1} - \delta_{\alpha a})^{-1}, \quad (4.50)$$

with the reduced Gaudin matrix given by

$$\Phi^r_{j\alpha,k\beta} = \begin{cases} N \frac{d}{d \lambda_{\alpha}^j} \theta_j(\lambda_{\alpha}^j) - \sum_{l\gamma}^{l\gamma \neq (j, \alpha)} \frac{d}{d \lambda_{\alpha}^j} \Theta_j(\lambda_{\alpha}^j - \lambda_{\beta}^l) & \text{if } (j, \alpha) = (k, \beta) \\ \frac{d}{d \lambda_{\alpha}^j} \Theta_{jk}(\lambda_{\alpha}^j - \lambda_{\beta}^k) & \text{if } (j, \alpha) \neq (k, \beta). \end{cases} \quad (4.51)$$

We will call $\|\lambda\|_r := |\det \Phi^r|$ the reduced norm of a string state $|\{\lambda\}\rangle$. 

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Chapter 4. Dynamical correlations in finite chains

**H, H⁻, and P matrices**

We will now consider the determinants of $\mathbf{H}$ and $\mathbf{H} - 2\mathbf{P}$. Again, let us move the $(n \times n)$-block corresponding to the $n$-string under consideration to the top left, and continue counting to $M$ with the other elements.

Using the Bethe equations, we can write $\mathbf{H}$ as

$$H_{ab} = K_{ab}^- G_b^- + K_{ab}^+ G_b^+ / F_b^-,$$  \hspace{1cm} (4.52)

where

$$F_b^c := \prod_{1 \leq k \leq M} \phi_{2c}(\lambda_b - \lambda_k)$$  \hspace{1cm} (4.53)

$$G_b^c := \prod_{1 \leq k \leq M} \phi_{2c}(\mu_k - \lambda_b)$$  \hspace{1cm} (4.54)

$$K_{ab}^\pm := \phi_{0} - 1(\mu_a - \lambda_b)\phi_{\pm 2}(\mu_a - \lambda_b),$$  \hspace{1cm} (4.55)

Note that the second term in (4.52) now has a plus sign, because the product (4.53) includes the factors for $k = b$.

For convenience, let us work with the matrix $h^{(1)}$ given by

$$h_{ab}^{(1)} := \frac{\tilde{F}_b^- H_{ab}}{F_b^+ G_b^+} = K_{ab}^- \tilde{F}_b^- G_b^- + K_{ab}^+$$  \hspace{1cm} (4.56)

For small string deviations $\delta$, for $b < n$, the vanishing factors are

$$\phi_{-2}(\lambda_b - \lambda_{b+1}) = -\phi_{2}(\lambda_{b+1} - \lambda_b) = d_b + O(d_b^2).$$  \hspace{1cm} (4.57)

where $d_b := i(\delta_b - \delta_{b+1})$ for $0 < b < n$.

Let us make these factors explicit by taking them out of the $F-$product (4.53).

We define

$$F_b^c := \prod_{1 \leq k \leq M} \phi_{2c}(\lambda_b - \lambda_k)$$  \hspace{1cm} (4.58)

Notably,

$$d_b F_b^- = \tilde{F}_b^-$$  \hspace{1cm} for $1 \leq b < n$  \hspace{1cm} (4.59)

$$-d_{b-1} F_b^+ = \tilde{F}_b^+$$  \hspace{1cm} for $1 < b \leq n$  \hspace{1cm} (4.60)

$$F_b^\pm = \tilde{F}_b^\pm$$  \hspace{1cm} otherwise.  \hspace{1cm} (4.61)

With these definitions, consider the elements of $h^{(1)}$ corresponding to a string,

$$h_{a1}^{(1)} = K_{a1}^+ + K_{a1}^- d_1 \frac{F_{n}^- G_{n}^-}{F_{1}^- G_{1}^-}$$

$$h_{an}^{(1)} = K_{an}^+ - K_{an}^- d_{n-1} \frac{F_{n}^- G_{n}^-}{F_{n}^+ G_{n}^+}$$

$$h_{ab}^{(1)} = K_{ab}^+ - K_{ab}^- d_b d_{b-1}^{-1} \frac{F_{b}^- G_{b}^-}{F_{b}^+ G_{b}^+}$$  \hspace{1cm} for $1 < b < n$  \hspace{1cm} (4.62)
Noting that for small $\delta$, for $b < n$, to leading order
\[ K^-_{a,b+1} - K^+_{ab} = d_b \partial_{\mu_a} K^+_{ab} =: d_b L_{ab} , \]  \hspace{1cm} (4.63)
we perform the following $n - 1$ column operations, leaving the determinant invariant,
\[ h^{(b)}_{ab} = h^{(b-1)}_{ab} + d_b d_{b-1}^{-1} F^-_{b} G^-_{b} h^{(b-1)}_{a,b-1} \]
for $1 < b < n$ , \hspace{1cm} (4.64)
concluded by
\[ h^{(n)}_{an} = h^{(n-1)}_{an} + d_{n-1}^{-1} F^-_{n} G^-_{n} h^{(n-1)}_{a,n-1} . \] \hspace{1cm} (4.65)

The resulting matrix $h^{(n)}$ is
\[ h^{(n)}_{a1} = K^+_{a1} + d_1 K^-_{a1} \]
\[ h^{(n)}_{ab} = K^+_{ab} + d_b \left[ K^-_{a1} \sum_{c=1}^{b} F^-_{c} G^-_{c} + \sum_{c=1}^{b} L_{ac} \prod_{d=c+1}^{b} F^-_{d} G^-_{d} \right] \]
\[ h^{(n)}_{an} = K^+_{an} + K^-_{a1} \prod_{c=1}^{n} F^-_{c} G^-_{c} + \sum_{c=1}^{n-1} L_{ac} \prod_{d=c+1}^{n} F^-_{d} G^-_{d} \]

Now that the $n$ columns of the matrix $h^{(n)}$ corresponding to the string all have elements that are $O(1)$, we may neglect the terms of $O(d)$, so that $h^{(n)}_{ab} = K^+_{ab}$ for $1 \leq b < n$. The column $h^{(n)}_{an}$ can be simplified by the following considerations. To leading order,
\[ F^\pm_n = F^0_{d\mp 1} \]
so that
\[ \prod_{d=c+1}^{n} F^-_{d} = \prod_{d=c+1}^{n} F^0_{d} = \prod_{d=c+1}^{n-1} \frac{F^0_n F^0_{n+1}}{F^0_{c} F^0_{c+1}} ; \] \hspace{1cm} (4.67)
\[ G^\pm_n = G^0_{d\mp 1} \]
so that
\[ \prod_{d=c+1}^{n} G^-_{d} = \prod_{d=c+1}^{n} G^0_{d} = \prod_{d=c+1}^{n-1} \frac{G^0_c G^0_{c+1}}{G^0_n G^0_{n+1}} . \] \hspace{1cm} (4.68)

Note that these relations also hold when $c = n - 1$ or $c = n$ and we understand the empty product as $\prod_{a=1}^{0} = 1$, and we have extended the definition (2.57) of the string roots to include the non-root values $\lambda^j_{\alpha 0} := \lambda^j_{\alpha} + i(n+1)\zeta/2$, $\lambda^j_{\alpha,n+1} := \lambda^j_{\alpha} - i(n+1)\zeta/2$.

This gives us
\[ h^{(n)}_{an} = K^+_{an} + K^-_{a1} \frac{F^0_n F^0_{n+1}}{F^0_{n} F^0_{1}} \frac{G^0_c G^0_{c+1}}{G^0_n G^0_{n+1}} + \sum_{c=1}^{n-1} L_{ac} \frac{F^0_n F^0_{n+1}}{F^0_{c} F^0_{c+1}} \frac{G^0_c G^0_{c+1}}{G^0_n G^0_{n+1}} \] \hspace{1cm} (4.69)
Finally multiplying the finite part of the factors we took out of the first \( n \) columns at the start back into the \( n \)th column, such that

\[
H^r_{an} := h^{(n)}_{an} \prod_{b=1}^{n} \frac{F^+_b G^+_b}{F^-_b} = h^{(n)}_{an} \left[ \frac{F^0_0 F^0_1}{F^0_n} \prod_{c=2}^{n+1} G^0_c \right],
\]

we arrive at the reduced matrix \( H^r \), given by

\[
H^r_{ab} = K^+_a b \quad \text{for } 1 \leq b \leq n - 1
\]

\[
H^r_{an} = \left[ \frac{F^0_0 F^0_1}{G^0_n} \prod_{j=2}^{n} G^0_j \right] \sum_{b=0}^{n} \frac{G^0_b G^0_{b+1}}{F^0_b F^0_{b+1}} \left[ (\delta_{b0} + \delta_{bn} - 1) L_{ab} + (\delta_{b0} + \delta_{bn}) K^+_a b \right]
\]

and

\[
\det H^r = \det H \prod_{b=1}^{n} \frac{F^+_b F^-_b}{F^+_b F^-_b} = (-1)^{n-1} \det H
\]

Since we need \( \det(H - 2P) \), we must apply the same sequence of operations to the matrix \( P \). As

\[
P_{ab} = -\phi^{-1}_1(\mu_a) \phi^{-1}_1(\mu_a) \tilde{F}^-_b
\]

this leads to

\[
P_{ab} = 0 \quad \text{for } 1 \leq b < n, \quad \text{(4.74)}
\]

\[
P_{an} = \left[ \frac{F^0_0 F^0_1}{G^0_n} \prod_{j=2}^{n} G^0_j \right] \phi^{-1}_1(\mu_a) \phi^{-1}_1(\mu_a) \sum_{b=1}^{n} \frac{G^0_b}{F^0_b}
\]

The \( M \)th column of \( H^- \) remains unchanged.

**Reduced determinant expressions**

Going back to the expressions (4.37, 4.36) for the form factors, we see that the divergencies in the Gaudin matrix exactly cancel those in the prefactors. Therefore, we can calculate form factors for string states using these expressions, but replacing the Gaudin matrix \( \Phi \) and the matrices \( H - 2P \) and \( H^- \) with the reduced versions we just calculated and leaving the divergent factors out of the prefactor.

**4.5.1 Form factors for lower-weight states**

On the isotropic chain, one or more of the rapidities may be infinite (i.e., one or more momenta may be zero). Let us suppose we have a single such rapidity, say \( \lambda_M = \infty \). The infinite rapidity is added by acting with a total-spin lowering
operator, \(|\{\lambda, \infty\}\rangle \propto S_0^- |\{\lambda\}\rangle\). We assume the state \(|\{\mu\}\rangle\) is a highest-weight state (e.g. the ground state), therefore \(S^+ |\{\mu\}\rangle = 0\). Explicitly writing the normalisation, 

\[
F_q^+ (\{\mu\}, \{\lambda, \infty\}) = \frac{\langle \{\mu\} | [S_q^a, S_0^-] | \{\lambda\} \rangle}{\sqrt{\langle \{\mu\} | \{\mu\} \rangle \langle \{\lambda\} | S_0^+ S_0^- | \{\lambda\} \rangle}} \tag{4.75}
\]

For a highest weight state, \(\langle S_0^+ S_0^- \rangle = 2 \langle S_0^+ \rangle\) so that the norm is given by 

\[
\langle \{\lambda\} | S_0^+ S_0^- | \{\lambda\} \rangle = \frac{1}{N} (N - 2M_\lambda) \langle \{\lambda\} | \{\lambda\} \rangle \tag{4.76}
\]

where \(M_\lambda\) is understood to be the number of roots in \(\{\lambda\}\), excluding the infinite rapidity. From this and \([S_q^a, S_0^-] = 2S_q^a/\sqrt{N}\), \([S_q^a, S_0^-] = -S_0^-/\sqrt{N}\), and obviously \([S_q^a, S_0^-] = 0\), we derive the following very useful relations, which can also be found in [85]:

\[
|F^+ (\{\mu\}_M, \{\lambda, \infty\}_{M+1})|^2 = \frac{4 |F^z (\{\mu\}, \{\lambda\})|^2}{N - 2M_\mu} \tag{4.77}
\]

\[
|F^z (\{\mu\}_M, \{\lambda, \infty\}_M)|^2 = \frac{|F^- (\{\mu\}, \{\lambda\})|^2}{N - 2(M_\mu - 1)} \tag{4.78}
\]

\[
|F^- (\{\mu\}_M, \{\lambda, \infty\}_{M-1})|^2 = 0 \tag{4.79}
\]

where \(M_\mu\) is the number of roots in the set \(\mu\).

When two rapidities are infinite, the only nonzero form factor is \(F^+\); here, we have to use the normalisation 

\[
\langle \{\lambda\} | S_0^+ S_0^+ S_0^- S_0^- | \{\lambda\} \rangle = \frac{2}{N^2} (N - 2M_\lambda)(N - 2M_\lambda - 1) \langle \{\lambda\} | \{\lambda\} \rangle \tag{4.80}
\]

so that 

\[
|F^+ (\{\mu\}_M, \{\lambda, \infty, \infty\}_{M+1})|^2 = \frac{2 |F^- (\{\mu\}, \{\lambda\})|^2}{(N - 2M_\mu + 2)(N - 2M_\mu + 1)} \tag{4.81}
\]

**Determinant expressions with infinite rapidities**

It is, however, instructive to see how these relations arise from the determinant expressions. Again, we have to be careful when calculating the determinants, as columns, to lowest order, become equal. We need the determinant of the matrix \(H - 2P\), as defined above, this time written as 

\[
[H - 2P]_{ab} = K_{ab}^- G_b^- - K_{ab}^+ G_b^+ W_b + 2(\mu_\lambda^2 + 1/4)^{-1} \tilde{F}_b^- \tag{4.82}
\]

where \(W_b := [\frac{\lambda_\gamma + i/2}{\lambda_\gamma - i/2}]^N\). Performing the operations 

\[
[H - 2P]_{ab}^{(1)} = [H - 2P]_{ab} - \frac{\tilde{F}_b^-}{F_M} [H - 2P]_{aM} \quad \text{for } b < M \tag{4.83}
\]

77
we now have a matrix with the same determinant,

\[
[H - 2P]^{(1)}_{ab} = (K_{ab}^- G_b^- - K_{ab}^+ G_b^+ W_b) + \tilde{F}_b^- D_{ab}^- (K_{aM}^- G_{aM}^- - K_{aM}^+ G_{aM}^+ W_{aM}) \quad \text{for } b < M
\]

\[
[H - 2P]^{(1)}_{aM} = (K_{aM}^- G_{aM}^- - K_{aM}^+ G_{aM}^+ W_{aM}) + 2(\mu_b^2 + 1/4)^{-1} \tilde{F}_M^- .
\]

As \(\lambda_M \to \infty\),

\[
\tilde{F}_b^- = -\lambda_M + O(1) \quad \tilde{F}_M^- = -i\lambda_M^{-1} + O(\lambda_M^{-2}) \quad (4.85)
\]

Furthermore,

\[
K_{aM}^- G_{aM}^- - W_b K_{aM}^+ G_{aM}^+ = i(-\lambda_M)^{M-3}[N - 2M + 2] + O(\lambda_M^{-4}) \quad (4.86)
\]

We may conclude that to lowest order,

\[
[H - 2P]^{(1)}_{ab} = (K_{ab}^- G_b^- - K_{ab}^+ G_b^+ W_b) = H_{ab}^- \quad \text{for } b < M
\]

\[
[H - 2P]^{(1)}_{aM} = 2(\mu_a^2 + 1/4)^{-1} \tilde{F}_M^- = H_{aM}^- \tilde{F}_M^- ,
\]

and therefore

\[
|\det[H - 2P]|^2 = \lambda_M^{2M-2} |\det H^-|^2 + O(\lambda_M^{2M-3}) \quad (4.88)
\]

It is easy to see

\[
\det \Phi = [N - 2M + 2] \lambda_M^{-2} \det \Phi_{M-1} + O(\lambda_M^{-4}) \quad (4.89)
\]

where \(\Phi_{M-1}\) consists of the Gaudin matrix without its last row and column. Using these expressions in (4.37), taking care of the prefactors, we find relation (4.78).

