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Frustrated XYZ spin-1/2 chain and its continuum limit

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Abstract

The XYZ spin-$\frac{1}{2}$ model describes a completely anisotropic spin chain, which is the most generic nearest neighbor quantum magnet in one dimension. It describes a truly interacting many-body system, but it is also known to be integrable in the Bethe ansatz framework, which, despite its complexity, allows to extract most of the thermodynamic properties. This is done by obtaining the solution for a finite chain and then taking the thermodynamic limit to describe a macroscopic system. Peculiarly, all techniques proposed in the second half of the 20^{th} century for this system are valid only for chains with an even number of sites. Although in general such boundary conditions are not expected to affect the thermodynamic properties of a system, recent literature has shown that an odd number of sites, by inducing frustration, can expose a different sector of the model. In this project, we retrieve and analyze the very convoluted recent literature dealing with the extension of the solution of the model to the case of an odd number of sites. The analysis then moves to the study of its thermodynamic limit. In the continuum limit, the XYZ chain maps in the famous sine-Gordon model, but, once again, this mapping is non-trivial. Applying frustrated boundary conditions to the chain grants access to the sector of the sine-Gordon model with an odd number of topological excitations. In particular, the chain's ground state corresponds to a single soliton, whose dispersion relation allows us a match between the two models.

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Contents

Introduction

One of the most fascinating aspects of theoretical physics is the irrepressible ambition to generalize: to take a system or phenomenon, to try to describe it through the language of mathematics, with the aim of analyzing and hopefully predicting its behaviors; then, although there was no compelling need, to try to extend our theory as far as possible. We want to make it as usable as feasible with the aim of describing the physical entity through a general model. Then, its particular cases can be recovered with a careful and appropriate choice of parameters. The same aspiration is perpetuated in the field of statistical physics. In parallel, the theoretical physicist must place a stark realism alongside this desire for abstraction. In particular, he must remain aware that mathematical tools are very powerful but still limited. One could focus on the development of new techniques, more effective for specific aims. Otherwise, pragmatism can lead us to optimize the use of existing methods to get as much information as possible, even resorting to ruses and approximations. This may appear to disagree with what was said before, but it is actually our job, always driven by the pursuit of abstract beauty but still in touch with the stark reality. Focusing on statistical physics, for example, in our real world we deal with three-dimensional systems. The mathematical tools we currently have at our disposal do not allow us to treat a macroscopic system analytically in a simple way. Even two-dimensional systems complicate things very quickly. With this in mind, statistical physics in the 1900s sought to formalize a method for mapping the physics of a macroscopic system into relatively elementary one-dimensional models. This sentence is definitely reductive to describe what *Conformal Field Theory* consists of but it is definitely a way to narrate its philosophy. Actually, only a small number of these one-dimensional models can assume this role, but their importance leads us to investigate all their variety and characteristics. The starting point is the well-known Ising model, and we would like to end up with the analytic solution of the most general spin chain, from which all the others can be recovered: the XYZ.

Although this solution has existed since the 1970s, it originated as limited to the even-numbered case, and many physicists in subsequent decades have attempted to extend it to the odd N case. The absence, as yet, of experimental evidence to show a distinction between the two cases for macroscopic systems may have limited research in this area. The complexity of the objective has certainly not helped, and many of the attempts have stalled. To get a satisfactory description, we will have to wait nearly 50 years, with the creation of a new technique, a variant of the Bethe ansatz, valid for both parities of the chain. Our first task will be to reconstruct the backbone connecting the texts dealing with the subject, in order to show their continuity. We will struggle with the multiple notations used in the literature, and with the difficulties coming from the nature of the techniques used, trying to overcome them.

The relevance of frustrated systems

The reader might wonder why there is so much interest in odd-numbered chains. As mentioned above, the desire to obtain a solution with broader validity, one that does not exclude odd-numbered chains, would itself be a noble expedient. Actually, we are moved by recent studies on the so-called *frustrated systems*, which could mark a breakthrough in the field of statistical physics. In spin chains, the phenomenon of geometrical *frustration* occurs when we choose an odd number of sites while selecting periodic boundary conditions, together *frustrated boundary conditions* (FBC): when a dominant anti-ferromagnetic regime is in force, one bond needs to display ferromagnetic alignment, as shown in fig.(1). In finite systems, it has been experimentally observed and reproduced; in particular, in small systems, it is very evident. This happens because frustration is carried by the boundary conditions, that affect directly two sites only. The common belief has been that by increasing the number of the sites, its effects vanish completely, and making an odd-numbered system identically equivalent to an even-numbered one. This notion has been theoretically formalized by Landau in its famous prescription, on which the whole Statistical Field Theory is based. In particular, among other points, it states that, for a macroscopic system, the thermodynamic properties are not influenced by the boundary conditions.

Our work aims to analyze the thermodynamic limit of both XYZ chains with even and odd number of sites, in order to identify potential differences. The choice of the XYZ model is dictated by the notoriety of its mapping into the sine-Gordon model, a fascinating connection between spin chains and field theories. Frustration in the chain could be

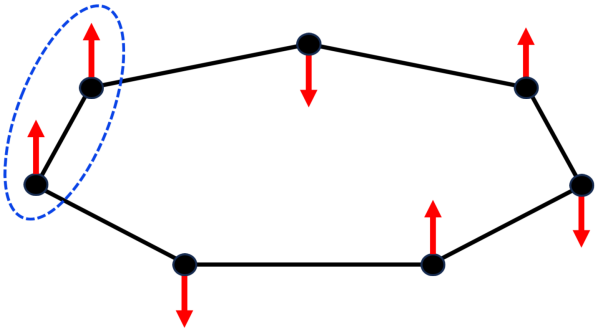


Figure 1: Intuitive example of a frustrated system: a ring-shaped chain (PBC) with $N = 7$ sites. Only one coupling is switched on, to make clear the nature of frustration: in this configuration, two adjacent spins must have the same direction.

connected with the emergence of a particular quasi-particle excitation in the continuum theory. With this in mind, we will look for the difference between the N odd and N even cases. In the event that we find it, in it we will search for the quasi-particle. Even this plan harbors pitfalls but many interesting insights will emerge.

Content structure

The first part of this work is a hard journey through the varied and convoluted literature on the integrability of the XYZ model. The introduction to integrability, in Chapter 1, is preparatory to understanding the formalism and methodologies used to deal with the more generic totally anisotropic chain. After that, in Chapter 2, we go into the meanderings of techniques for solving XYZ, introducing the eight-vertex model, the QISM, and the TQ relations. A great achievement has been to trace the common thread that connects the work of our predecessors in this field. In Chapter 3, then, we describe the recent new method called "off-diagonal Bethe ansatz" for extending the solution of the XYZ to the odd-numbered case. This formalism is particularly complex but turns out to have, in some of its variations, applications to other systems as well, mainly spin chains. Although this technique does not return the eigenstates of the model, it can give the spectrum and interesting cues in the thermodynamic limit. Indeed, the analysis of the string solutions allowed us to investigate the ground state of the frustrated chain and the elementary excitations. In particular, we are interested in the differences between the ground state energies in the odd and even N case. Our hope, which becomes action in chapter 4, is to identify in this discrepancy the emergence of the sine-Gordon soliton. Finally, in the last chapter, we extract conclusions, considerations, and possible insights.

Chapter 1

Integrability techniques

Even if *solvability* and *integrability* often go together, they are not the same thing. While the former lies in our ability and computational power, the latter is a property of the system. In statistical physics, by integrability of a system, we mean the possibility of getting its exact solution; but even the concept of "exact solution" is not self-defined. For classical systems the distinction between integrable and non-integrable systems is sharp: an integrable system has a number of conserved charges, or first integrals, scaling like the number of degrees of freedom. In the case of quantum systems, the classification is not so straightforward. For example, an exact solution for some (few) many-body quantum systems is achievable, in the sense that each eigenstate can be uniquely characterized by a set of quantum numbers. However, this solution can in principle emerge from different techniques, and the integrability of the system may acquire consistency inside the technique itself, such as Bethe ansatz or Quantum Inverse Scattering method, through the rise of those quantum numbers.

Notice that the concept of integrability lives in many fields, such as differential geometry or fluid mechanics for its classical version, and condensed matter or string theory for its quantum counterpart. Our work will focus on the integrability of one-dimensional quantum systems in statistical physics. One can refer to these models also as (1+1)-dimensional models: 1 space + 1 time directions. In these integrable systems, the analytic solution is based on the fact that any scattering event between quasi-particles can be decomposed into a series of two-body scatterings. The direct consequence is that the elementary excitations cannot be created nor destroyed in a scattering event ruled by an integrable Hamiltonian. Anyway, due to the huge field we are diving in, let us first introduce the kind

of models we are dealing with, and remark differences and connections between classical and quantum ones.

1.1 Classical-quantum mapping

The quantum nature of a system in principle requires the use of quantum tools to deal with it, with the complications it entails, such as the exponential growth of the Hilbert space. However, if we find a way of encoding the quantum component of a model into classical degrees of freedom, the problem can be faced in a more skilled way. We do not expect to be thrown into an easy work environment, but the relatively deep knowledge of classical statistical systems would guarantee us significant facilitation to solve the quantum ones. In order to get familiar with this procedure, let us start by describing the classical-quantum mapping for the most famous chain in statistical physics: the Ising model.

1.1.1 One-dimensional Ising model

The introductory model to statistical physics is the Ising model [1], first introduced by Lenz in 1920. Then it was theoretically described in 1925 by one of his Ph.D. students in Hamburg, Ernst Ising, who showed the absence of a phase transition in the one-dimensional case. Its simplicity and its several applications make it very useful to get the fundamental notions about our subject. It is in the basement of magnetic phenomena and we can complicate it in many ways to get each time a different and specific system. The Hamiltonian of the classical Ising model is:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i, \quad \sigma_i = \pm 1. \tag{1.1}$$

The notation $\langle i, j \rangle$ means that we consider just neighboring sites, and we can do it even in more than one dimension. Here the spins σ_i are taken as scalar quantities, which can take only values $+1$ or -1, namely without any quantum nature. The parameter J identifies the strength of the spin-spin interaction while B is the external magnetic field. When $B = 0$ the system has Z_2 symmetry, which consists in the simultaneous flip of all the spins. In the absence of B, we can get the exact solution using a recursive method, which consists of computing the partition function Z_{N+1} in terms of the previous Z_N. An alternative way, good also for $B \neq 0$, is the transfer matrix method. It relies on the relationship that

links classical systems of statistical mechanics in d dimensions with quantum systems in $(d-1)$ and is based on the observation that the sum over the spin configurations can be equivalently expressed in terms of products of 2×2 matrices.
For example, if we consider a chain with N sites, we have:

$$H = -J\sum_{i=1}^{N-1}\sigma_i\sigma_j - B\sum_{i=1}^{N}\sigma_i, \quad \sigma_i = \pm 1. \tag{1.2}$$

Assuming periodic boundary conditions, i.e., $\sigma_i = \sigma_{N+i}$, the chain has ring geometry. Using the transfer matrix method, the partition function, i.e. the sum over all the possible configurations which can be used to obtain the main quantities characterizing the system, is:

$$H = \sum_{\{\sigma\}} T(\sigma_1,\sigma_2)T(\sigma_2,\sigma_3)\cdots T(\sigma_N,\sigma_1). \tag{1.3}$$

The T's are 2 by 2 transfer matrices acting on a two-dimensional vector space with basis elements corresponding to the spin-up and spin-down states, and it has matrix elements

$$T(\sigma,\sigma') = \exp\left[\beta J\sigma\sigma' + \frac{1}{2}\beta B(\sigma+\sigma')\right], \qquad \beta = \frac{1}{k_B T} \tag{1.4}$$

Thus V can be written as

$$T(\sigma,\sigma') = \begin{pmatrix} e^{\beta J}+e^{\beta B} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J-\beta B}\end{pmatrix} = e^{\beta J}\cosh(\beta B)\begin{pmatrix} 1+\tanh(\beta B) & e^{-2\beta J} \\ e^{-2\beta J} & 1-\tanh(\beta B)\end{pmatrix} \tag{1.5}$$

and it is easy to see that the product of V's correctly reproduces the Boltzmann weights of the Ising model configurations. Indeed, the transfer matrices have the role of connecting adjacent sites along the chain. Taking the limits $\beta B \to 0, \beta J \to \infty$ while keeping $\alpha = e^{2\beta J}\tanh(\beta B)$ finite, we get

$$T \simeq \text{const.} \times (I + e^{-2\beta J}(\sigma^x + \alpha\sigma^z)), \tag{1.6}$$

where I is the identity matrix in two dimensions and σ^x and σ^z are the Pauli matrices. The

associated quantum Hamiltonian is now easy to extract by identifying $\delta\tau = e^{-2\beta J}$, i.e. τ as quantum time-direction, yielding $H = -\sigma^x - \alpha\sigma^z$. These matrices are two-dimensional, so the Hilbert space for the associated quantum system is two-dimensional. Thus, this is the simplest non-trivial quantum system, often called a "two-state" quantum system. This can be seen as a sort of mapping onto a (0+1)-dimensional model. The terms are typically known respectively as a "transverse magnetic field" and just plain "magnetic field". The off-diagonal transverse field arises in the quantum Hamiltonian because in the classical model the spins of course can vary as one moves from slice to slice. In this simple case, it is easy to check that $[T, H] = 0$, so the transfer matrix and the Hamiltonian have the same eigenvectors. Although having a transfer matrix commute with the Hamiltonian is not typical behavior, such behavior occurs frequently in certain models in 1+1 dimensions. Such models are called integrable, and as a consequence, some quantities can be computed exactly by using techniques such as the Bethe ansatz.

1.1.2 Classical two-dimensional Ising model

The quantum-classical mapping can be described better considering a 2-dimensional Ising model on a square lattice, without external magnetic fields. Its Hamiltonian is:

$$H = -\frac{1}{2}\sum_{i=1}^{N-1} \sigma_{i,j}\left[J_x\left(\sigma_{i,j+1} + \sigma_{i,j-1}\right) + J_y\left(\sigma_{i+1,j} + \sigma_{i-1,j}\right)\right]. \tag{1.7}$$

The transfer matrix acts on a one-dimensional slice of spins, the vector space spanned by the set of all spins along the slice. Thus the resulting quantum Hamiltonian will act on a many-body system of spins in a row, so that this and similar one-dimensional quantum systems are typically referred to as "chains".

Going into details, consider the two directions in the square lattice: x (horizontal) and y (vertical). The horizontal one is conventionally the "principal" one, along which the global transfer matrix will act connecting adjacent columns. Anyway, this global transfer matrix is a composition of two transfer matrices: one acting along the horizontal axis and the other along the vertical axis, both connecting adjacent sites. We take different couplings, J_x and J_y, in the two directions for completeness. We remark that, in the classical Ising model, the spin variables are simply boolean. This means that here J_x and

J_y are not couplings between different components of the spin vectors, precisely because the spins are not vectors, and neither are operators. Only the following mapping will make them assume that role, due to the emergence of new σ's with a quantum nature, i.e. Pauli matrices. Thus, for a link along x, the situation is the same of the one-dimensional example, which consisted entirely of horizontal links. So, for each row, the "x"-transfer matrix is

$$W_i = \begin{pmatrix} e^{\beta J_x} & e^{-\beta J_x} \\ e^{-\beta J_x} & e^{\beta J_x} \end{pmatrix} = e^{\beta J_x}(I + e^{-2\beta J_x}\sigma_i^x). \tag{1.8}$$

For a link in the vertical direction, the transfer matrix is diagonal, measuring whether or not the two adjacent spins are the same:

$$V_{i,i+1} = e^{\beta J_y \sigma_i^z \sigma_{i+1}^z} = \cosh(\beta J_y) + \sigma_i^z \sigma_{i+1}^z \sinh(\beta J_y). \tag{1.9}$$

Considering periodic boundary conditions ($\sim$ all indices mod N) in the y-direction, the global transfer matrix that connects a whole column with N sites with the adjacent one is

$$T = \left(\prod_{i=1}^{N} V_{i,i+1} \right) \left(\prod_{i=1}^{N} W_j \right). \tag{1.10}$$

For M sites and periodic boundary conditions along the horizontal axis ($N \cdot M$ sites in the lattice totally) the partition function is

$$Z = \mathrm{tr}(T)^M. \tag{1.11}$$

At this point, we can connect this two-dimensional classical model with a one-dimensional quantum one. In order to achieve this, we find a limit where T is near the identity, i.e. $e^{-2\beta J_x} \to 0$, $\tanh(\beta J_y) \to 0$, while keeping $\lambda \equiv e^{2\beta J_x} \tanh(\beta J_y)$ finite. This limit sends $J_x \to \infty$ whereas $J_y \to 0$. Thus, the quantum Ising Hamiltonian is

$$H = -\lambda \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^{N} \sigma_i^x. \tag{1.12}$$

This object identifies a one-dimensional quantum system, because, doing our mapping, we singled out the x-direction as imaginary time. The fact that the limit sent J_x to ∞ can be seen as the sites in this direction became effectively close to each other like they are now overlapped, constituting a single site belonging to a one-dimensional chain of N sites along the y-direction. The same method can be generalized to higher-dimensional lattices.

From now on, we will focus on one-dimensional quantum systems. Indeed, there are several examples of degrees of freedom effectively constrained to move along a chain, since the transverse directions are energetically blocked. Therefore, the study of these systems will allow us to have a clever description of many physical models. But in doing this, we will keep in mind the possibility of this bilateral mapping between a d-dimensional classical system and a $(d-1)$-dimensional quantum one.

1.2 The Heisenberg model

The Heisenberg, or XXX, chain is a quantum one-dimensional system that well represents a one-dimensional quantum magnet. So, this time we are starting directly with a quantum model. Along the chain, each site hosts a spin variable which is now described by a three-dimensional vector $\mathbf{S}$ and that interacts with the adjacent sites. In the case of spin $\frac{1}{2}$ ($S_n^\alpha = \frac{\sigma_n^\alpha}{2}$ where σ_n^α are the Pauli matrices), the Heisenberg chain with N sites and p.b.c. has Hamiltonian:

$$H = -J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} = -J \sum_{i=1}^{N} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right). \tag{1.13}$$

Due to the overall minus sign, $J > 0$ identifies a FM regime, while $J < 0$ an AFM one. In terms of eigenstates of H, the value of J does not affect their structure, i.e. they will be the same in every regime and for any magnitude of the energy scale J. The ground state nature and the low-energy excitations will be sensitively affected by J, though. Considering H as an operator acting on a 2^N Hilbert space, the orthogonal basis elements are $|\sigma_1 \cdots \sigma_N\rangle$.

Let us see how this model is integrable in terms of Bethe ansatz technique, briefly introducing the aspects of the coordinate Bethe ansatz approach that will be useful in our work. It is based on the intuition that superpositions of plane waves would be exact eigenstates of the system, taking into account its symmetries. For example, the Heisenberg model has two main symmetries: SU(2) (rotational symmetry around all three axes) and translational (discrete and allowed by periodic boundary conditions). The ladder is due to the structure of the chain with equispaced sites. The former is evident since the Hamiltonian is just a sum of scalar products. At the moment, we will use only the U(1) rotational symmetry around one axis, the z one by convention, because the model remains integrable even if we apply an external magnetic field (say along z). Then, obviously, the full SU(2) symmetry will manifest itself making the spectrum degenerate for states in the same multiplet. Since the z-component of the total spin $S^z = \sum_{i=1}^{N} S_i^z$ is the generator of the aforementioned U(1) symmetry, then $[S^z, H] = 0$, i.e. S^z is a conserved quantum number. This allows us to consider a sector associated with each value of $S^z = \frac{N}{2} - R$. From this perspective, we can take $R = 0$, i.e. $S^z = \frac{N}{2}$, hosting the single reference state $|0\rangle = |\uparrow \cdots \uparrow\rangle$, since each $\uparrow$ contributes with $+\frac{1}{2}$. R is the number of flipped (down) spins, thus the $R = 1$ sector hosts N states $|n\rangle = S_n^-|0\rangle$ where n identifies which spin of the chain is flipped. While $|0\rangle$ is an eigenstate of H, $|i\rangle$ is not because it does not share with the Hamiltonian the property of being translationally invariant. Thus, we need to build linear combinations

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn}|n\rangle, \qquad k = \frac{2\pi m}{N}, \quad m = 0, ..., N-1, \tag{1.14}$$

which are now eigenstates of H. They represent the so-called ***magnon*** excitations, i.e. $\Delta S = 1$ excitations. They are an example of the quasi-particles that we introduced before, having a crucial role in the Bethe ansatz framework. It is relevant to keep in mind this classification of states in terms of the sector they live in, which is in turn identified by the number of spins flipped with respect to a reference state.

1.2.1 Ingredients of CBA

In this section, without going into details of the Coordinate Bethe ansatz, following [2] and [3], we would like to introduce some quantities that will become useful also in the Algebraic Bethe ansatz and in the Quantum Inverse Scattering Method. Let us start by saying that a magnon can be seen as a collective excitation of the chain which assumes, in our description, the role of a spin-1 quasi-particle. When we add another magnon, for example taking $R = 2$ we cannot take a mere superposition of magnons but we need to write a generic eigenstate of H in which 2 spins are flipped, which has the form:

$$|\psi\rangle = \sum_{1 \leq n_1 \leq n_2 \leq N} f(n_1, n_2)|n_1, n_2\rangle, \tag{1.15}$$

where $f(n_1, n_2)$, in the Bethe's ansatz, assumes the form of a superposition of two plane waves:

$$(n_1, n_2) = A\, e^{i(k_1 n_1 + k_2 n_2)} + A'\, e^{i(k_1 n_2 + k_2 n_1)}. \tag{1.16}$$

Imposing the eigenvalue equation $H|\psi\rangle = E|\psi\rangle$, with $E = E_0 + J\sum_{j=1,2}(1 - \cos k_j)$, we get the scattering phase relation:

$$\frac{A}{A'} \equiv e^{i\theta} = -\frac{e^i(k_1 + k_2) + 1 - 2e^{ik_1}}{e^i(k_1 + k_2) + 1 - 2e^{ik_2}}. \tag{1.17}$$

where θ is the scattering phase. We are describing the situation with the two magnons scattering with each other acquiring a phase shift on their momenta. So, k_1 and k_2, the quasi-momenta of the Bethe ansatz wavefunction are not the free magnon wave numbers. k_1 and k_2 can be determined by imposing p.b.c. $f(n_1, n_2) = f(n_2, n_1 + N)$ getting $e^{ik_1 N} = e^{i\theta}$ and $e^{ik_2 N} = e^{-i\theta}$. These are the *Bethe equations*, usually written in logarithmic form. So, taking the logarithm and summing the two identities we get

$$K = k_1 + k_2 = \frac{2\pi}{N}(I_1 + I_2), \tag{1.18}$$

where the momentum K is the quantum number associated with the translational symmetry of the Hamiltonian, really observable, whereas k_1 and k_2, and consequently the so-called Bethe numbers I_1 and I_2, identify the state, i.e., the Bethe ansatz wavefunction. Depending on their values, the solution can be real or complex. In the first case, the dispersion relation forms a continuum, highlighting the presence of an internal d.o.f. ($k = k_1 - k_2$). The complex solution, instead, is a bound state of two magnons, behaving

like a single object, without internal degrees of freedom.
This argument can be extended to $R > 2$ flipped spins, getting R relations between the phase shifts and the quasi-momenta:

$$Nk_j = 2\pi \hat{I}_j + \sum_{l \neq j} \theta(k_j, k_l), \qquad j = 1, ..., R, \tag{1.19}$$

where $\hat{I}_j \in \{0, 1, ..., N-1\}$.
Since $\theta(k_j, k_l) \neq \theta(k_j - k_l)$, in this form we do not have translational invariance in the momenta. To restore it we can introduce another fundamental quantity: the *rapidity* λ. It is a reparametrization of the momenta through the relation

$$k_j = \frac{1}{i} \ln \frac{\lambda_j + i}{\lambda_j - i} = \pi - \theta_1(\lambda_j), \quad \text{i.e.} \quad \lambda_j = \cot \frac{k_j}{2}, \tag{1.20}$$

through which

$$\theta(k_j, k_l) = -\theta_2(\lambda_j - \lambda_l) + \pi \, \mathrm{sgn}[\mathcal{R}(\lambda_j - \lambda_l)], \tag{1.21}$$

where

$$\theta_n(\lambda) \equiv 2 \arctan \frac{\lambda}{n}. \tag{1.22}$$

In terms of the rapidities, the Bethe equations (1.19) become

$$N\theta_1(\lambda_j) = 2\pi I_j + \sum_{l=1}^{R} \theta_2(\lambda_j - \lambda_l), \qquad j = 1, ..., R. \tag{1.23}$$

where $\{I_j\}$ are Bethe numbers intricately related to $\{\hat{I}_j\}$ but fortunately, for our purposes, we can use them without making explicit the relation. Indeed, our need is just that they give the proper counting of the states, as they do.