Similarly, we can derive relation (4.79) from the determinant expressions.

### 4.5.2 Form factors for singular states vanish

In the case of singular states (as in chapter 3), the reduced determinant expressions for correlators become degenerate. However, we can show that the form factors must vanish in this case with the following simple argument, based on their symmetry properties under lattice shifts and inversion.

**Translation symmetry**

All singular states have a symmetric rapidity distribution, which implies their total momentum must be either 0 or \(\pi\). The former implies symmetry under lattice shifts, and corresponds to the case with an odd number of finite roots aside from \(\pm i/2\). The latter implies antisymmetry when shifting the lattice by one site, and corresponds to the case where there is an even number of such roots.
Parity symmetry

Let us now turn our attention to the symmetry properties under lattice inversion (the parity operation). Under parity, the wave function $\chi_\{\lambda\}(j_1, \ldots, j_M)$ is taken to $\chi_\{\lambda\}(N - j_M + 1, \ldots, N - j_1 + 1)$. Inserting this in the Bethe wave function, we get

$$\chi_\{k\}(N - j_M + 1, \ldots, N - j_1 + 1) = e^{i \sum_\alpha k_\alpha (N + 1)} A_0 \sum_\mathcal{P} (-1)^{\mathcal{P}} e^{\frac{1}{2} i \sum_{\alpha < \beta} \Phi(k_{\mathcal{P} \alpha}, k_{\mathcal{P} \beta})} e^{i \sum_\alpha -k_{\mathcal{P} \alpha} j_{M - \alpha}}$$

(4.90)

Now let us set $k'_{M - \alpha} := -k_\alpha$, so that

$$\chi_\{k\}(N - j_M + 1, \ldots, N - j_1 + 1) = e^{i \sum_\alpha k_\alpha (N + 1)} A_0 \sum_\mathcal{P} (-1)^{\mathcal{P}} e^{\frac{1}{2} i \sum_{\alpha < \beta} \Phi(k'_{\mathcal{P} \alpha}, k'_{\mathcal{P} \beta})} e^{i \sum_\alpha k'_{\mathcal{P} \alpha} j_{\alpha}}$$

(4.91)

where $\mathcal{V}$ is the inversion permutation, such that $\mathcal{V} \mathcal{P} \mathcal{V} = \mathcal{P}(M - \alpha)$. Realising that $[\mathcal{V} \mathcal{P} \mathcal{V}] = [\mathcal{P}]$, we see that we recover the Bethe wave function for the set of momenta $\{k'\}$, with a prefactor $e^{i \sum_\alpha k_\alpha (N + 1)} = e^{i \sum_\alpha k_\alpha}$. Therefore, a Bethe wave function with $\{k\} = \{-k\}$ is either symmetric (if $\sum_\alpha k_\alpha = 0$) or antisymmetric (if $\sum_\alpha k_\alpha = \pi$) under parity; conversely, if a state $\chi_\{k\}$ is an eigenfunction of parity at eigenvalue $v$, we must have $\chi_\{k\} = v \chi_\{-k\}$.

Consider, however, a singular Bethe wave function; take for instance $\chi_{\pm i/2}(j_1, j_2) = (-1)^{j_1} \delta_{j_1, j_2} + (-1)^{j_2} \delta_{j_1 + N, j_2 + 1}$. It is easily seen that this state is symmetric under parity, but antisymmetric under a single-site shift. In [69] the above argument is taken to imply that singular states cannot be Bethe states. However, even though $\{\lambda\} = \{-\lambda\}$, the momenta for the singular complex are $k_\pm = \pi/2 \pm i \infty$; the limit that needs to be taken to arrive as this point is such that at no point $\lambda_\pm = -\lambda_\pm$ except at the limit itself. The opposite momenta $k_\pm = -\pi/2 \pm i \infty$ yield, in the limit, the same wave function; but $\{k\} \neq \{-k\}$ and therefore singular Bethe states do not satisfy the symmetry relation above.

Applying the above argument to the singular-state wave function of (3.83), we see that lattice inversion takes the finite momenta to their opposites; but the part of the wave function corresponding to the singular complex is taken to itself. (Note that the extra scattering factor for opposite momenta surrounding a pair does not change, as the property of surrounding something is invariant under parity). Thus the eigenvalue under parity from a singular state is $-e^{i \sum_\alpha k_\alpha}$. Indeed, for a general singular state, symmetry under shifts implies antisymmetry under parity and vice versa.

Symmetry and form factors

Now it is easy to show that form factors of singular states with the ground state vanish. Consider an even singular state, i.e. of momentum $\pi$. The ground state for
even \( M \) has momentum 0. Therefore, the only possibly nonvanishing form factor operates at momentum \( \pi \),

\[
F_\pi^\alpha (\text{GS}, \{\pm i/2, \lambda\}) = \langle \text{GS} | \sum_j (-1)^j S_j^\alpha |\{\pm i/2, \lambda\}\rangle
\]  

(4.92)

As we have shown, the state \(|\{\pm i/2, \lambda\}\rangle\) is symmetric under parity. Since \( N \) is even, the state \( \sum_j (-1)^j S_j^\alpha |\{\pm i/2, \lambda\}\rangle \) is antisymmetric under parity. But the ground state \(|\text{GS}\rangle\) is symmetric; therefore, their overlap (which is the form factor) must be zero. The converse argument holds when we consider odd singular states; again, the form factor is zero.

### 4.6 Sum rules

The form factors (squared) satisfy a set of sum rules, viz.:

\[
\frac{1}{N} \sum_q \sum_{\{\lambda\}} |F_q^z (\{\mu\}, \{\lambda\})|^2 = \frac{1}{4}
\]  

(4.93)

\[
\frac{1}{N} \sum_q \sum_{\{\lambda\}} |F_q^{-} (\{\mu\}, \{\lambda\})|^2 = \frac{1}{2} - \langle S^z \rangle_{\{\mu\}} = \frac{M_\mu}{N}
\]  

(4.94)

\[
\frac{1}{N} \sum_q \sum_{\{\lambda\}} |F_q^{+} (\{\mu\}, \{\lambda\})|^2 = \frac{1}{2} + \langle S^z \rangle_{\{\mu\}} = \frac{N - M_\mu}{N}
\]  

(4.95)

For the structure factor, we need the connected sum rule for \( F^z \),

\[
\frac{1}{N} \sum_q \sum_{\{\lambda\} \neq \{\mu\}} |F_q^z (\{\mu\}, \{\lambda\})|^2 = \frac{1}{4} - \langle S^z \rangle_{\{\mu\}}^2 = \frac{1}{4} \left[ 1 - \left( 1 - \frac{2M_\mu}{N} \right)^2 \right]
\]  

(4.96)

These sum rules play a crucial role in any approach based on summing over a limited number of intermediate states: since every term in the sum is positive, the sum provides a very easy check on the accuracy of the approximation; the idea being that the further the sum rule is satisfied, the better the approximation is. Obviously, erratic contributions that do not push the sum rule contribution over 100% go unnoticed. However, if one knows the contributions to be correct, the saturation gives an impression of the amount of contribution missing; if on the other hand, the sum rule is over-satisfied, we know that there must be an error. For these reasons we will always state the sum rule saturation of a structure factor calculation.

The above sum rules only work if the contributions are known over all of \((k, \omega)\) space. Sometimes we want to restrict the region in \(k\)-space where we calculate contributions, so that we can go to higher chain lengths in a given amount of calculation time. In some cases additional sum rules are known: for instance, in the isotropic model at zero field, the integral of the first energy moment of the structure factor is known for every value of the momentum (see also chapter 5. Such sum rules provide additional checks on the results.
4.7 Calculation scheme

With these expressions for the form factors, we can calculate the structure factor by approximating the sum (4.1). This is possible because, as it turns out, the vast majority of the spectral weight is carried by a relatively limited number of form factors, thus obviating the need to calculate the full Hilbert space of $2^N$ states. Such a method was employed in [86, 87], where the two-spinon contribution to the structure factor at fixed momentum was calculated.

In general, it is expected that the two-spinon part should carry the bulk of the spectral weight, with lesser and decreasing contributions from higher-spinon states. The rationale is that spinons can be seen as kinks in the spin configuration between an A and a B Néel state; although they are dressed kinks, which have acquired some spatial extension, they are still rather localised objects. This picture is only rigorously valid in the gapped phase $\Delta > 1$, where in the Ising limit the Néel states are true ground states. In the gapless phases, this is of course not the case; however, spinons retain their localised nature. The excitation created by a local spin operator can decomposed into a series of spinon excitations; the canonical example is a spin flip in a Néel background which can be seen as two directly adjacent kinks. Because of the dressing of the spinons, there will also be higher-spinon terms in the expansion; these will however be much smaller than the two-spinon term.

Although, as argued, the two-spinon part carries the bulk of the spectral weight, a non-negligible part is carried by more complex excitations. Including these contributions, we will show that in most cases it is possible to saturate the sum rule over 99%.

4.7.1 Principal contributions

The form factors are matrix elements of operators working on a single site, which therefore only locally change the wave function. As a consequence, states with higher overlap with the ground state are expected to have higher form factors. Based on this rationale and the known two-particle contribution [85], we expect the lowest-lying excitations to be individually the most important. However, as the higher-lying states vastly outnumber the lower-lying ones; the density of states diverges toward the upper boundary of the two-spinon continuum, so that individually modest contributions of states may amount to a large signal on the upper boundary. Indeed, in the XY model ($\Delta = 0$ case), the structure factor itself diverges towards that boundary [88, 85]. Accordingly, it may be necessary to solve a large number of Bethe states and calculate a large number of determinants to capture the contribution on this side of the continuum.

4.7.2 Adaptive algorithm

It is favourable to calculate the largest individual contributions first, so that when the calculation is stopped one can reasonably expect that the contribution of the
states not calculated (typically, the overwhelming majority) have a small contribution. We follow the enumeration scheme outlined in section 2.7.3, in which the states are largely ordered by decreasing contribution. As an illustration, figure 4.1 shows how this works out in a specific case.

However, this reasoning is far from rigorous, and in many cases there is no monotonous decrease. It often happens that a group of states with more particles moved outward have higher contributions than the states with only one outward particle, but one that is moved further out. However, we do not know a way of ordering the states such that their contributions decrease monotonously. It also depends on which of the form factors is calculated. Therefore, we introduce an adaptive scanning algorithm, in which the current row of the diagram is extended by two blocks at a time, until the contribution drops below a given threshold. The remaining states that could be accessed by extending this row are skipped and the scanning continues with an extra particle moved one position outward. It is useful to keep track of which states have been visited and which have not, so that it is possible to come back at a later stage and extend the calculation with a lower threshold.

4.7.3 Solving Bethe’s equations

When the quantum numbers are distributed symmetrically and there exist even strings with quantum number zero, we can immediately decide to skip the state: its contribution must be zero by symmetry, as derived in section 4.5.2. For other states, we first solve the Bethe–Takahashi equations iteratively. Simple iteration of the equations is generally a good method. The number of iteration steps required to reach convergence can be lowered by applying an extrapolation scheme: after four
iteration steps, if $\lambda^{(n)}$ is the value found in the $n$th iteration step, the polynomial going through the points $(1/n, \lambda^{(n)})$ is calculated. Its value at the y axis gives then the next approximation, after which the procedure is repeated. For not-too-large systems (e.g. $N \sim 100$), convergence can be reached faster by the Newton–Raphson method. However, as the latter involves computing the Jacobian determinant (i.e. the determinant of the Gaudin matrix (4.33)) at every step, an $O(N^3)$ calculation, for really large systems (e.g. $N \sim 1000$) simple iteration is preferable: each iteration is an $O(N)$ computation, and the number of iterations necessary seems to be between $O(N)$ and $O(N^2)$. However, one single Newton–Raphson step at the end can be done for free, since we need to know Gaudin’s matrix anyway, to calculate the norm of the wave function. It is advantageous to alternate between the various methods to avoid getting stuck in a loop.

We use the first-order deviations to check whether this solution is close enough to an actual solution of the Bethe equations. If this is not the case, the full Bethe equations must be solved. Using the solution of the Bethe–Takahashi equations as initial values, this can again be done iteratively, as outlined in section 3. When convergence is reached, the determinants for the form factors must be calculated. At $O(N^3)$ (using LU decomposition, see e.g. [64]), this is the bottleneck of the computation. While for pure strings we can use the reduced determinants, for deviated strings, we need to insert the full complex solution. This we can only do if we insert it as the left-hand state $\{\mu\}$, for otherwise we run into the same degeneracies to avoid which the reduced determinants were introduced. A consequence of this is that we cannot compute the contribution of deviated strings to the $F^-$ form factor. Fortunately, in this case, real states and pure two-strings together satisfy the sum rule to an extremely high degree.

### 4.8 Results for the DSF

To show the power of this method, let us give a few results. Figures 4.8.1–4.6 give a variety of structure factors on a number of systems with different parameters, which we will discuss in the following sections.

The dynamical structure factor for a finite chain, being the sum of a finite number of form factors (squared), is a collection of delta peaks. Experimental measurements, on the other hand, obviously have a finite resolution. To compare the two, the delta functions need to be smoothed out to nonzero width one way or another. This makes it also easier to compare the results to those for an infinite chain (see chapter 5).

In the figures of this section, the $\delta$ function is smoothened in the $\omega$ direction by

$$
\delta(\omega - \omega_0) \rightarrow \frac{1}{2\epsilon\sqrt{\pi}} e^{-\frac{(\omega - \omega_0)^2}{4\epsilon^2}}.
$$

(4.97)

In choosing the width $\epsilon$ we must compromise between, on the one hand, the desire to get a smooth graph in which the individual delta functions are no longer visible,
Chapter 4. Dynamical correlations in finite chains

4.8.1 Isotropic chain at zero field

The obvious first graph to show here is the structure factor for the original Heisenberg model, the isotropic model at zero field. Because of the rotation symmetry, structure factors in all directions are equal,

$$S^{zz}(q, \omega) = S^{yy}(q, \omega) = S^{xx}(q, \omega)$$ (4.98)

and as a consequence $S^{-+}(q, \omega) = S^{+-}(q, \omega) = 2S^{zz}(q, \omega)$. This structure factor is shown in figure 4.8.1 as a function of momentum $q$ and energy $\omega$, calculated on a chain of $N = 500$ sites. About 0.9% of the sum rule is not accounted for, which gives an estimate for the accuracy of the plot. Note that one can go to higher saturation levels by keeping the chain shorter—for instance, on $N = 200$, we can easily go to 99.5%—but at the expense of a cruder plot made up of less momentum modes and less form factors in the energy direction, so that a wider smoothening is necessary.
4.8. Results for the DSF

Figure 4.3: Structure factors for $\Delta = 1$ at $N = 200$ at various values of external field. The columns show, from left to right, $S^{-+}$, $S^{zz}$, and $S^{+-}$. The rows show, from top to bottom, $M = 75$, $M = 50$, and $M = 25$. The sum rule saturations for these plots are given in table 4.1. It should be noted that in the two graphs in the top right a sizeable contribution to the sum rule is missing.

<table>
<thead>
<tr>
<th>$\Delta = 1$</th>
<th>$S^{-+}$</th>
<th>$S^{zz}$</th>
<th>$S^{+-}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M = 75$</td>
<td>99.49%</td>
<td>97.37%</td>
<td>81.40%</td>
</tr>
<tr>
<td>$M = 50$</td>
<td>99.92%</td>
<td>98.54%</td>
<td>89.21%</td>
</tr>
<tr>
<td>$M = 25$</td>
<td>99.99997%</td>
<td>99.60%</td>
<td>96.25%</td>
</tr>
</tbody>
</table>

Table 4.1: Sum rule saturations for the $\Delta = 1$ structure factors of figure 4.3.
Chapter 4. Dynamical correlations in finite chains

<table>
<thead>
<tr>
<th>( \Delta = 0.75 )</th>
<th>( S^{-+} )</th>
<th>( S^{zz} )</th>
<th>( S^{+-} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M = 100 )</td>
<td>98.8%</td>
<td>97.8%</td>
<td>—</td>
</tr>
<tr>
<td>( M = 75 )</td>
<td>99.85%</td>
<td>98.46%</td>
<td>93.60%</td>
</tr>
<tr>
<td>( M = 50 )</td>
<td>99.97%</td>
<td>99.40%</td>
<td>94.52%</td>
</tr>
<tr>
<td>( M = 25 )</td>
<td>99.36%</td>
<td>99.94%</td>
<td>97.95%</td>
</tr>
</tbody>
</table>

Table 4.2: Sum rule saturations for the \( \Delta = 0.75 \) structure factors of figure 4.4.

of down spins \( M \). The number of down spins \( M \) is always given for the ground state with respect to which we measure; note that we can find the field for which such a state with given \( M \) has lowest energy by using \( \partial_h (E - M h) = 0 \). The intermediate states which carry the correlations have either one more down spin (for \( S^{-+} \)), an equal number, or one less (for \( S^{+-} \)).

As the field gets stronger, we move towards the saturation transition, after which the ground state is aligned with the field and coherent spin waves (magnons) with dispersion relation \( \omega = J \cos q \) describe the excitations of the system. This can be seen as the graph for \( S^{-+} \) (which becomes the magnon propagator) approaches the dispersion relation. Obviously, \( S^{-+} \) becomes zero at saturation as the ground state there has all spins down.

### 4.8.3 Anisotropic chains

Now let us break the isotropy by introducing a \( \Delta \neq 1 \). The longitudinal and transverse structure factors at zero field are no longer equal. By reflection symmetry, we do still have \( S^{-+} = S^{+-} \) at zero field; though this quantity can only be calculated through the latter formulation as applying \( S^- \) to a state with \( M = N/2 \) pushes it ‘through the equator’ to the side that is not reachable by Bethe ansatz from an all-up reference state.

Figure 4.4 shows the three structure factors for the anisotropic Heisenberg chain with \( \Delta = 0.75 \), whereas figure 4.5 shows them for \( \Delta = 0.25 \). As a function of magnetic field, roughly the same behaviour is visible as for the isotropic chain; however, comparing the various graphs at different anisotropies, the transition from the \( XXX \) to the \( XX0 \) model becomes visible: the spectral weight in the longitudinal structure factor becomes more evenly distributed with lower \( \Delta \) (in \( XX0 \), the distribution is flat) whereas the transverse structure factors become more sharply peaked.

### 4.8.4 Two-string contribution

In figure 4.6 the contribution to the transverse structure factor at zero field of states involving one two-string is shown for the two anisotropic cases studied. It is clearly non-negligible, with a sum rule contribution of around 6.5\%. In fact, states with a single two-string are classified (in the isotropic case) as two-spinon states;
Figure 4.4: Structure factors for $\Delta = 0.75$ at $N = 200$ at various values of external field. Same configuration as figure 4.3. At the top, two graphs are added for $S^{-+}$ and $S^{zz}$ at $M = 100$. 
Figure 4.5: Structure factor for $\Delta = 0.25$, and $N = 200$ at various values of external field. Same configuration as figure 4.5.
4.8. Results for the DSF

\[
\begin{array}{|c|ccc|}
\hline
\Delta = 0.75 & S^{++} & S^{zz} & S^{+-} \\
M = 100 & 94.6\% & 99.8\% & - \\
M = 75 & 99.66\% & 99.82\% & 92.65\% \\
M = 50 & 99.95\% & 99.85\% & 93.93\% \\
M = 25 & 99.99995\% & 99.991\% & 97.73\% \\
\hline
\end{array}
\]

Table 4.3: Sum rule saturations for the $\Delta = 0.25$ structure factors of figure 4.5.

Figure 4.6: Two-string contributions to the transverse structure factor at zero magnetic field for anisotropies $\Delta = 0.25$ (left) and 0.75, at chain length $N = 200$. Note that the colour scale has been enhanced as compared to that used in the previous figures. The sum rule contribution from these states is 7.2% and 6.3% respectively.

their importance is therefore not unexpected. In fact, deviated strings, which are not included in these plots might push the two-string contribution further up.

4.8.5 Real space

For small distances, equal-time correlation functions of Heisenberg chains at zero field in real space can be calculated analytically. This is done in the thermodynamic limit on the basis of the multidimensional integral representation [89]. The expressions resulting from this representation are very hard to evaluate; progress in this respect was made first for a special correlation function known as the emptiness formation probability [90, 91, 92, 93, 94, 95] which is directly related to the neighbour correlators.

For the isotropic chain the first two neighbour correlators have been known for a long time [96, 97]; five more were found more recently [98, 99, 100, 101]. For anisotropic chains results are known up to three neighbours [102, 103, 104]. These exact results give an extra check on the accuracy of our results, which are easily Fourier transformed to real space. In tables 4.4–4.6 we compare our results to these
exact values. The order of magnitude of the error turns out to be what is expected from the sum rule saturation.

Figure 4.7 gives the real-space equal-time structure factor for the isotropic chain for all values of distance between sites; in this plot the algebraic decrease of correlation functions with distance is clearly visible, until the point where finite-size effects set in.

4.8.6 Sum rule saturation

Throughout the plots shown, the sum rule saturation is generally decent; exceptions to this are mostly in the region near the isotropic point and close to (but not at) zero field. The missing contributions are most strongly felt in the $S^+\!\!-$ structure factor. In fact, the worst results can be found by choosing the smallest possible field (e.g., $M = 99$ at $N = 200$). This is precisely the region where the string hypothesis is at its worst (see also chapter 3). We therefore guess that it is due to strings that are either strongly deviated or degenerated into pairs of real solutions; neither is as of yet incorporated into the form factor algorithm for anisotropic chains. In principle it should be possible to include these, provided we can solve the Bethe equations with high enough precision.

4.9 Discussion

We have shown that, using determinant formulas for form factors derived from the Bethe ansatz, it is possible to compute two-point spin–spin correlation functions for all combinations of local spin operators, for the isotropic and the gapless anisotropic regime of the Heisenberg chain. By checking our results against sum rules and known results in various limits, we have established that they are highly accurate. We have tried a similar technique for the gapped regime, but we have not obtained satisfactory saturation of the sum rules; it is not clear yet where to look for the missing part, so more study is required to find a solution in this region.

One of the things that can be noted from the solutions we have found is that configurations which include two-strings give a nonnegligible contribution. This is expected in the isotropic zero-field case, where states with one two-string are the spin-0 excitations that, together with a triplet of spin-1 excitations, form the two-spinon states. Although it is less clear what a two-spinon state is away from the isotropic zero-field point, the correlation functions are still dominated by excitations without bound states and by states that only have two-strings. Apart from a few anomalous symmetric configurations, configurations with higher strings give only negligible contributions.

In the isotropic regime, it should also be noted that bound states which have deviated from their string-hypothesis shape give an important contribution, at least at the chain lengths accessible to this method.
Figure 4.7: Absolute value of equal-time correlation functions for the isotropic chain as a function of distance, for two values of the chain length, \( N = 200 \) and \( N = 500 \).

Table 4.4: Comparison of equal-time correlation functions \( \langle S^z_j S^z_{j+l} \rangle \) for the isotropic chain \( \Delta = 1 \) at zero field for small distances \( l \in \{1 \ldots 7\} \). The left column gives the distance between the two sites. The second column gives the exact value obtained from the polynomial representation (the numbers in square brackets are references to the papers in question). The third column gives results found by summing form factors on \( N = 500 \) sites, with a sum rule saturation of rule to 99.09\%, whereas the fourth column corresponds to form factor results for a chain of \( N = 200 \) sites, achieving sum rule saturation to 99.54\%.

<table>
<thead>
<tr>
<th>( l )</th>
<th>( S^z_{p} )</th>
<th>( S^z_{N=500} )</th>
<th>( S^z_{N=200} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.14771572685 [96]</td>
<td>-0.1468136115</td>
<td>-0.1473014000</td>
</tr>
<tr>
<td>2</td>
<td>0.06067976996 [97]</td>
<td>0.0608307920</td>
<td>0.0607489482</td>
</tr>
<tr>
<td>3</td>
<td>-0.05024862726 [98]</td>
<td>-0.0499557263</td>
<td>-0.0501865200</td>
</tr>
<tr>
<td>4</td>
<td>0.03465277698 [99]</td>
<td>0.0345879961</td>
<td>0.0346686176</td>
</tr>
<tr>
<td>5</td>
<td>-0.03089036665 [100]</td>
<td>-0.0308175221</td>
<td>-0.0309084391</td>
</tr>
<tr>
<td>6</td>
<td>0.02444673833 [101]</td>
<td>0.0244777086</td>
<td>0.0244682130</td>
</tr>
<tr>
<td>7</td>
<td>-0.02249822276 [101]</td>
<td>-0.022458141</td>
<td>-0.0225365414</td>
</tr>
</tbody>
</table>

Table 4.5: Comparison of equal-time correlation functions \( \langle S^a_j S^a_{j+l} \rangle \) at zero field for \( \Delta = 0.75 \) for small distances \( l \in \{1, 2, 3\} \). The left column gives the distance between the two sites. Subscript \( p \) refers to the exact polynomial representation following [102, 103, 104], whereas \( N=200 \) refers to our results obtained by summing form factors for a chain of \( N = 200 \) sites, achieving sum rule saturation to 98.73\% (\( S^{zz} \)) and 98.89\% (\( S^{-+} \)).

<table>
<thead>
<tr>
<th>( l )</th>
<th>( S^a_{p} )</th>
<th>( S^a_{N=200} )</th>
<th>( S^{-+}_{p} )</th>
<th>( S^{-+}_{N=200} )</th>
</tr>
</thead>
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<td>-0.305461</td>
<td>-0.304906</td>
</tr>
<tr>
<td>2</td>
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<td>0.043427</td>
<td>0.140331</td>
<td>0.140553</td>
</tr>
<tr>
<td>3</td>
<td>-0.035605</td>
<td>-0.035911</td>
<td>-0.117158</td>
<td>-0.117201</td>
</tr>
</tbody>
</table>
Chapter 4. Dynamical correlations in finite chains

Table 4.6: Comparison of equal-time correlation functions $\langle S^a_j S^\bar{a}_{j+1} \rangle$ at zero field for $\Delta = 0.25$ for small distances $l \in \{1, 2, 3\}$. The left column gives the distance between the two sites. Subscript $p$ refers to the exact polynomial representation following [102, 103, 104], whereas $N=200$ refers to our results obtained by summing form factors for a chain of $N = 200$ sites, thereby achieving saturation of the sum rule to 99.88% ($S^{zz}$) and 95.61% ($S^{-+}$).

<table>
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<tr>
<th></th>
<th>$S^z_p$</th>
<th>$S^z_{ff}$</th>
<th>$S_p^{-+}$</th>
<th>$S_{ff}^{-+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.113489</td>
<td>-0.113337</td>
<td>-0.316807</td>
<td>-0.311455</td>
</tr>
<tr>
<td>2</td>
<td>0.012979</td>
<td>0.012961</td>
<td>0.180965</td>
<td>0.180967</td>
</tr>
<tr>
<td>3</td>
<td>-0.016396</td>
<td>-0.016397</td>
<td>-0.152364</td>
<td>-0.152466</td>
</tr>
</tbody>
</table>

Table 4.6: Comparison of equal-time correlation functions $\langle S^a_j S^\bar{a}_{j+1} \rangle$ at zero field for $\Delta = 0.25$ for small distances $l \in \{1, 2, 3\}$. The left column gives the distance between the two sites. Subscript $p$ refers to the exact polynomial representation following [102, 103, 104], whereas $N=200$ refers to our results obtained by summing form factors for a chain of $N = 200$ sites, thereby achieving saturation of the sum rule to 99.88% ($S^{zz}$) and 95.61% ($S^{-+}$).
5. The thermodynamic limit

In this chapter we discuss the infinite isotropic Heisenberg chain. This limit was first studied by Hultén [96], who derived its ground state energy. Much later, des Cloizeaux and Pearson [105] found the spinon excitation spectrum. Other thermodynamic properties were found shortly thereafter [106, 42, 107, 108, 109, 47]. The approach to the dynamical structure factor in the infinite chain is completely different and complementary to the approach we have discussed for the finite chain. In the first sections, we will introduce some background on the thermodynamic Bethe ansatz approach, after which we go on to the calculation of dynamical structure factors in this approach.¹

5.1 The thermodynamic Bethe ansatz

In the thermodynamic limit, we let the chain length go to infinity while keeping the magnetisation constant. Thus, the number of down spins increases with the chain length. For the quantum numbers we now define the parameter $x := I/N$. Defining particles and holes as before, as quantum number positions that are occupied/unoccupied where they are not in the ground state, we must now define particle $\rho$ and hole $\bar{\rho}$ densities, such that $\rho + \bar{\rho} = 1$,

\[\rho(x) = \frac{1}{N} \sum_{l \in \{I\}} \delta(x - l/N) \quad \bar{\rho}(x) = \frac{1}{N} \sum_{m \not\in \{I\}} \delta(x - m/N) \quad (5.1)\]

The Bethe equations for the isotropic Heisenberg chain become

\[\theta_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' \theta_2(\lambda - \lambda')\rho(\lambda') = 2\pi x(\lambda), \quad (5.2)\]

¹This work was done in collaboration [110] with Jean-Sébastien Caux.
Taking the derivative of (5.2) with respect to the rapidity $\lambda$, we get the equation
\[
a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda')\rho(\lambda') = \rho(\lambda) + \bar{\rho}(\lambda),
\]
(5.3)

5.1.1 Ground state rapidity distribution

Knowing that for all $N$ in the finite chain, in the ground state all quantum number positions are filled in an uninterrupted interval symmetric around the origin, we set $B$ as the boundaries of the rapidity distribution in the ground state: within the interval $|\lambda| < B$, the hole density $\bar{\rho}$ vanishes; without, the particle density $\rho$ vanishes. This way, Hulthén [96] found the equation for the ground state density $\rho_0$ in the isotropic model in zero field; in general, it reads
\[
\rho_0(\lambda) + \int_{-B}^{B} d\lambda' a_2(\lambda - \lambda')\rho(\lambda') = a_1(\lambda),
\]
(5.4)
with the magnetisation given by
\[
\int_{-B}^{B} d\lambda \rho_0(\lambda) = M/N.
\]
(5.5)

This can be solved numerically or, in the isotropic case for zero field, where $B \to \infty$, analytically by Fourier transformation. Taking the following convention for the Fourier transform,
\[
\tilde{\rho}(\omega) = \int_{-\infty}^{\infty} d\lambda e^{i\omega\lambda} \rho(\lambda) \quad \rho(\lambda) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\lambda} \tilde{\rho}(\omega)
\]
(5.6)
and using the convolution theorem, the expression for the ground state density becomes
\[
\rho_0(\lambda) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\tilde{a}_1(\omega)}{1 + \tilde{a}_2(\omega)},
\]
(5.7)
As $\tilde{a}_n(\omega) = e^{-n|\omega|}$, this gives $\rho_0(\lambda) = \frac{1}{4 \cosh(\pi \lambda)}$.