In the case of a single magnon, the solution is real and we can express the bare momentum and energy of the quasi-particle in terms of the quasi-momentum k entering the wave-function:

$$p_0(\lambda) = \frac{1}{i} \ln \frac{\lambda + i}{\lambda - i} = k \tag{1.24}$$

$$\epsilon_0(\lambda) = -J \frac{\mathrm{d}k}{\mathrm{d}\lambda} = \frac{2J}{\lambda^2 + i} = J(1 - \cos k). \tag{1.25}$$

Notice that the classification of complex solutions is not easy, even numerically, and it is still an open problem. However, in the thermodynamic limit ($N \to \infty$, system size $\to \infty$, while their ratio remains finite) we can assume the so-called *string hypotesis*: the complex solutions are arranged into strings in the complex plane, characterized by the same real part and equispaced imaginary components. For example, in (1.24) and (1.25) the subscript 0 stands for a 0-type string, corresponding to real solutions: the rapidity λ belongs to the real axis. Using these bare quantities, we can express the momentum and the energy of the eigenstates as:

$$K = \left[\sum_{j=1}^{R} p_0(\lambda_j)\right] \bmod 2\pi = \left[\pi\, R - \frac{2\pi}{N}\sum_{j=1}^{R} I_j\right] \bmod 2\pi, \tag{1.26}$$

$$E = E_0 + J\sum_{j=1}^{R} \epsilon_0(\lambda_j), \tag{1.27}$$

Notice that, in the quantization equations like (1.23), when I_j is an admissible quantum number, the corresponding solution k_j is said to be a *root* and, in the TD limit, we can denote the density of these solutions around k with the function $\rho^{(r)}(k)$. Anyway, these equations admit solutions in k_j also for integer values of $\bar{I}_j$, that are not admissible quantum numbers. The solutions associated with them are called *holes* and their density around k is $\rho^{(h)}(k)$.

1.2.2 String hypothesis

Now let us analyze the string hypothesis for the complex roots introduced in subsection (1.2.1). The word *hypothesis* stands for the fact that we do not know if the emerging solutions exhaust the whole Hilbert space. Anyway, we believe that they describe very well the thermodynamics of the chain: solutions "out" of the strings are less relevant for the analysis of systems at equilibrium.
Take the first interesting case $R = 2$, well described in [3], and write the Bethe equations:

$$\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^N = \frac{\lambda_1 - \lambda_2 + 2i}{\lambda_1 - \lambda_2 - 2i}, \tag{1.28}$$

$$\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^N = \frac{\lambda_2 - \lambda_1 + 2i}{\lambda_2 - \lambda_1 - 2i}. \tag{1.29}$$

and, consequently

$$\left(\frac{\lambda_1+i}{\lambda_1-i}\right)^N\left(\frac{\lambda_2+i}{\lambda_2-i}\right)^N=1. \tag{1.30}$$

Now, if $\mathrm{Im}(\lambda_1)\neq 0$, the LHS in eq.(1.28) increases (or decreases) exponentially as $N\to\infty$; so, to compensate, we need that

$$\lambda_1-\lambda_2=\pm 2i, \quad \text{i.e.} \quad \lambda_{1,2}\equiv\lambda_{\frac{1}{2}}\pm i. \tag{1.31}$$

The fact of having complex conjugated pairs as Bethe roots is actually a trademark of the Bethe ansatz, and it happens always, also for higher R.
The total energy and momentum of this state are real:

$$p_{\frac{1}{2}}=p_0(\lambda+i)+p_0(\lambda-i)=\frac{1}{i}\ln\frac{\lambda+2i}{\lambda-2i}, \tag{1.32}$$

$$\epsilon_{\frac{1}{2}}=\epsilon_0(\lambda+i)+\epsilon_0(\lambda-i)=\frac{4J}{\lambda^2+4}, \tag{1.33}$$

and give the dispersion relation

$$\epsilon_{\frac{1}{2}}(p)=\frac{J}{2}(1-\cos p_{\frac{1}{2}}). \tag{1.34}$$

If we take $R>2$, we assume that complex solutions can be organized into vertical *complexes* (or *strings*) of $2M+1$ rapidities in the complex plane, where M identifies the string, characterized by the same real value for all the rapidities. The admissible values for M are $0,\frac{1}{2},1,...$ and the rapidities associated with each M are:

$$\lambda_m^{(M)}+2im, \qquad m=-M,-M+1,...,M-1,M. \tag{1.35}$$

A state can have more than one complex of type M: the number of such M-complexes "inside" a state is denoted by ν_M. So, if we now take a state with a fixed magnetization, it has to satisfy the identity:

$$R=\sum_M(2M+1)\nu_M. \tag{1.36}$$

A string, containing $2M+1$ roots, can be seen as a group of spins that move together since they have the same real rapidity. Thus, in this framework, they can be considered as

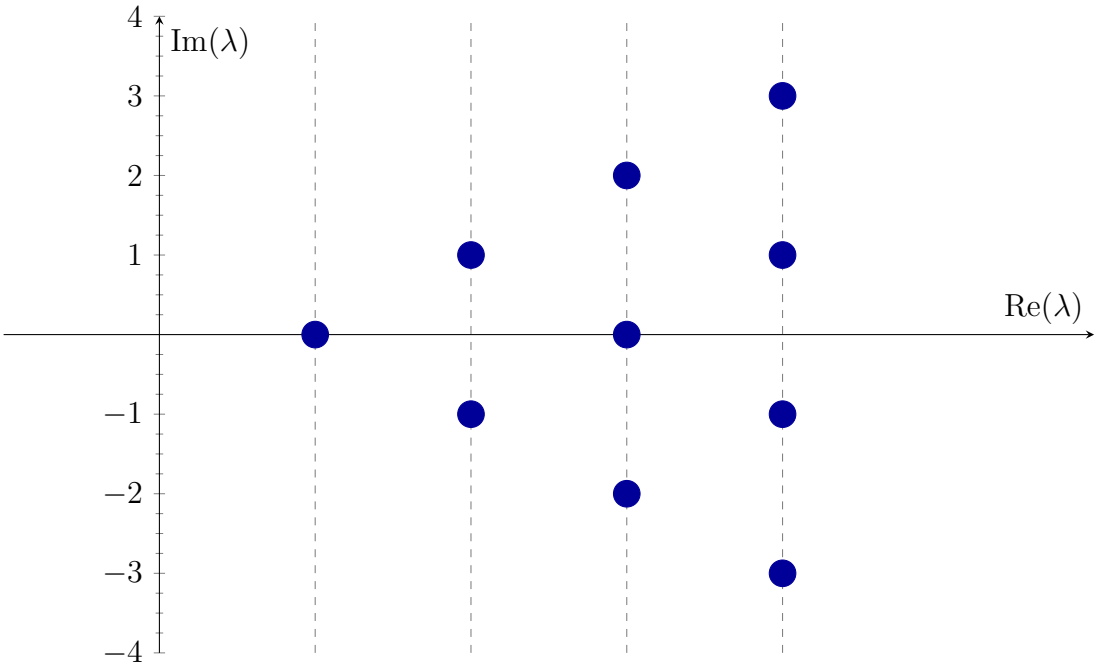


Figure 1.1: The figure shows how the strings lay on the complex plane. The rapidities (points) with the same real part belong to the same string. The first point on the left constitutes the whole 0-complex ($M = 0$) and it is a real solution. On its right, we find the $\frac{1}{2}$-complex ($M = \frac{1}{2}$) with two complex rapidities, equispaced by $2i$. The 1-complex comprehends a real root and two complex ones, still at the same distance. The $\frac{3}{2}$ complex has two pairs of complex rapidities, and this scheme repeats for higher M.

a single entity with precise momentum and energy, given by the sum of these quantities over all the rapidities within one string:

$$p_M(\lambda_M) = \sum_{m=-M}^{M} p_0(\lambda + 2im) = \frac{1}{i} \ln \frac{\lambda_M + i(2M+1)}{\lambda_M - i(2M+1)} \tag{1.37}$$

$$\epsilon_M(\lambda_M) = \sum_{m=-M}^{M} \epsilon_0(\lambda + 2im) = \frac{2J(2M+1)}{\lambda_M^2 + (2M+1)^2} = \frac{J}{2M+1}(1 - \cos p_M). \tag{1.38}$$

For example, in the previous $R = 2$ case, to satisfy eq.(1.36), we needed just one $\frac{1}{2}$-complex (i.e. $M = \frac{1}{2}$ and $\nu_{\frac{1}{2}} = 1$); thus, to get the whole momentum and energy of the state, we just had to sum along this single string constituted of two roots: $p_{\frac{1}{2}} = \sum_{m=-\frac{1}{2}}^{\frac{1}{2}} p_0(\lambda_{\frac{1}{2}} + 2im)$ and $\epsilon_{\frac{1}{2}} = \sum_{m=-\frac{1}{2}}^{\frac{1}{2}} \epsilon_0(\lambda_{\frac{1}{2}} + 2im)$.

Notice that the Bethe ansatz techniques are known to be powerful to solve many systems but, the string hypothesis, still being an hypothesis, is not completely clear how much

it can describe the reality. What we expect is that, it should be a good approximation of reality if ν_0, i.e. the number of single-particle (real) solutions, dominates over all the other complexes in the sum (1.36).

In any case, the facts that a spin chain's Hilbert space is finite and that momenta are constrained within a Brillouin zone impose some other constraints on the solutions. The first implies that not all quantum numbers are allowed: for example, the Bethe numbers associated with roots among the same M-complex must be different ($I_{M,j} \neq I_{M,j'}$), otherwise we get a vanishing solution. The second tells us that Bethe numbers are bounded: it can be computed that the maximum quantum number that characterizes a finite rapidity is

$$I_M^{max} = \frac{N-1}{2} - \sum_{M'} J(M,M')\nu_{M'} \qquad \text{where} \quad J(M,M') \equiv \begin{cases} 2\min(M,M') + 1 & M \neq M' \\ 2M + \dfrac{1}{2} & M = M' \end{cases} \tag{1.39}$$

Then, since all the scattering phases are odd functions of their argument, we have that

$$I_M^{min} = -I_M^{max}, \tag{1.40}$$

which implies that there exists an amount P_M of vacancies for a M-complex equal to

$$P_M = 2I_M^{max} + 1 = N - 2\sum_{M'} J(M,M')\nu_{M'}. \tag{1.41}$$

It can be proven that the number of states accessible within the string hypothesis scales like 2^N. Thus, only a few states are neglected in this framework: they are the ones that have a large number of complex rapidities that are not organized in strings, but are still able to satisfy the Bethe equations (1.19). This can happen because in these equations, the exponential growth/decay on the RHS can accidentally compensate the same behavior on the LHS. We remark that these solutions are not significant for the TD of the model but they can become useful to determine the completeness of the Bethe approach and for other investigations.

1.2.3 AFM case: $J = -1$

This brief recap on the CBA for the XXX model was useful to look at the backbone of the string hypothesis, which will be crucial for our investigation of the XYZ chain. Another fundamental ingredient in the Bethe ansatz approach is the identification of the ground state (or, more generally, of a reference state), in order to "build on it" the excited states, identified by specific quasi-particle excitations.

In this sense, the FM case is quite trivial. In fact, we can choose as ground state the completely polarized one $|0\rangle$ characterized by all the spins aligned, i.e. with overall spin $S = \frac{N}{2}$. Such a state is degenerate with all the other members of the $S = \frac{N}{2}$ multiplet. They can be obtained from $|0\rangle$ just by adding zero-momentum magnons, which possess zero bare momentum and zero bare energy (see eqs.(1.24),(1.25)), so they cannot change the energy of the system, keeping it in the ground state. If we want to get lower excited states from the vacuum, we can add bound state complexes, so we can refer to the ground state as a magnon-vacuum with quadratic dispersion relation for the excitations. In this case, lower excitations are not multiple-magnon excitations because it can be shown that the latter have higher energy than bound state complexes.

The AFM regime is instead very interesting, both for physical applications and to describe some new features of the Bethe ansatz technique. In particular, a new quasi-particle will emerge to describe the system: the ***spinon***.

The ground state in this regime has to be a state with all the spins flipped with respect to its neighbors. For the moment we are considering chains with an even number of sites N. So, the ground state has total spin $S = 0$, i.e., it lives in the $R = \frac{N}{2}$ sector. In the FM case, bounded states had lower energy than unbound magnons because that regime obviously favors the clustering of flipped spins. The opposite regime instead, implies the contrary hierarchy: unbound magnons have now lower energy and they will constitute the lower excitations. Actually, since we begin from the $R = 0$ reference state, we need these quasi-particle excitations even to get the ground state. What we do is add $\frac{N}{2}$ 0-complexes (unbound magnons), i.e., R real single quasi-particle excitations. In our notation:

$$\nu_0 = \frac{N}{2} \qquad \text{while} \quad \nu_M = 0, \text{ for} \quad M \geq \frac{1}{2} \qquad \xrightarrow{\text{eq.(1.36)}} \; R = \frac{N}{2}. \tag{1.42}$$

The total number of vacancies is given by (1.41):

$$P_0 = N - 2J(0,0)\nu_0 = N - \frac{N}{2} = \frac{N}{2}, \tag{1.43}$$

which coincides with the number of particle states. Thus, this time, the Bethe numbers occupy all the allowed vacancies (from (1.39) and (1.40)):

$$-\frac{N}{4} + \frac{1}{2} \leq I_{0,k} \leq \frac{N}{4} - \frac{1}{2} \tag{1.44}$$

and they are clearly integer for $\frac{N}{2}$ odd, while half-integer for $\frac{N}{2}$ even. The fact that the vacancies are all occupied means that there exists only one state with $\frac{N}{2}$ real magnons, which is the antiferromagnetic ground state $|\text{AFM}\rangle$.
Now, if we want to build excited states, we can take the ground state and substitute the real quasi-particles with complexes. The number of 0-complexes removed will be called κ and it will label the excited states:

$$\nu_0 = \frac{N}{2} - \kappa. \tag{1.45}$$

The example for κ=1 can be explicative on how we proceed in this framework: since we have just one quasi-particle to relocate, we cannot excite a M-complex with $M \geq 0$, hence we have $R = \frac{N}{2} - 1$, i.e., $S^z = 1$. Re-using eq.(1.41) we get the number of vacancies:

$$P_0 = N - 2 \cdot 2 \cdot \frac{1}{2}\left(\frac{N}{2} - 1\right) = \frac{N}{2} + 1 \Rightarrow P_0 = R + 2. \tag{1.46}$$

This means that we will place each quasi-particle, choosing R Bethe numbers among the P_0 possible ones, but two vacancies will remain empty. These two holes have to be chosen and this choice selects the excited state.
For higher κ the scheme is the same, but the situation becomes quickly complicated since we can populate also the complexes, and the way we do it characterizes the excitations above the ground state.

1.2.4 The emergence of the spinon in the TD limit

Fortunately, the Bethe equations simplify drastically in the thermodynamic limit ($N \to \infty$): the real roots become quasi-continuous and we can evaluate the density distribution of the state's rapidities.

Let us begin with the ground state, where all the roots are real the corresponding Bethe numbers fill the vacancies without holes. Assume $\frac{N}{2}$ to be odd, so that

$$I_{0,j} \equiv j, \qquad \text{with} \quad j = -\frac{N}{4} + \frac{1}{2}, -\frac{N}{4} + \frac{3}{2}, ..., \frac{N}{4} - \frac{1}{2}. \tag{1.47}$$

so that the BAE's take the form

$$\arctan \lambda_j = \pi \frac{j}{N} + \frac{1}{N} \sum_l \arctan \left(\frac{\lambda_j - \lambda_l}{2} \right). \tag{1.48}$$

As the variable $x = \frac{j}{N}$ becomes continuous and limited in $\left[-\frac{1}{4}, \frac{1}{4}\right]$ in the limit $N \to \infty$, the set of roots λ_j turns into the function $\lambda(x)$. The equation (1.48) becomes

$$\arctan \lambda(x) = \pi x + \frac{1}{N} \int_{-\frac{1}{4}}^{\frac{1}{4}} \arctan \left(\frac{\lambda(x) - \lambda(y)}{2} \right) \mathrm{d}y. \tag{1.49}$$

Now, since in this framework, the eigenvalues of local observables take the form of sums over roots, we change variables in order to integrate over λ, and not over x (the continuous form of the quantum numbers). The mapping $x \to \lambda(x)$ consists in sending the interval $-\frac{1}{4} \leq x \leq \frac{1}{4}$ into the whole real axis $-\infty \leq \lambda \leq \infty$, and the correspondence between the sum, the integral in $\mathrm{d}x$ and the one in $\mathrm{d}\lambda$ is:

$$\frac{1}{N} \sum_j f(\lambda_j) = \int_{-\frac{1}{4}}^{\frac{1}{4}} f(\lambda(x)) \mathrm{d}x = \int_{-\infty}^{\infty} f(\lambda) \rho_0(\lambda) \mathrm{d}\lambda. \tag{1.50}$$

The quantity $\rho_0(\lambda)$ is the density of real rapidities and it correspond to the Jacobian of the change of variable:

$$\rho_0(\lambda) = \frac{\mathrm{d}x}{\mathrm{d}\lambda} = \left. \frac{1}{\lambda'(x)} \right|_{x=\lambda^{-1}(\lambda)} \tag{1.51}$$

Differentiating eq.(1.49) with respect to λ we get a linear integral equation:

$$\frac{2}{1+4\lambda^2} = \pi \rho_0(\lambda) + \int_{-\infty}^{\infty} \frac{\rho(\mu)}{1+(\lambda-\mu)^2} \mathrm{d}\mu, \tag{1.52}$$

that can be conveniently written in the recurrent form

$$\rho_0(\lambda) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{K}(\lambda - \mu) \rho_0(\mu) \mathrm{d}\mu = \frac{1}{2\pi} \theta_1'(\lambda) \tag{1.53}$$

where $\mathcal{K}(\lambda-\mu)$ is the "kernel"

$$\mathcal{K}(\lambda-\mu) \equiv \frac{\mathrm{d}}{\mathrm{d}\lambda}\theta_2(\lambda) = \frac{4}{(\lambda-\mu)^2+4}. \tag{1.54}$$

Equation (1.52) can be solved by Fourier transform getting

$$\rho_0(\lambda) = \frac{1}{4\cosh(\frac{\pi\lambda}{2})}. \tag{1.55}$$

The momentum and energy of the g.s. are given by

$$K = N\int p_0(\lambda)\rho_0(\lambda)\mathrm{d}\lambda = \frac{\pi}{2}N \mathrm{mod} 2\pi \equiv K_{AFM}, \tag{1.56}$$

$$E = E_0 + N\int \epsilon_0(\lambda)\rho_0(\lambda)\mathrm{d}\lambda = N\left(\frac{1}{4}-\ln 2\right) \equiv E_{AFM}, \tag{1.57}$$

where p_0 and ϵ_0 are defined in (1.24) and (1.25).

Now take the case κ=1, i.e. $\nu_0 = \frac{N}{2}-1$ and $\nu_M = 0$ for $M \geq \frac{1}{2}$. The emerging states are characterized by two holes: we can select among the vacancies which quantum numbers are empty. Let us choose j_1 and j_2: the Bethe numbers are no longer $I_{0,j} \equiv j$ but

$$I_{0,j} = j + \theta_H(j-j_1) + \theta_H(j-j_2), \qquad \text{where} \quad \theta_H(j) = \begin{cases} 1 & j \geq 0 \\ 0 & j < 0 \end{cases} \tag{1.58}$$

We can now map $x_1 = \frac{j_1}{N}$ and $x_2 = \frac{j_2}{N}$ into λ_1 and λ_2 respectively, and recover the integral equation in this case for the real roots rapidity density $\rho_t(\lambda)$ (t stands for "triplet"):

$$\rho_t(\lambda) + \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathcal{K}(\lambda-\mu)\rho_t(\mu)\mathrm{d}\mu = \frac{1}{\pi(1+\lambda^2)} - \frac{1}{N}[\delta(\lambda-\lambda_1)+\delta(\lambda-\lambda_1)]. \tag{1.59}$$

Since we are dealing with linear equations, the solution of eq.(1.59) can be written as

$$\rho_t(\lambda) = \rho_0(\lambda) + \frac{1}{N}[\tau(\lambda-\lambda_1)+\tau(\lambda-\lambda_2)], \tag{1.60}$$

where $\tau(\lambda)$ is solution of the equation

$$\tau(\lambda) + \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathcal{K}(\lambda-\mu)\tau_t(\mu)\mathrm{d}\mu = \delta(\lambda). \tag{1.61}$$

Its Fourier transform is

$$\tilde{\tau}(\omega) = \frac{1}{1+\exp^{-2|\omega|}}. \tag{1.62}$$

Working directly in Fourier space we can compute its contribution to the momentum and energy of the states. Remember that the bare momentum and energy of the real 0-complexes (the only ones that can be populated for κ=1) are still p_0 and ϵ_0; what changes is the way they are occupied, i.e. the density distribution is now ρ_t. So we have:

$$K = N\int p_0(\lambda)\rho_t(\lambda) \;=\; K_{AFM} + k(\lambda_1) + k(\lambda_2), \tag{1.63}$$

$$E = N\int \epsilon_0(\lambda)\rho_t(\lambda) \;=\; E_{AFM} + \epsilon(\lambda_1) + \epsilon(\lambda_2), \tag{1.64}$$

where

$$k(\lambda) \equiv \frac{\pi}{2} - \arctan\sinh\frac{\pi\lambda}{2}, \tag{1.65}$$

and

$$\epsilon(\lambda) \equiv \frac{\pi}{2\cosh\frac{\pi\lambda}{2}}, \tag{1.66}$$

are the functions that identify the excitation that a hole generates in the system. It is clear that in our case, having two holes, the state we constructed (but equivalently also the others with κ=1 even if with a different choice of the position of the holes) has two excitations over the ground states. They are identified as collective excitations over the ground states, and they are called ***spinons***. Notice that they can exist only as collective excitations of the system in the TD limit, in the sense that they cannot be generated by a spin flip, since flipping a spin-$\frac{1}{2}$ creates a spin-1 excitation, and consequently, a finite number of flips generates integer spin excitations. They are typical of the AFM regime because they exist over a ground state ($|AFM\rangle$) that is far from a vacuum state ($|0\rangle$). We can imagine it as generated by flipping every spin after a given reference point along the chain. It is fascinating that this physical instance goes along with the mathematical identity $\sum_{n=1}^{\infty}(-1)^n = -\frac{1}{2}$ obtained by analytical continuation.

Combining (1.65) and (1.66) we can also get the dispersion relation of the single spinon excitation:

$$\epsilon(k) = \frac{\pi}{2}\sin k \qquad \text{with} \quad -\frac{\pi}{2} \le k \le \frac{\pi}{2}. \tag{1.67}$$

which can approximated to be linear for small k. The dispersion relations of two spinons are very different from the one of a pure spin-1 excitation made by one magnon since the former makes a band due to its composite nature, while the latter is a simple curved line.

Now we highlight the direct jump from zero to two spinons. Indeed it is a direct consequence of considering a chain with an even number of sites. In the case of N odd instead, individual spinons can exist due to the degeneracy between states belonging to two different sectors: $R = \frac{N-1}{2}$ and $R = \frac{N+1}{2}$. Remember this occurrence, because it will be fundamental for the purposes of this work.

Another interesting aspect of the AFM Heisenberg model is that if we consider the case K=2 we can have two situations:

1. we can keep $\nu_M = 0$ for $M \geq \frac{1}{2}$ getting a state with $S_z = 2$ and generating 4 holes;
2. we take $\nu_0 = \frac{N}{2} - 2$, and we start to populate a complex, the one with $M = \frac{1}{2}$ ($\nu_{\frac{1}{2}} = 1$ while $\nu_M = 0$ for $M \geq 1$). This keeps $R = \frac{N}{2}$ and $S_z = 0$.

In this last case, using 1.41 the vacancies are:

$$P_0 = \frac{N}{2} \qquad \text{and} \qquad P_{\frac{1}{2}} = 1. \tag{1.68}$$

This means that, having $\nu_0 = \frac{N}{2} - 2$ to be inserted among the $P_0 = \frac{N}{2}$ vacancies, we are left with 2 holes; while the $\frac{1}{2}$-complex has no freedom: its state is fixed since $\nu_{\frac{1}{2}} = 1$ fits exactly in the only $P_{\frac{1}{2}} = 1$ vacancy.
In the TD limit, solving the linear equation for the density of real roots $\rho_s(\lambda)$, we get the exact same expressions (1.65) and (1.66) we got for the momentum and energy in the K=1 case. This fact is a general feature in our framework: the contributions from the complex cancel out and the state has the same momentum, energy, and dispersion relation computed in the case without complexes, but with the same number of holes. Indeed, notice that we called the distribution density $\rho_s(\lambda)$ because this state is degenerate with the one with $\rho_t(\lambda)$, and while the former has magnetization $S^z = 0$ (singlet), the latter has $S^z = 1$ (triplet). So, also for higher K=1, it remains that the contribution of M-complexes to the momentum and energy identically vanishes, i.e., these quantities depend only on the number of particles ($\leftrightarrow$ real roots).
Anyway, we need to remark that these multiplets are exactly degenerate only at the

Heisenberg point and get split as we add anisotropy (e.g. XXZ or XYZ), associated with the SU(2) symmetry breaking.

1.3 The XXZ chain

A straightforward generalization of the XXX chain can be obtained by introducing the anisotropy along one of the axes, namely we modify one of the three couplings, say the one along z, getting a different magnitude and/or sign with respect to the other two. The model clearly loses its SU(2) symmetry but keeps the U(1) around the z-axis, i.e. on the XY plane. This means that the integrability of the model is still intact. Indeed, as you can remember, the construction of the Bethe ansatz solution for the XXX chain was based just on the U(1) symmetry, with the presence of the bigger SU(2) giving the degeneracy between states belonging to different R-sectors seen in the last paragraph.
This means that the CBA methodology remains the same, but the classification of the complex roots is more complicated, and the nature of the low-energy excitations changes.

1.3.1 Hamiltonian and possible regimes

The Hamiltonian of the XXZ model in the absence of an external magnetic field is:

$$H = -J \sum_{n=1}^{N} \left[S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z \right], \tag{1.69}$$

where we select periodic boundary conditions. Notice that if $|\Delta| = 1$ we recover the Heisenberg chain.
The various regimes are selected by the combinations of the two parameters J and Δ. We cite the most interesting ones for our purposes. Let us assume $J > 0$, namely *ferromagnetic* order preferred on the XY plane. The parameter Δ fixes the strength of the uniaxial anisotropy along the z direction, competing with the planar term: $|\Delta| < 1$ sets a planar regime, while $|\Delta| > 1$ an axial one. In the axial regime, if also Δ is positive, we have an axial ferromagnet, and an axial anti-ferromagnet if Δ is negative. This last regime is the crucial one for our aims.

In particular, for $\Delta < -1$, the phase is dominated by the Ising AFM along z of the $\Delta \to -\infty$ limit. Its ground states are the two degenerate Néel states $|N_1\rangle \equiv |\uparrow\downarrow\uparrow\downarrow\cdots\rangle$

and $|N_2\rangle \equiv |\downarrow\uparrow\downarrow\uparrow\cdots\rangle$. The low-energy excitations are constructed in terms of *domain walls*, i.e., regions where one type of Néel order changes into the other, thus creating two consecutive aligned spins. These states can be created by flipping a potentially macroscopic number of spins, but their energy cost only lies at the boundaries and does not depend on the number of flipped spins: this phenomenon generates fractionalized excitations (seen before for XXX), and each domain wall carries spin $S = \frac{1}{2}$, i.e. the simplest example of a spinon.

For $|\Delta| < 1$ we have a paramagnetic phase, reached passing through $\Delta = -1$, where happens a BKT (Berezinsky-Kosterliz-Thouless) type phase transition: the excitation spectrum goes from massive to gapless, but the ground state energy and all its derivatives are continuous across the point.

Having discussed the phenomenology of the system, let us solve the system analytically using the CBA approach.

1.3.2 Coordinate Bethe ansatz solution

As said before, we proceed with this solution exactly as for the isotropic case. Due to the U(1) symmetry, the magnetization along the z-axis

$$S^z \equiv \sum_{n=1}^{N} S_n^z \tag{1.70}$$

is a conserved quantity, commuting with H. This allows us to divide the problem into sectors of defined magnetization, considering only the case $0 \leq S^z \leq \frac{N}{2}$ since the negative magnetization solution can be recovered just by flipping all the spins.
Again, the reference state $|0\rangle$ is the ferromagnetic one with all spins up ($S^z = \frac{N}{2}$), it is unique in that sector and it is an eigenstate of the Hamiltonian. Considering magnetization $S^z = \frac{N}{2} - R$, the number of states in this sector is equivalent to all the possible configurations ($\{n_l\}$) that the system can assume by placing the R spin-flips. A generic state in this sector can be written as

$$|\Psi\rangle = \sum_{\{n_l\}} f(n_1, n_2, ..., n_R)|n_1, n_2, ..., n_R\rangle, \tag{1.71}$$

with

$$|n_1, n_2, ..., n_R\rangle \equiv S^-_{n_1} S^-_{n_2} \cdots S^-_{n_R} |0\rangle \tag{1.72}$$

the state with R spins flipped at the positions $\{n_l\}$. Since we took $S^z \geq 0$ without loss of generality, then $R \leq \frac{N}{2}$ and we mention that only for *even* N we can have $S^z = 0$ while for *odd* number of sites the magnetization is always a half-integer. The state (1.71) is obviously too generic, thus we have to impose some constraints to get proper eigenstates of H (1.69). With this in mind, we can directly analyze the eigenvalue equation for the Hamiltonian, i.e. applying directly H to the state (1.71):

$$\begin{aligned}(H - E)\Psi = &- \frac{J}{2} \sum_{j=1}^{R} (1 - \delta_{n_j+1, n_{j+1}}) \left[f(n_1, ..., n_j + 1, n_{j+1}, ..., n_R) + f(n_1, ..., n_j, n_{j+1} - 1, ..., n_R) \right] \\ &+ \left[E_0 - E + J\Delta R - J\Delta \sum_{j=1}^{R} \right] f(n_1, n_2, ..., n_R) \; = \; 0.\end{aligned} \tag{1.73}$$

Then, the ansatz consists again of writing the "amplitude" function in (1.71) as a superposition of plane waves. In subsection (1.2.1), we did it explicitly for $R = 2$, here we propose the version for any $0 \leq R \leq \frac{N}{2}$:

$$f(n_1, ..., n_R) \equiv \sum_{\mathcal{P}}^{R!} A[\mathcal{P}] \, e^{\sum_{j=1}^{R} k_{\mathcal{P}_j} n_j} = \Omega_R \sum_{\mathcal{P}}^{R!} \exp \left[\sum_{j=1}^{R} k_{\mathcal{P}_j} n_j + \frac{i}{2} \sum_{j<l}^{R} \tilde{\Theta}(k_{\mathcal{P}_j}, k_{\mathcal{P}_l}) \right], \tag{1.74}$$

where $\mathcal{P}$ is a permutation of the quasi-momenta k_j. The sum of all these momenta k_j gives the total momentum of the Bethe wave function (1.74): $K = \left(\sum_{j=1}^{R} \text{mod} 2\pi \right)$. Inserting (1.74) into (1.73), and after a few computations, we fix the scattering phases as

$$\Theta(k, k') \equiv \tilde{\Theta}(k, k') - \pi = 2 \left(\arctan \frac{\Delta \sin(\frac{k-k'}{2})}{\cos(\frac{k+k'}{2}) - \Delta \cos(\frac{k-k'}{2})} \right), \tag{1.75}$$

so that (1.74) is an eigenfunction of (1.73) with eigenenergy:

$$E = E_0 + J\Delta R - \sum_{l=1}^{R} \cos k_l. \tag{1.76}$$

Then, by imposing periodic boundary conditions, we get the following quantization relations on the scattering phases:

$$e^{ik_jN} = \prod_{j\neq l} e^{i\tilde{\Theta}(k_j,k_l)} = (-1)^{R-1} \prod_{j\neq l} \frac{e^{i(k_j+k_l)} + 1 - 2\Delta e^{ik_j}}{e^{i(k_j+k_l)} + 1 - 2\Delta e^{ik_l}}, \qquad j = 1, ..., R. \tag{1.77}$$

In their logarithmic form, they are the Bethe equations for our system:

$$Nk_j = 2\pi \tilde{I}_j - \sum_{l=1}^{R} \Theta(k_j, k_l), \qquad j = 1, ..., R, \tag{1.78}$$

where the $\{\tilde{I}_j\}$ are the quantum numbers defining the state.
Again, let us reparametrize the quasi-momenta k_j in terms of the rapidities $\tilde{\lambda}_j$ as

$$e^{ik_j} = \frac{\sin\frac{\phi}{2}(\tilde{\lambda}_j + i)}{\sin\frac{\phi}{2}(\tilde{\lambda}_j - i)}, \tag{1.79}$$

where the parameter ϕ is fixed by requiring the coveted translational invariance of the scattering phase, i.e., being a function of rapidity difference only; this constraint sets

$$\cosh\phi = \Delta. \tag{1.80}$$

Now, rewriting the Bethe equations (1.78) in terms of these new variables, we have:

$$N\tilde{\theta}_1(\tilde{\lambda}_j) = 2\pi I_j + \sum_{l\neq j}^{R} \tilde{\theta}_2(\tilde{\lambda}_j - \tilde{\lambda}_l), \qquad j = 1, ..., R, \tag{1.81}$$

where

$$\tilde{\theta}_n(\tilde{\lambda}) \equiv 2\arctan\left[\coth\left(\frac{n\phi}{2}\right)\tan\left(\frac{\tilde{\lambda}\phi}{2}\right)\right]. \tag{1.82}$$

At this point, we can also write the momentum and energy of the system, in terms of rapidities:

$$K = 2\sum_{j=1}^{R} \cot^{-1}\frac{\tan(\frac{\phi\tilde{\lambda}_j}{2})}{\tanh\frac{\phi}{2}}, \tag{1.83}$$

$$E = E_0 + \sum_{j=1}^{R} \tilde{\epsilon}(\tilde{\lambda}_j), \tag{1.84}$$

where

$$\tilde{\epsilon}(\tilde{\lambda}) \equiv -J\frac{\sinh^2\phi}{\cosh\phi - \cos(\phi\tilde{\lambda})} \tag{1.85}$$

is the quasi-particle energy.

We can observe that the phase $\tilde{\theta_1}(\tilde{\lambda}_j)$ is actually the original quasi-momentum k_j. Thus we can write also the quasi-particle momentum in terms of $\tilde{\lambda}_j$ as

$$p(\tilde{\lambda}_j) \equiv \tilde{\theta_1}(\tilde{\lambda}_j) = k_j \tag{1.86}$$

and the associated dispersion relation as

$$\tilde{\epsilon}(\tilde{\lambda}) = -\frac{\sinh\phi}{\phi}\frac{\mathrm{d}}{\mathrm{d}\tilde{\lambda}}p(\tilde{\lambda}) = J(\Delta - \cos k). \tag{1.87}$$

In order to study better the string solutions of the XXZ, it is worth going through another reparametrization of the rapidities:

$$\lambda = \phi\tilde{\lambda} \tag{1.88}$$

that sends us from $\tilde{\theta_1}(\tilde{\lambda}_j) = k_j$ to

$$\theta_1(\lambda_j) = k_j, \tag{1.89}$$

and allows us to rewrite the last expression (1.81) for the Bethe equations as

$$N\theta_1(\lambda_j) = 2\pi I_j + \sum_l \theta_2(\lambda_j - \lambda_l), \qquad j = 1, ..., R. \tag{1.90}$$

where functions θ_n depend now also on ϕ, and they are different depending on the regime selected.

So far, we have introduced the basic elements for our description of the XXZ, namely the nature of its quasi-particle excitations. Though, we know that the CBA solution has its own features in each regime of the system, in turn, selected by Δ, or equivalently by ϕ. Therefore, let us focus on the solution of the two most interesting regimes for our needs: the paramagnetic ($|\Delta| < 1$) and the uni-axial antiferromagnet ($\Delta = 1$).

1.3.3 Paramagnetic regime: $|\Delta| < 1$

In this phase, the magnitude of the couplings in the XY plane is greater than the one along z, and we will focus on the $\Delta < 0$ regime. The most relevant aspect is that it hosts gapless excitations, while the uni-axial ferromagnet ($\Delta > 1$), for example, has gapped

magnon excitations: $\epsilon_M(p_M = 0) \neq 0$.
Using the relation (1.89), we notice that real rapidities (as we know, associated with the ground state) generate real quasi-momenta constrained in an interval $k \in [-(\pi-\gamma), \pi-\gamma]$ depending on a parameter $\gamma = -i\phi$ which goes to 0 as $\Delta \to -1$ and goes to π as $\Delta \to -1$. If the quasi-momenta are outside this interval, they correspond to rapidities lying on the $i\pi$ horizontal axis. The "problem" for this phase is that the function $k(\lambda)$ is periodic in the imaginary axis, in the sense that $k_j = k(\lambda_j) = k(\lambda_j + i2\pi)$.
The ground state is given by pure, real rapidities, filling the Fermi sea, whose density, in the TD limit, is the solution of the integral equation (1.53):

$$\rho_0(\lambda) + \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathcal{K}(\lambda-\mu)\rho_0(\mu)\mathrm{d}\mu = \frac{1}{2\pi}\theta_1'(\lambda). \tag{1.91}$$

which comes from the Bethe equations (1.90). With respect to the XXX version (1.53) we have a different kernel function:

$$\mathcal{K}(\lambda) \equiv \frac{\mathrm{d}}{\mathrm{d}\lambda}\theta_2(\lambda) = \frac{\sin(2\gamma)}{\cosh\lambda - \cos(2\gamma)}. \tag{1.92}$$

The magnetization of this state, in the usual scheme, is

$$S^z = \frac{N}{2} - N\int_{-\infty}^{\infty} \rho_0(\lambda)\mathrm{d}\lambda, \tag{1.93}$$

and its energy is

$$E = E_0 + N\int_{-\infty}^{\infty} \epsilon_0(\lambda)\rho_0(\lambda)\mathrm{d}\lambda \tag{1.94}$$

where

$$\epsilon_0(\lambda) \equiv -J\sqrt{1-\Delta^2}\,\theta_1'(\lambda) = -J\frac{\sin^2\gamma}{\cosh\lambda - \cos\gamma}. \tag{1.95}$$

is the (bare) single magnon energy.
Assuming N even, the lowest energy state has zero magnetization, and thus is given by $\frac{N}{2}$ real rapidities (*half filled* sector), which exhausts the allowed vacancies.

1.3.4 Spectra of spinons and magnons in the paramagnetic phase

Following the approach proposed in subsection (1.2.4), we can analyze the elementary excitations of the XXZ chain. Similarly, these low-energy excitations are obtained by removing κ real rapidities from the ground state contribution. Each removal leaves two

holes among the allowed vacancies: these holes are the already introduced *spinons*. Using the "new" kernel function, we can perform the same kind of computations done for the Heisenberg chain, obtaining the momentum and energy carried by each spinon:

$$k(\lambda) \equiv \frac{\pi}{2} - \arctan\left(\sinh\frac{\pi\lambda}{2\gamma}\right), \tag{1.96}$$

$$\epsilon(\lambda) \equiv J\frac{\pi}{2}\frac{\sin\gamma}{\gamma}\frac{1}{\cosh\frac{\pi\lambda}{2\gamma}}, \tag{1.97}$$

yielding the dispersion relation

$$\epsilon(k) = J\frac{\pi}{2}\frac{\sin\gamma}{\gamma}\sin k. \tag{1.98}$$

One interesting feature of the XXX chain was the degeneracy between the singlet and triplet states, i.e. pairs of spinon excitations had the same energy as solutions with other M-complexes. That relied on the SU(2) symmetry of the isotropic chain, now broken in the XXZ. Thus, in the latter, for each state one has to determine the contributions from each excitation separately.

Another novelty of this model is the fact that additional real excitations (k real) can be generated by placing on the $i\pi$ axis some of the κ rapidities just removed from the real axis. The associated spectrum can be computed through the usual techniques, getting

$$\epsilon(k) = J\pi\frac{\sin\gamma}{\gamma}\left|\sin\frac{k}{2}\right|\sqrt{1+\cot^2\left[\left(\frac{\pi}{\gamma}-1\right)]\frac{\pi}{2}\right]\sin^2\frac{k}{2}}. \tag{1.99}$$

Each of these excitations carries $S^z = 1$ and this reminds us of a magnon, but we have to be careful. For example, in the $\Delta \to 1$ ($\gamma \to \pi$) limit, they approach the magnonic dispersion relation, but they are physical only for $0 < \Delta < 1$. Indeed, for $\Delta > 0$ their contribution vanishes in the linear approximation, and magnons can only appear in high-energy states. At low momentum, their dispersion relation is the same as individual spinons, but since the latter appear in pairs and are composite excitations, they are actually distinguishable. Moreover, their momentum range is complementary to that of the spinon excitations. To sum up, low-momentum magnons can only appear close to $\Delta = 1$.

1.3.5 String solutions in the paramagnetic phase

Real solutions (i.e., $\mathrm{Im}(\lambda) = 0$) are the basis of the thermodynamics of the system. The influence of (non-0)-complexes instead, depends on the nature of the system itself and is actually still difficult to evaluate. In any case, we must take them into account, since their effects could always be structural. In the XXZ case, in the paramagnetic phase, string solutions are higher energy states compared to unbound states. However, due to their number and structure, they contribute significantly to the dynamics of the model. Moreover, unlike its isotropic counterpart, here not all complexes are allowed in the paramagnetic phase. This makes the problem of accounting for them very controversial.

The fundamental constraint for the strings comes from the normalizability of the wave function. To show it, consider a M-complex, with overturned spins at positions $n_1 < n_2 < \cdots < n_{2M+1}$. The relevant parts of the wave function can be written as

$$f(n_1, ..., n_{2M+1}) = (z_1 z_2 \cdots z_{2M+1})^{n_1} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} \left[\prod_{j<l} \sinh \frac{1}{2}(\lambda_{\mathcal{P}_j} - \lambda_{\mathcal{P}_l} + 2i\gamma) \right] \prod_{n=1}^{2M} \left(\prod_{nl=+1}^{2M+1} z_{\mathcal{P}_l} \right)^{n_{j+1}-n_j} \tag{1.100}$$

where $z_j \equiv e^{ik_j} = \frac{\sinh \frac{1}{2}(i\gamma - \lambda_j)}{\sinh \frac{1}{2}(i\gamma + \lambda_j)}$.
When $\mathrm{Im}(\lambda_j) \neq 0$, then $|z_j| \neq 1$; so, assuming $\mathrm{Im}(k_j) \geq \mathrm{Im}(k_{j+1})$, for the wave function not to explode we need to require

$$|z_1 z_2 \cdots z_{2M+1}| = 1 \qquad \text{and} \qquad \left| \prod_{l=n+1}^{2M+1} z_l \right| < 1 \qquad n = 1, ..., 2M. \tag{1.101}$$

These conditions guarantee that one of the permutations yields a normalizable wave function. We still have to force all the others to vanish. To do this we can select the following string structure for bound states:

$$\lambda_{M,j} = \lambda_M + \frac{1-\eta}{2}\pi + i\,2(M-j)\gamma \qquad j = 0, ..., 2M, \tag{1.102}$$

where we introduced the parameter $\eta = \pm 1$, which identifies the "*parity*" of the string and divides the complexes into two types: the ones with the center of mass lying on the real axis ($\eta = +1$) and lying on the $i\pi$ axis ($\eta = -1$).

We can compute the momentum and energy of these M-complexes:

$$p_M(\lambda_M) = \frac{1}{i} \ln \frac{\sinh \frac{1}{2}\left[i(2M+1)\gamma - \lambda_M - i\frac{1-\eta}{2}\pi\right]}{\sinh \frac{1}{2}\left[i(2M+1)\gamma + \lambda_M + i\frac{1-\eta}{2}\pi\right]}, \tag{1.103}$$

$$\epsilon_M(\lambda_M) = -J \frac{\sin\gamma \, \sin[(2M+1)\gamma]}{\eta \cosh\lambda_M - \cos[(2M+1)\gamma]}. \tag{1.104}$$

and their dispersion relation:

$$\epsilon_M(p_M) = -J \frac{\sin\gamma}{\sin[(2M+1)\gamma]} \left[\cos[(2M+1)\gamma] + \cos p_M\right]. \tag{1.105}$$

In addition, concerning the accounting problem we mentioned earlier, we can extract the range limitation for the momenta of the strings:

$$\cos p_M > -\cos[(2M+1)\gamma] \qquad \text{for } \eta = +1, \tag{1.106}$$

$$\cos p_M < -\cos[(2M+1)\gamma] \qquad \text{for } \eta = -1, \tag{1.107}$$

showing that it depends on the length M and parity η of the string, and on γ (i.e. Δ). We also have other constraints coming from the second equation in (1.101):

$$\eta \, \sin[(2M+1-n)\gamma] \, \sin[n\gamma] > 0 \qquad n = 1, ..., 2M. \tag{1.108}$$

At *roots of unity*, i.e. points at which $\gamma = \frac{p}{q}\pi$ with p and q co-prime numbers, these constraints mean that only strings shorter than q are allowed. Irrational values of $\frac{\gamma}{\pi}$ can be approximated by continued fractions to work out the selection rules. Although the cumbersome nature of this solution, the results are in good agreement with the actual behavior of the systems.

1.3.6 Uni-axial antiferromagnet: $\Delta < -1$

We close this section on the CBA describing the other possible antiferromagnetic situation: the uni-axial antiferromagnet. In this regime, the ground state has zero magnetization $S^z = 0$ and is given by $\frac{N}{2}$ magnons lying on the $|0\rangle$ ferromagnetic reference state. Then, we proceed as usual, solving the integral equation (1.91) for the density of real rapidities obtained in the TD limit. To do so, we need to point out that $\Delta < -1$ imposes a precise range on the quasi-momentum k, i.e. on λ, as said at the beginning of subsection (1.3.3).

In this phase $Re(k) \in (-\pi, \pi)$ and this interval is mapped into $Re(\lambda) \in (-\pi, \pi)$; this means that this time the integral in (1.91) goes from $-\pi$ to π. Moreover, the Kernel function $\mathcal{K}(\lambda) \equiv \frac{\mathrm{d}}{\mathrm{d}\lambda}\theta_2(\lambda)$ assumes the form

$$\mathcal{K}(\lambda) = \frac{\sinh(2\phi)}{\cosh(2\phi) - \cos\lambda}. \tag{1.109}$$

Thanks to periodicity, the integral equations can be solved through Fourier transform, getting a situation in which, for $\frac{N}{2}$ real rapidities, the number of vacancies allowed is $\frac{N}{2}+1$. This gives a singular behavior: the ground state configuration generated by a symmetric distribution of quantum numbers turns out to be nearly degenerate with one in which these numbers are shifted by one unity. But while the first has zero momentum, the second has π: in the $\Delta \to -\infty$ limit these two states become the the symmetric/antisymmetric combination of the two Néel states: $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle \pm |\downarrow\uparrow\downarrow\uparrow\cdots\rangle$.
Instead, low-energy excitations are 2K spinons generated by removing K rapidities from the ground states. Each spinon contributes with energy [4] [5]

$$\epsilon(k) = J\frac{\sinh\phi}{\pi} I(k)\sqrt{1 - k^2\cos^2 k} \tag{1.110}$$

where

$$I(k) \equiv \int_0^{\frac{\pi}{2}} \frac{\mathrm{d}\theta}{\sqrt{1 - k^2\sin^2\theta}} \tag{1.111}$$

is the *complete elliptic integral* of the first kind.

Even if we will not make use of the Coordinate Bethe ansatz in the following, the description of this method is fundamental to fixing in mind the concept of the string hypothesis and to understanding its "second quantized version" called *Algebraic Bethe ansatz* (ABA).

1.4 Recap on classical and quantum integrability

In the case of classical systems and in quantum field theories, what makes a system integrable is an infinite number of conserved charges. For a discrete (1+1)-dimensional quantum system like the XXZ spin chain, this condition is not sufficient since, for any quantum mechanical system, the set of projectors onto the eigenstates of a Hamiltonian is a complete set of charges in convolution with one-another and with the Hamiltonian itself. This sort-of-integrability is the reflection of the fact that the Schrödinger equation

is essentially a linear differential equation. For this reason, the actual integrability relies on the technique we used to solve the system. What emerged was the possibility of identifying its integrability in the Coordinate Bethe ansatz framework. What we can say now is that Ising, Heisenberg, and XXZ, for example, *are known to be* integrable. If we insert another anisotropy, therefore selecting the XYZ model, for all we know so far, we must appeal to the previously enhanced quantum-classical mapping. Indeed, we leverage the mapping of the quantum 1D chain into the 2D classical 8-vertex model, that we are about to introduce. There, we make use of the Quantum Inverse Scattering Method techniques, relying on the manipulation of one fundamental object: the transfer matrix, already introduced in the Ising model section (1.1). Since this transfer matrix commutes with the Hamiltonian of the original quantum system, searching for its spectrum we also recover the eigenenergies of the physical model. Notice that this method can be used also to solve the XXZ chain, through its mapping into the 6-vertex model [2] [3]. Anyway, in the case of XYZ, this can be seen not only as a solving technique but as the basis of the quantum integrability of our system. At this point, we know that we can, in principle, recover its spectrum and its eigenstates. Thus, in general, a quantum system is said to be integrable when we use a technique and it technically happens to be integrated.

1.5 Algebraic Bethe ansatz

The Algebraic Behte-ansatz can be seen as the second quantization of CBA in the sense that we will deal directly with operators instead of wave functions. Actually, wave functions will still lie under our talk, but the direct work will be done on matrices operating on an enlargement of the physical space. The ABA is in one-to-one correspondence with the Quantum Inverse Scattering Method (QISM) [6], introduced by Bogoliubov, Izergin, and Korepin, and whose name will be clear soon.
The ABA is based on the previously remarked relation between two-dimensional classical integrable systems and one-dimensional quantum ones. The former are based on the formalism of the *transfer matrices* that allow us to construct the partition function of the model, known to encode all the thermodynamics. If we want to summarize it, in ABA we apply certain operators to a reference state (called *pseudo-vacuum*) to generate other states (wave functions), and to do so, we use the Yang-Baxter algebra that these transfer matrices obey.

1.5.1 Technicalities of the ABA

The previously mentioned enlargement of the physical space is the first main feature of this approach. Indeed, the introduction of some auxiliary space or variable allows us to decouple the interaction: the physical d.o.f.s do not interact among themselves, but only with the entities in the auxiliary space. Then, after getting the solution for the whole enlarged space, we can trace out the auxiliary variables and recover the physical original model solution. This auxiliary space's insertion corresponds to the addition of a probe that propagates inside the real system and interacts with the physical variables.

Talking in operators, the most relevant entity is the *transfer matrix* $\mathbf{T}(\lambda)$ of the system, whose role and construction will be clear when built specifically for our XYZ spin chain. By now, we can say that it depends on the *spectral parameter* λ, which can be seen as the rapidity of the probe injected in the system. The transfer matrix operates in the physical Hilbert space $\mathcal{H}$, i.e. $\mathbf{T}(\lambda) : \mathcal{H} \to \mathcal{H}$, and commutes with the Hamiltonian. If we add the auxiliary space $\mathcal{V}_a$ (subscript a in case we need more than one copy of the aux. space), we introduce an operator, strictly connected to the transfer matrix, that acts in the enlarged space: the *monodromy matrix* $\mathcal{T}_a(\lambda) : \mathcal{H} \times \mathcal{V}_a \to \mathcal{H} \times \mathcal{V}_a$. This connection consists of the possibility of recovering the transfer matrix just by tracing over the ancillary space: $\mathbf{T}(\lambda) = \mathrm{tr}_a \mathcal{T}_a(\lambda)$.
The freedom on the value of λ is necessary to define a whole family of $\mathbf{T}$'s, commuting with one another independently of λ. The integrability of the model is strictly bound to these commutation relations. Indeed, they guarantee the transfer matrix to be a generating function of a series of conserved charges, among which we can find the Hamiltonian of the original system. Therefore, if we diagonalize the transfer matrix we consequently get the eigenvectors of the Hamiltonian, too.