5.1.2 Energy

The energy of a state described by the density $\rho(\lambda)$ is
\[
E = -J |\phi_2| \pi \int_{-\infty}^{\infty} \rho(\lambda) d\lambda a_1(\lambda) - h(N/2 - M)
\]
(5.8)
With the ground state solution $\rho_0(\lambda)$ this yields Hulthén’s value for the ground state energy density of the infinite chain,
\[
E_0/N = -J (\log 2 - \frac{1}{4})
\]
(5.9)
5.2 Spinons

In the finite chain, we generated particle–hole pairs by removing a quantum number from the ground state interval and replacing it outside of the interval. The analogue of this in the thermodynamic limit, removing a particle at \( \bar{J} \) and putting it at \( J \), yields the distribution

\[
\rho(x) = \rho_0(x) + \frac{1}{N} \delta(x - J/N) - \frac{1}{N} \delta(x - \bar{J}/N) \tag{5.10}
\]

\[
\bar{\rho}(x) = \bar{\rho}_0(x) - \frac{1}{N} \delta(x - J/N) + \frac{1}{N} \delta(x - \bar{J}/N) \tag{5.11}
\]

The density as a function of the rapidities, with particle rapidity \( \mu \) and hole rapidity \( \bar{\mu} \), is then

\[
\rho(\lambda) = dx(\lambda) \rho_0(\lambda) + \frac{1}{N} \delta(\lambda - \mu) - \frac{1}{N} \delta(\lambda - \bar{\mu}) \tag{5.12}
\]

The response of the density to the introduction of the particle–hole pair is encoded in the backflow function,

\[
K(\lambda; \mu, \bar{\mu}) := N \rho_0(\lambda) \left[ \frac{dx(\lambda)}{dx_0(\lambda)} - 1 \right], \tag{5.13}
\]

so that the equation for the density becomes

\[
\rho(\lambda) = \rho_0(\lambda) + \frac{1}{N} \left[ K(\lambda; \mu, \bar{\mu}) + \delta(\lambda - \mu) - \delta(\lambda - \bar{\mu}) \right] \tag{5.14}
\]

Subtracting integral equation 5.3 applied to the ground state from same applied to the particle–hole state, we get an equation for the backflow function

\[
K(\lambda; \mu, \bar{\mu}) + \int_{-B}^{B} d\lambda' a_2(\lambda - \lambda') K(\lambda'; \mu, \bar{\mu}) = -a_2(\lambda - \mu) + a_2(\lambda - \bar{\mu}) \quad \text{for } \lambda \in [-B, B]
\]

\[
K(\lambda; \mu, \bar{\mu}) = 0 \quad \text{for } \lambda \notin [-B, B].
\]

Following [111], this equation can be inverted if we define the even function \( b_2(\lambda - \lambda') \) such that

\[
\int d\lambda' \left[ \delta(\lambda - \lambda') + b_2(\lambda - \lambda') \right] \left[ \delta(\lambda' - \bar{\lambda}) + a_2(\lambda' - \bar{\lambda}) \right] = \delta(\lambda' - \bar{\lambda}) \tag{5.16}
\]

Applying (5.16) on both sides of (5.15), we get the expression

\[
K(\lambda; \mu, \bar{\mu}) = -a_2(\lambda - \mu) - \int_{-B}^{B} d\lambda' b_2(\lambda - \lambda') a_2(\lambda' - \mu) - b_2(\lambda - \bar{\mu}). \tag{5.17}
\]
Chapter 5. The thermodynamic limit

The energy and momentum of a particle–hole state with respect to the ground state are given by

\[
\omega := E - E_0 = \epsilon_0(\mu) - \epsilon_0(\bar{\mu}) + \int_{-B}^{B} d\lambda \, \epsilon_0(\lambda) K(\lambda; \mu, \bar{\mu}) \tag{5.18}
\]

\[
k := K - K_0 = -\phi_1(\mu) + \phi_1(\bar{\mu}) - \int_{-B}^{B} d\lambda \, \phi_1(\lambda) K(\lambda; \mu, \bar{\mu}) \pmod{2\pi}, \tag{5.19}
\]

where \(\epsilon_0(\lambda) := h - \pi J a_1(\lambda) \sin \zeta\) is the energy of a bare magnon.

If we now define the particle energy

\[
\epsilon(\lambda) := \epsilon_0(\lambda) + \int_{-B}^{B} d\lambda' \, b_2(\lambda - \lambda') \epsilon_0(\lambda') \tag{5.20}
\]

we see that the energy and momentum with respect to the ground state of the mode with particle \(\lambda\) and hole \(\bar{\lambda}\) are given by an expression that strongly suggests two independent excitations, called \textit{spinons}, that always show up in pairs:

\[
\omega = \epsilon(\mu) + \epsilon(\bar{\mu}) \tag{5.21}
\]

\[
k = k(\mu) + k(\bar{\mu}) \pmod{2\pi}. \tag{5.22}
\]

At zero field, the spinon energy and momentum are given by

\[
\epsilon(\mu) = \frac{\pi J}{2} |\sin k(\mu)| \tag{5.23}
\]

\[
k(\mu) = \pi + \theta_1(\mu), \tag{5.24}
\]

which defines a dispersion relation \(\epsilon(k)\).

### 5.2.1 Two-spinon continuum

The boundaries of the region in energy space reached at a given momentum are found as follows. By symmetry, we need only consider \(0 \leq k_1 + k_2 < \pi\). This means, in particular, that both spinon momenta are in \([0, \pi)\), and hence the energy can be written

\[
\omega = \pi \sin \frac{k_1 + k_2}{2} \cos \frac{k_1 - k_2}{2}. \tag{5.25}
\]

We see that the energy is minimised if \(k_1 - k_2\) is maximised, and maximised if it equals zero. Therefore, the \textit{two-spinon continuum} is given by

\[
\frac{\pi}{2} |\sin k| =: \omega_{2l} \leq \omega \leq \omega_{2u} := \pi \sin k/2. \tag{5.26}
\]

The two-spinon continuum is shown in figure 5.2. The lower boundary of this continuum, which is by construction the lowest-lying excitation of the model, is called the \textit{des Cloizeaux–Pearson mode} [105].
5.2. Spinons

5.2.2 Completeness of spinons

The spinon picture is rigorous in the thermodynamic limit. It is conjectured that multiple-spinon states completely span the Hilbert space [112, 58, 113, 89], diagonalising the Hamiltonian as

$$H |\{\xi\}\rangle_{\{\sigma\},i} = \sum_{j=1}^{n} \epsilon(\xi_j) |\{\xi\}\rangle_{\{\sigma\},i}, \quad (5.27)$$

for a finite number $n$ of spinons. Here $\xi$ is a spectral parameter associated to each spinon. Spinons are spin-$\frac{1}{2}$ particles; their spin is labelled by the $\sigma = \pm$. In fact a spinon can be identified [112, 58] with a kink in the spin distribution: in the limit of infinite distance, it connects the Néel state with up spins on the A sublattice to that with up spins on the B sublattice. This is the reason they only show up in pairs on an even periodic chain. The two values for the index $i$ correspond to two choices for the up sublattice that are available for every configuration of an even number of kinks.

The completeness relation for the spinon basis is conjectured by Jimbo and Miwa [89] to be

$$1 = \sum_{n \geq 0} \sum_{i,\{\sigma\}} \frac{1}{n!} \oint \frac{d\xi_1}{2\pi i \xi_2} \cdots \frac{d\xi_n}{2\pi i \xi_2} |\{\xi\}\rangle_{\{\sigma\},i} \langle \{\xi\}|, \quad (5.28)$$

where the unit circle is the contour for the integral.

Thus, every state can be described by its spinon content, completely ignoring the presence or absence of bound states. This decomposition is rather surprising in the light of what we know about the finite chain. It indicates that the energy associated to bound states must go to zero as $1/N$. This is the case if the number of higher strings remains finite while the number $M_1$ of real rapidities goes to infinity with $N$. However, if the higher-string content is macroscopic, it is hard to see how their energy can vanish.

In the finite chain, for a given momentum, the lowest excitations form a group of four: a $S = 1$ triplet, given by the state with $M - 1$ finite real rapidities and one infinite rapidity (at $S^z = 0$), the states with $M - 1$ real rapidities ($S^z = \pm \frac{1}{2}$) and the corresponding state with $M + 1$ down spins, which has $S^z = -\frac{1}{2}$ and is only reachable by the Bethe ansatz starting from the all-down reference state; and a $S = 0$ singlet, consisting of the state with $M - 2$ finite real rapidities and a two-string at zero. As the string rapidity goes to zero, these excitations all get the same energy; they form two doublets represented by two spin-$\frac{1}{2}$ spinons. Thus the $S = 0$ state must be identified with an antisymmetric spinon–antispinon superposition while the $S = 1$ state equals the symmetric superposition.

5.2.3 Four-spinon continuum

Let us give special attention to the four-spinon continuum, mainly because it has been misidentified in the literature [114, 115] and because a correct description of
Chapter 5. The thermodynamic limit

the continuum is important for the calculation of the dynamical structure factor. Again, we need only consider \(-\pi \leq k_1 + k_2 + k_3 + k_4 < 0\), and each \(k_n \in [-\pi, 0]\). However, since we're adding four momenta, there are two ways to end up in the interval \([-\pi, 0]\) modulo \(2\pi\). Define sectors \(m = 0\) and \(m = 1\) by

\[
2\pi m = k + \sum_{n=1}^{4} k_n
\] (5.29)

(note that this equation should not be taken modulo \(2\pi\)).

We change variables to a more physical notation of internal \((k, \omega)\) and external \((K, \Omega)\) momenta and energies, i.e.,

\[
K := -k_1 - k_2
\]

\[
\Omega := -\frac{\pi}{2} (\sin k_1 + \sin k_2)
\] (5.31)

We then have \(K = k + k_3 + k_4 + 2\pi m\), and the transformation can be written out in full as

\[
k_1 = -\frac{K}{2} + \acos \frac{\Omega}{\omega_{2u}(K)}
\]

\[
k_2 = -\frac{K}{2} - \acos \frac{\Omega}{\omega_{2u}(K)}
\] (5.32)

\[
k_3 = -\pi m + \frac{K - k}{2} + \acos \frac{\omega - \Omega}{\omega_{2u}(k - K)}
\]

\[
k_4 = -\pi m + \frac{K - k}{2} - \acos \frac{\omega - \Omega}{\omega_{2u}(k - K)}
\]

The four-spinon continuum is the area in \((k, \omega)\) space that we can reach if we let the internal energy and momentum take on all their allowed values. This can be represented graphically by taking two two-spinon continua, one turned upside down, which are displaced by the external momentum and energy \((k, \omega)\). The logic is here that the external four-spinon momentum must internally be carried by two two-spinon pairs, which can only take energy–momentum values within the two-spinon continuum. Therefore, we can find the four-spinon continuum by analysing the intersections of the boundaries of the two two-spinon continua. As a bonus, we will get information about the shape of the intersection of the continua themselves, which is extremely useful when calculating structure factors (see section 5.3). This procedure is illustrated in figure 5.1.

Lowering the upside-down continuum from above, we see that a given momentum \(k\) has a solution from the moment the upper boundaries cross until the moment the lower boundaries cross. Although crossings of upper boundaries with lower boundaries do influence the shape of the overlap, they do not alter the region in \(k\)-space for which solutions exist. Therefore, we only need to know the intersection of upper boundary with upper boundary and of lower boundary with lower boundary. The former gives the equation

\[
2\pi |\sin K_u/2| = \omega - 2\pi |\sin K_u/2|.
\] (5.33)
In the region $K \in [0, 2\pi)$, this has the solutions
\[ K_{\text{au}}^\pm = \frac{k}{2} \pm 2 \cos \frac{\omega}{4\pi \sin k/4} \] \[ K_{\text{au}}^\pm \in [0, k] , \] (5.34)
existing if $2\pi \sin k/2 \leq \omega \leq 4\pi \sin k/4$; and
\[ K_{\text{bu}}^\pm = \frac{k}{2} + (1 \mp 1)\pi \pm 2 \sin \frac{\omega}{4\pi \cos k/4} \] \[ K_{\text{bu}}^\pm \in [k, 2\pi] , \] (5.35)
existing if $2\pi \sin k/2 \leq \omega \leq 4\pi \cos k/4$.

Intersections of lower boundary and lower boundary are given by the equation
\[ \pi |\sin K_l| = \omega - \pi |\sin k - K_l| . \] (5.36)

In the region $K \in [0, \pi]$—the other half Brillouin zone can be found by symmetry—this has the solutions
\[ K_{\text{al}}^\pm = \frac{k}{2} \pm \cos \frac{\omega}{2\pi \sin k/2} \quad (\text{mod } \pi) \] \[ K_{\text{al}}^\pm \in [k - \pi, k] \] (5.37)
existing if $\pi \sin k \leq \omega \leq 2\pi \sin k/2$; and
\[ K_{\text{bl}}^\pm = \frac{k}{2} \pm \sin \frac{\omega}{2\pi \cos k/2} \quad (\text{mod } \pi) \] \[ K_{\text{bl}}^\pm \in [0, k - \pi] \cup [k, 2\pi] \] (5.38)
existing if $\pi \sin k \leq \omega \leq 2\pi \cos k/2$. Figure 5.2 shows the regions in $(k, \omega)$ space in which these inequalities are satisfied. The grey area in this figure is the region in which at least one of them is satisfied; this is the four-spinon continuum.

### 5.3 Dynamical structure factor

As in the case for the finite chain, the dynamic structure factor is calculated by inserting a resolution of the identity between the two spin operators; in the thermodynamic limit, the spinon basis (5.28) is the appropriate one to insert. This gives an expression in terms of spinon form factors. Bosonisation of the quantum affine algebra [116, 117, 118, 89] of spinon creation and annihilation operators allows these to be calculated.

Thus, the dynamical structure factor is written
\[
S(k, \omega) = \sum_{n \geq 0} \frac{2\pi}{n!} \sum_{m} \frac{\pm}{i, \{\epsilon\}} \oint \frac{d\xi_1}{2\pi i \xi_1} \cdots \frac{d\xi_n}{2\pi i \xi_n} \times
\]
\[ \times e^{im(k + \sum_{j=1}^{n} k_j)} \delta(\omega - \sum_{j=1}^{n} \epsilon_j) \langle 0 | S_0^z(0) | \{\xi\} \rangle_{i, i, \{\epsilon\}} S_0^z(0) | 0 \rangle_i , \]
where the $n$th term in the $n$-sum represents the $n$-spinon contribution. The two terms $i = \pm$ are equal, so the sum can be replaced by a factor of 2.
Chapter 5. The thermodynamic limit

Figure 5.1: The integration region is given by the intersection of two two-spinon continua, one turned upside down. The displacement between the two is given by \((k, \omega)\). This leads to six classes of integration regions, each of which is illustrated here. Labelled 1–3 top left to right, 4–6 bottom left to right, they correspond to the sectors indicated in figure 5.2.