1.5.2 Yang-Baxter equation

From now on, we need to get familiar with the concept of *consistency relations*, as they are fundamental in this framework. In the Coordinate Bethe ansatz we worked directly with the eigenfunctions of the system. Instead, the ABA structure, and then the integrability itself, relies on the properties of some peculiar operators. For example, in the CBA, the Bethe equations came from quantization relations, explicitly imposed on the ansatz wave function. In this sense, they were probably more physically intuitive than their ABA

counterpart. Indeed, at some point they will emerge, as trademarks of Bethe ansatz techniques; but they will just descend from the consistency relations involving those matrices. In particular, the integrability of the model is encoded in the property that the order of application of two monodromy matrices is related by a similarity transformation. The latter is realized by another operator: the *intertwiner* or $\mathcal{R}$-*matrix* $\mathcal{R}_{a,b}(\lambda) : \mathcal{V}_a \times \mathcal{V}_b \to \mathcal{V}_a \times \mathcal{V}_b$, and the identity can be written as

$$\mathcal{T}_a(\lambda)\,\mathcal{T}_b(\mu)\,\mathcal{R}_{a,b}(\mu-\lambda) = \mathcal{R}_{a,b}(\mu-\lambda)\,\mathcal{T}_b(\mu)\,\mathcal{T}_a(\lambda). \tag{1.112}$$

This relation owes its existence to another equation satisfied by the R-matrix on its own, the so-called *Yang-Baxter equation* (YBE):

$$\mathcal{R}_{1,2}(\lambda-\mu)\,\mathcal{R}_{1,3}(\lambda-\nu)\,\mathcal{R}_{2,3}(\mu-\nu) = \mathcal{R}_{2,3}(\mu-\nu)\,\mathcal{R}_{1,3}(\lambda-\nu)\,\mathcal{R}_{1,2}(\lambda-\mu), \tag{1.113}$$

where the subscripts indicate on which two out of the three copies of the auxiliary space the intertwiner acts.
Here comes the explanation of the word *inverse* in the name Quantum Inverse Scattering Problem: intuitively, we should take a quantum system and look for its intertwiner matrix, since each solution of the YBE (1.113) generates a family of integrable models. Actually, the aim of recovering the R-matrix starting from the system is quite complicated to pursue. For this reason, in practice, we travel in the opposite direction: first, we look for solutions of eq.(1.113), and then we recover which integrable model they are associated with. The word *scattering* is to remind us that the probe pictorially scatters with the degrees of freedom of the physical chain. The other two words' meaning is pretty clear.

After this brief smattering about ABA, we do not expect that the method is clear, but this section was useful in introducing the cornerstones of this new technique. Now, it is time to enter the model on which this work is about, the XYZ spin chain: you will see that the Algebraic approach will be much clearer when directly seen on the battlefield.

Chapter 2

The XYZ spin chain

Among the family of the one-dimensional spin-$\frac{1}{2}$ chain, we can decide to switch on all the nearest-neighbor interactions. This is what happens in the Heisenberg model. Looking back at its Hamiltonian in eq.(1.13), it is clear that the coupling is the same for the interaction between each component of the vector spin. If we want to introduce anisotropy along one of the three axes, we can select a different coupling between the z-component, for example, getting the XXZ model. When all three couplings are different, the anisotropy is complete, giving us the XYZ spin chain. This is the most general model since the previously introduced chains can be recovered from it just by performing the appropriate limit.

In this chapter, we are going to introduce the physics of this chain and show in which sense it is integrable in the Algebraic Bethe ansatz framework.

2.1 The Hamiltonian

Let us start by introducing the Hamiltonian of the quantum XYZ spin chain with N sites [7]:

$$H = \sum_{i=1}^{N} \left(J_x \sigma_i^x \sigma_{i+1}^x + J_y \sigma_i^y \sigma_{i+1}^y + J_z \sigma_i^z \sigma_{i+1}^z \right) \tag{2.1}$$

In order to be clear, let us recap the basic features of the model, even at the risk of being redundant: J_x, J_y and J_z are real parameters, while, as usual, σ_j^α is the appropriate Pauli matrix as acting on site. We assume *periodic boundary conditions* (PBC), i.e. $\sigma_{L+1}^\alpha = \sigma_1^\alpha$.

When J_x, J_y and J_z are all unequal we have the XYZ model, but we can recover the XXZ by selecting $J_x = J_y = 1$, $J_z = \Delta$ and the XXX by choosing $J_x = J_y = J_z = 1$, except for a common multiplying factor. We remark that the XYZ is integrable with the following techniques for arbitrary values of the couplings J_α, but integrability would be broken if we added an external arbitrary magnetic field. Notice that, by now, no assumption on the number of sites has been made: N is finite and, if not specified, it can be either even or odd. Distinctions will be made when necessary.

As from the Heisenberg to the XXZ chain we lost the SU(2) symmetry to remain with the U(1), introducing another anisotropy we threw the U(1) to keep the Z_2 only. Indeed, there is no rotational symmetry left, but if we reverse every spin with respect to one of the three principal planes, the system remains the same. However, you can remember that the U(1) symmetry was crucial for the CBA approach, both in the XXX and in the XXZ model. Thus, remember the lack of this symmetry, because we will need a trick to overcome it.

Historically, the first physicist to solve this model, for N even, was Baxter in 1972 [8]. In section (2.2) we are going to introduce, mainly following [9], the fundamental elements the solution cannot bypass.

2.2 8-vertex transfer matrix construction

As we said, nowadays, the integrability of this one-dimensional quantum chain is obliged to pass through the mapping into the classical two-dimensional 8-vertex model. So, the first step, for every attempt to integrate the XYZ is this mapping. Notice that the connection is not immediately intuitive, but will be clear later.

First, we have to select the 8-vertex model: take a two-dimensional square lattice with M rows and N columns (N sites per row). Each site of the lattice is a vertex that can assume a particular configuration, depending on how it is connected with its nearest neighbors. In fig.(2.1) we show the eight possible configurations. Then, we have to build the $2^N \times 2^N$ transfer matrix which connects two successive rows of the lattice. This is realized by summing over all the possible configurations along one row. Its elements are:

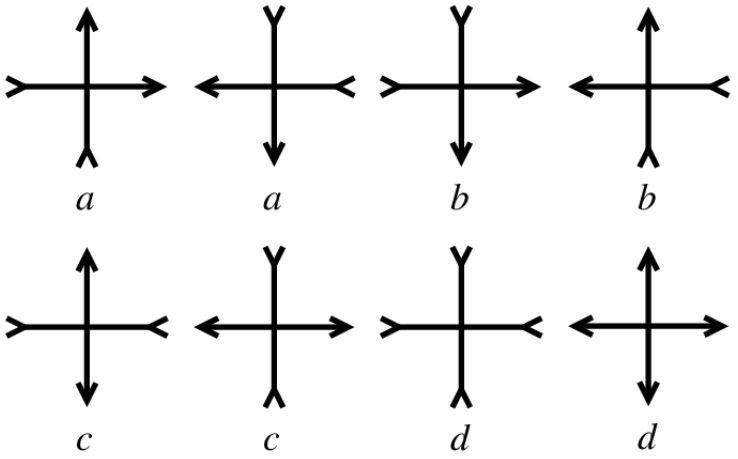


Figure 2.1: The figure shows the 8 possible configurations each vertex can assume in the 8-vertex model. The letters (a, b, c, or d) under each vertex correspond to the energy contribution of that precise configuration. If two vertices are associated with the same letter, then they carry the same energy. Notice that, to recover the 6-vertex model, we need to remove the d-type vertices, leaving only the six allowed ones.

$$\mathrm{T}_{\alpha|\alpha'} = \sum_{\text{all config.}}^{\text{one row}} \exp\left(-\beta \sum_{j=1}^{8} n_j \epsilon_j\right) \tag{2.2}$$

where n_j is the number of vertices of type j and ϵ_j is the energy brought by one vertex of type j. The subscript $\alpha|\alpha'$ stands for the two rows that are being connected. Assuming that the interaction is invariant under simultaneous inversion of the directions of all the arrows on the lattice, the eight-vertex model has that

$$\begin{aligned} \epsilon_1 &= \epsilon_2, \\ \epsilon_3 &= \epsilon_4, \\ \epsilon_5 &= \epsilon_6, \\ \epsilon_7 &= \epsilon_8. \end{aligned} \tag{2.3}$$

This justifies that in fig.(2.1) the configurations are clustered in couples with the same energy (same subscript a, b, c or d). We can then write the vertex weights

$$\omega_j = \exp(-\beta \epsilon_j) \tag{2.4}$$

having consequently

$$\begin{aligned}\omega_1 &= \omega_2 = a,\\ \omega_3 &= \omega_4 = b,\\ \omega_5 &= \omega_6 = c,\\ \omega_7 &= \omega_8 = d.\end{aligned} \tag{2.5}$$

A related set of quantities that we are going to use are

$$\begin{aligned}\mathrm{w}_1 &= \frac{1}{2}(c+d),\\ \mathrm{w}_2 &= \frac{1}{2}(c-d),\\ \mathrm{w}_3 &= \frac{1}{2}(a-b),\\ \mathrm{w}_4 &= \frac{1}{2}(a+b).\end{aligned} \tag{2.6}$$

They become particularly useful to individuate explicitly the symmetries of the partition function Z, obtained "summing over" all the M rows:

$$Z = \sum_{a_1} \cdots \sum_{a_M} \mathrm{T}_{a_1|a_2} \mathrm{T}_{a_2|a_3} \cdots \mathrm{T}_{a_M|a_1} = \mathrm{tr}(\mathbf{T}^M) \tag{2.7}$$

where this trace is taken in the physical space $\mathcal{H} = (\mathcal{H}_C)^N = (\mathbb{C}^2)^N$ in which the square matrix $\mathbf{T}$ works.

The utility is clear when we write

$$Z(\mathrm{w}_1, \mathrm{w}_2, \mathrm{w}_3, \mathrm{w}_4) \;=\; Z(\pm\mathrm{w}_i, \pm\mathrm{w}_j, \pm\mathrm{w}_k, \pm\mathrm{w}_l) \tag{2.8}$$

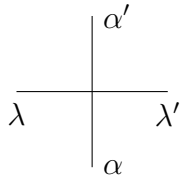
for any permutation (i, j, k, l) of $(1, 2, 3, 4)$. This identity is valid and means that Z is invariant by negating or interchanging any of the w's.

Now introduce another parameter $\lambda_j = \pm 1$ according to whether the arrow along the horizontal bond between columns $(j-1)$ and (j) points right or left, respectively. It has nothing to do with the spectral parameter λ used in the previous chapter. Notice that

the indices α, α' and λ, λ' play different roles. The former are the "quantum" indices identifying the vertical arrows, while the latter are the "auxiliary" indices identifying the horizontal arrows. Both can take only values ± 1 giving all the possible combinations. The auxiliary ones can be also seen as the matrix indices of a 2×2 matrix $\mathbf{R}_{\alpha}^{\alpha'}$, which numbers its entries. Thus, a matrix $\mathbf{R}_{\alpha}^{\alpha'}(\lambda, \lambda')$ is associated with each vertex, exploiting its configuration. It has elements:

$$\mathrm{R}_{\alpha}^{\alpha'}(\lambda, \lambda') = \begin{cases} 0 & \text{if the configuration is NOT allowed} \\ \omega_j & \text{if the configuration is allowed} \end{cases} \tag{2.9}$$

We can intrepret this expression in this way: we first select a vertex in the lattice, then we choose λ and λ'. This fixes the direction of the horizontal arrows exiting from the vertes, for example $\lambda \equiv \lambda_j$ on the left of the vertex, and $\lambda' \equiv \lambda_{j+1}$ on its right. At this point the "quantum" indices α and α' choose the vertical arrows above and under the vertex. The fact that we are using λ's as indices implies that, in practice, dealing with each vertex, we are working in an enlarged space $\mathcal{H}_C \otimes \mathcal{V}_a$ with respect to the physical one $\mathcal{H}_C$ that we have for each site of the chain. In particular, we chose them to be both of dimension 2, i.e., also the auxiliary space is $\mathbb{C}^2$. And the 2×2 matrix $\mathbf{R}$ lives in this auxiliary space. These assumptions and the equations (2.2)-(2.9) establish the link between problems of quantum mechanics on one-dimensional chains a problems of classical statistical physics on two-dimensional lattices.



No worries if in principle we could get 16 vertices, i.e. also non-allowed ones, from these combinations: the R-matrix (2.9) is designed to vanish in that case, leaving us only with the vertices permitted in the eight-vertex model, depicted in fig.(2.1).

At this point, keeping in mind the different role of α and λ, we can modify a bit the notation for $\mathbf{R}$ and we can write

$$\mathrm{T}_{\alpha|\alpha'} = \sum_{\lambda_1} \cdots \sum_{\lambda_N} \left(\mathrm{R}(\alpha_1, \alpha_1') \, \mathrm{R}(\alpha_2, \alpha_2') \cdots \mathrm{R}\left(\alpha_N, \alpha_N'\right) \right) \tag{2.10}$$

where it is assumed λ_1=λ_{N+1}. Treating explicitly the λ's as indices, can rewrite the sum as a trace, and (2.10) becomes:

$$\mathrm{T}_{\alpha|\alpha'} = \mathrm{tr}_a \left(\mathbf{R}(\alpha_1, \alpha'_1)\mathbf{R}(\alpha_2, \alpha'_2) \cdots \mathbf{R}(\alpha_N, \alpha'_N)\right) \tag{2.11}$$

where the trace has the subscript $_a$ since it is now taken in the auxiliary space $\mathcal{V}_a = \mathbb{C}^2$. Indeed, tracing out the ancillary space, we recover an operator working on the physical space, as we want for $\mathbf{T}$.

There exist four possible $\mathbf{R}(\alpha, \alpha')$:

$$\begin{aligned}
\mathbf{R}(+,+) &= \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \\
\mathbf{R}(+,-) &= \begin{pmatrix} 0 & d \\ c & 0 \end{pmatrix} \\
\mathbf{R}(-,+) &= \begin{pmatrix} 0 & c \\ d & 0 \end{pmatrix} \\
\mathbf{R}(-,-) &= \begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix}.
\end{aligned} \tag{2.12}$$

Notice that using the usual 2×2 Pauli operators (calling here $\sigma^4 = \mathrm{Id}$), we can write a compact expression for R:

$$\mathrm{R}(\alpha, \alpha'|\lambda, \lambda') \;=\; \sum_{j=1}^{4} \mathrm{w}_j \sigma_{\alpha,\alpha'} \sigma_{\lambda,\lambda'} \tag{2.13}$$

For our aims, it is convenient to introduce also the (local) so-called Lax-operator $\mathcal{L}_n$ (or local transition matrix) defined by

$$\mathcal{L}_n \;=\; \sum_{j=1}^{4} \mathrm{w}_j \, \sigma^j \otimes \sigma_n^j \;=\; \begin{pmatrix} \mathrm{w}_4\sigma_n^4 + \mathrm{w}_3\sigma_n^3 & \mathrm{w}_1\sigma_n^1 - \mathrm{w}_2\sigma_n^2 \\ \mathrm{w}_1\sigma_n^1 + \mathrm{w}_2\sigma_n^2 & \mathrm{w}_4\sigma_n^4 - \mathrm{w}_3\sigma_n^3 \end{pmatrix} \tag{2.14}$$

which lives in the auxiliary space as a 2×2 matrix, but each of its four entries acts on the local physical space $\mathcal{H}_C$. Using these operators, we can write the transfer matrix T as

$$\mathbf{T} \,=\, \mathrm{tr}_a(\mathcal{L}_N \cdots \mathcal{L}_1). \tag{2.15}$$

To make it even more compact, we can define the monodromy matrix $\mathcal{T}$ as

$$\mathcal{T} \,=\, \mathcal{L}_N \cdots \mathcal{L}_1 \,=\, \prod_{n=1}^{N} \mathcal{L}_n \tag{2.16}$$

in this expression, the trace can be seen as reconnecting the $(N+1)$ columns, in order to build the transfer operator which characterizes the transition between two adjacent entire rows.
Then the identity (2.15) takes the form

$$\mathbf{T} \,=\, \mathrm{tr}_a \mathcal{T}. \tag{2.17}$$

Now, we already said that solutions of exactly-solvable two-dimensional models are based on the commutation relations between transfer matrices; in particular transfer matrices with different values of the coefficients w_j, i.e., of a, b, c, d. From this perspective, we anticipate here that we will parametrize them using some constants and one only variable (u). Notice that the u takes the place of the λ adopted in the previous chapter when we briefly introduced the ABA. This means that by changing u we get in principle different matrices $\mathrm{T}(u)$. Hence, we have to investigate under what conditions on the w_j the transfer matrices commute.
Let us look at two monodromy matrices $\mathcal{T}$ and $\mathcal{T}'$ having two different sets of coefficients w_j and w'_j. The corresponding transfer matrices **T** and **T'** commute if there exists a non-singular 4 by 4 numerical matrix $\mathcal{R}$ such that

$$\mathcal{R}\,(\mathcal{T} \bigotimes \mathcal{T}') \,=\, (\mathcal{T}' \bigotimes \mathcal{T})\,\mathcal{R}. \tag{2.18}$$

We remark that this $\mathcal{R}$ is different from **R** in 2.9. This $\mathcal{R}$ is the matrix introduced in subsection (1.5.2) that must be solution of the Yang-Baxter equation.
Then, eq.(2.18) is true if the analogous relation is satisfied by the Lax-matrices $\mathcal{L}_n$:

$$\mathcal{R}\,(\mathcal{L}_n \bigotimes \mathcal{L}'_n) \,=\, (\mathcal{L}'_n \bigotimes \mathcal{L}_n)\,\mathcal{R}. \tag{2.19}$$

since the product can be taken out of the tensor product and vice-versa. This identity can be actually seen as another way of writing the YBE. It has been found that eq.(2.18) is satisfied if and only if, for all permutations (j,k,l,n) of (1,2,3,4), the following relation holds:

$$\mathrm{w}_n\mathrm{w}'_l\mathrm{w}''_j \;-\; \mathrm{w}_l\mathrm{w}'_n\mathrm{w}''_k \;+\; \mathrm{w}_n\mathrm{w}'_j\mathrm{w}''_l \;-\; \mathrm{w}_j\mathrm{w}'_k\mathrm{w}''_n \;=\; 0. \tag{2.20}$$

Eq.(2.20) is a way of writing six independent equations that correspond to the so-called *"Star-Triangle relations"* of the eight-vertex model.

2.2.1 Parametrization via elliptic functions

The complicated solution of the Star-Triangle relations, concurrently with the YBE, gives the structure of the $\mathcal{R}$ matrix

$$\mathcal{R} = \begin{pmatrix} a(u) & 0 & 0 & d(u) \\ 0 & b(u) & c(u) & 0 \\ 0 & c(u) & b(u) & 0 \\ d(u) & 0 & 0 & a(u) \end{pmatrix}, \tag{2.21}$$

of the $\mathcal{L}$ matrix

$$\mathcal{L} = \begin{pmatrix} \alpha(u) & 0 & 0 & \delta(u) \\ 0 & \beta(u) & \gamma(u) & 0 \\ 0 & \gamma(u) & \beta(u) & 0 \\ \delta(u) & 0 & 0 & \alpha(u) \end{pmatrix}, \tag{2.22}$$

and the required parametrization of its coefficients α, β, γ, and δ in order to satisfy eq.(2.19). These parametrizations are not unique, and even less are the notations. Indeed, every source is likely to adopt a different one. Beyond dispute is the need for a specific type of function, the only one with a peculiar quasi-periodic behavior, required from the previous identities: the *elliptic functions*. We refer you to Appendix A for explanations of these functions. In our case we report the parametrization used in two papers by Cao et al. ([10] and [11]):

$$\alpha(u) \;=\; \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \quad \beta(u) \;=\; \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \tag{2.23}$$

$$\gamma(v) = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \quad \delta(v) = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \quad (2.24)$$

where u is the spectral parameter, η is the crossing parameter, and τ is a generic complex number such that $\mathrm{Im}(\tau) > 0$. We will see the crossing parameter has the role of setting the anisotropy between the three couplings of the quantum Hamiltonian (2.1), for example $\eta = 0$ would mean $J_x = J_y = J_z$, while $\eta = 0.5$ selects the XY chain ($J_z = 0$). The complex number τ can tune the amplitude of the couplings.

The choice of this parametrization is not random: these papers are the hub of this work and conforming with their notation is useful. Moreover, it is very convenient since it is very general. Indeed,

$$\theta\begin{bmatrix}a_1\\ a_2\end{bmatrix}(u,\tau) = \sum_{m=-\infty}^{\infty} \exp\{i\pi[(m+a_1)^2\tau] + 2(m+a_1)(u+a_2)]\}, \quad (2.25)$$

and its combinations can assume the form of every elliptic function we need in our work. It is also useful to define two other functions connected to the θ's:

$$\sigma(u) = \theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,\tau), \quad (2.26)$$

and

$$\zeta(u) = \frac{\partial}{\partial u}\{\ln\sigma(u)\}. \quad (2.27)$$

We use some other lines to connect from the beginning the elliptic functions' notations adopted by several sources. The u used by now is the spectral parameter in [11]. Its correspondent in [9] and [12] is instead its rescaling:

$$z \equiv \pi u. \quad (2.28)$$

Moreover, they use a different notation for the elliptic functions. Here we report the one present in [12] since it is the most suitable for numerical computations (the same as

"Wolfram Mathematica"'s):

$$\begin{aligned}
\theta_1(z,q) &\equiv -\theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} (u,\tau), \\
\theta_2(z,q) &\equiv \theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} (u,\tau), \\
\theta_3(z,q) &\equiv \theta \begin{bmatrix} 0 \\ 0 \end{bmatrix} (u,\tau), \\
\theta_4(z,q) &\equiv \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} (u,\tau).
\end{aligned} \tag{2.29}$$

where $q = e^{i\pi\tau}$. The notation used in [9] is actually quite the same as [12], and their connection is exploited in Appendix A.

2.2.2 Connection with the XYZ Hamiltonian

Now that we have the Lax-matrices, we can use eq.(2.16) to recover the monodromy matrix. More explicitly we can write:

$$\mathcal{T}(u) = \mathcal{L}_N(u-\xi_N)\mathcal{L}_{N-1}(u-\xi_{N-1})\cdots\mathcal{L}_1(u-\xi_1). \tag{2.30}$$

where we allow each site to be endowed with a different spectral parameter. We remember that u identifies the rapidity of the probe injected into the system. Even if transfer matrices and monodromy matrices do not have a direct interpretation in the one-dimensional quantum chain, each ξ_j can be seen as the rapidities of the degree of freedom placed at site j. The ξ_j's are often called inhomogeneous parameters.

Consequently, we can use eq.(2.15) to obtain the transfer matrix. The crucial property is that transfer matrices identified by different coefficients, for example generated by different values of the spectral parameter, but still obeying that parametrization, commute:

$$[\mathbf{T}(u), \mathbf{T}(v)] = 0 \qquad \forall\, u, v. \tag{2.31}$$

This commutation relation has a fundamental meaning: $\mathbf{T}(u)$, varying u, constitute a whole family of operators, commuting with each other. Thus, $\mathbf{T}(u)$ can be seen itself as a

generating function for a family of commuting operators. Each of these can be regarded as a Hamiltonian for a quantum system with many integrals of motion. The remarkable thing is that the Hamiltonian of the XYZ spin chain is contained in this family.
In particular, we can extract the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N}\left(J_x\sigma_i^x\sigma_{i+1}^x + J_y\sigma_i^y\sigma_{i+1}^y + J_z\sigma_i^z\sigma_{i+1}^z\right), \tag{2.32}$$

which is exactly (2.1) with just an overall factor $\frac{1}{2}$, from the transfer matrix using

$$H = \frac{\sigma(\eta)}{\sigma'(0)}\left(\frac{\partial \ln T(u)}{\partial u}\Big|_{u=0,\,\xi_j=0} - \frac{1}{2}N\zeta(\eta)\right), \tag{2.33}$$

where $\sigma'(0) = \frac{\partial}{\partial u}\sigma(u)\big|_{v=0}$ and the function $\zeta(\eta)$ is defined in (2.27). The identity (2.33) leads us to the following parametrization of the coupling constants

$$J_x = e^{i\pi\eta}\frac{\sigma(\eta+\frac{\tau}{2})}{\sigma(\frac{\tau}{2})}, \quad J_y = e^{i\pi\eta}\frac{\sigma(\eta+\frac{1+\tau}{2})}{\sigma(\frac{1+\tau}{2})}, \quad J_x = \frac{\sigma(\eta+\frac{1}{2})}{\sigma(\frac{1}{2})}. \tag{2.34}$$

where the crossing parameter η and the complex number τ find their physical meaning. We remark that the formulae (3.33) are not restrictions on J_x, J_y, and J_z, but they give their parametrization up to an insignificant common factor. It is worth remarking that by playing with the parameters inside, in principle we can select any regime of our system. As always, we will be primarily interested in cases with one or more couplings that are anti-ferromagnetic. Notice, anyway, that there will be no longer a planar regime and each axis will be by itself: the one with greatest magnitude is referred to as dominant.

At this point, we recovered the connection between the transfer matrix of the 8-vertex model and the XYZ spin chain Hamiltonian. The presence of H among the family of operators commuting with $\mathbf{T}$, in practice tells us what we wanted to hear:

$$[H, \mathbf{T}(u)] = 0 \qquad \forall u. \tag{2.35}$$

This means that by diagonalizing $\mathbf{T}$ we are simultaneously finding the eigenvalues and eigenstates of H. Unfortunately, we are still far from having the luxury of shouting that the work is done. Indeed, the diagonalization of the transfer matrix is actually very cum-

bersome. In the case of N even, we can adopt two methods to do it: the *Generalized Algebraic Bethe ansatz* and the *TQ-relations*. The first is more physically intuitive, the second is more flexible. In the following, we are going to introduce them both. Let us start with the Generalized Algebraic Bethe ansatz.

2.3 ABA approach to the eight-vertex model

The ABA procedure involves the direct construction of the monodromy matrix through eq.(2.30). In particular, when the dimension of the auxiliary space $\mathcal{V}_a$ is chosen to be 2 (i.e. $\dim(\mathcal{V}_a) = \dim(\mathcal{H}_j) = 2$), the monodromy operator can be represented as a 2×2 matrix where each entry is an operator acting on the whole Hilbert space $\mathcal{H} = (\mathcal{H}_j)^N$:

$$\mathcal{T} = \begin{pmatrix} \mathbf{A}(z) & \mathbf{B}(z) \\ \mathbf{C}(z) & \mathbf{D}(z) \end{pmatrix}. \tag{2.36}$$

For notation's sake, we adopt the rescaling of the spectral parameter announced in subsection (2.2.1):

$$z \equiv \pi u. \tag{2.37}$$

Then, tracing out the ancillary space, we get the transfer matrix:

$$\mathbf{T}(z) \equiv \mathrm{tr}_a\, \mathcal{T}(z) = \mathbf{A}(z) + \mathbf{D}(z). \tag{2.38}$$

The operators $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$ can be represented as $2^N \times 2^N$ matrices. Their expressions are not simple but we do not actually need them. Indeed, if we insert (2.36) in (2.18), the Yang-Baxter equation for the monodromy matrix provides a series of generalized commutation relations between the $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ matrices at different spectral parameters. Then, by making use of these relations, still ignoring the explicit expressions of the operators involved, we can generate eigenstates of the system. At least, the last sentence refers to what we are able to do in the standard Algebraic Bethe ansatz, used to solve the XXZ chain.

2.3.1 Step back to the XXZ chain

What we have done until now is good both for XXZ and XYZ, nothing must be thrown away. The difference in the preliminary phases of the method is that the latter maps into the 6-vertex model, instead of the 8-vertex one. At first glance, this distance could seem unbridgeable, and maybe cause of even more differences in the subsequent steps of the method. Actually, looking back at fig.(2.1), to recover the 6-vertex model it is sufficient to remove the last two vertex configurations, labeled by d. The consequence of this removal can be found quite intuitively in the matrices $\mathcal{R}$ and $\mathcal{L}$: their structure is the same but the entries $d(z)$ and $\delta(z)$ are now identically zero. This will give a different parametrization of $\alpha(z)$, $\beta(z)$ and $\gamma(z)$, but we still end up with the form 2.36 for the monodromy matrix, following the same steps. Obviously, the operators $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ have different expressions, and consequently different commutation relations. In particular, the expression for $\mathbf{C}(z)$ allows us to identify a state which is annihilated by $\mathbf{C}(z)$ for any spectral parameter z:

$$\mathbf{C}(z)|0\rangle = 0 \qquad \forall\, z. \tag{2.39}$$

In this expression, $|0\rangle$ assumes the role of reference state and it is called *pseudo-vacuum*, because it hosts no quasi-particle excitations. This approach with operators acting on a reference state to create other eigenstates of the transfer matrix is also called *Quantum Inverse Scattering Method* (QISM).
The issue for the XYZ model is that the reference state $|0\rangle$ cannot be found for its expression of $\mathbf{C}(z)$, and this is strictly linked to the lack of U(1) of the totally anisotropic chain.

2.3.2 Extension to the XYZ

At this point, we need to find a trick to overcome this obstacle. First of all, let us focus again on the implications of the lack of U(1) symmetry of the XYZ spin chain. The pseudo-vacuum is defined as the state without excitations. The ability to count and classify these excitations comes from the presence of conserved quantities that identify them. In the method used so far, the fundamental quantity is the total spin S_z. Since U(1) symmetry is generated by just such a spin, the absence of the former does not allow us to use the latter as a conserved quantity.

Consider the local $\mathcal{L}$-matrix (2.14) as a 2×2 matrix in the auxiliary space, but with

elements acting on the local physical space $\mathcal{H}_j = \mathbb{C}^2$. We can rewrite it in a form similar to $\mathcal{T}$, since the latter is the N-times ordered product of the former:

$$\mathcal{L}_n(z) = \begin{pmatrix} \alpha_n(z) & \beta_n(z) \\ \gamma_n(z) & \delta_n(z). \end{pmatrix} \tag{2.40}$$

This form appears to be in discord with (2.22), because that was 4×4 instead of 2×2. Actually, it just depends on how we "play" with the auxiliary space. Here, in fact, the elements of $\mathcal{L}$ are not numerical entries but, as we said, operators acting on the physical space. We admit that the notation, with the Greek letters already used in that case, is very inconvenient. But we kept it in order to be as coherent as possible with the sources [9] [12]. The subscript $_n$ is there to remark that, in this case, we deal with a physical operator locally acting at row n (site n in the chain).

Anyway, the relevant part of this formulation lives in the operator $\gamma_n(z)$: for the 8-vertex model, it is non-degenerate for almost all z. Hence, we cannot obtain a local vacuum, either for $\mathcal{L}_n(z)$ or for a finite product of such matrices. Namely, for $\mathcal{T}(z)$ it is not possible to find $C(z)$ that annihilates a state for all z.

Still in the QISM framework, Takhadzhan and Faddeev in [9] performed a very clever trick to overcome the hump. Instead of using the generating vector (2.39), they used a family of generating vectors, and instead of the commutation relations between $\mathbf{A}(z)$, $\mathbf{B}(z)$, $\mathbf{B}(z)$ and $\mathbf{D}(z)$ in (2.36), they used a series of permutation relations for various linear combinations of these operators.

The construction of this family of generating vectors starts by applying a local gauge transformation to the local transition matrix $\mathcal{L}_n$:

$$\mathcal{L}'_n(z) \;=\; M^{-1}_{n+1}(z)\mathcal{L}_n M_n(z), \tag{2.41}$$

where the $M_n(z)$ are arbitrary non-singular 2 by 2 numerical matrices. Thus, the new monodromy matrix

$$\mathcal{T}'(z) \;=\; \prod_{n=1}^{N} \mathcal{L}'_n(z) \tag{2.42}$$

differs from $\mathcal{T}(z)$ only by the simple linear transformation

$$\mathcal{T}'(z) \;=\; M_{N+1}^{-1}(z)\mathcal{T}(z)M_1(z). \tag{2.43}$$

Actually, we can admit that there exists a whole family of gauge transformations

$$M_{n+l-1}(z) \;\equiv\; M_n^l(z) \tag{2.44}$$

depending on an integer l. The corresponding transformed local transition matrices are $\mathcal{L}_n^l$ and they are denoted by

$$\mathcal{L}_n^l(z) \;=\; M_{n+l}^{-1}(z)\mathcal{L}_n(z)M_{n+l-1}(z) \;=\; \begin{pmatrix} \alpha_n^l(z) & \beta_n^l(z) \\ \gamma_n^l(z) & \delta_n^l(z), \end{pmatrix} \tag{2.45}$$

where s and t can be omitted since they are assumed to be fixed for our aims. Similarly, the monodromy matrix $\mathcal{T}_N^l(z)$ can be written in terms of the original $\mathcal{T}\,(z)$:

$$\mathcal{T}_N^l(z) \;=\; M_{N+l}^{-1}(z)\mathcal{T}\,(z)M_l(z) \equiv \begin{pmatrix} \mathbf{A}^l(z) & \mathbf{B}^l(z) \\ \mathbf{C}^l(z) & \mathbf{D}^l(z). \end{pmatrix} \tag{2.46}$$

and we can clearly recover $\mathcal{T}'\,(z)$ selecting $l = 1$.
Now M_k can be chosen in such a way, that there exists a local reference state at each site, that is annihilated by $\gamma_n^l(z)$, for all values of v, namely

$$\gamma_n^l(z)\,\omega_n^l \;=\; 0 \qquad \forall z, \tag{2.47}$$

even if, with respect to the six-vertex model, this reference state is not an eigenvector of neither $\alpha_n^l(z)$ nor $\delta_n^l(z)$. To achieve this, M_k can be defined as:

$$M_k(z;\, s,t) = \begin{pmatrix} \theta_1(s+k\eta-z) & \frac{1}{g(\tau_k)}\theta_1(t+k\eta+z) \\ \theta_4(s+k\eta-z) & \frac{1}{g(\tau_k)}\theta_4(t+k\eta+z). \end{pmatrix} \tag{2.48}$$

where $g(z) = \theta_1(z)\,\theta_4(z)$, $\tau_k = \frac{s+t}{2} + k\eta - \frac{\pi}{2}$, and s and t are two arbitrary but fixed complex parameters, not reported again the following. Now that identity (2.47) is satisfied, the vectors

$$\Omega_N^l \;=\; \omega_1^l \otimes \cdots \otimes \omega_N^l \tag{2.49}$$

are annihilated by $\mathbf{C}_N^l(z)$, and the action of $\mathbf{A}_N^l(z)$ and $\mathbf{D}_N^l(z)$ is known, namely

$$\begin{cases} \mathbf{C}_N^l(z)\Omega_N^l = 0, \\ \mathbf{A}_N^l(z)\Omega_N^l = \Omega_N^{l-1}, \\ \mathbf{D}_N^l(z)\Omega_N^l = \left(\frac{h^N(z)}{h^N(z+\eta)}\right)\Omega_N^{l+1}, \end{cases} \tag{2.50}$$

where $h(z) = \theta_4(0)\,\theta_4(z)\,\theta_1(z)$. Hence, $\{\Omega_N^l\}_{l=-\infty}^{l=+\infty}$ constitutes a family of generating vectors (i.e., on which the actions of the elements of the transformed monodromy matrix are known) for the transfer matrix of the eight-vertex model.
Anyway, to generate the eigenvectors of the model is better to consider more general transformations of $\mathcal{T}$, by not restricting the indexes of the gauge transformation matrices, namely not imposing l as subscript for both M's:

$$\mathcal{T}^{\,k,l}(z) \;=\; M_k^{-1}(z)\mathcal{T}\,(z)M_l(z) \equiv \begin{pmatrix} \mathbf{A}_{k,l}(z) & \mathbf{B}_{k,l}(z) \\ \mathbf{C}_{k,l}(z) & \mathbf{D}_{k,l}(z) \end{pmatrix}. \tag{2.51}$$

Notice that the transfer matrix, being the trace of the monodromy matrix, can be still recovered as

$$\mathbf{T}(z) \;=\; \mathbf{A}(z) \,+\, \mathbf{D}(z) \;=\; \mathbf{A}_{l,l}(z) \,+\, \mathbf{D}_{l,l}(z), \tag{2.52}$$

and that the monodromy matrix $\mathcal{T}_N^{\,l}(z)$ can be written in the new notation as $\mathcal{T}_{k=N+l,l}^{\,l}\,(z)$. Now, these new elements of $\mathcal{T}_{k,l}$ have well-defined and relatively simple commutation relations, that can be recovered from the RTT-relation (2.18). Then, they can be used, in particular $\mathbf{B}_{k,l}$, to build the eigenstates of the model. We refer below to the procedure.

The needed commutation relations are:

$$\begin{aligned} &\mathbf{B}_{k,l+1}(z)\mathbf{B}_{k+1,l}(\mu) = \mathbf{B}_{k,l+1}(\mu)\mathbf{B}_{k+1,l}(z), \\ &\mathbf{A}_{k,l}(z)\mathbf{B}_{k+1,l-1}(\mu) = \alpha(z,\mu)\,\mathbf{B}_{k,l-2}(\mu)\mathbf{A}_{k+1,l-1}(z) - \beta(z,\mu)\,\mathbf{B}_{k,l-2}(z)\mathbf{A}_{k+1,l-1}(\mu), \\ &\mathbf{D}_{k,l}(z)\mathbf{B}_{k+1,l-1}(\mu) = \alpha(\mu,z)\,\mathbf{B}_{k+2,l}(\mu)\mathbf{D}_{k+1,l-1}(z) + \beta(z,\mu)\,\mathbf{B}_{k+2,l}(z)\mathbf{D}_{k+1,l-1}(\mu), \end{aligned} \tag{2.53}$$

where the functions $\alpha(z,\mu)$ and $\beta_k(\lambda,\mu)$ are defined as

$$\alpha(z,\mu) = \frac{h(z-\mu-\eta)}{h(z-\mu)} \qquad \beta_k(z,\mu) = \frac{h(\eta)\,h(\tau_k+\mu-z)}{h(\mu-z)\,h(\tau_k)}. \tag{2.54}$$

At this point, we are able to construct the transfer matrix eigenstates. First, take the vector

$$\Psi_l(z_1,...,v_n) \;=\; \mathbf{B}_{l+1,l-1}(z_1)\cdots\mathbf{B}_{l+n,l-n}(z_n)\,\Omega_{l-n}, \tag{2.55}$$

where the rapidities $\{z_k\}_{k=1}^n$ are to be determined.

By using the commutation relations (2.53), we can obtain the actions of $A_{l,l}(z)$ and $D_{l,l}(z)$ on the state (2.55):

$$\begin{aligned}
\mathbf{A}_{l,l}(z)\Psi_l(z_1,...,z_n) &= \hat{\Lambda}(z|z_1,...,z_n)\Psi_{l-1}(z_1,...,z_n) + \sum_{j=1}^{n}\hat{\Lambda}_j^l(z|z_1,...,z_n)\Psi_{l-1}(z_1,...,z_{j-1},z,z_{j+1},...,z_n),\\
\mathbf{D}_{l,l}(z)\Psi_l(z_1,...,z_n) &= \tilde{\Lambda}(z|z_1,...,z_n)\Psi_{l+1}(z_1,...,z_n) + \sum_{j=1}^{n}\tilde{\Lambda}_j^l(z|z_1,...,z_n)\Psi_{l+1}(z_1,...,z_{j-1},z,z_{j+1},...,z_n)
\end{aligned} \tag{2.56}$$

where

$$\begin{aligned}
\hat{\Lambda}(z|z_1,...,z_n) &= \prod_{k=1}^{n}\alpha(z,z_k),\\
\hat{\Lambda}_j^l(z|z_1,...,z_n) &= -\beta_{l-1}(z,z_j)\prod_{k=1,k\neq j}^{n}\alpha(z_j,z_k),\\
\tilde{\Lambda}(z|z_1,...,z_n) &= \frac{h(z)}{h(z+\eta)}\prod_{k=1}^{n}\alpha(z_k,z),\\
\tilde{\Lambda}_j^l(z|z_1,...,z_n) &= \beta_{l+1}(z,z_j)\left(\frac{h(z_j)}{h(z_j+\eta)}\right)\prod_{k=1,k\neq j}^{n}\alpha(z_j,z_k).
\end{aligned} \tag{2.57}$$

Until now, we seem to be happy about the procedure. However, a problem emerges at this stage. If we consider the vector (2.55), the action (2.56) is actually realized only consistently with the commutation relations between A and B in (2.53), since

$$\mathbf{A}_{l,l}(z)\Psi_l(z_1,...,z_n) = \mathbf{A}_{l,l}\,\mathbf{B}_{l+1,l-1}(z_1)\cdots\mathbf{B}_{l+n,l-n}(z_n)\,\Omega_{l-n}. \tag{2.58}$$

Indeed, $\mathbf{A}_{l,l}(z)$ has to be commuted through all the $\mathbf{B}(z_k)$, and finally we need to evaluate $\mathbf{A}_{l,l}(z)\Omega_{l-n}$ using (2.50). But this is only possible if $n=\frac{N}{2}$. This restriction puts a big brake on our ambitions: the generalized Bethe ansatz method only works for chains of even length.

Anyway, for completeness, we report the last steps of this procedure. We multiply (2.55) by $e^{2\pi i l\theta}$ with $0 \leq \theta \leq 1$ and sum it over all the integers l obtaining the vector:

$$\Psi_\theta(z_1, ..., z_n) = \sum_{l=-\infty}^{\infty} e^{2\pi i l\theta} \Psi_l(z_1, ..., z_n). \tag{2.59}$$

This state, using (2.56), can be seen to be an eigenstate of the eight-vertex transfer matrix, with eigenvalue

$$\Lambda_f(z) = e^{2\pi i\theta} \hat{\Lambda}(z|z_1, ..., z_n) + e^{-2\pi i\theta} \tilde{\Lambda}(z|z_1, ..., z_n), \tag{2.60}$$

if the rapidities z_j satisfy the Bethe equations:

$$\left(\frac{h(z_j)}{h(z_j + \eta)}\right)^N = e^{4\pi i\theta} \prod_{k=1, k\neq j}^{n} \frac{\alpha(z_j, z_k)}{\alpha(z_k, z_j)}. \tag{2.61}$$

Let us conclude by saying that the infinite sum in (2.59) requires a special investigation. Indeed, it is summable to zero for all θ except for finitely many values of θ_j. For these θ_j the numbers (2.60) are the eigenvalues of $\mathbf{T}(z)$. Results by Baxter show that 0 is among these θ_j. Anyway, the situation simplifies if we impose restrictions on the range of η, which, however, allow us to select all the regimes of the system. Without going into details, the restriction is

$$K\eta = m_1\, 2\pi + m_2\, \pi\tau \tag{2.62}$$

with K, m_1 and m_2 being integers. Since the elliptic theta functions are quasi-periodic by definition, $M_k(z)$, $\mathcal{T}^{k,l}(z)$ and $\Psi_l(z_1, ..., z_n)$ are all quasi-periodic functions of k and l in this case. If we choose appropriately a common normalizing factor, it can be shown that they become periodic in k and l with period K. As a result, the infinite sum in (2.59) becomes finite with the values $\theta = \frac{k}{K}$ for $k = 0, 1, ..., K - 1$.
In any case, despite the elegance of this method, we anticipate that we cannot use it for our aims, i.e., for frustrated chains. Thus, with the tools we know to date, the only other possibility is to bring into play the TQ relations.

2.4 TQ relations

Baxter's famous solution to the 8-vertex model has been the origin of a long series of works [7], [9], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22], from McCoy, Fabricius, Klümper, and among the others, Baxter himself. In particular, over the years, there have been reformulations of this solution also in the framework of Algebraic Bethe ansatz and of the Quantum Inverse Scattering Method [9]. Summarizing the previous section, it is well-known that the Algebraic Bethe ansatz technique can be successfully applied to the XXZ model. In the XYZ chain case, the total anisotropy removes the residual U(1) symmetry of the model. This does not allow us to make use of ABA in the same direct way. Anyway, we can apply some preliminary gauge transformations to "prepare the field" for the ABA. However, this precise technique requires the existence of a reference state to build the other eigenstates, and such a state is not identifiable in the case of an odd number of sites. An extension to the case N odd has been proposed by Niccoli and Terras in [23].

Anyway, the original solution of the even-length XYZ chain was based on a smart idea conceived by Baxter [8]. Instead of thinking in terms of the monodromy matrix, he focused on the construction of an additional operator $\mathbf{Q}(z)$, this time acting in the same space as $\mathbf{T}$. This Q-matrix allows for an easy derivation of the Bethe equations and of the spectrum of the transfer matrix. Indeed, it is built as an operator that commutes with $\mathbf{T}$:

$$[\mathbf{T}(z), \mathbf{Q}(z')] = [\mathbf{Q}(z), \mathbf{Q}(z')] = 0 \tag{2.63}$$

and that satisfies the following equation:

$$\mathbf{T}(z)\,\mathbf{Q}(z) = \mathbf{Q}(z)\,\mathbf{T}(z) \;= \phi(z-\eta')\mathbf{Q}(z+2\eta') + \phi(z+\eta')\mathbf{Q}(z-2\eta') \tag{2.64}$$

with $\phi(v) = [\rho\, h(\frac{v}{2})]^N$, where ρ is a normalization factor. We add that this construction was also instrumental in the development of the algebraic version of the thermodynamic Bethe ansatz. [1] The commutation relation tells us that $\mathbf{T}$ and $\mathbf{Q}$ commute, namely they

[1] We are not digging into the first Q-matrix construction but you can consult Appendix C of [8] to get more details on its construction. We can say though, that he actually started from the eigenvalue version of (2.64). Then, with non-trivial considerations, he extended that to an operator identity: since $\mathbf{T}(y)$ and $\mathbf{T}(z)$ commute, there exists a representation independent of z in which $\mathbf{T}(z)$ is diagonal $\forall z$. Thus, we can build a matrix $\mathbf{Q}(v)$ which is also diagonal in the same representation, with diagonal elements $Q(v)$. In this perspective can look at eq.(2.65) as a matrix equation in this representation. So, we can in principle go back to the original representation, getting the generalized matrix equation (2.64).

share the same eigenvectors. For the eigenvectors of $\mathbf{T}(z)$, we can obtain the identity

$$T(z)\,Q(z) \;=\; \phi(\eta - z)\,Q(z + 2\eta') \;+\; \phi(\eta + z)\,Q(z - 2\eta') \tag{2.65}$$

for the eigenvalues $\Lambda(z)$ associated with the eigenvectors. In this expression, $\eta' = \eta - 2I$, where I is the complete elliptic integral, namely one of the two half-periods of the (quasi-periodic) elliptic functions. Look at Appendix A for an in-depth analysis of the elliptic functions. The subsequent analysis relies on the peculiar nature of elliptic functions. The requirement of $\Lambda(z)$ and $Q(z)$ being entire functions of z (since the operators $\mathbf{T}$ and $\mathbf{Q}$ are) leaves us, after many computations [24], with an ansatz for $Q(z)$:

$$Q(z) = e^{\tau z} \prod_{j=1}^{n} h\left(\frac{z - z_j}{2}\right). \tag{2.66}$$

where $h(z)$ has been defined in section (2.3.2) as $h(z) = \theta_4(0)\,\theta_4(z)\,\theta_1(z)$ and with a complicated but unnecessary to exploit definition of τ (not to be confused with the imaginary number that enters the elliptic θ's). What is relevant in this expression is the fact that the function $h(x)$ has a simple zero at $x = 0$, so setting $z = z_j$ in (2.65) causes the LHS to vanish, leaving

$$\left(\frac{h[\frac{1}{2}(\eta - z_j)]}{h[\frac{1}{2}(\eta + z_j)]}\right)^N = -e^{-4\tau\eta'} \prod_{l=1}^{n} \frac{h[\frac{1}{2}(z_j - z_l - 2\eta')]}{h[\frac{1}{2}(z_j - z_l + 2\eta')]} \qquad j = 1, ..., n. \tag{2.67}$$

which are the Bethe equations for the XYZ chain. They determine the rapidities $z_1, ..., z_n$ and they have many solutions corresponding to the different eigenvalues. Now, if we substitute the roots just found in the expression for $q(z)$ it is vanishing by construction. So, plugging it into (2.65), we obtain the eigenvalues $\Lambda(z)$ of the transfer matrix $\mathbf{T}(z)$.

This approach is very general because it relies on the Q-operator construction, which can be mathematically manipulated in order to obey the desired commutation relations. The whole procedure can be as always extended to the XXZ chain with a consequent simplification of some expressions, getting parametrizations in terms of hyperbolic functions instead of elliptic ones. Moreover, in the generalized ABA we had to extend the 6-vertex method to the 8-vertex through a gauge transformation trick. In this case, the building of Q directly guarantees the reliability of the method, since Q is based on the eight-vertex model requirements from the beginning. However, even this approach conceals a problem

if we search for a solution of an odd-length chain. The issue is represented by the number n which enters the products and corresponds to the number of roots. In fact, the most careful readers could have noticed that we did not exploit its limitations. We remedy saying that Baxter set

$$n = \frac{N}{2}. \tag{2.68}$$

Indeed, following the properties of the elliptic functions, $Q(z)$ ends up having $\frac{N}{2}$ zeros per period rectangle. This precisely constitutes the limitation we had to avoid to have a valid method for N odd since n must be an integer.

Actually, also for even-N this approach has a disadvantage: we obtained the spectrum of the transfer matrix and consequently we can get all the information contained in the partition function, but we cannot access directly to the eigenvectors of the system. This is quite the opposite of the Algebraic Bethe ansatz, which started from the eigenstates of the transfer matrix to characterize the system. Anyway, the TQ-relations are more powerful if we want to develop the *Thermodynamic Bethe ansatz*. This last aspect drives us to try to extend the TQ-relations method to N odd.

Chapter 3

Extension to N odd: "off-diagonal Bethe ansatz"

3.1 First TQ relations for N odd

In a series of works, McCoy and Fabricius [17], [18], [20], [21], performed several manipulations on the Baxter's TQ relations with the aim of extending them to the odd N case. In their papers, this description appears to be possible, but only for particular values of the eight-vertex model parameters. They demonstrate that the location of zeros of the Q-matrix is qualitatively different from the case of even N. In particular, such rapidities satisfy a previously unknown equation which is more general than the Bethe equation. Let us discuss briefly their work.