Figure 5.2: The four-spinon continuum, indicated by the grey area, including the two-spinon continuum, indicated by the dark grey area. Also shown are the six sectors that yield differently shaped integration regions. Sector 1) \(K_{\alpha u}^\pm\) exist; 2) \(K_{\alpha u}^\pm, K_{b\ell}^\pm\) exist; 3) \(K_{\alpha u}^\pm, K_{b\ell}^\pm\) exist; 4) \(K_{a\ell}^\pm\) exist; 5) \(K_{\alpha u}^\pm, K_{b\ell}^\pm, K_{b\ell}^\pm\) exist; 6) \(K_{a\ell}^\pm, K_{b\ell}^\pm\) exist.
5.3. Dynamical structure factor

5.3.1 Two-spinon contribution

The expression (5.39) is rather difficult. It has a contour integral for every spinon present in the expansion, and these contour integrals are notoriously hard to evaluate. However, the bulk of the structure factor is expected to arise from the two-spinon contribution alone, and in this case the expression becomes much simpler: there are only two contour integrals and the delta functions in (5.39), which represent conservation of energy and momentum, take care of them. This was done in [119, 120] for the isotropic chain, and in [121] for the gapped anisotropic chain. For the isotropic model, the resulting expression for the two-spinon contribution reads

\[ S_2(k, \omega) = \frac{1}{2} \frac{e^{-I(\rho(k, \omega))}}{\sqrt{\omega^2_{2u}(k) - \omega^2}} \Theta(\omega_{2u}(k) - \omega) \Theta(\omega - \omega_{2l}(k)) \],

(5.40)

where the parameter \( \rho \) is given by

\[ \cosh(\pi \rho(k, \omega)) = \sqrt{\frac{\omega^2_{2u}(k) - \omega^2_{2l}(k)}{\omega^2 - \omega^2_{2l}(k)}} \]

(5.41)

and \( I(\rho) \) is the integral

\[ I(\rho) := \int_0^\infty dt \ t^{-1} e^t \cosh 2t \cos 4\rho t - 1 \cosh t \sinh 2t \]

(5.42)

These expressions lead to a total two-spinon contribution of 72.89\% [120] of the sum rule (4.93).

A sum rule that is convenient to gauge single-momentum lineshapes of the structure factor is the first frequency moment sum rule,

\[ K_1(q) := \int_0^\infty d\omega \frac{\omega}{2\pi} S(q, \omega) = \frac{2E_0}{3N} (1 - \cos q) \],

(5.43)

where \( E_0 \) is the ground-state energy (5.9). For each value of the momentum \( k \), two-spinon states satisfy the first frequency moment sum rule to 71.30\%. An example of a two-spinon lineshape calculated this way is given in figure 5.4, where it is compared to finite-size two-spinon calculations.

Finite-size scaling

It is interesting to see what happens as we approach the thermodynamic limit with finite chains. As we have seen, four two-spinon excitations of different spin correspond to four excitations in the finite chain; of these, however, only one contributes to the structure factor. Of the total spin-one spinons, two have a spin in the z direction, i.e. the wrong number of down spins, and therefore the \( S^z \) matrix element vanishes. Spin-zero spinons correspond to states with a single two-string
whose quantum number is fixed at the origin; the contribution of these states is numerically zero. This is consistent with the fact that, by isotropy, the $S_{zz}$ form factor equals twice the $S^{-+}$ form factor; in the finite-size form factor expansion for $S^{-+}$ only the states with $S = 1$, $S^z = 0$ appear. Assuming the spinon expansion is the same in this case, this implies the $S = 0$, $S^z = 0$ states must have vanishing form factor.

The class of states corresponds to the set of states with one infinite rapidity and all other rapidities finite and real. At zero field, these are the only non-bound states to give a nonzero contribution to the structure factor. As they can be constructed by picking $N/2 - 1$ distinct quantum numbers out of a set of $N/2$, the number of such states equals $N(N + 2)/8$.

In Fig. 5.3 we compare our results for finite chains of increasing lengths to these infinite-chain results. On the left we show that contributions decrease with chain length in a way that is consistent with the limit value, although the convergence is very slow. On the right, we go to higher chain lengths (up to 8000 sites) by calculating the contribution to the first moment sum rule (5.43) at $k = \pi/5$. In the thermodynamic limit, this contribution density is 0.17229. In Fig. 5.4, on the left, the longitudinal structure factor is shown as a function of energy. The density of states, shown on the right, is virtually unchanging with system size, which shows that the dependence on chain length must be accounted for by the two-spinon transition rate.

From these graphs it is clear that, even at considerable chain lengths, finite-size effects play an important role. The approach to the thermodynamic limit is extremely slow; in terms of the field theory, it is tempting to interpret this as an effect of the logarithmic corrections due to marginal operators that appear in the
5.3. Dynamical structure factor

Dynamical structure factor

\[ S^{(2)}(\pi/5, \omega) \]

\[ D^{(2)}(\pi/5, \omega) \]

**Figure 5.4:** Two-spinon contribution to longitudinal structure factor at zero field, at \( k = \pi/5 \). The inset magnifies a region of the plot to show more clearly the slow convergence of the finite-size curves to the limit curve. (Since the contributing states are all in the same family, their energies form a smooth curve. Hence, instead of using the delta function smoothing 4.97 to get a smooth curve, we scaled all data points by the density of peaks and interpolated. This has the advantage that it leaves the sharp lower edge as it is.)

zero-field isotropic model. To find out whether this is the case, a similar study should be made of the two-spinon excitations in the anisotropic chain, where such marginal operators are absent.

It should be noted, however, that the two-spinon contribution is not a physical quantity; the full dynamical structure factor is. Therefore, these results do not necessarily imply that physically observable quantities have such a slow dependence on system size. For instance, while this shows that the contribution to the structure factor due to more-spinon intermediate states is lower in shorter chains, this contribution lies to a large extent within the two-spinon continuum. Higher-spinon contributions are only clearly distinguishable as such if they lie above the lower-spinon continuum. In that region, however, the total contribution is very low.

5.3.2 Four-spinon contribution

It is much more difficult to get a manageable expression for the four-spinon contribution. The problem was attacked in [122, 123], in which an expression for the dynamical structure factor was derived in terms of a double integral over an infinite series. In a later article [124] it was attempted to derive some of the properties of the four-spinon contribution; however, in this work the four-spinon continuum was misidentified as the periodicity of \( k \)-space was not correctly taken into account.

As a result, further attempts to numerically calculate the four-spinon contribution [123, 124, 114] did not produce satisfactory results; in particular the contribution to the sum rule was estimated to be between 1% and 2.5% [115], which is quite
inconsistent with the picture of a series expansion in spinons. With a correct identification of the four-spinon continuum, however, and with improved numerics, the figure becomes a much more credible 27%, as we will now show.

As shown in [123] (up to a few errors corrected in [110], the four-spinon contribution to the dynamical structure factor is given by

\[
S_4(k, \omega) = C_4 \int_{-\pi}^{0} dk_1 \cdots dk_4 \delta[(k + \sigma_i k_i) \text{mod} 2\pi] \delta[\omega + \sum_i \epsilon(k_i)] J(\{k\}),
\]

where the prefactor is

\[
C_4 = 3^{-1} 2^{-9} \Gamma(\frac{1}{4})^{-8} A(\frac{i\pi}{2})^{-8}
\]

with

\[
A(z) := \exp \left[ - \int_0^\infty dt t^{-1} e^{t \sinh^2 \left[ t(1 + iz/\pi) \right]} \frac{\sinh 2t \cosh t}{\sinh 2t} \right].
\]

The correlation weight \( J(\{p\}) \) is

\[
J(\{p\}) := e^{-\sum_{i<j}^4 t(p_i - p_j)} \sum_{l=1}^4 |g_l(\{p\})|^2,
\]

with the momentum parameter \( \rho \) given by \( \cot \rho_i = \sinh 2\pi \rho_i \); \( g_l \), at its turn, is given by

\[
g_l = (-1)^{l+1} \sum_{j=1}^4 \cosh 2\pi \rho_j \sum_{m=\Theta_-(j-l)}^{\infty} \prod_{i \neq j} \Gamma(m - \frac{1}{2} + i \rho_{ji}) \prod_{i=1}^4 \frac{\Gamma(m - \frac{1}{2} + i \rho_{ji})}{\Gamma(m + 1 + i \rho_{ji})}.
\]

Note that we use a nonstandard step function given by \( \Theta_-(n) = 0 \) if \( n \leq 0 \), \( \Theta_-(n) = 1 \) if \( n > 0 \).

In terms of the physical variables \( k, \omega, K, \Omega \) and the integration domain \( D(k, \omega) \) defined in subsection 5.2.3, the four-spinon contribution to the structure factor can now be written

\[
S_4(k, \omega) = \int_{D(k, \omega)} dKd\Omega \frac{J(k, \omega; K, \Omega)}{\sqrt{\omega_{2u}(K - \Omega)^2 (\omega_{2u}^2 (k - K) - (\omega - \Omega)^2)}}
\]

The integral can now be evaluated numerically, using a Romberg method (see e.g. [64]) in which the integration region is successively, recursively, and adaptively split into three sections. Divergencies show up at the boundary of the integration region, which can be dealt with by transformations of variables—this is one reason why it is important to know the integration domain exactly. In figure 5.5 some results are shown for the four-spinon contribution at various values of the external momentum.
5.4. The Müller ansatz

The Müller ansatz is a phenomenological approximation to the correlation function of the Heisenberg chain that has been of great value to experimental physicists, due
Figure 5.6: The two- and four-spinon parts of the dynamical structure factor at momenta $k = \pi/4$, $k = \pi/2$, $k = 3\pi/4$, and $k = \pi$.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$K_1^{2\text{-sp}}(q)$</th>
<th>$K_1^{4\text{-sp}}(q)$</th>
<th>$K_1^{2+4\text{-sp}}(q)$</th>
</tr>
</thead>
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<tr>
<td>$\pi/8$</td>
<td>71.30%</td>
<td>27.2%</td>
<td>98.5%</td>
</tr>
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<td>71.30%</td>
<td>27.3%</td>
<td>98.6%</td>
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<tr>
<td>$3\pi/8$</td>
<td>71.30%</td>
<td>27.3%</td>
<td>98.6%</td>
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<tr>
<td>$\pi/2$</td>
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<td>98.4%</td>
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<tr>
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<td>97.8%</td>
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<td>97.5%</td>
</tr>
<tr>
<td>$7\pi/8$</td>
<td>71.30%</td>
<td>25.9%</td>
<td>97.2%</td>
</tr>
<tr>
<td>$\pi$</td>
<td>71.30%</td>
<td>26.6%</td>
<td>97.9%</td>
</tr>
</tbody>
</table>

Table 5.1: Relative contribution of two- and four-spinon intermediate states in terms of the first frequency-moment sum rule (5.43) for various values of momentum, to an accuracy of about 1% of the value shown. The two-spinon contribution is always 71.30%, so that the values shown here, being all around 27%, account for most of the leftover weight, as expected. The third column gives the sum rule contribution of two- and four-spinon states combined.
to the lack of exact results and the fact that it is very simple. It was developed by Müller, Bonner and others [125, 85] on the basis of exact results in the XY (free-fermion) model [88], the two-spinon structure factor as and numerical computations on small chains, and is constructed in such a way as to satisfy the sum rules.

The Müller ansatz approximation to the structure factor is

$$S_M(q, \omega) = \frac{\Theta(\omega - \omega_{21}) \Theta(\omega_{2u} - \omega)}{\sqrt{\omega^2 - \omega_{21}^2}}. \quad (5.50)$$

The step functions guarantee that this expression only has contributions in the two-spinon region. Near and above the two-spinon upper boundary it does not catch the correct behaviour of the structure factor: obviously, it misses out on any of the four-spinon signal above the two-spinon boundary; it also shows a sharp cutoff at that boundary instead of the square-root cusp. In general, however, this approximation does remarkably well in capturing the overall shape of the contribution. One reason for this is that, as we have shown, higher-spinon excitations contribute mostly in the two-spinon region.

5.5 Discussion

Provided one takes into account the correct shape of the four-spinon continuum, it is possible to calculate the four-spinon part of the dynamical structure factor of the zero-field isotropic Heisenberg model in the thermodynamic limit. It turns out that its contribution is most important within the two-spinon continuum, but it falls of smoothly at the upper edge.

A comparison of two-spinon contributions in finite chains of different length to that in the thermodynamic limit shows that the distribution of contributions varies
significantly but very slowly with increasing \( N \). Consequently, even chains of very large length (thousands of sites) cannot be considered to be thermodynamic in this respect.
The structure factor at low momentum

At low momentum, a completely different approach is available to describe the excitations of the system. In this region, the two-spinon continuum approaches a linear dispersion relation; this observation can be used to construct an effective bosonic field theory for the excitations in this region, a method known as bosonis-ation. This field theory can then be used to gain an analytic understanding of the structure of the structure factor at low momentum as computed from the Bethe ansatz. Specific features of the dynamical structure factor that have been addressed are the width of the two-spinon peak and the tail of the structure factor at high energies.

6.1 Field theory setup

The construction of a bosonic field theory for the Heisenberg chain is explained in e.g. [5, 127]. One starts with a map of the spin raising and lowering operators to spinless fermion creation and annihilation operators. The dispersion relation is then linearised around the Fermi points and the continuum limit is taken. The particle–hole excitations of the linear fermion theory are then represented as boson fields. The construction is based on the free-fermion limit. Afterwards, interactions can be treated as renormalisations and perturbations. This is the theory of the Luttinger liquid, developed by Haldane [128, 129, 130] on the basis of the ideas of Luther and Emery [131] and Efetov and Larkin [132].

We first give a short overview and try to establish a consistent notation for the scope of this chapter. Then, we compare a proposed field-theory description of...
some features of the structure factor to Bethe ansatz results calculated by the methods of chapter 4.

6.1.1 Fermion model

A fermion interpretation comes naturally for a spin-1/2 lattice: the fact that only two states are possible on each site is reminiscent of the Pauli exclusion principle. In the context of the coordinate Bethe ansatz we thought of the state with all spins down as a vacuum and of up spins as particles. However, spins on different sites commute, whereas fermions anticommute, so it is not obvious how to make this analogy rigorous. The solution is to introduce an operator that keeps track of fermion exchanges and compensates for the sign: the Jordan–Wigner string. This leads to the Jordan–Wigner transformation [133]

\[
S_j^+ = : \psi_j^\dagger e^{i\pi \sum_{i<j} \psi_i^\dagger \psi_i} \quad S_j^- = : e^{-i\pi \sum_{i<j} \psi_i^\dagger \psi_i} \psi_j \quad S_j^z = : \psi_j^\dagger \psi_j - \frac{1}{2} .
\]

(6.1)

where the operators \( \psi^\dagger \), \( \psi \) have regular fermionic anticommutation relations. The Jordan–Wigner string is a nasty thing; consequently, this transformation would not be very successful in treating Heisenberg chains if not for the fact that the strings attached to adjacent sites cancel. Indeed, on a higher-dimensional lattice or on a lattice with next-nearest neighbour interactions this transformation is not nearly as useful as in the present case.

Let us first look at the limit \( \Delta \to 0 \). In the spin language, this is called the XX0 model, which is the isotropic case of the XY model [12]. In the fermion language, the XX0 Hamiltonian reads

\[
H_0 := J \sum_j \frac{1}{2} (\psi_{j+1}^\dagger \psi_j + \psi_j^\dagger \psi_{j+1}) - h \psi_j^\dagger \psi_j ,
\]

(6.2)

i.e. it is a model of fermions that hop to an adjacent site with probability amplitude \( J \). The magnetic field takes the role of a chemical potential. In zero field, the symmetry between up and down spins translates to a particle–hole symmetry. This is a free-fermion model (the tight-binding model) which can be readily diagonalised by a lattice Fourier transformation \( \psi_k := \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{iak_j} \psi_j \), leading to

\[
H_0 = \sum_{n=1}^N (J \cos aq_n - h) \psi_q^\dagger \psi_q ,
\]

(6.3)

with \( aq_n = 2\pi n/N \) and the lattice spacing is given by \( a \). The Fermi points are at \( \pm k_F \) with \( ak_F = \cos(-h) \); at zero field this is \( ak_F = \pi/2 \).

We take the continuum limit \( N \to \infty \), \( a \to 0 \) such that the length \( L := Na \) is constant; the Brillouin zone becomes the full real line, \( q_n = 2\pi n/L \). To prevent notational overload we will write the mode indices as function values. We concentrate
6.1. Field theory setup

on the excitations of lowest energy: the particle–hole excitations close to the left and right Fermi points. These excitations are called left (−) and right (+) movers, respectively. With a momentum cutoff Λ, and momentum expanded around the Fermi points, the Hamiltonian becomes

\[ H_0 \approx -Ja \left( \sum_{|q-k_F|<\Lambda} (q-k_F) \psi_q^\dagger \psi_q - \sum_{|q+k_F|<\Lambda} (q+k_F) \psi_q^\dagger \psi_q \right) \]

\[ =: v \sum_{|k|<\Lambda} k \left[ \psi_+^\dagger (k) \psi_+(k) - \psi_-^\dagger (k) \psi_-(k) \right] , \]

where \( v = Ja \) is the Fermi speed.

The next step is to identify these low-energy excitations with those of a model with strictly linear excitations, given by the Hamiltonian above but with the momentum sum running over full \( k \)-space.

In real space, the Hamiltonian takes the form of free Dirac fermions on a circle (the Luttinger model [134]),

\[ H_0 = v \int_0^L dx \psi_+^\dagger (x)i\partial_x \psi_+(x) - \psi_-^\dagger (x)i\partial_x \psi_-(x) . \]

6.1.2 Bosonisation

The idea behind bosonisation is to represent the particle–hole excitation, which is created by two fermionic operators, as a single boson. More precisely, with a particle–hole excitation created by the fermion current operator

\[ J_\mp (q) := \sum_k \psi_\mp^\dagger (k+q) \psi_\mp (k) , \]

the following operators, defined for \( q \neq 0 \),

\[ b_q^\dagger = \sqrt{\frac{2\pi}{L |q|}} \sum_k \left[ \Theta(-q) \psi_-^\dagger (k+q) \psi_- (k) + \Theta(q) \psi_+^\dagger (k+q) \psi_+ (k) \right] \]

\[ b_q = \sqrt{\frac{2\pi}{L |q|}} \sum_k \left[ \Theta(-q) \psi_-^\dagger (k-q) \psi_- (k) + \Theta(q) \psi_+^\dagger (k-q) \psi_+ (k) \right] \]

have bosonic commutation relations \([b_q^\dagger, b_{q'}] = \delta_{q,q'}\). Amazingly, as was shown by Haldane [129], these bosonic operators completely span the Fock space of the one-dimensional fermion.

The real-space expression is usually given in terms of the fields

\[ \varphi (x) = -\frac{\pi}{L} \left( (m_+ + m_-)x + i \sum_{q \neq 0} \sqrt{\frac{L |q|}{2\pi}} \frac{e^{-a|q|/2-ix}}{q} \left( b_q^\dagger + b_{-q} \right) \right) \]

\[ \vartheta (x) = \frac{\pi}{L} \left( (m_+ - m_-)x + i \sum_{q \neq 0} \sqrt{\frac{L |q|}{2\pi}} \frac{e^{-a|q|/2-ix}}{|q|} \left( b_q^\dagger - b_{-q} \right) \right) . \]
where \( m_\mp \) are the numbers of left- and right-moving fermions in excess of the ground state. The fermion operator can be expressed in terms of these fields by the bosonisation identity

\[
\psi_\mp(x) = U_\mp \lim_{a \to 0} (2\pi a)^{-1/2} e^{i x (k_F - \pi/L)} e^{-i [\varphi(x) - \vartheta(x)]},
\]

(6.12)

where the Klein factor \( U_\mp \), which accounts for the anticommutation of different fermion species, is for us of no further importance. Note that in terms of the boson operators \( b^\dagger, b \) this expression is a product of coherent-state operators [135]. This rather magical identity is a consequence of the commutation relation

\[
[J_\mp(q), \psi_\mp(x)] = -e^{iqx} \psi(x),
\]

which is easily derived.

Since the fermion operators, which fully describe the system, are given by exponentials of the boson fields \( \varphi(x), \vartheta(x) \), the latter take their value on a unit circle and satisfy the quasiperiodic boundary conditions

\[
\varphi(L) = \varphi(0) - \pi(m_+ + m_-) \quad \vartheta(L) = \vartheta(0) + \pi(m_+ - m_-)
\]

(6.13)

with \((m_+ + m_-)\) and \((m_+ - m_-)\) playing the role of winding numbers.

Applying the bosonisation identity (6.12) after the the Jordan–Wigner transformation (6.1), we find for the spin operators at \( x = ja \)

\[
S^z(x) := \frac{S^z_j}{a} = -\frac{\partial_x \varphi(x)}{\pi} + \frac{\cos(2\varphi(x) - 2k_F x)}{\pi a} + \cdots
\]

(6.14)

\[
S^+(x) := \frac{S^+_j}{\sqrt{a}} = \frac{e^{-i\vartheta(x)}}{\sqrt{2\pi a}} [(-1)^x + \cos(2\varphi(x))] + \cdots
\]

(6.15)

\[
S^-(x) := \frac{S^-_j}{\sqrt{a}} = \frac{e^{i\vartheta(x)}}{\sqrt{2\pi a}} [(-1)^x + \cos(2\varphi(x))] + \cdots
\]

(6.16)

Perhaps even more surprising than the bosonisation identity (6.12) is the expression of the Hamiltonian in terms of the boson fields: it is simply a free-boson Hamiltonian

\[
H_0 = \frac{v}{2\pi} \int dx \ (\partial_x \vartheta)^2 + K^{-1}(\partial_x \varphi)^2.
\]

(6.17)

This is known as the Luttinger liquid Hamiltonian, as it is the basis of Luttinger liquid theory, which is to one-dimensional fermions as Fermi liquid theory is to higher-dimensional fermions. The parameter \( K \) is known as the Luttinger parameter. For the free theory it equals \( K = 1 \); however, as we will see in the next section, interactions will give different relative weights to the two terms in the Hamiltonian, which renormalises \( K \) and \( v \).

This is quite nontrivial, but most easily seen by considering the commutation relation \([b_q, H_0] = vq b_q\) which implies that \( H_0 \), up to operators commuting with \( b_q \), must be of the form \( v \sum_{q \neq 0} |q\rangle b^\dagger_q b_q \).
Indeed, in terms of the operators $b, b^\dagger$, the Luttinger liquid Hamiltonian (6.17) can be written

$$H_0 = \frac{v\pi}{2L} \left[ K(m_+ - m_-)^2 + K^{-1}(m_+ + m_-)^2 \right]$$

$$+ \frac{v}{4} \sum_{q \neq 0} |q| \left( \frac{b_q^\dagger}{b_{-q}} \right) \cdot \left( \frac{K^{-1} + K}{K^{-1} - K} \right) \left( \frac{b_q}{b_{-q}} \right).$$

For $K = 1$, the sum over boson operators equals the above simple form; for non-unity $K$ it can be brought onto this form by Bogolyubov transformation

$$\begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} := \begin{pmatrix} \cosh \gamma/2 & \sinh \gamma/2 \\ \sinh \gamma/2 & \cosh \gamma/2 \end{pmatrix} \begin{pmatrix} b_q \\ b_{-q}^\dagger \end{pmatrix},$$

where $\gamma := -\log K$. Thus the ground state of this Hamiltonian is the vacuum of Bogolyubov quasiparticles $c, c^\dagger$.

### 6.1.3 Interaction terms

We are now ready to consider the interaction term induced by a nonzero anisotropy $\Delta$. This becomes a nearest-neighbour interaction of strength $J\Delta$,

$$H_\Delta := J\Delta(\psi_{j+1}^{\dagger}\psi_{j+1} - \frac{1}{2})(\psi_j^{\dagger}\psi_j - \frac{1}{2}).$$

In the continuum limit, in terms of the boson fields, it becomes

$$H_\Delta = v\Delta \int dx \left[ \frac{1}{\pi} \partial_x \varphi (x + a) + \frac{e^{-2ik_F(x+a)}}{2\pi a} e^{2i\varphi(x+a)} + \text{H.c.} \right] \times$$

$$\times \left[ \frac{1}{\pi} \partial_x \varphi (x) + \frac{e^{-2ik_Fx}}{2\pi a} e^{2i\varphi(x)} + \text{H.c.} \right].$$

Discarding the oscillating terms, the Hamiltonian becomes, to leading order in derivatives,

$$H_\Delta = v\Delta \int dx \frac{1}{\pi^2} [1 - \cos(2k_Fa)](\partial_x \varphi)^2 + \left[ \frac{e^{-4ik_Fx-2ik_Fa}}{(2\pi a)^2} e^{2i[\varphi(x+a)+\varphi(x)]} + \text{H.c.} \right].$$

The latter term is only non-oscillating at zero field, where $4k_Fx(j) = 2\pi j$. In this case, we get a contribution $\cos 2(\varphi(x+1) + \varphi(x)) \approx \cos 4\varphi(x)$; this term represents the umklapp process in the fermion model. Thus we write the interaction Hamiltonian as

$$H_\Delta = v\Delta \int dx \frac{1}{\pi^2} [1 - \cos 2k_Fa](\partial_x \varphi)^2 - \frac{\cos 4\varphi(x)}{2\pi^2 a^2}.$$
expression shows the power of the bosonisation approach: in essence, an interacting theory of fermions has been rewritten as a free theory of bosons.

The Luttinger parameter $K$ and the Fermi speed $v$ are renormalised by other terms (such as band curvature) and field theory can only give an approximate expression. However, their exact values for the interacting model can be determined from the Bethe ansatz by comparing quantities accessible to both methods \[136, 128\]

\[
\frac{1}{2K} = 1 - \frac{\zeta}{\pi} \quad (6.24)
\]

\[
v = \frac{J\pi}{2\zeta} \sin \zeta \quad (6.25)
\]

(where $\zeta = \cos \Delta$).

### 6.2 Correlation functions

The ground-state spin–spin correlation functions are now (to leading order) easy to determine, as the ground state is the vacuum of quasiparticles $c, c^\dagger$. The easiest is the longitudinal structure factor at nonzero field, which is just the density–density correlator

\[
S_{zz}(q, \omega) = \frac{1}{L} \int dt \, e^{i\omega t} \langle \rho_q(t) \rho_{-q}(0) \rangle \quad (6.26)
\]

with

\[
\rho_q = \sqrt{\frac{L|q|}{2\pi}} (b_{-q} + b_q) = \sqrt{\frac{L|q|}{2\pi}} e^{-\gamma/2} (c_{-q} + c_q) \quad (6.27)
\]

where $e^{-\gamma/2} = \sqrt{K}$, so that immediately follows

\[
\langle \rho_q(t) \rho_{-q}(0) \rangle = \frac{LK|q|}{2\pi} \langle e^{itH_0} (c_{-q} + c_q) e^{-itH_0} (c_{-q} + c_q) \rangle = \frac{LK|q|}{2\pi} e^{-ivt|q|/2} \quad (6.28)
\]

The longitudinal structure factor equals

\[
S_{zz}(q, \omega) = \frac{1}{L} \int dt \, e^{i\omega t} \langle \rho_q(t) \rho_{-q}(0) \rangle = K|q| \delta(\omega - v|q|) \quad (6.29)
\]

Therefore, without perturbations, field theory predicts a single peak for the structure factor. This is because all excitations are carried by a single coherent excitation: the particle–hole excitations of the Jordan–Wigner fermion. As we have just seen, these have a dispersion relation $\omega = v|k|$, reflecting the Lorentz invariance of the Luttinger model \(6.17\). Note that this result already includes interactions on the level of the Luttinger parameter. To get a more realistic expression for the structure factor in the spin chain, it is therefore necessary to include perturbations
6.2. Correlation functions

arising from band curvature and higher orders in the interaction. In zero field, the umklapp term also needs to be taken into account.

The transverse correlation function, though somewhat harder to obtain, can also be found via the expressions (6.14) (see e.g. [127, 5]). In both the longitudinal and the transverse case this leads to an operator expansion where the coefficients are non-universal and therefore renormalised by all sorts of perturbation terms. As for the Luttinger liquid parameters, the exact value of these coefficients must be found by other means.

The correlators for the boson fields are

\[
\begin{aligned}
\langle [\varphi(x, t) - \varphi(x', t')]^2 \rangle &= \frac{K}{2} \log \left( \frac{(x - x')^2 + (v |t - t'| + a)^2}{a^2} \right) \quad (6.30) \\
\langle [\vartheta(x, t) - \vartheta(x', t')]^2 \rangle &= \frac{1}{2K} \log \left( \frac{(x - x')^2 + (v |t - t'| + a)^2}{a^2} \right) \quad (6.31) \\
\langle \varphi(x, t) \vartheta(x', t') \rangle &= \frac{1}{2} \text{Arg}[v(t - t') + a \text{sign}(t - t') + i(x - x')] \quad . \quad (6.32)
\end{aligned}
\]

6.2.1 Long-distance space–time correlators

The coefficients for the large-distance expansion of the spin–spin correlation functions in the anisotropic model were derived by Lukyanov [137, 138],

\[
\begin{aligned}
\langle S_j^{z+}(t) S_j^{z+}(0) \rangle_c &= (-1)^l \frac{A/2}{(l^+_\eta)^{2/\eta}} \left[ 1 - \frac{B}{(l^-\eta)^{-2+2/\eta}} + \cdots \right] \\
&\quad - \frac{\tilde{A}/2}{(l^+_\eta)^{2+1/2\eta}} \left[ \frac{1}{2} \left( \frac{l^-}{l^+} + \frac{l^+}{l^-} \right) + \frac{\tilde{B}}{(l^-\eta)^{-1+1/\eta}} + \cdots \right] , \quad (6.33)
\end{aligned}
\]

\[
\begin{aligned}
\langle S_j^{z+}(t) S_j^{z+}(0) \rangle_c &= \frac{1}{4\pi^2 \eta l^+} \left[ \frac{1}{2} \left( \frac{l^-}{l^+} + \frac{l^+}{l^-} \right) + \frac{\tilde{B}_z}{(l^-\eta)^{-2+2/\eta}} \left( 1 + \frac{2 - \eta}{4(1 - \eta)} \left( \frac{l^-}{l^+} + \frac{l^+}{l^-} \right) + \cdots \right) \right] \\
&\quad + \frac{(-1)^l A_z/4}{(l^-\eta)^{2/\eta}} \left[ 1 - \frac{B_z}{(l^-\eta)^{1/\eta - 1}} + \cdots \right] , \quad (6.34)
\end{aligned}
\]

where \( l^\pm := l \pm t/\epsilon \), and \( \epsilon \) is an anisotropy-dependent time scale [139]. In the isotropic model, the umklapp term leads to logarithmic corrections to the correlation function.