Rodney Baxter spent a lot of time and papers to get the final version of the solution of the 8-vertex model. The first paper approaching this theme dates back to 1972. After ten years, in 1982, he recollected all the material concerning exactly solved statistical models in his book [24]. In the previous chapter, we reported the solution written in the book. However, recently, McCoy and Fabricius analyzed the steps that brought the Q-matrix to assume the form (2.66), proposed by Baxter in his book. They focused on the fact that this definition applies only to N even and they wondered which which step imposed this limitation. They found out that it came from the will to make the definition of $Q(z)$ valid for any η. In fact, the proceeding that brings the solution of many statistical models passes by the analysis of the freedom left to their parameters. What must be preserved is the possibility of recovering every physically accessible regime. Namely, we are allowed

to restrict one or more parameters to a narrower domain, but every physical phase still has to be selectable. In our case, the crossing parameter η is the one under examination.

McCoy and Fabricius recovered the first version of the Q-matrix defined in 1972 in [8] as

$$Q_{72}(z) = \mathcal{K}(q, z_k)\, e^{-i\nu\pi z/2I} \prod_{j=1}^{N} \theta_1(z - z_j) \tag{3.1}$$

where $\mathcal{K}(q, z_k)$ keeps its normalization. Notice that the subscript $_{72}$ is the same as that used by McCoy and refers to the year in which the matrix was introduced by Baxter. The expression (3.1) is the most general function that satisfies the quasi-periodicity properties

$$\begin{aligned} Q_{72}(z + 2I) &= (-1)^{\nu'} Q_{72}(z) \\ Q_{72}(z + 2iI') &= q^{-N} e^{-iN\pi z/I} Q_{72}(z) \end{aligned} \tag{3.2}$$

required by the 8-vertex model and the TQ relation in the form

$$\mathbf{T}(z)\mathbf{Q}(z) = [\rho\, \theta_1(0)\bar{h}(z - \eta)]^N \mathbf{Q}(z + \eta) + [\rho\, \theta_1(0)\bar{h}(z + \eta)]^N \mathbf{Q}(z - \eta). \tag{3.3}$$

where $\bar{h} \equiv \theta_1(z)\theta_4(z)$. They are actually the same as Baxter's, just written in a different way. The parameters ν and ν' in (3.2) are related by the constraint $\nu' + \nu + N = \textit{even integer}$, and I is the complete elliptic integral of the first type. We note that under the spin inversion, $\sigma_j^z \to -\sigma_j^z$ the eigenvalues of the transfer matrix are invariant but the total spin $S^z \to (-1)^N S^z$. Thus, when N is odd, each eigenvalue of $\mathbf{T}(z)$ is doubly degenerate, with one eigenvector in each of the two sectors S^z and $-S^z$, one with $\eta' = 0$ and one with $\eta' = 1$, due to the so-called Kramer's degeneracy. This phenomenon does not happen for N even. So, this aspect clearly separates the two situations. Anyway, what we want to remark is that this solution is restricted to the so-called *root of unity condition* [25] for the crossing parameter:

$$\eta = \frac{mI}{L} \tag{3.4}$$

where m and L are two integers. This restriction is consistent with the expression of Q_{72} in (3.1), where the product goes from 1 to N. Namely, it is extended to N roots, not just $\frac{N}{2}$. At this point, Baxter wanted to propose a method with a simpler expression for $Q(z)$ and more powerful in the search for the eigenvectors. Thus, he presented the new Q-matrix (2.66), which is valid for every η but only for N even.

To avoid this limitation, and to approach odd-length chains, McCoy and Fabricius rehashed the matrix $\mathbf{Q}_{72}$. Making use of the TQ relation, in the case $\eta = \frac{mI}{L}$ with m odd and L even or odd, they recovered a more different type of the Bethe equations:

$$\left(\frac{h(z_l-\eta)}{h(z_l+\eta)}\right)^N = e^{2\pi i\nu\eta/I} \prod_{j=1,\, j\neq l}^{N} \frac{\theta_1(z_l-z_j-2\eta)}{\theta_1(z_l-z_j+2\eta)}, \tag{3.5}$$

which mainly differ from the Bethe equations (2.67) for even N in two features: the function $\theta_1(z)$ appearing on the RHS instead of $h(z)$ and the number of terms in the products, now N. For the N emerging roots, as they admit, it is very tough to find a scheme in terms of the string hypothesis. Therefore, probably for this reason, their speculation has stalled, but it was the first commendable attempt to reach a solution for the frustrated case.

3.2 Introduction to inhomogeneous TQ relations

In section (1.5), we introduced the concept of consistency relations between matrices. It is fundamental to fix the picture that more than one parametrization or definition can be correct as long as they describe the system *consistently* with the previous constraints. The ancestor of these restrictions is the Yang-Baxter equation (1.113), on which the quantum integrable models are defined. Then, in this framework, each model collects particular characteristics depending on its own nature. From this perspective, the TQ relation is a perfect example of our approach. Indeed, it is a ploy, theorized by Baxter, to diagonalize the transfer matrix making use of an auxiliary one. As we have seen, the form of the Q-matrix is not fixed, being subject to changes. Moreover, even the TQ relations themselves can be reviewed to adapt them to our issues, provided that we obey all the required consistency relations.

Recently, Cao et al. proposed a new method, still based on the TQ relations, which allows us to treat the N even and the N odd case in the same framework: the "off-diagonal Bethe ansatz" [26].

Going back to the most general form of the TQ relations, we can write

$$\Lambda(u) = a(u)\frac{Q(u-\eta)}{Q(u)} + d(u)\frac{Q(u+\eta)}{Q(u)}. \tag{3.6}$$

that encodes Baxter's intuition that the eigenvalues $\Lambda(u)$ of the transfer matrix $\mathbf{T}(u)$ take a unified shape for all the eigenstates. It can be rewritten in the matrix form

$$\mathbf{Q}(u)\mathbf{T}(u) = a(u)\mathbf{Q}(u-\eta) + d(u)\mathbf{Q}(u+\eta). \tag{3.7}$$

where $a(u)$ and $d(u)$ are two known model-dependent functions. This operator relation is not affected by the representation basis and, since $[\mathbf{T}(u), \mathbf{T}(v)] = 0$, the eigenstates of the transfer matrix do not depend on u. At this point, suppose that $|\Psi\rangle$ is a common eigenstate of the transfer matrix and the Q-operator (such an eigenstate exists since $\mathbf{T}$ and $\mathbf{Q}$ commute by hypothesis) with eigenvalues

$$\begin{aligned} \mathbf{T}(u)|\Psi\rangle &= \Lambda(u)|\Psi\rangle \\ \mathbf{Q}(u)|\Psi\rangle &= Q(u)|\Psi\rangle. \end{aligned} \tag{3.8}$$

Substituting in (3.7), we recover the scalar equation (3.6). For these reasons, the TQ relation is universal for most of the integrable models, but only if owners of a proper reference state. In general, $Q(u)$ is a polynomial of some entire function $f(u)$ and can be parametrized as

$$Q(u) = \prod_{j=1}^{M} f(u-\mu_j) \tag{3.9}$$

with $f(0) = 0$, where the parameters $\{\mu_j | \, j = 1, ..., M\}$ are the Bethe roots. They are the solutions of the BAEs

$$\frac{a(\mu_j)}{d(\mu_j)} = -\frac{Q(\mu_j+\eta)}{Q(\mu_j-\eta)} \tag{3.10}$$

deriving from the constraint that $\Lambda(u)$ is also an entire function about u, and the regularity of eq.(3.6) requires that all the residues about μ_j must be zero. Thus, the simplicity of the "poles" μ_j is crucial to derive the above BAEs, and it is a common feature of the Bethe roots.

Now, for most of the integrable models without U(1) symmetry, this relation does not allow polynomial solutions of $Q(u)$. Thus, an extended version of (3.6), namely an *inhomogeneous* TQ relation should be used [27]. In the following, we give a concise introduction to this method.

3.2.1 Basic ingredients of the ODBA

The absence of the U(1) symmetry, i.e. of a proper reference state, induces difficulties in the research of the eigenstates of the transfer matrix. This practically comes from the fact that some off-diagonal elements of the monodromy matrix enter the expression of the transfer matrix. For example, we saw it in the Algebraic Bethe ansatz, which followed the scheme of constructing the eigenvectors to recover the eigenvalues; but the use of the more versatile TQ relation seemed to help us. Indeed, a reference state is not needed for getting the spectrum, if we use the functional TQ relation. In any case, note that expressions like (2.66) for $Q(u)$, obtained by Baxter for the XYZ (that lacks U(1) symmetry), were not polynomials of some entire function, due to the exponential term depending on z.
We would like to get the eigenvalue $\Lambda(u)$ as a degree N polynomial of some entire function $f(u)$ and factorized as

$$\Lambda(u) = \Lambda_0 \prod_{j=1}^{N} f(u - x_j) \tag{3.11}$$

where Λ_0 is a constant to be determined by the asymptotic behavior of $\mathbf{T}$. If there are N equations for the N unknowns x_j, then $\Lambda(u)$ can be determined completely. The central idea of the ODBA is to derive the functional TQ relation based on N operator identities which determine the N unknowns in (3.11).

3.2.2 Functional relations of the XXX chain

Here we propose an example of solution for the XXX spin chain to show more clearly how this method is consistent: for other integrable models, even when owners of U(1) symmetry.
Let us show the OBDA clearly, starting from the $\mathcal{L}$-matrix for the periodic XXX spin chain:

$$\begin{aligned} \mathcal{L}_{0,j}(u) &= u + \eta P_{0,j} \\ &= u + \frac{1}{2}\eta(1 + \sigma_j \cdot \sigma_0), \end{aligned} \tag{3.12}$$

where η is the crossing parameter ($\eta = 1$ in this case), $\sigma_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ are the Pauli matrices and $P_{i,j}$ is the permutation operator possessing the properties

$$P_{i,j}O_j = O_j P_{i,j}, \qquad P_{i,j}^2 = Id, \qquad \mathrm{tr}_j P_{i,j} = \mathrm{tr}_i P_{i,j} = Id, \tag{3.13}$$

for an arbitrary operator O in the corresponding tensor space. We can also show that the L-matrix also satisfies the following relations:

$$\begin{aligned}
&\cdot \text{Initial condition:} \quad \mathcal{L}_{1,2}(0) = P_{1,2}, \\
&\cdot \text{Unitary relation:} \quad \mathcal{L}_{1,2}(u)\mathcal{L}_{2,1}(u) = -\phi(u) \times Id, \text{ with } \phi(u) = u^2 - 1, \\
&\cdot \text{Crossing relation:} \quad \mathcal{L}_{1,2}(u) = -\sigma_1^y \mathcal{L}_{1,2}^{t_1}(-u-1)\sigma_1^y, \\
&\cdot \text{PT-symmetry:} \quad \mathcal{L}_{1,2}(u) = \mathcal{L}_{2,1}(u) = \mathcal{L}_{1,2}^{t_1,t_2}(u), \\
&\cdot \text{Z}_2\text{-symmetry:} \quad \sigma_1^\alpha \sigma_2^\alpha \mathcal{L}_{1,2}(u) = \mathcal{L}_{2,1}(u)\sigma_1^\alpha \sigma_2^\alpha \quad \alpha = x, y, z, \\
&\cdot \text{Fusion condition:} \quad \mathcal{L}_{1,2}(\pm 1) = \pm 1 + P_{1,2} = \pm 2 P_{1,2}^{(\pm)},
\end{aligned} \tag{3.14}$$

where $P_{1,2}^{(\pm)}$ are the symmetric/antisymmetric projection operators. With the above properties, the following crossing-unitary relation holds, too:

$$\mathcal{L}_{1,2}^{t_1}(u)\mathcal{L}_{1,2}^{t_1}(-u-2) = \mathcal{L}_{1,2}^{t_1}(-u-2)\mathcal{L}_{1,2}^{t_1}(u) = -\phi(u+1) \times Id. \tag{3.15}$$

Then we can, as usual, recover the monodromy and the transfer matrix as

$$\begin{aligned}
&\mathcal{T}_0(u) = \mathcal{L}_{0,N}(u - \xi_N) \cdots R_{0,1}(u - \xi_1), \\
&\mathbf{T} = \text{tr}_0 \mathcal{T}_0(u)
\end{aligned} \tag{3.16}$$

where $\{\xi_j \,| j = 1, ..., N\}$ are the inhomogeneity parameters. Notice that we left explicit the subscript 0 which identifies the auxiliary space on which the trace is performed.
In order to get some functional relations involving the transfer matrix, we evaluate $\mathbf{T}(u)$ at the particular points $u = \xi_j$ and $u = \xi_j - 1$. Applying the initial condition among (3.14) of the $\mathcal{L}$-matrix we can express the transfer matrix at $u = \xi_j$ as:

$$\begin{aligned}
\mathbf{T}(\xi_j) &= \text{tr}_0\{\mathcal{L}_{0,N}(\xi_j - \xi_N) \cdots \mathcal{L}_{0,j+1}(\xi_j - \xi_{j+1}) \cdot P_{0,j} \cdot \mathcal{L}_{0,j-1}(\xi_j - \xi_{j-1}) \cdots \mathcal{L}_{0,1}(\xi_j - \xi_1)\} \\
&= \mathcal{L}_{j,j-1}(\xi_j - \xi_{j-1}) \cdots \mathcal{L}_{j,1}(\xi_j - \xi_1) \times \text{tr}_0\{\mathcal{L}_{0,N}(\xi_j - \xi_N) \cdots \mathcal{L}_{0,j+1}(\xi_j - \xi_{j+1})\} \\
&= \mathcal{L}_{j,j-1}(\xi_j - \xi_{j-1}) \cdots \mathcal{L}_{j,1}(\xi_j - \xi_1) \cdot \mathcal{L}_{j,N}(\xi_j - \xi_N) \cdots \mathcal{L}_{j,j+1}(\xi_j - \xi_{j+1}).
\end{aligned} \tag{3.17}$$

The initial condition has been crucial in allowing us to rewrite the transfer matrix ate the special spectral parameter points ξ_j as a product of $\mathcal{L}$-matrices. The transfer matrix $\mathbf{T}(\xi_j)$ assumes the form of a reduced monodromy matrix if the j^{th} quantum space is treated as the auxiliary space.

The crossing relation among (3.14) makes it possible to express the transfer matrix $\mathbf{T}(\xi_j - 1)$ as:

$$\begin{aligned}\mathbf{T}(\xi_j - 1) &= \mathrm{tr}_0\{\mathcal{L}_{0,N}(\xi_j - \xi_N - 1)\cdots\mathcal{L}_{0,1}(\xi_j - \xi_1 - 1)\} \\ &= (-1)^N \mathrm{tr}_0\{\sigma_0^y \mathcal{L}^{t_0}_{0,N}(-\xi_j + \xi_N)\cdots\mathcal{L}^{t_0}_{0,1}(-\xi_j + \xi_1)\sigma_0^y\} \\ &= (-1)^N \mathrm{tr}_0\{\mathcal{L}_{0,1}(-\xi_j + \xi_1)\cdots\mathcal{L}_{0,N}(-\xi_j + \xi_N)\} \\ &= (-1)^N \mathcal{L}_{j,j+1}(-\xi_j + \xi_{j+1})\cdots\mathcal{L}_{j,N}(-\xi_j + \xi_N)\cdot\mathcal{L}_{j,1}(-\xi_j + \xi_1)\cdots\mathcal{L}_{j,j-1}(-\xi_j + \xi_{j-1}).\end{aligned} \tag{3.18}$$

Then, using the unitary relation among (3.14), we have

$$\mathbf{T}(\xi_j)\mathbf{T}(\xi_j - 1) = a(\xi_j)d(\xi_j - 1)\, Id, \qquad j = 1, ..., N, \tag{3.19}$$

with

$$a(u) = \prod_{j=1}^{N}(u - \xi_j + 1), \qquad d(u) = \prod_{j=1}^{N}(u - \xi_j). \tag{3.20}$$

Thus, applying (3.19) to an eigenstate of $\mathbf{T}(u)$, the corresponding eigenvalue Λ satisfies

$$\Lambda(\xi_j)\Lambda(\xi_j - 1) = a(\xi_j)d(\xi_j - 1) \qquad j = 1, ..., N. \tag{3.21}$$

From the definition of the transfer matrix (3.16) it is easy to show that $\Lambda(u)$ is a degree N polynomial of u, as expected for a model with U(1) symmetry, with the asymptotic behavior $\Lambda(u) = 2u^N + \cdots$.
Moreover, it can be proven that each solution of (3.20) can be parametrized in terms of the TQ relation (3.6) with a polynomial Q-function.

3.2.3 Inhomogeneity's takeover

Baxter's TQ relation (3.6) gives a convenient parametrization of the eigenvalues of the transfer matrix, but it is obvious that it is not unique. We could demonstrate that for *any* given parameter ϕ, the inhomogeneous TQ relation

$$\Lambda(u) = e^{i\phi}a(u)\frac{Q(u-1)}{Q(u)} + e^{-i\phi}d(u)\frac{Q(u+1)}{Q(u)} + 2(1 - \cos\phi)\frac{a(u)d(u)}{Q(u)}, \tag{3.22}$$

with

$$Q(u) = \prod_{j=1}^{N}(u - \mu_j), \tag{3.23}$$

satisfies (3.21), and therefore characterizes the spectrum of $\mathbf{T}(u)$ of the periodic XXX chain completely, provided that the Bethe roots $\{\mu_j \,|j = 1, ..., N\}$ satisfy the BAEs

$$e^{i\phi}a(\mu_j)Q(\mu_j - 1) + e^{-i\phi}d(\mu_j)Q(\mu_j + 1) = 2(\cos\phi - 1)a(\mu_j)d(\mu_j), \tag{3.24}$$

and the selection rules $\mu_j \neq \mu_l$ and $\mu_j \neq \xi_l, \xi_l - 1$.

For most of the spin-$\frac{1}{2}$ models, the operator identity (3.19) and its functional version hold, but with a different crossing parameter:

$$\mathbf{T}(\xi_j)\mathbf{T}(\xi_j - \eta) = a(\xi_j)d(\xi_j - \eta)\, Id, \qquad j = 1, ..., N, \tag{3.25}$$

$$\Lambda(\xi_j)\Lambda(\xi_j - \eta) = a(\xi_j)d(\xi_j - \eta), \qquad j = 1, ..., N, \tag{3.26}$$

where $a(u)$ and $d(u)$ are two known functions with zeros $\{\xi_j - \eta\}$ and $\{\xi_j\}$, respectively. It can be shown that the functional relations together with the analytic properties of the transfer matrix constitute the necessary and sufficient conditions to determine the N unknowns of the $\Lambda(u)$ polynomial (as we have proven for the XXX) and allow us to construct the more general functional TQ relation

$$\Lambda(u) = e^{i\phi(u)}a(u)\frac{Q(u-\eta)Q_1(u-\eta)}{Q(u)Q_2(u)} + e^{-i\phi(u+\eta)}d(u)\frac{Q(u+\eta)Q_2(u+\eta)}{Q(u)Q_1(u)} + c(u)\frac{a(u)d(u)}{Q(u)Q_1(u)Q_2(u)}, \tag{3.27}$$

with $Q(u)$ being a degree M polynomial, and $Q_1(u)$ and $Q_2(u)$ degree M_1 polynomials. $c(u)$ is a polynomial adjust function of degree n which matches the asymptotic behavior of $\Lambda(u)$. The phase $\phi(u)$ can be determined using the initial condition of the transfer matrix. By definition of $a(u)$ and $d(u)$ at the special points $u = \xi_j$, $\xi_j - \eta$, the last term vanishes. This is the crucial property of the inhomogeneous TQ relation: makes it possible for the generalized functional TQ relation to satisfy the scalar eq.(3.26) automatically, for arbitrary Q-functions and $c(u)$. Namely, eq.(3.27) leads to

$$\Lambda(\xi_j) = e^{i\phi(\xi_j)}a(\xi_j)\frac{Q(\xi_j - \eta)Q_1(\xi_j - \eta)}{Q(\xi_j)Q_2(\xi_j)}, \tag{3.28}$$

$$\Lambda(\xi_j) = e^{-i\phi(\xi_j)} d(\xi_j - \eta) \frac{Q(\xi_j) Q_2(\xi_j)}{Q(\xi_j - \eta) Q_1(\xi_j - \eta)} \tag{3.29}$$

and these two equations identically give eq.(3.21).
Our last task is to ensure $\Lambda(u)$ to be a polynomial of degree N. For this aim, we need three conditions:

1. $M + 2M_1 - n = N$:
2. the asymptotic behavior of the RHS of eq.(3.27) must coincide with the one of $\mathbf{T}(u)$;
3. the RHS of eq.(3.27) must be regular.

The last constraint gives the Bethe ansatz equations.
Then, since eq.(3.27) is valid for all the eigenvalues, we naturally conclude that also its operator version holds:

$$\mathbf{T}(u) = e^{i\phi(u)} a(u) \frac{\mathbf{Q}(u-\eta)\mathbf{Q}_1(u-\eta)}{\mathbf{Q}(u)\mathbf{Q}_2(u)} + e^{-i\phi(u+\eta)} d(u) \frac{\mathbf{Q}(u+\eta)\mathbf{Q}_2(u+\eta)}{\mathbf{Q}(u)\mathbf{Q}_1(u)} + c(u) \frac{a(u)d(u)}{\mathbf{Q}(u)\mathbf{Q}_1(u)\mathbf{Q}_2(u)}, \tag{3.30}$$

with all Q-operators being commutative with each other. Notice that this is the most general TQ relation for spin-$\frac{1}{2}$ quantum integrable systems derived from the operator product identities. We remark that there is actually an infinite number of choices for the Q-functions and for $c(u)$. For example, for the XXX chain, a $n = 0$ or $n = 1$ were both sufficient to parametrize $\Lambda(u)$ completely. Conversely, some systems are very sensitive to the choice of M_1. For instance, the eigenvalues of the XYZ spin chain with an odd number of sites N cannot be characterized correctly by a TQ relation with $M_1 = 0$; thus, we need to choose $M_1 \neq 0$.
We mention that, even if it is very powerful in getting the eigenvalues, an important problem in the ODBA scheme is to retrieve the eigenstates, that are known to be crucial to compute correlation functions and dynamical properties.

3.2.4 Brief remark on Bethe roots

As we mentioned before, in order to get a self-consistent set of BAEs, the poles μ_j must be simple. For example, examining the Bethe states emerging from the Coordinate Bethe ansatz, we can deduce the Pauli principle for the Bethe roots: the eigenvector is zero as long as $\mu_j = \mu_l$ for $j \neq l$. In fact, to preserve the regularity of $\Lambda(u)$, doubly degenerate

μ_j (if they exist) must satisfy the condition

$$\text{res}\{(u-\mu_j)\Lambda(u)\}|_{u=\mu_j}=0 \tag{3.31}$$

and this gives rise to an additional equation and makes the $M-1$ Bethe roots overdetermined.

3.3 ODBA for the XYZ model

In this section, we introduce how to apply ODBA to obtain the solution of the fully anisotropic spin chain with periodic boundary conditions. Check out how this technique simplifies the derivation process for the XYZ, and, in particular, provides the exact solution for the odd-N case. The first subsection is devoted to reviewing the Hamiltonian and the properties of the matrices involved in the eight-vertex model.

3.3.1 Recap on the Hamiltonian

Take the usual Hamiltonian

$$H=\frac{1}{2}\sum_{i=1}^{N}\left(J_x\sigma_i^x\sigma_{i+1}^x+J_y\sigma_i^y\sigma_{i+1}^y+J_z\sigma_i^z\sigma_{i+1}^z\right), \tag{3.32}$$

with coupling constants

$$J_x=e^{i\pi\eta}\frac{\sigma(\eta+\frac{\tau}{2})}{\sigma(\frac{\tau}{2})},\quad J_y=e^{i\pi\eta}\frac{\sigma(\eta+\frac{1+\tau}{2})}{\sigma(\frac{1+\tau}{2})},\quad J_z=\frac{\sigma(\eta+\frac{1}{2})}{\sigma(\frac{1}{2})}. \tag{3.33}$$

parameterized in terms of the elliptic functions defined in (2.25). The associated $\mathcal{L}$-matrix was

$$\mathcal{L}=\begin{pmatrix}\alpha(u) & 0 & 0 & \delta(u)\\ 0 & \beta(u) & \gamma(u) & 0\\ 0 & \gamma(u) & \beta(u) & 0\\ \delta(u) & 0 & 0 & \alpha(u)\end{pmatrix}, \tag{3.34}$$

with entries

$$\alpha(u) = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \quad \beta(u) = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \tag{3.35}$$

$$\gamma(v) = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}, \quad \delta(v) = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\eta,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\eta,2\tau)}. \tag{3.36}$$

We remind that u is the spectral parameter, η is the crossing parameter, and τ is a generic complex number such that $\mathrm{Im}(\tau) > 0$.

For convenience's sake, we report again the two other functions connected to the θ's:

$$\sigma(u) = \theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,\tau), \tag{3.37}$$

and

$$\zeta(u) = \frac{\partial}{\partial u}\{\ln\sigma(u)\}. \tag{3.38}$$

Again, using (2.30) we can obtain the monodromy matrix, and subsequently the transfer matrix. At this point, the Hamiltonian can be recovered by making use of the relation (2.33).

Now, to dive into the ODBA, we need to write the properties of this $\mathcal{L}$, as we did in subsection (3.2.2) for the XXX chain.