This result is for a chain of infinite length. However, as the Luttinger liquid is a conformal field theory and \( \partial_x \varphi \) a primary operator of dimension \( \eta = 1 \), we can compare the infinite-chain expression to our finite-size results by applying a conformal mapping of the space-time plane \( z = (x, it) \) to a cylinder \( w \), where the space direction is periodic; i.e., \( z = e^{2\pi i w/L} \) [140, 40]. The two-point function for a primary field \( \eta \) of dimension \( \eta \),

\[
\langle \eta(z_1) \eta(z_2) \rangle = (z_1 - z_2)^{-2\eta} \quad , \quad (6.35)
\]

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maps under this transformation as

\[
\langle \eta(w_1)\eta(w_2) \rangle = \left( \frac{dw}{dz} \right)_{w_1}^{-h} \left( \frac{dw}{dz} \right)_{w_2}^{-h} \langle \eta(z_1)\eta(z_2) \rangle = \left[ \frac{L}{\pi} \sin \frac{\pi}{L}(w_1 - w_2) \right]^{-2h}
\]

so that we can take finite-size effects into account by setting

\[
l_{\pm} := \frac{L}{\pi} \sin \left[ \frac{\pi}{L}(l \pm t/\epsilon) \right].
\]

We compare equal-time correlation functions calculated from this field-theoretical expression to those found by Fourier transforming the structure factor as calculated by the Bethe ansatz methods of chapter 4. In tables 6.1 and 6.2, results of both approaches, for the longitudinal as well as the transverse structure factor, are compared side-to-side for two values of the anisotropy $\Delta$. Figure 6.1 shows plots as a function of distance.
6.3. Peak width

As we have seen from the Bethe ansatz results in earlier chapters, in the spin chain the peak of the dynamical structure factor widens with increasing (but low) momentum. This is known exactly in the XX0 model, where the exact structure

\[ \langle S^z_i S^z_j \rangle = \begin{cases} \frac{-1}{L} & \text{for } l \langle S^z_0 S^z_l \rangle = 1e^{-05} \\ \frac{-1}{L} & \text{for } l \langle S^z_0 S^z_l \rangle = 1e^{-04} \\ \frac{-1}{L} & \text{for } l \langle S^z_0 S^z_l \rangle = 0.001 \\ \frac{-1}{L} & \text{for } l \langle S^z_0 S^z_l \rangle = 0.01 \\ \frac{-1}{L} & \text{for } l \langle S^z_0 S^z_l \rangle = 0.1 \\ \frac{-1}{L} & \text{for } l \langle S^z_0 S^z_l \rangle = 0 \end{cases} \]

\[ \frac{1}{L} \sum_{i=0}^{L-1} \frac{1}{L} \sum_{j=0}^{L-1} \langle S^z_i S^z_j \rangle = \left( \frac{-1}{L} \right)^2 \]

\[ \langle S^z_i S^z_j \rangle = \sum_{q=0}^{\infty} n_q |q| \]

\[ k_{(n)} = 2k_F (m_+ - m_-) + \sum_{q \neq 0} n_q q , \] (6.39)

\[ E_{(n)} = \frac{\pi v}{2L} [K(m_+ - m_-)^2 + K^{-1}(m_+ + m_-)^2] + v \sum_{q \neq 0} n_q |q| \] (6.38)

In nonzero magnetic field, there is no umklapp term, so that right-movers remain right-movers and left-movers remain left-movers. Figure 6.3 shows the contributions for finite field; indeed, all contributions lie around \( m_+ = m_- = 0 \).

For zero field, the umklapp term allows the exchange of left- and right-movers; however, the total number of fermions is a constant; thus \( m_+ + m_- = 0 \). In figure 6.4 it can be seen how the form factors we found numerically do indeed cluster around the values for \( m_+ - m_- = 0 \) and \( m_+ - m_- = 2 \). This allows to separate the contributions that must be associated to the umklapp term from those generated by other perturbations.

6.2.2 Energy levels

For the boson states, we have the energies and momenta [141, 142]

\[ E_{(n)} = \frac{\pi v}{2L} [K(m_+ - m_-)^2 + K^{-1}(m_+ + m_-)^2] + v \sum_{q \neq 0} n_q |q| \] (6.38)

\[ k_{(n)} = 2k_F (m_+ - m_-) + \sum_{q \neq 0} n_q q , \] (6.39)

\[ E_{(n)} = \frac{\pi v}{2L} [K(m_+ - m_-)^2 + K^{-1}(m_+ + m_-)^2] + v \sum_{q \neq 0} n_q |q| \]

\[ k_{(n)} = 2k_F (m_+ - m_-) + \sum_{q \neq 0} n_q q , \]

Figure 6.1: Equal-time spin-spin correlation functions as a function of lattice distance, for anisotropies \( \Delta = 0.25 \) and \( \Delta = 0.75 \), for chains of \( N = 200 \) sites. Form factor results are compared to the asymptotics from field theory, adapted to finite size. The deviations are well within those expected from the sum rules and finite size effects for the form factors, and subleading corrections to the field theory result.

\[ E_{(n)} = \frac{\pi v}{2L} [K(m_+ - m_-)^2 + K^{-1}(m_+ + m_-)^2] + v \sum_{q \neq 0} n_q |q| \]

\[ k_{(n)} = 2k_F (m_+ - m_-) + \sum_{q \neq 0} n_q q , \] (6.39)

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Chapter 6. The structure factor at low momentum

factor is known and only has contributions between $\omega_{U,L}(q) = 2J \sin q/2 \sin (k_F \pm q/2)$.

It has been attempted to derive the functional dependence of the width on momentum in field theory; however, this has given contradictory results [143, 144]. The main underlying problem is that perturbation theory fails near the ‘light cone’ $\omega = v |q|$, where perturbative corrections become divergent. This means that chances of getting a good result are strongly dependent on finding a way to do the resummation of diagrams.

In the Bethe ansatz, one can get an expression for the width by looking at the two-spinon region, which yields the main peak. For $\Delta \ll 1$, we start from the XX0 model, where the Bethe equations simply become

$$k_\alpha = 2\pi J_\alpha / N.$$ (6.40)

with energy still given by $E_\alpha = J \cos k_\alpha - h$. In this limit, all contributions to the structure factor come from single particle–hole excitations. A particle at momentum $k$ and a hole at momentum $\bar{k}$ form a quasiparticle of momentum and energy

$$q = \bar{k} - k \quad \quad \omega = J(\cos k - \cos \bar{k}) = 2J \sin \frac{k + \bar{k}}{2} \sin \frac{q}{2}.$$ (6.41)

The width is given by the difference between lowest and highest values for the energy, found for $k_F \neq \pi/2$ at $(k + \bar{k})/2 = k_F \pm q/2$ (assuming $|q| < |k_F - \pi/2|$). Their difference gives the line width

$$\delta \omega_{\Delta=0,h\neq0}(q) = 4J \cos k_F \sin^2 q/2 = q^2/m + O(q^4),$$ (6.42)
where \( m := 1/J \cos k_F \) is an effective mass. At \( h = 0 \), where \( k_F = \pi/2 \), the highest energy is found at \( (k + \bar{k})/2 = \pi/2 \) and the difference is
\[
\delta \omega_{\Delta=0,h=0}(q) = 4J(\sin q/2)(1 - \cos q/2) = Jq^3/8 + O(q^5) \ .
\]
This \( q^3 \) scaling persists at all \(-1 < \Delta \leq 1\), which follows from the boundaries of the two-spinon continuum found by des Cloizeaux and Gaudin [145]. At small but nonzero anisotropy \( \Delta \) and nonzero field \( h \), expansion of the scattering term in the Bethe equations leads to a correction of the effective mass,
\[
\delta \omega_{\Delta=0,h\neq0}(q) = 4J \left( 1 + \frac{2\Delta}{\pi} \sin k_F \right) \cos k_F \sin^2 q/2 \ ,
\]
i.e. the peak widens with momentum as \( q^2 \). To compare this result to the form factor calculation, we calculate the particle–hole lineshape at a set of low momenta for increasing chain length \( N \), and extrapolate to the infinite chain. The result is shown in figure 6.3; both approaches are in complete agreement.

### 6.3.1 High-energy tail

As we have seen in the four-spinon calculation in section 5.2, higher excitations not only add to the structure factor in the two-spinon continuum, but also produce a contribution above it; in principle all the way to infinity as long as we keep increasing the number of spinons involved. In field theory this contribution must come from corrections to the Luttinger model due to band curvature and interaction terms. A lowest-order result was derived by Pustilnik et al. [146].

---

**Figure 6.3:** Nonzero-field high-energy tail of the dynamic structure factor for \( \Delta = 0.75, M/N = 0.4, N = 600, \) and \( q = 2\pi/50 \). The dots represent the structure factor calculated from the Bethe ansatz as described in chapter 4, the line is the structure factor as calculated from the field theory, equation (6.46). The inset shows the fine structure of the form factors, which group in clusters around energy levels \( \omega = 2\pi vl/N \).
It is found \[126, 137\] that the leading irrelevant operators are

\[
\delta H(x) = \eta_- \left[ \left( \frac{\partial}{\partial x} \varphi_L \right)^3 - \left( \frac{\partial}{\partial x} \varphi_L \right)^3 \right] + \eta_+ \left[ \left( \frac{\partial}{\partial x} \varphi_L \right)^2 \frac{\partial}{\partial x} \varphi_R - \left( \frac{\partial}{\partial x} \varphi_R \right)^2 \frac{\partial}{\partial x} \varphi_L \right] + \zeta_- \left[ \left( \frac{\partial}{\partial x} \varphi_L \right)^4 + \left( \frac{\partial}{\partial x} \varphi_R \right)^4 \right] + \zeta_+ \left( \frac{\partial}{\partial x} \varphi_L \right)^2 \left( \frac{\partial}{\partial x} \varphi_R \right)^2 + \zeta_3 \left[ \left( \frac{\partial}{\partial x} \varphi_L \right)^3 \frac{\partial}{\partial x} \varphi_R + \left( \frac{\partial}{\partial x} \varphi_R \right)^3 \frac{\partial}{\partial x} \varphi_L \right] + \lambda \cos(4\sqrt{\pi K} \varphi + 4k_F x) .
\]

(6.45)

The \( \lambda \)-term, which represents umklapp scattering, is only important at \( h = 0 \), as it oscillates for \( k_F \neq \pi/2 \). Quadratic terms are left out of this expression: they modify the dispersion relation but do not yield contributions above the two-spinon continuum. The \( \eta_- \) term is responsible for the widening of the peak \[147\]. The \( \eta_+ \) term dominates the high-energy tail at nonzero field; the correction term is found to be

\[
\delta S_{zz}^{zz}(q, \omega) = \frac{K\eta_+^2 q^4}{v\pi} \frac{\Theta(\omega - v|q|)}{\omega^2 - v^2 q^2} .
\]

(6.46)

In figure 6.3 the prediction of this formula is compared to the structure factor as found from the Bethe ansatz by the methods of chapter 4. At zero field, the \( \eta_\pm \) terms are excluded by particle–hole symmetry, and the \( \zeta \) and \( \lambda \) terms need to be included. The \( \zeta_3 \) term is excluded \[126\] by conservation of the

\[2v S_{zz}^{zz}(q, \omega)\]

Figure 6.4: Zero-field high energy tail of the dynamic structure factor for \( \Delta = 0.25 \), \( N = 600 \), and \( q = 2\pi/50 \). The contributions from the two correction terms are shown separately. The solid line corresponds to the umklapp (\( \lambda \)) term (6.47) and is compared to the sum of form factors near \( \omega = 2\pi v(l + 4K)/N \), represented by the dots. The dotted line includes finite-size corrections to the solid line. The lower, dashed line corresponds to the \( \zeta \) term (6.48) and is compared to the sum of form factors near \( \omega = 2\pi vl/N \), represented by the squares.
first of the nontrivial conserved quantities produced by the algebraic Bethe ansatz, viz. the heat current [148]. The corrections at zero field are then found to be

\[ \delta S_{\zeta+}^{zz}(q, \omega) = \frac{K \eta_+^2}{48v^2 \pi^2} q^2 (\omega^2 - v^2 q^2) \Theta(\omega - v |q|) \] (6.47)
\[ \delta S_{\lambda}^{zz}(q, \omega) = 8 \lambda^2 K^2 (2v)^3 \sin^2(4\pi K) \Gamma^2(1 - 4K) q^2 (\omega^2 - v^2 q^2) 4K^{-3} \Theta(\omega - v |q|) , \] (6.48)

where the latter result was found in [149]. Figure 6.4 compares this formula to the structure factor as found from the Bethe ansatz.

### 6.4 Discussion

Bethe ansatz methods, such as the form factor method of chapter 4, prove to be a good tool in finding corrections to the field theory description of the Heisenberg chain. We have shown how to analyse the widening of the coherent peak in the low-momentum line shape of the dynamic structure factor. Furthermore, we have seen how the high-energy corrections can be described both by irrelevant-operator corrections in field theory, and by numerical form factor methods. Again, numerics and field theory are in excellent agreement.
Chapter 6. The structure factor at low momentum
7.

Conclusion

I count not myself to have apprehended: but this one thing I do, forgetting those things which are behind, and reaching forth unto those things which are before, I press toward the mark.

— Philippians 3:13–14

In the preceding chapters I have shown how to use the Bethe ansatz to extract dynamical correlation functions from the Heisenberg model in the isotropic and gapless anisotropic phase. This is made possible by the fact that the bulk of the correlation function is carried by a relatively small number of intermediate states. Most of these are two-spinon states; yet, a significant part of the correlation function is carried by higher-spinon states. In terms of the classification of states in the finite lattice, it turns out to be important to be able to solve bound states. The two-strings, especially, carry some weight but higher strings cannot be ignored either. Luckily, it is possible to solve the Bethe equations in all these cases: starting from the Bethe–Takahashi string solution, an iterative procedure has been outlined to find solutions in the complex plane. The dynamical structure factors calculated this way satisfy the sum rules to a degree between excellent and decent; we hope that they will be applicable to description of inelastic neutron scattering data on realistic materials.

However, there is still much room for improvement on this method. For one thing, we cannot yet achieve saturation of the sum rule for small magnetic fields; especially the $S^{+−}$ structure factor yields disappointing results in this region. But for the other structure factors, too, some non-negligible part of the sum rule remains missing and it would be interesting to know where this comes from. Possible sources are deviated strings and pairs of real roots of the EKS type.

For further improvement, first and foremost, we need to be able to find all solutions of the Bethe ansatz. I have shown that, taking deviations into account, most of the solutions of the Bethe equations take the form of strings. For given small magnon number $M$, the fraction of solutions that do not fit into this picture decreases with
increasing chain length, though their number increases; the functional dependence of the number of missing solutions on chain length is consistent with a picture where EKS-type pairs are the only non-string solutions. Whether these pairs derive only from narrow two-strings of from larger strings as well can as of yet not be inferred. What happens at small magnetic field, with $M$ close to $N/2$, is another open question. Should the problem of finding all solutions be overcome, another obstacle arises: in many cases, special solutions lead to degeneracies in the determinant formulas for form factors. In cases where these special solutions have nonzero contributions, such degeneracies must be removed by rewriting the determinants. All in all, perfecting the computation of structure factors for the gapless Heisenberg chains will still lead to a sizeable number of technical challenges, though the ground has been broken and we can already obtain very promising results.

The logical next step forward is to apply this method to the region of parameter space not covered in this thesis: the gapped antiferromagnetic and the ferromagnetic phases of the Heisenberg chain. Since these phases have an altogether different physical character, many unexpected problems are expected to arise.

After that, one can think of doing finite-temperature calculations. Theoretically, this is pretty straightforward, as it involves only a Boltzmann sum; however, the computational challenge of solving yet another big sum on top of what we already do is huge. Aside from that, it will be necessary to solve matrix elements between two general states, not just those for which one of the states is the ground state. This will open a Pandora’s box of its own; for instance, it is quite unclear whether the singular states I discussed, which so conveniently have zero matrix elements with the ground state, will give a contribution, and if so, how to calculate this.

Another thing to consider is possible applications of the structure factor as a computational tool. One application that comes to mind is treating the coupling between multiple chains as a perturbation on the integrable single chain. The connection to field theory has already yielded rather promising results, and more is to be expected. Many things remain not completely understood here, such as the $N$-dependence of the various contributions to the structure factor and how this fits into the field theoretical picture.

Further research might go into extending the approach discussed in this thesis to other integrable models. Indeed, a very similar approach has already been applied to the Lieb-Liniger model of locally interacting bosons in one dimension, which is relevant to the study of elongated Bose-Einstein condensates [150, 151]. Other models that may be attacked are integrable spin chains of higher spin, and spin chains with boundaries. The ultimate goal in this respect would be to be able to solve the dynamics of the one-dimensional Hubbard model using this technique. It is clear that considerable difficulties will have to be overcome to get there.