3.3.2 Properties of the $\mathcal{L}$-matrix and Operator Product Identities

The L-matrix defined above satisfies the YBE and possesses the following properties:

$$
\begin{aligned}
&\cdot \text{Initial condition:} \quad \mathcal{L}_{1,2}(0) = P_{1,2}, \\
&\cdot \text{Unitary relation:} \quad \mathcal{L}_{1,2}(u)\mathcal{L}_{2,1}(-u) = -\xi(u) \times Id, \quad \text{with} \quad \xi(u) = \frac{\sigma(u-\eta)\sigma(u+\eta)}{\sigma(\eta)^2}, \\
&\cdot \text{Crossing relation:} \quad \mathcal{L}_{1,2}(u) = (-i\sigma_1^y)\mathcal{L}_{1,2}^{t_2}(-u-\eta)(-i\sigma_1^y), \\
&\cdot \text{PT-symmetry:} \quad \mathcal{L}_{1,2}(u) = \mathcal{L}_{2,1}(u) = \mathcal{L}_{1,2}^{t_1,t_2}(u), \\
&\cdot \text{Z}_2\text{-symmetry:} \quad \sigma_1^\alpha\sigma_2^\alpha\mathcal{L}_{1,2}(u) = \mathcal{L}_{2,1}(u)\sigma_1^\alpha\sigma_2^\alpha \quad \alpha = x, y, z, \\
&\cdot \text{Fusion condition:} \quad \mathcal{L}_{1,2}(-\eta) = -(1+P_{1,2}) = -2P_{1,2}^{(-)},
\end{aligned}
\tag{3.39}
$$

The XYZ transfer matrix satisfies the following operator identities:

$$
\mathbf{T}(\xi_j)\mathbf{T}(\xi_j - \eta) = a(\xi_j)d(\xi_j - \eta)\, Id, \qquad j = 1, ..., N, \tag{3.40}
$$

with

$$
\begin{aligned}
a(u) &= \prod_{l=1}^{N} \frac{\sigma(u - \xi_l + \eta)}{\sigma(\eta)}, \\
d(u) &= a(u-\eta) = \prod_{l=1}^{N} \frac{\sigma(u - \xi_l)}{\sigma(\eta)}.
\end{aligned}
\tag{3.41}
$$

The quasi-periodicity of the elliptic function $\sigma(u)$

$$
\sigma(u+\tau) = -e^{2i\pi(u+\frac{\tau}{2})}\sigma(u), \qquad \sigma(u+1) = -\sigma(u), \tag{3.42}
$$

directly induces the quasi-periodic properties of the R-matrix:

$$
\begin{aligned}
\mathcal{L}_{1,2}(u+1) &= -\sigma_1^z\mathcal{L}_{1,2}(u)\sigma_1^z \\
\mathcal{L}_{1,2}(u+\tau) &= -e^{2i\pi(u+\frac{\eta}{2}+\frac{\tau}{2})}\sigma_1^x\mathcal{L}_{1,2}(u)\sigma_1^x.
\end{aligned}
\tag{3.43}
$$

Consequently, the transfer matrix possesses the following quasi-periodicity properties:

$$\begin{aligned}\mathbf{T}(u+1) &= (-1)^N \mathbf{T}(u) \\ \mathbf{T}(u+\tau) &= (-1)^N e^{-2\pi i\{Nu+N(\frac{\eta+\tau}{2})-\sum_{j=1}^N \xi_j\}} \mathbf{T}(u).\end{aligned} \tag{3.44}$$

In addition, the operator identity

$$\prod_{j=1}^{N} \mathbf{T}(\xi_j) = \prod_{j=1}^{N} a(\xi_j) \times Id \tag{3.45}$$

can be obtained from the unitary relation among (3.39) combined with the form of the transfer matrix.
The quasi-periodicity properties (3.44), and the relations (3.40) and (3.45) are sufficient to determine the spectrum of $\mathbf{T}(u)$, and accordingly the one of the Hamiltonian.

3.3.3 Inhomogeneous TQ relation

Applying $\mathbf{T}(u)$ to an arbitrary eigenstate $|\Psi\rangle$, we can verify that the corresponding eigenvalue $\Lambda(u)$ has properties similar to those of $\mathbf{T}(u)$:

$$\begin{aligned}\Lambda(u+1) &= (-1)^N \mathbf{T}(u) \\ \Lambda(u+\tau) &= (-1)^N e^{-2\pi i\{Nu+N(\frac{\eta+\tau}{2})-\sum_{j=1}^N \xi_j\}} \Lambda(u),\end{aligned} \tag{3.46}$$

and the analytic properties of the $\mathcal{L}$-matrix indicate that

$$\Lambda(u) \text{ is an entire function of } u. \tag{3.47}$$

This last property and the quasi-periodicity features tell us that $\Lambda(u)$ is, as desired, an elliptic polynomial of degree N. Similarly, (3.40) and (3.45) lead to

$$\Lambda(\xi_j)\Lambda(\xi_j-\eta) = a(\xi_j)d(\xi_j-\eta)\, Id, \qquad j=1,...,N, \tag{3.48}$$

$$\prod_{j=1}^{N} \Lambda(\xi_j) = \prod_{j=1}^{N} a(\xi_j). \tag{3.49}$$

The equations (3.46)-(3.48) provide sufficient conditions to determine the function $\Lambda(u)$ and allow us to construct the inhomogeneous TQ relation

$$\Lambda(u) = e^{2i\pi l_1 u + i\phi} a(u) \frac{Q_1(u-\eta)}{Q_2(u)} + e^{-2i\pi l_1 (u+\eta) - i\phi} d(u) \frac{Q_2(u+\eta)}{Q_1(u)} + c \frac{\sigma^{L_1}\left(u+\frac{\eta}{2}\right) a(u) d(u)}{\sigma^{L_1}(\eta) Q_1(u) Q_2(u)}, \tag{3.50}$$

where l_1 is an integer, ϕ and c are two constants to be determined, and M and m are two non-negative integers that satisfy the relation

$$N + L_1 = 2M. \tag{3.51}$$

In the following, keep in mind that the integer L_1 appears only in the last term of (3.50); thus it is necessary only when $c \neq 0$, and even in those cases it can be unnecessary, but here we keep it for generality's sake. The functions $Q_1(u)$ and $Q_2(u)$ are specularly parametrized by $2M$ Bethe roots divided into two sets both with M elements, $\{\mu_j | j = 1, ..., M\}$ and $\{\nu_j | j = 1, ..., M\}$, as follows:

$$Q_1(u) = \prod_{j=1}^{M} \frac{\sigma(u-\mu_j)}{\sigma(\eta)}, \qquad Q_2(u) = \prod_{j=1}^{M} \frac{\sigma(u-\nu_j)}{\sigma(\eta)}. \tag{3.52}$$

Now, $\Lambda(u)$ given by the functional TQ relation (3.50) satisfy the eq.s (3.46)-(3.48), provided that the $2M+2$ parameters entering the TQ relation (namely, the $2M$ Bethe roots, c, and ϕ) satisfy the $2M+2$ Bethe ansatz equations:

$$\left(\frac{N}{2} - M\right)\eta - \sum_{j=1}^{M} (\mu_j - \nu_j) = l_1 \tau + m_1, \qquad l_1,\, m_1 \in \mathbb{Z}, \tag{3.53}$$

$$M\eta - \sum_{l=1}^{N} \xi_l + \sum_{j=1}^{M} (\mu_j + \nu_j) = m_2, \qquad m_2 \in \mathbb{Z}, \tag{3.54}$$

$$\frac{c\, e^{2i\pi(l_1\mu_j + l_1\eta) + i\phi} \sigma^{L_1}(\mu_j + \frac{\eta}{2})}{\sigma^{L_1}(\eta)} a(\mu_j) = -Q_2(\mu_j) Q_2(\mu_j + \eta), \tag{3.55}$$

$$\frac{c\, e^{2i\pi l_1 \nu_j - i\phi} \sigma^{L_1}(\nu_j + \frac{\eta}{2})}{\sigma^{L_1}(\eta)} d(\nu_j) = -Q_1(\nu_j) Q_1(\nu_j - \eta). \tag{3.56}$$

Notice that (4.4) and (3.54) are two equations and they come from the required quasi-periodicity of $\Lambda(u)$. Equations (4.2) and (3.56) are $M + M\,(= 2M)$ identities and they are derived from the constraint on the analyticity of $\Lambda(u)$.

We open a small parenthesis to remark that the "inhomogeneity" of the TQ relations is not

the same "inhomogeneity" of the inhomogeneous parameters ξ_j. The former is due to the presence of the last term in eq.(3.50), while the latter was discussed when we introduced the monodromy matrix of the XYZ chain in subsection (2.2.2). We needed this difference between spectral parameters at different sites for the technique's sake. But now, we need a "homogeneous limit" to recover the physical behavior of the system. Practically, it corresponds to setting all the sites at the same rapidity, sending $\xi_j \to 0\,(j = 1, ..., N)$. Performing this limit, which affects the functions $a(u)$ and $d(u)$, the inhomogeneous TQ relation is reduced to

$$\begin{aligned}\Lambda(u) =& e^{2i\pi l_1 u + i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q_1(u-\eta)}{Q_2(u)} + e^{-2i\pi l_1(u+\eta)-i\phi}\frac{\sigma^N(u)}{\sigma^N(\eta)}\frac{Q_2(u+\eta)}{Q_1(u)} \\ &+ c\,\frac{\sigma^{L_1}\left(u+\frac{\eta}{2}\right)}{\sigma^{L_1}(\eta)Q_1(u)Q_2(u)}\frac{\sigma^N(u+\eta)\sigma^N(u)}{\sigma^N(\eta)\sigma^N(\eta)},\end{aligned} \tag{3.57}$$

and the BAES are modified into

$$\left(\frac{N}{2} - M\right)\eta - \sum_{j=1}^{M}(\mu_j - \nu_j) = l_1\tau + m_1, \qquad l_1,\, m_1 \in \mathbb{Z}, \tag{3.58}$$

$$M\eta + \sum_{j=1}^{M}(\mu_j + \nu_j) = m_2, \qquad m_2 \in \mathbb{Z}, \tag{3.59}$$

$$\frac{c\,e^{2i\pi(l_1\mu_j + l_1\eta)+i\phi}\sigma^{L_1}(\mu_j+\frac{\eta}{2})}{\sigma^{L_1}(\eta)}\frac{\sigma^N(\mu_j+\eta)}{\sigma^N(\eta)} = -Q_2(\mu_j)Q_2(\mu+\eta), \tag{3.60}$$

$$\frac{c\,e^{2i\pi l_1\nu_j - i\phi}\sigma^{L_1}(\nu_j+\frac{\eta}{2})}{\sigma^{L_1}(\eta)}\frac{\sigma^N(\nu_j)}{\sigma^N(\eta)} = -Q_1(\nu_j)Q_1(\nu_j-\eta). \tag{3.61}$$

The equation (3.49) is a selection rule:

$$\Lambda(0) = e^{i\phi}\prod_{j=1}^{M}\frac{\sigma(\mu_j+\eta)}{\sigma(\nu_j)} = e^{\frac{2i\pi k}{N}}, \qquad k = 1, ..., N. \tag{3.62}$$

Finally, the eigenvalue of the Hamiltonian with PBC is given by

$$E = \frac{\sigma(\eta)}{\sigma'(0)}\left(\sum_{j=1}^{M}[\zeta(\nu_j) - \zeta(\mu_j+\eta)] + \frac{1}{2}N\zeta(\eta) + 2i\pi l_1\right). \tag{3.63}$$

3.3.4 Even N case

The inhomogeneous TQ relations for the XYZ have been introduced especially for the odd N case, but they are designed to be general, and then valid for N even, as well. Let us show what happens if we select N as an even number.

We can prove that, from the eq.s (3.60) and (3.61), either the choices $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$ leads to $c = 0$. This means that for $c = 0$ a one-to-one correspondence between the two sets $\{\mu_j\}$ and $\{\nu_k\}$ (that have the same number of elements M) is induced, namely either $\mu_j = \nu_k$ or $\mu_j = \nu_k - \eta$. Thus, looking back at (3.51) and using (3.58), we conclude that for a generic spectral parameter η and $c = 0$, we can set $L_1 = 0$ in (3.51), and the parameters have to obey the relations

$$l_1 = 0, \qquad N = 2M, \qquad \{\mu_j\} = \{\nu_k\} \equiv \{\lambda_j\}. \tag{3.64}$$

This means that now the spectrum of the system can be obtained from $M = \frac{N}{2}$ Bethe roots, making use of the TQ relation (3.57), at this point reduced to a conventional one:

$$\Lambda(u) = e^{i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q(u-\eta)}{Q(u)} + e^{-i\phi}\frac{\sigma^N(u)}{\sigma^N(\eta)}\frac{Q(u+\eta)}{Q(u)} \tag{3.65}$$

where the functions $Q_1(u)$ and $Q_2(u)$ are melted into the same function

$$Q(u) = \prod_{l=1}^{M}\frac{\sigma(u-\lambda_l)}{\sigma(\eta)}. \tag{3.66}$$

The parameters to be determined are now $M+1$, namely $\{\lambda_j\}$ and ϕ, and they satisfy the BAEs and the selection rule:

$$\frac{\sigma^N(\lambda_j+\eta)}{\sigma^N(\lambda_j)} = -e^{-2i\phi}\frac{Q(\lambda_j+\eta)}{Q(\lambda_j+\eta)}, \qquad j = 1, ..., M, \tag{3.67}$$

$$e^{i\phi}\prod_{j=1}^{M}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)} = e^{\frac{2i\pi k}{N}}, \qquad k = 1, ..., N. \tag{3.68}$$

Notice that the BAEs (3.67) coincide exactly with the ones obtained by Baxter in [24] with his standard TQ relations and by Takhtadzhan and Faddeev in [9] with the QISM. Thus, our TQ relations are back to being homogeneous. The fact that the eigenvalues can be determined by $M = \frac{N}{2}$ Bethe roots had been already proven by Baxter in [28]. In this sense, $c = 0$ must not lead to new solutions but just to different parametrizations

of the eigenvalues. Finally, the selection rule (3.68) determines the parameter ϕ and, accordingly, the amplitude of $\Lambda(u)$.
When N is odd, the BAEs (3.58)-(3.61) do not admit any solutions for $c = 0$ and generic η. Thus, we can follow two paths: keep generic η but remaining with an inhomogeneous TQ relation ($c \neq 0$) or select degenerate values of η.

3.3.5 Odd N case: generic η and $c \neq 0$

The first option is accomplished by considering the most general form of the eigenvalue $\Lambda(u)$, i.e. another TQ relation:

$$\Lambda(u) = e^{2i\pi l_1 u + i\phi} a(u) \frac{Q_1(u-\eta)}{Q_2(u)Q(u)} + e^{-2i\pi l_1 (u+\eta) - i\phi} d(u) \frac{Q_2(u+\eta)}{Q_1(u)Q(u)} + c \frac{\sigma^{L_1}\left(u+\frac{\eta}{2}\right) a(u)d(u)}{\sigma^{L_1}(\eta) Q_1(u) Q_2(u) Q(u)}, \tag{3.69}$$

where $Q_1(u)$ and $Q_2(u)$ are the same as always (3.52), whereas $Q(u)$ has the usual form but now is a product of M_1 terms instead of M:

$$Q(u) = \prod_{l=1}^{M_1} \frac{\sigma(u-\lambda_l)}{\sigma(\eta)}. \tag{3.70}$$

where M_1 has to satisfy $N + L_1 = 2M + M_1$. For convenience, we put again $L_1 = 0$, relying on the numerical simulations [26] showing that any choice of L_1 might give a complete set of eigenvalues. After the homogeneous limit, the TQ relation right above becomes:

$$\begin{aligned} \Lambda(u) = & e^{2i\pi l_1 u + i\phi} a(u) \frac{Q_1(u-\eta)Q(u-\eta)}{Q_2(u)Q(u)} \\ & + e^{-2i\pi l_1 (u+\eta) - i\phi} d(u) \frac{Q_2(u+\eta)Q(u+\eta)}{Q_1(u)Q(u)} \\ & + c \frac{a(u)d(u)}{Q_1(u)Q_2(u)Q(u)}. \end{aligned} \tag{3.71}$$

The associated BAEs are:

$$\left(\frac{N}{2}-M-M_1\right)\eta-\sum_{j=1}^{M}(\mu_j-\nu_j)=l_1\tau+m_1,\qquad l_1,\,m_1\in\mathbb{Z}, \tag{3.72}$$

$$\frac{N}{2}\eta+\sum_{j=1}^{M_1}(\lambda_j)+\sum_{j=1}^{M}(\mu_j+\nu_j)=m_2,\qquad m_2\in\mathbb{Z}, \tag{3.73}$$

$$ca(\mu_j)+e^{-2i\pi l_1(\mu_j+\eta)-i\phi}Q_2(\mu_j+\eta)Q_2(\mu_j)Q(\mu_j+\eta)=0, \tag{3.74}$$

$$cd(\nu_j)+e^{2i\pi l_1\nu_j+i\phi}Q_1(\nu_j-\eta)Q_1(\nu_j)Q(\nu_j-\eta)=0, \tag{3.75}$$

$$\begin{aligned}ca(\lambda_j)d(\lambda_j)+e^{2i\pi l_1\lambda_j+i\phi}a(\lambda_j)Q_1(\lambda_j-\eta)Q_1(\lambda_j)Q(\lambda_j-\eta)\\ +e^{-2i\pi l_1(\lambda_j+\eta)-i\phi}d(\lambda_j)Q_2(\lambda_j+\eta)Q_2(\lambda_j)Q(\lambda_j+\eta)=0,\end{aligned} \tag{3.76}$$

$$e^{i\phi}\prod_{j=1}^{M}\frac{\sigma(\mu_j+\eta)}{\sigma(\nu_j)}\prod_{j=1}^{M_1}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)}=e^{\frac{2i\pi k}{N}},\qquad k=1,...,N. \tag{3.77}$$

Notice that, since N is odd, M_1 must be odd and M takes the possible values

$$M=1,...,\frac{N-1}{2}. \tag{3.78}$$

and we need in total N Bethe roots to determine the spectrum of the transfer matrix, while $\frac{N}{2}$ were sufficient for even N. Finally, the energy eigenvalues of the XYZ chain can be recovered using:

$$E=\frac{\sigma(\eta)}{\sigma'(0)}\left(\sum_{j=1}^{M}[\zeta(\nu_j)-\zeta(\mu_j+\eta)]+\sum_{j=1}^{M_1}[\zeta(\lambda_j)-\zeta(\lambda_j+\eta)]+\frac{1}{2}N\zeta(\eta)+2i\pi l_1\right). \tag{3.79}$$

3.3.6 Numerical check of ODBA solution via exact diagonalization for small N

This method has promising power for odd N systems due to its generality. However, it is not very easy in terms of analytical computations. Thus, our first objective is to evaluate its goodness verifying the results obtained by Cao et al. with our own method of exact diagonalization. This computation is also performed to make it more clear the match between the method and the actual physics of the system.

First of all, we used the notation (2.29) to rewrite all the elliptic theta functions in a form compatible with *Wolfram Mathematica* [29]. We took the smallest non-trivial system for N odd for convenience, i.e. $N=3$, and we considered $M=M_1=1$ with their exact same

E_n	n
-1,4087	0
-1,4087	0
-1,4087	0
-1,4087	0
1.1847	1
1.1847	1
1.6326	2
1.6326	2

Table 3.1: Spectrum of the XYZ spin chain with $N = 3$ sites with couplings $J_x = 1.06536$, $J_y = 0.94502$, $J_z = 0.80693$ and $N = 3$, obtained using a Lanczos algorithm. The subscript n stands for the energy level.

choices of the parameters:

$$\eta = 0.20, \qquad \tau = i, \qquad l_1 = m_1 = m_2 = 0. \tag{3.80}$$

Using the identities (3.33), we computed the values of the parameters we are selecting with the choice $\eta = 0.20$, $\tau = i$. The results are:

$$J_x = 1.06536, \qquad J_y = 0.94502, \qquad J_z = 0.80693, \tag{3.81}$$

so, since the Hamiltonian has no overall minus sign, these couplings yield an antiferromagnetic regime along all three axes, as desired to make frustration emerge. In general, due to the properties of the elliptic functions, it can be observed that every real $\eta \in \left(0, \frac{1}{2}\right]$ gives the same exact regime. Once we verified this, we implemented on *GNU Octave* [30] a *Lanczos algorithm* [31] to obtain the first eigenvalues of the system, inserting the obtained J's as couplings. This algorithm is powerful and efficient in estimating the largest eigenvalue of a system described by a Hermitian matrix. When, as in our case, we search for the ground state, i.e. the state with the lowest energy, it is sufficient to put an overall minus sign and restore the correct hierarchy in the end. We made use of the Z_2 symmetry of the system to optimize the efficiency of the computation, working in one sector only and duplicating the results for the other sector. The results coincide with the ones obtained by the cited authors, and they are shown in (3.1). They satisfy the phenomenology expected from a frustrated system: each excited state is doubly degenerate due to the Z_2 symmetry, while the ground state is four-time degenerate due to the combined effect of the Z_2 and time-inversion symmetries.

We repeated the same proceeding for $N = 5$ with the same parameters as before, and we got the results reported in table (3.2). These results match again with the ones obtained by Cao et al. It is interesting to analyze the characteristics of the spectra obtained. Indeed, we note that all states turn out to be double or four times degenerate. One of these degeneracies is given by the presence of Z_2 symmetry, connected to the parity in the magnetization, and it is the one that unites all the energy levels. According to [32] [33], the other degeneracy is associated with Kramer's theorem. In fact, it states that such degeneracy is responsible for ground state manifolds at least two-fold degenerate, and it occurs in systems possessing total half-integer spin and time-reversal symmetry. These hypotheses are satisfied by our frustrated system. To give a taste of it, we can say that it consists of the emergence of states with non-zero total momentum. Another way to see the appearance of this degeneracy is to notice that the parity of the magnetization along the three directions commute with the Hamiltonian, but anti-commute with one another. In addition to this symmetry, the model is also clearly symmetric under a mirror symmetry passing through any of its sites. While states with 0 (or π) momentum are singlet under this symmetry, any state with non-zero momentum has to be degenerate with the state with opposite momentum. In [33], it was shown that topological frustration can promote a finite (non-extensive) momentum in the ground state and in these cases the ground state manifold's degeneracy is doubled. Again, this happens always for the ground state while only under certain conditions for the excited states.
For completeness, and to investigate the complexity of the equations they derived, we solved the system of BAEs (3.72)-(3.77) for $N = 3$ using Mathematica and we obtained the exact same results reported in [26]; we show them in table (3.3). We remark that the μ's, the ν's, and the λ's are all Bethe roots with the same attributes; in the sense that there is no hierarchy or distinction of roles between them. The different letters are just the heritage of the notation we used for the Q-functions (Q_1, Q_2, Q).

It could be interesting to evaluate the goodness of this method for higher dimensions of the system. However, the difficulty increases with the number of sites N. Already for $N = 5$, the algorithm struggles to find the roots, and for higher N a much more precise method would be required. Anyway, the comparison would be with exact diagonalization results, which are known to be limited to systems of small dimensions. Moreover, for finite N, the scheme of the Bethe roots is not so clear since we cannot read them through the string hypothesis. For this reason, let us consider the other case that allows us to

E_n	n
-3.5134	0
-3.5134	0
-3.5134	0
-3.5134	0
-1.4219	1
-1.4219	1
-1.2506	2
-1.2506	2
-1.2506	2
-1.2506	2
-0.8624	3
-0.8624	3
-0.8624	3
-0.8624	3
0.7043	4
0.7043	4
0.7043	4
0.7043	4
1.0235	5
1.0235	5
1.0235	5
1.0235	5
1.0813	6
1.0813	6
1.0813	6
1.0813	6
2.0062	7
2.0062	7
2.3593	8
2.3593	8
2.6910	9
2.6910	9

Table 3.2: Spectrum of the XYZ spin chain with $N = 5$ sites with couplings $J_x = 1.06536$, $J_y = 0.94502$, $J_z = 0.80693$, obtained using a Lanczos algorithm. The subscript n stands for the energy level.

μ_1	μ_1	λ_1	c	ϕ	k	E_n	n
$0.35000 + 0.02632i$	$0.45000 + 0.02632i$	$-1.10000 - 0.05263i$	$-0.08948 + 0.00000i$	$-0.08501 + 0.00000i$	1	-1.40865	0
$0.35000 - 0.02632i$	$0.45000 - 0.02632i$	$-1.10000 + 0.05263i$	$-0.08948 + 0.00000i$	$0.08501 + 0.00000i$	2	-1.40865	0
$-0.15000 + 0.08693i$	$0.05000 + 0.08693i$	$-0.10000 - 0.17387i$	$3.04065 + 0.00000i$	$4.10893 + 0.00000i$	2	-1.40865	0
$-0.15000 - 0.08693i$	$0.05000 - 0.08693i$	$-0.10000 + 0.17387i$	$3.04065 + 0.00000i$	$4.10893 + 0.00000i$	1	-1.40865	0
$-0.65000 - 0.27875i$	$0.55000 - 0.27875i$	$0.90000 + 0.55749i$	$-0.28951 + 0.00000i$	$0.35925 + 0.00000i$	0	1.18468	1
$-0.28066 + 0.31196i$	$-0.18066 + 0.31196i$	$0.16133 - 0.62392i$	$-0.61188 + 0.36729i$	$0.27657 + 0.04967i$	0	1.18468	1
$0.15828 + 0.12139i$	$0.25828 + 0.12139i$	$-0.71655 - 0.24279i$	$-0.09303 - 0.16695i$	$-0.29190 + 0.31832i$	0	1.63263	2
$-0.42198 + 0.50000i$	$-0.32198 + 0.50000i$	$0.44397 - 1.00000i$	$3.33371 - 7.57925i$	$-0.94248 + 0.14392i$	0	1.63263	2

Table 3.3: Numerical solutions for the BAEs (3.72)-(3.77) for system dimension $N = 3$, integers $M = M_1 = 1$, and parameters $\eta = 0.20$, $\tau = i$, $l_1 = m_1 = m_2 = 0$. On the right, we reported the eigenenergies obtained from the Bethe roots using the relation (3.79).

get solutions of the BAEs, the one for degenerate values of η, that turns out to be more suitable to take the thermodynamic limit.