With this thesis, I hope to have convinced the reader that the Bethe ansatz is not only an elegant branch of mathematical physics and a tool to find energy spectra, but it can also be realistically used to calculate dynamics. As such, what is presented in this thesis is only the very beginning; there is a world of possibility out there.
A.

Complete Bethe ansatz solutions of finite XXX chains

Доверяй, но проверяй

— Russian adage

In tables A.1–A.4 we give the rapidities for all highest-weight eigenstates of the isotropic Heisenberg chain at 8 sites, except the reference state (which has no rapidities). Lower-weight states can be formed by adding the appropriate number of infinite rapidities.

At this size, the model is easily completely diagonalisable and therefore we do not need the Bethe ansatz to solve it. However, while constructing the complete solution from the Bethe ansatz solutions is easy for this number of particles, mapping the exactly diagonalised wave functions to solutions of the Bethe equations is not. Therefore, we believe it valuable to have an exhaustive list at hand. The solutions are found by the methods of chapter 3. The quantum numbers are determined from the rapidities, thereby providing a valuable check on their accuracy as solutions to the Bethe equations. We have also checked these solutions against a complete diagonalisation, and found full agreement.

One thing one can easily see is that these solutions neatly satisfy the classification in terms of the string hypothesis: the states can be associated one-to-one with string states, with small but significant deviations, and with quantum numbers that satisfy the bound (2.88).
Chapter A. Complete Bethe ansatz solutions of finite XXX chains

Table A.1: Highest-weight Bethe ansatz solutions for $N = 8$, $M = 1$

<table>
<thead>
<tr>
<th>$2J$</th>
<th>$2J_1$</th>
<th>$\lambda$</th>
<th>$E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>0</td>
<td>0.174124 50490717</td>
<td>-3.801937735804284</td>
</tr>
<tr>
<td>2.</td>
<td>-2</td>
<td>-0.820250609262081</td>
<td>-3.267035698361317</td>
</tr>
<tr>
<td>3.</td>
<td>-3</td>
<td>-0.130438947345799</td>
<td>-3.144122805653573</td>
</tr>
<tr>
<td>4.</td>
<td>-4</td>
<td>-0.0382603981905997</td>
<td>-3.144122805653573</td>
</tr>
<tr>
<td>5.</td>
<td>-5</td>
<td>-0.0539607683954299</td>
<td>-2.437016024448842</td>
</tr>
<tr>
<td>6.</td>
<td>-6</td>
<td>-0.0820036908620831</td>
<td>-2.258562022054145</td>
</tr>
<tr>
<td>7.</td>
<td>-7</td>
<td>-0.130438947345799</td>
<td>-2.437016024448842</td>
</tr>
<tr>
<td>8.</td>
<td>-8</td>
<td>-0.150704301237499</td>
<td>-2.258562022054145</td>
</tr>
<tr>
<td>9.</td>
<td>-9</td>
<td>-0.150704301237499</td>
<td>-2.258562022054145</td>
</tr>
</tbody>
</table>

Table A.2: Highest-weight Bethe ansatz solutions for $N = 8$, $M = 2$. There are 15 states with all real solutions, and 5 with a single two-string.

<table>
<thead>
<tr>
<th>$2J$</th>
<th>$2J_1$</th>
<th>$\lambda$</th>
<th>$E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.</td>
<td>-10</td>
<td>-0.39873669441202</td>
<td>-2.44504186791263</td>
</tr>
<tr>
<td>11.</td>
<td>-11</td>
<td>-0.39873669441202</td>
<td>-2.44504186791263</td>
</tr>
<tr>
<td>12.</td>
<td>-12</td>
<td>-0.428405998277582</td>
<td>-1.5629397551186</td>
</tr>
<tr>
<td>13.</td>
<td>-13</td>
<td>-0.428405998277582</td>
<td>-1.5629397551186</td>
</tr>
<tr>
<td>14.</td>
<td>-14</td>
<td>-0.288675134594813</td>
<td>-2.6662540378448438</td>
</tr>
</tbody>
</table>

Table A.3: Highest-weight Bethe ansatz solutions for $N = 8$, $M = 3$. There are 15 states with all real solutions, and 5 with a single two-string.
Table A.3: Highest-weight Bethe ansatz solutions for $N = 8$, $M = 3$. There are 10 solutions with all reals, 15 with one two-string, and 3 with a single three-string. We give both Bethe $J$ and Bethe–Takahashi $I$ quantum numbers. The latter are subscripted by the length of the string for which they are quantum numbers.
Table A.4: Highest-weight Bethe ansatz solutions for $N = 8$, $M = 4$. There is 1 state with all real solutions, 6 with one two-string, 5 with one three-string, 1 single four-string, and 1 with two two-strings.
Table A.6: Highest-weight Bethe ansatz solutions for \( N = 10, \ M = 2 \). There are 28 states with only real roots and 7 two-strings.
Table A.7: Highest-weight Bethe ansatz solutions for $N = 10$, $M = 3$. There are $45$ states with only real roots, $35$ states with one twostring and $5$ three-strings.
Table A.8: Highest-weight Bethe ansatz solutions for $N = 10$, $M = 4$. Real: 15, one two-string: 46, one three-string: 21, one four-string: 4, two two-strings: 6.
Table A.9: Highest-weight Bethe ansatz solutions for $N = 10$, $M = 5$. Real: 1; one two-string: 10; one three-string: 14; one four-string: 7; one five-string: 1; two two-strings: 5; one two- and one three-string: 3.
Bibliography


[34] L. Van Hove, Phys. Rev. 95, 249 (1954).


Samenvatting

Het lijkt simpel
en dat is het ook

— Loesje

Dynamica van Heisenberg-spinketens

In dit proefschrift bestudeer ik de dynamica van het eendimensionele Heisenberg-model. Het Heisenbergmodel beschrijft een systeem van lokale magnetische momenten, meestal spins genoemd. Spin is een eigenschap van elementaire deeltjes zoals elektronen, die soms als een tolbeweging wordt voorgesteld. De quantum-mechanica beperkt die beweging echter tot maar twee mogelijkheden: linksom of rechtsom. Het is gebruikelijk om deze richtingen als op (↑) en neer (↓) aan te duiden, naar de richting van het magnetisch veld dat de spin produceert. In het Heisenbergmodel wisselwerken de spins alleen met hun naaste buren; de precieze vorm van de wisselwerking kan variëren. Eventueel kan er een extern magnetisch veld aanwezig zijn dat met alle spins interageert.

Dit model werd geïntroduceerd door Werner Heisenberg in 1928 met als doel om ferromagnetische ordening van materialen te bestuderen. Dit is een ordening, waarin alle spins spontaan dezelfde kant gaan wijzen. Gezamenlijk produceren ze zo een sterk magnetisch veld. De alledaagse magneten, ondermeer op ijskastdeuren te vinden, zijn ferromagneten. Een minder direct opvallende, maar zeker zo opmerkelijke ordening is de antiferromagnetische, waarin de spins om en om tegen elkaar inwijzen en zo elkaars magnetisch veld opheffen. Een antiferromagneet produceert dus geen sterk magnetisch veld om zich heen, wat de reden is dat het zo lang heeft geduurd voordat het verschijnsel van antiferromagnetisme ontdekt werd: waar ferromagnetisme al in de Griekse oudheid bekend was, werd antiferromagnetisme pas rond de jaren dertig van de twintigste eeuw gevonden. Het Heisenbergmodel kan zowel ferro- als antiferromagnetisme beschrijven.

Als je het model beperkt tot één ruimtelijke dimensie heb je een rij van spins; dit wordt een spinketen genoemd. In een dimensie is het effect van wisselwerkingen veel sterker dan in bijvoorbeeld drie. Intuïtief is dat makkelijk te begrijpen voor iedereen die wel eens in een file gestaan heeft: in een dimensie kunnen deeltjes niet langs elkaar heen, en bewegingen nemen dus de vorm aan van collectieve golven.
In drie dimensies bewegen alle deeltjes door elkaar heen zonder veel van elkaar te merken. Als gevolg daarvan is in drie dimensies een beschrijving in termen van losse deeltjes vaak nog een goede manier om iets over het systeem te zeggen, terwijl het in een dimensie noodzakelijk is te denken in termen van het collectief gedrag. Dit betekent dat de gebruikelijke benaderingsmethoden niet meer werken, en er aan nieuwe (en dus interessante) methoden gewerkt moet worden. Dit is een van de redenen waarom zulke systemen voor theoretisch fysici interessant zijn.

**Experimentele relevantie**

Er is ook een experimenteel belang van de studie van eendimensionale systemen. In sommige materialen is de wisselwerking in een gegeven richting veel sterker dan in de andere twee, zodat ze zich, bij de juiste temperatuur beschouwd, als eendimensionaal gedragen. De magnetische eigenschappen van zo’n materiaal kunnen worden bestudeerd met neutronen. Aangezien een neutron elektrisch ongeladen is, kan het diep in een materiaal doordringen, tot het verstrooid wordt door wisselwerking met elektronen en atoomkernen. Een deel van de energie en impuls van het neutron wordt dan overgedragen aan excitaties in het systeem. Dit kunnen bijvoorbeeld geluidsgolven (fononen) zijn, die ontstaan wanneer een neutron met een atoomkern botst; voor ons is echter de wisselwerking tussen de spin van neutron en elektron, die magnetische excitaties veroorzaakt, van belang. Na de verstrooiing wordt het neutron opgevangen door detectoren. De verandering van energie en impuls van het neutron die zo bepaald kan worden correspondeert met de energie en impuls van een excitatie in het systeem. Op deze manier geeft neutronenverstrooiing dus een beeld van de interne dynamica van het bestudeerde materiaal. Deze interne dynamica is wat ik in dit proefschrift theoretisch tracht te beschrijven op basis van het Heisenbergmodel. De grootheid die de connectie tussen theorie en experiment maakt is de dynamische structuurfactor. Deze beschrijft de correlaties en excitaties van het model en is evenredig met de intensiteit van neutronen die in een verstrooiingsexperiment bij een bepaalde energie- en impulsoverdracht worden aangetroffen. De waarde van de structuurfactor voor een bepaalde impuls en energie geeft dus aan hoe waarschijnlijk het is dat een neutron dat botst op het onderzochte materiaal een magnetische golf aanslaat met precies die impuls en energie.

**De Bethe-ansatz voor het Heisenbergmodel**

Voor het bepalen van deze grootheid in het eendimensionale Heisenbergmodel zijn, zoals hierboven opgemerkt, de gebruikelijke benaderingsmethoden ongeschikt. De keerzijde is dat het model een grote rijkdom aan wiskundige structuur vertoont. Deze structuur maakt het mogelijk om de energieniveaus van het systeem exact te bepalen; iets wat zeer uitzonderlijk is in de natuurkunde van veeldeeltjessystemen, waar benaderingen normaliter de dienst uitmaken. Deze methode wordt de Bethe-ansatz genoemd, naar Hans Bethe die haar in 1931 ontwikkelde. Deze methode gaat
uit van een referentietoestand van het systeem, waarbij alle spins een bepaalde kant
opwijzen. Spins die de andere kant opwijzen kunnen dan als deeltjes beschouwd
worden. De Bethe-ansatz is nu gebaseerd op de aanname dat de wisselwerking
 tussen deze deeltjes volledig bepaald wordt door de interactie tussen paren van
deeltjes. Met deze aanname kan het model opgelost worden. Vervolgens kan worden
bewezen dat de gevonden oplossing exact geldig is. Ik bespreek de Bethe-ansatz
voor het Heisenbergmodel in het tweede hoofdstuk van dit proefschrift.

Wortels van de Bethevergelijkingen in het complexe vlak

In het derde hoofdstuk ga ik nader in op de structuur van de oplossingen van
Bethes vergelijkingen. Deze vergelijkingen hebben zowel oplossingen op de reële
lijn als in het complexe vlak. De reële oplossingen zijn eenvoudig numeriek te
vinden, maar dit gaat niet op voor de complexe oplossingen. Er bestaat echter een
benadering die uitgaat van een veronderstelling over hoe de oplossingen eruitzien:
de stringhypothese. Het argument voor deze hypothese is dat ze exact is in de limiet
voor een oneindige keten met een eindig aantal deeltjes. Op een eindige keten zijn
er echter afwijkingen van de hypothese. In dit hoofdstuk leid ik vergelijkingen
af om deze afwijkingen te vinden, zodat de exacte oplossingen in het complexe
vlak gevonden kunnen worden. Het blijkt dat niet alle oplossingen op deze manier
gevonden kunnen worden, omdat de stringhypothese niet voor alle oplossingen
opgaat.

Dynamische correlaties in eindige ketens

Hoewel de Bethe-ansatz inmiddels 75 jaar oud is, was het tot voor kort niet mo-
gelijk om hiermee informatie over dynamische grootheden te verkrijgen, waardoor
de toepasbaarheid beperkt bleef. In de afgelopen jaren heeft de wiskunde van in-
tegereerbare modellen echter een stormachtige ontwikkeling doorgemaakt. Nieuwe
analytische vergelijkingen geven een sterke vereenvoudiging van het probleem om
de dynamische structuurfactor te bepalen, waardoor een benadering mogelijk wordt
die het probleem binnen het bereik van numerieke berekeningen op de computer
brengt. Dit is van belang omdat exacte wiskundige uitdrukkingen lang niet altijd
berekenbaar zijn, gegeven de beperkingen van processortijd en geheugenruimte. De
methode die we hebben ontwikkeld om de dynamische structuurfactor in benade-
ring te berekenen beschrijf ik in het vierde hoofdstuk van dit proefschrift.

De thermodynamische limiet

De methode van hoofdstuk vier werkt op ketens met een eindig aantal spins. Het is
echter ook mogelijk het systeem te beschouwen in de limiet waar het aantal spins
naar oneindig gaat. Dit vergt een totaal andere wiskundige aanpak, maar ook hier
zo zijn exacte wiskundige uitdrukkingen beschikbaar. De aanpak in deze limiet, be-
sproken in het vijfde hoofdstuk, beschouwt het systeem in termen van spinons. Dit
zijn excitaties die vrij eenvoudig intuitief begrepen kunnen worden in termen van

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de antiferromagnetische ordening. Er zijn namelijk twee gelijkwaardige antiferromagnetische toestanden die elkaars spiegelbeeld zijn. Een spinon is een overgang tussen deze twee toestanden. Zo’n overgang kost energie omdat twee spins dezelfde kant op moeten wijzen. Deze energie is echter lokaal geconcentreerd rond de positie van de overgang, en op grote afstand is er niets van te merken. Daardoor gedragen spinons zich als deeltjes. De dynamische structuurfactor kan uitgedrukt worden als een reeksonwikkeling in termen van toestanden met toenemend aantal spinons, waarbij de termen steeds ingewikkelder worden. Wederom zijn de mathematische uitdrukkingen niet op een eenvoudige manier uit te rekenen, als gevolg waarvan in het verleden onjuiste berekeningen gepubliceerd zijn voor de bijdrage van vier-spinontoestanden. In dit hoofdstuk worden de correcte resultaten gegeven.

**De structuurfactor bij lage impuls**

In het zesde hoofdstuk bespreek ik een andere manier om de Heisenbergketen aan te pakken. Voor excitaties met lage impuls is het namelijk mogelijk om een quantumveldtheorie op te stellen. Het voordeel van de veldtheoretische aanpak is, dat hij niet afhangt van de specifieke wiskundige structuur van integreerbaarheid, die in de vorige hoofdstukken zo’n belangrijke rol speelde. Daardoor maakt deze aanpak het mogelijk om resultaten uit te breiden naar een grotere groep modellen. Het is echter zeer moeilijk om de juiste waarden voor parameters in zo’n veldtheorie te vinden, en de resultaten van de eerdere hoofdstukken zijn van grote waarde bij het zoeken daarnaar.
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