3.3.7 Odd N case: degenerate values of η

It was shown in [10] [26] that only at the discrete points of the spectral parameter

$$\eta = \frac{2l_1}{N-2M}\tau + \frac{2m_1}{N-2M} \qquad l_1,\, m_1 \in \mathbb{Z}. \tag{3.82}$$

we can put $c = 0$ and the BAEs (3.58)-(3.61) admit solution. Then, the inhomogeneous TQ relation (3.57) is reduced to a conventional homogeneous one:

$$\Lambda(u) = e^{2i\pi l_1 u + i\phi}\frac{\sigma^N(u+\eta)}{\sigma^N(\eta)}\frac{Q(u-\eta)}{Q(u)} + e^{-2i\pi l_1(u+\eta)-i\phi}\frac{\sigma^N(u)}{\sigma^N(\eta)}\frac{Q(u+\eta)}{Q(u)}, \tag{3.83}$$

where

$$Q(u) = \prod_{l=1}^{M}\frac{\sigma(u-\lambda_l)}{\sigma(\eta)}, \tag{3.84}$$

and the $M+1$ parameters $\{\lambda_j\}$ and ϕ satisfy the associated BAEs:

$$e^{2i\pi(2l_1\lambda_j + l_1\eta)+2i\phi}\,\frac{\sigma^N(\lambda_j+\eta)}{\sigma^N(\lambda_j)} = -\frac{Q(\lambda_j+\eta)}{Q(\lambda_j-\eta)} \qquad j = 1, ..., M, \tag{3.85}$$

$$e^{i\phi}\prod_{j=1}^{M}\frac{\sigma(\lambda_j+\eta)}{\sigma(\lambda_j)} = e^{\frac{2i\pi k}{N}}, \qquad k = 1, ..., N. \tag{3.86}$$

It should be emphasized that, since $c = 0$, the relation (3.51) does not need to be satisfied, and we can make the "safe" choice $M = N$, which gives a complete set of solutions, as emerged from some numerical analyses [26]. Another crucial aspect is that in the thermodynamic limit ($N \to \infty$) the degenerate points given by eq.(3.82) become dense in the whole complex η-plane. The latter ensures the covering of all the possible regimes of the physical system and allows us to obtain the thermodynamic properties (up to the order of $O(N^{-2})$) of the XYZ for generic values of η. This analysis has been realized in [11] and will be reported in the following section (3.4).

3.4 Thermodynamic limit: ground state and elementary excitations

As announced in the last paragraph of subsection (3.3.7), since the degenerate values of the crossing parameter η become dense in the complex η-plane as $N \to \infty$, we can take the shortest path to analyze the system in the thermodynamic limit. Thus, consider $c = 0$ and η obeying (3.82). Then we can take $M = N$ and $m_1 = -m$ without losing generality [11], and we also choose $l_1 = -1$ to keep η depending on τ. Notice that the case $\eta \in \mathbb{R}$ can be easily recovered. The degenerate points become

$$\tilde{\eta}_m = \frac{\tau}{N} + \frac{2m}{N} \qquad m \in \mathbb{Z}. \tag{3.87}$$

It is also convenient to restrict to the case $0 < \frac{2m}{N} \leq \frac{1}{2}$, since the range $\frac{1}{2} < \frac{2m}{N} \leq 1$ is a straightforward extension but with slightly different distributions of the Bethe roots for the ground state and hole excitations.
If we redefine the λ's by $\lambda_j = \frac{i}{2}x_j - \frac{\tilde{\eta}_m}{2}$, we can consider the $\{x_j\}$ as our physical Bethe roots, frameable in terms of the string hypothesis, and solutions of the BAEs

$$e^{\pi x_j + 2i\phi}\frac{\sigma^N[\frac{i}{2}(x_j - i\tilde{\eta}_m)]}{\sigma^N[\frac{i}{2}(x_j + i\tilde{\eta}_m)]} = -\prod_{k\neq j}^{N}\frac{\sigma[\frac{i}{2}(x_j - x_k - 2i\tilde{\eta}_m)]}{\sigma[\frac{i}{2}(x_j - x_k - 2i\tilde{\eta}_m)]} \qquad j = 1, ..., N, \tag{3.88}$$

$$e^{i\phi}\prod_{j=1}^{M}\frac{\sigma[\frac{i}{2}(x_j - i\tilde{\eta}_m)]}{\sigma[\frac{i}{2}(x_j + i\tilde{\eta}_m)]} = e^{\frac{2i\pi k}{N}}, \qquad k = 1, ..., N. \tag{3.89}$$

simply derived from (3.85)-(3.86). Similarly, (3.63) becomes

$$E = \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)}\left(\sum_{j=1}^{N}\left[\frac{\sigma'[\frac{i}{2}(x_j + \tilde{\eta}_m i)]}{\sigma[\frac{i}{2}(x_j + \tilde{\eta}_m i)]} - \frac{\sigma'[\frac{i}{2}(x_j + \tilde{\eta}_m i)]}{\sigma[\frac{i}{2}(x_j + \tilde{\eta}_m i)]}\right] + \frac{N}{2}\frac{\sigma'(\tilde{\eta}_m)}{\sigma(\tilde{\eta}_m)}\right). \tag{3.90}$$

where we can insert the Bethe roots $\{x_j\}$ recovered from the BAEs to get the spectrum of the Hamiltonian (3.32). Since we are interested in the thermodynamic properties of the system, we shall evaluate the distribution of the Bethe roots in the thermodynamic limit, relying on the string hypothesis.

3.4.1 String hypothesis

Here, the string hypothesis consists in a general form for the solutions of the BAEs, proposed by Takahashi [4]:

$$x_\alpha^{j,k} = x_\alpha^j + (n_j + 1 - 2k)\eta\, i + \frac{1 - v_j}{2} i + O(e^{-\delta N}), \qquad 1 \le k \le n_j, \tag{3.91}$$

where x_α^j is the position of the j-string, k means the kth Bethe root scrolling the string, n_j is the length of the string, $v_j = \pm 1$ identifies the parity of the same string, and $O(e^{-\delta N})$ stands for the finite-size correction. If $v_j = 1$, the center of the j-string is the real axis, whereas if $v_j = -1$, the center of the string is the horizontal line with imaginary part i. Thus, we make this assumption also for our Bethe roots when N is large. The length n_j and the parity v_j, for example, are determined by the parameters of the system, just $\frac{2m}{N}$ in our case. It is convenient to expand $\frac{2m}{N}$ into a so-called simple continued fraction (SCF) of length l as done by Takahashi, too:

$$\frac{2m}{N} = \frac{c_2}{c_1} = \frac{1}{a_1 + \frac{1}{\cdots + \frac{1}{a_l}}} \equiv [a_1, \cdots, a_l], \qquad a_l \ge 2 \quad \text{and} \quad c_1, c_2 \,\text{co-primes}, \tag{3.92}$$

where $a_1 \ge 2$ since $0 < \frac{2m}{N} \le \frac{1}{2}$. Then we need to define the integers z_s and the quantities y_s as

$$z_0 = 0, \qquad z_k = \sum_{j=1}^{k} a_j, \qquad k = 1, 2, ..., l; \tag{3.93}$$

$$y_{-1} = 0, \qquad y_0 = 1, \qquad y_k = a_k y_{k-1} + y_{k-2}. \tag{3.94}$$

In terms of these new elements, the length n_j and parity v_j of string solutions should satisfy the following relations [4]:

$$\begin{aligned} &n_j = y_{s-1} + (j - z_s) y_s, \qquad s = 0, 1, ..., l, \qquad z_s \le j < z_{s+1}, \qquad j = 1, 2, \cdots, z_l; \\ &n_{z_l+1} = y_l; \\ &v_j = (-1)^{\lfloor (n_j - 1)\frac{2m}{N} \rfloor} \qquad j \ne z_1; \\ &v_{z_1} = -1. \end{aligned} \tag{3.95}$$

Here $\lfloor x \rfloor$ denotes the so-called $floor(x)$, that is the maximum integer less than or equal to x.

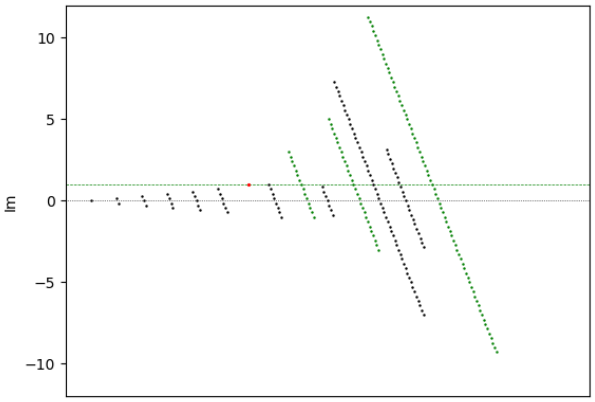


Figure 3.1: Disposition of the Bethe roots for $l_1 = -1$ as strings on the complex plane for $N = 73$, $\tau = i$, and $\frac{2m}{N} = \frac{10}{73}$. The strings are oblique due to the non-vanishing imaginary part of the crossing parameter. Notice that the centers of strings (3.91) with positive parity ($v_j = 1$) lay on the real axis, while the ones of strings with negative parity ($v_j = -1$) are on the shifted horizontal green line. The red point constitutes the whole 1-string for $j = 7$ and it represents a hole among the real roots.

From the eq.s (3.92)-(3.95) we obtain $y_l = c_1$ which corresponds to the length of the $(z_l + 1)$-string, and from eq.(3.95) we can deduce that the number of string types is $z_l + 1$.

Let us consider an example value for $\frac{2m}{N}$ in order to make the description of the string structure clearer. So, let us take $\frac{2m}{N} = \frac{10}{73} = [7, 3, 3]$. Substituting these values in (3.95) we obtain all the required quantities that, plugged into the string hypothesis expression (3.91), give us all the Bethe roots, clustered in strings. As $N = 73$, the value of the crossing parameter is $\tilde{\eta}_m = \frac{i}{73} + \frac{10}{73}$. We remark that, choosing $l_1 \neq 0$, the crossing parameter η would depend on τ. And if τ is chosen to be purely imaginary as usual, η will have an imaginary part. This is reflected in the structure of the strings making them oblique: they are not parallel to the imaginary axis. The disposition of the roots for $l_1 = -1$ is shown in fig.(3.1).

3.4.2 Distribution of Bethe roots

Now that we have the strings, we have to plug them into the BAEs (3.88). Then, omitting exponentially small corrections, and taking the product of the BAEs (3.89) for n_j

components of a j-string, we get the equation for the position x_α^j of the j-string:

$$e^{\varphi_j(x_\alpha^j)} g^N(x_\alpha^j; n_j, v_j) = (-1)^{n_j+1} \prod_{r=1}^{z_l+1} \prod_{\beta=1}^{M_r} \prod_{k=1}^{\min(n_r,n_j)-1} g(x_\alpha^j - x_\beta^r; n_r + n_j, v_r v_j)$$
$$\times\, g(x_\alpha^j - x_\beta^r; |n_r - n_j|, v_r v_j)\, g^2(x_\alpha^j - x_\beta^r; |n_r - n_j| + 2k, v_r v_j), \tag{3.96}$$

where M_r is the number of r-strings and

$$\varphi_j(x) = \pi n_j \left(x + i\frac{1 - v_j}{2} \right) + i2n_j\phi, \tag{3.97}$$

$$g(x; n, v) = \frac{\sigma[\frac{i}{2}(x - n\tilde{\eta}_m i + \frac{1-v}{2} i)]}{\sigma[\frac{i}{2}(x + n\tilde{\eta}_m i + \frac{1-v}{2} i)]}. \tag{3.98}$$

Taking the logarithm of eq.(3.96), we have

$$\frac{1}{i}\varphi_j(x_\alpha^j) + N\vartheta_j(x_\alpha^j) = 2\pi I_\alpha^j + \sum_{r=1}^{z_l+1} \sum_{\beta=1}^{M_r} \Theta_{jr}(x_\alpha^j - x_\beta^j), \qquad \alpha = 1, ..., M_r, \tag{3.99}$$

where I_α^j is an integer (half-integer) for $n_j + M_j + 1 - N\frac{1+v_j}{2}$ even (odd) and

$$\vartheta_j(x) \equiv \vartheta(x; n_j, v_j) = -i \ln[(-v_j)\, g(x; n_j, v_j)], \tag{3.100}$$

$$\Theta_{jr}(x) = \vartheta(x; n_r + n_j, v_j v_r) + \vartheta(x; |n_r - n_j|, v_j v_r) + 2 \sum_{k=1}^{\min(n_r,n_j)-1} \vartheta(x; |n_r - n_j| + 2k, v_j v_r). \tag{3.101}$$

In particular, $\vartheta_j(x)$ is an elliptic function with double quasi-periodicities $2i$ and $2\frac{\tau}{i}$, but it is sufficient to consider their values in one periodicity. In order to shift the variables into the domain $[-i, i]$, we define

$$\begin{aligned} q_j &\equiv (-1)^s (p_s - (j - z_s) p_{s+1}), \qquad s = 0, 1, ..., l, \quad j = 1, 2, ..., z_l, \quad z_s \le j \le z_{s+1}, \\ q_{z_l+1} &= (-1)^{l+1} p_{l+1}, \end{aligned} \tag{3.102}$$

where the $\{p_s\}$ constitute a series:

$$p_0 = \frac{N}{2m}, \quad p_1 = 1, \quad p_n = p_{n-2} - p_{n-1} a_{n-1}, \tag{3.103}$$

with

$$a_{n-1} = \left\lfloor \frac{p_{n-2}}{p_{n-1}} \right\rfloor, \qquad n = 2, 3, ..., l+1. \tag{3.104}$$

This makes the series completely determined by the SCF expansion (3.92), which yields $p_{l+1} = 0$. Moreover, from (3.102) we extract the range covered by the q's: $-1 \leq q_j \leq \frac{N}{2m} - 1$ for $j = 1, 2, ..., z_l + 1$ with internal ordering $|q_r| \leq |q_j|$ if $r > j$. It can also be proven that q_j can be parametrized as

$$q_j = \omega_j \frac{N}{2m} - n_j, \tag{3.105}$$

where

$$\omega_{z_1} = 0, \qquad \omega_j = \left\lfloor (n_j - 1)\frac{2m}{N} \right\rfloor + 1, \quad j \neq z_1. \tag{3.106}$$

From this expression, we notice that the integers ω_j, and consequently the quantities q_j, are only determined by the length n_j of the j-string.
These quantities allow us to express the function $\vartheta_j(x)$ as

$$\vartheta_j(x) = \frac{1}{i} \ln \frac{\theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} \left(\frac{i}{2}(x + (q_j \frac{2m}{N} i + \frac{n_j}{N} \frac{\tau}{i})) \right)}{\theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} \left(\frac{i}{2}(x - (q_j \frac{2m}{N} i + \frac{n_j}{N} \frac{\tau}{i})) \right)}. \tag{3.107}$$

This expression is useful to deduce that the behavior of the function $\vartheta_j(x)$ sensitively depends on the sign of q_j: it is monotonically increasing in x for $q_j > 0$ while monotonically increasing in x for $q_j > 0$.
At this point, we can go back to the string hypothesis (3.91), substitute it into the selection rule (3.89), and take the logarithm, obtaining

$$\sum_{j=1}^{z_l+1} \left\{ \frac{1}{2\pi} \vartheta_j(x_\alpha^j) \right\} = I + \frac{k_1}{2N} - \frac{\phi}{2\pi}, \qquad k_1 = 1, ..., 2N, \tag{3.108}$$

where I is an integer (half-integer) for $\sum_{j=1}^{z_l+1} M_j \frac{1+v_j}{2}$ even (odd). The function $\vartheta_j(x)$ has the role of quantifying the distribution of the Bethe roots. In particular, this equation tells us that the distribution and the value of ϕ are tied to each other, and consequently they are both fixed for each state.

These algebraically complicated steps were preparatory to defining the counting function

$Z_j(x)$ as

$$Z_j(x) = \frac{\varphi_j(x)}{2\pi N i} + \frac{1}{2\pi}\vartheta_j(x) - \frac{1}{N}\sum_{r=1}^{z_l+1}\sum_{\beta=1}^{M_r}\frac{1}{2\pi}\Theta_{jr}(x - x_\beta^r). \tag{3.109}$$

The imposition $Z_j(x_\alpha^j) = I_\alpha^j/N$ corresponds exactly to (3.99).
In the thermodynamic limit, x_α^j becomes a continuous variable and the counting function $Z_j(x)$ turns into a continuous function. Thus, we define

$$\frac{d}{dx}Z_j(x) = \text{sign}(q_j)[\rho_j(x) + \rho_j^h(x)], \tag{3.110}$$

where $\rho_j(x)$ is the density of states characterized by the j-string, while $\rho_j^h(x)$ is the density of the corresponding holes. Notice that the function $\text{sign}(q_j)$ is needed due to the different monotonicity of $\vartheta_j(x)$ depending on the sign of q_j.
At this point, we can plug (3.109) into the definition (3.110), namely we take the derivative of (3.109) with respect to x, and we obtain the integral equations for the densities of states:

$$\text{sign}(q_j)\rho_j^h(x) = a_j(x) + \frac{n_j}{2Ni} - \sum_{r=1}^{z_l+1}\int_{-Q}^{Q} A_{jr}(x-y)\rho_r(y)dy, \tag{3.111}$$

where the functions $a_j(x)$ and $A_{jr}(x)$, defined as

$$\begin{aligned} a_j(x) &\equiv a(x; n_j, v_j) = \frac{1}{2\pi}\frac{d}{dx}\vartheta_j(x) \\ &= -\frac{1}{4\pi}\left\{ \frac{\theta'\begin{bmatrix}\frac{1}{2}\\0\end{bmatrix}[\frac{i}{2}(x-(q_j\frac{2m}{i}+\frac{n_j}{N}\frac{\tau}{i}))]}{\theta\begin{bmatrix}\frac{1}{2}\\0\end{bmatrix}[\frac{i}{2}(x-(q_j\frac{2m}{i}+\frac{n_j}{N}\frac{\tau}{i}))]} - \frac{\theta'\begin{bmatrix}\frac{1}{2}\\0\end{bmatrix}[\frac{i}{2}(x+(q_j\frac{2m}{i}+\frac{n_j}{N}\frac{\tau}{i}))]}{\theta\begin{bmatrix}\frac{1}{2}\\0\end{bmatrix}[\frac{i}{2}(x+(q_j\frac{2m}{i}+\frac{n_j}{N}\frac{\tau}{i}))]} \right\}, \end{aligned} \tag{3.112}$$

$$\begin{aligned} A_{jr}(x) &= \frac{1}{2\pi}\frac{d}{dx}\Theta_j(x) + \delta_{jr}\text{sign}(q_j)\delta(x) \\ &= a(x; n_r + n_j, v_r v_j) + a(x; |n_r - n_j|, v_r v_j) + 2\sum_{k=1} a(x; |n_r - n_j| + 2k, v_r v_j) + \delta_{jr}\text{sign}(q_j)\delta(x), \end{aligned} \tag{3.113}$$

are elliptic functions with double-periods $2i$ and $2\frac{\tau}{i}$. Since the j-strings are distributed in the interval $\left[-\frac{\tau}{i}, \frac{\tau}{i}\right]$ on the real axis (remember that τ is pure imaginary) we can choose the extreme of the integral to be $Q = \frac{\tau}{i}$.

3.4.3 Ground state energy

All the functions computed until now become useful to calculate the physical quantities of the XYZ chain with odd N in the thermodynamic limit.

Let us focus on the ground state energy. Thus, our goal is to arrange the Bethe roots in a way that is allowed by all the previous considerations, but also choosing a configuration that minimizes the energy of the system. We know that the real Bethe roots contribute negative energies, so we want them to fill the real axis as far as possible. The first constraint is that, in general, the maximum number of real Bethe roots is $\frac{N}{2}$. This means that, as the first thing, imagine putting $\frac{N}{2}$ on the real axis for even N or $\frac{N}{2}-1$ for odd N; the remaining roots will be distributed on the complex plane with the shape of strings satisfying (3.95). In the following, the real roots will be expressed as 1-strings, corresponding to $n_j = 1$ and $v_j = +1$ in (3.95).

Therefore, substituting $n_j = 1$ and $v_j = +1$ in (3.113), we are selecting the function A_{1r} associated with the ground state:

$$A_{1r}(x) = a(x; n_r + 1, v_r) + a(x; n_r - 1, v_r) + \delta_{1r}\text{sign}(q_1)\delta(x). \tag{3.114}$$

This equation can be solved by Fourier transform. The FT of the function $A_{1r}(x)$ is

$$\tilde{A}_{1r}(k) = 2\cosh\left(\frac{i}{\tau}k\pi\tilde{\eta}_m\right)\frac{\sinh[\frac{i}{\tau}k\pi(q_r\frac{2m}{N} - n_r\frac{\tau}{N})]}{\sinh(\frac{i}{\tau}k\pi)}. \tag{3.115}$$

We make use of this expression by plugging it into the FT of the whole eq.(3.111) with $j = 1$. This yields the FT of the density of states at the ground state

$$\tilde{\rho}_1(k) = \frac{1}{2\cosh(\frac{i}{\tau}k\pi\tilde{\eta}_m)} - \frac{\tilde{\rho}_1^h(k)}{\tilde{A}_{11}(k)} - \frac{\tau\delta_{k0}}{N\tilde{A}_{11}(k)} - \sum_{r\neq 1}^{z_l+1}\frac{\sinh[\frac{i}{\tau}k\pi(q_r\frac{2m}{N} - n_r\frac{\tau}{N})]}{\sinh[\frac{i}{\tau}k\pi(1-\tilde{\eta}_m)]}\tilde{\rho}_r(k). \tag{3.116}$$

It is clear that real Bethe roots, holes, and strings are coupled together. In particular, it is interesting that the distribution of real Bethe roots depends on the densities of holes and strings.

Now, if we take a look back at the expression (3.90) for the eigenenergies of the system in terms of Bethe roots, and we make use of (3.112), we obtain that the energy of a r-string

is

$$\varepsilon_r(\tilde{\eta}_m) = \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} \left\{ \frac{\theta' \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} [\frac{i}{2}(x - (q_j \frac{2m}{i} + \frac{n_j}{N} \frac{\tau}{i}))]}{\theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} [\frac{i}{2}(x - (q_j \frac{2m}{i} + \frac{n_j}{N} \frac{\tau}{i}))]} - \frac{\theta' \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} [\frac{i}{2}(x + (q_j \frac{2m}{i} + \frac{n_j}{N} \frac{\tau}{i}))]}{\theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} [\frac{i}{2}(x + (q_j \frac{2m}{i} + \frac{n_j}{N} \frac{\tau}{i}))]} \right\}$$
$$= -4\pi \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} a_r(x). \tag{3.117}$$

Thus, from the last two eq.s and again (3.90), we get the expression for the ground state energy of the system

$$E_g^{\text{odd}}(\tilde{\eta}_m) = -4\pi N \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} \left\{ \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} a_1(x)\rho_1(x)dx + \sum_{r\neq 1}^{z_l+1} \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} a_r(x)\rho_r(x)dx \right\} + \frac{N}{2} \frac{\sigma'(\tilde{\eta}_m)}{\sigma'(0)}$$
$$= -\frac{2i\pi N}{\tau} \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \left\{ \frac{\tilde{a}_1(k)}{2\cosh(\frac{i}{\tau}k\pi\tilde{\eta}_m)} - \frac{\tilde{\rho}_1^h(k)}{2\cosh(\frac{i}{\tau}k\pi\tilde{\eta}_m)} \right\} + \frac{N}{2} \frac{\sigma'(\tilde{\eta}_m)}{\sigma'(0)}. \tag{3.118}$$

Then, exploiting the Fourier transform $\tilde{a}_1(k) = \frac{\sinh[\frac{i}{\tau}k\pi(1-\tilde{\eta}_m)]}{\sinh(\frac{i}{\tau}k\pi)}$, we can recollect the terms

$$e_0(\tilde{\eta}_m) = -\frac{i\pi}{\tau} \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{\sinh[\frac{i}{\tau}k\pi(1-\tilde{\eta}_m)]}{\sinh(\frac{i}{\tau}k\pi)\,\cosh(\frac{i}{\tau}k\pi\tilde{\eta}_m)} + \frac{1}{2} \frac{\sigma'(\tilde{\eta}_m)}{\sigma'(0)} \tag{3.119}$$

$$\epsilon_h(\tilde{\eta}_m) = \frac{i\pi N}{\tau} \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{\tilde{\rho}_1^h(k)}{\cosh(\frac{i}{\tau}k\pi\tilde{\eta}_m)} \tag{3.120}$$

to write

$$E_g^{\text{odd}}(\tilde{\eta}_m) = e_0(\tilde{\eta}_m)N + \epsilon_h(\tilde{\eta}_m). \tag{3.121}$$

Thus, we recognize $e_0(\tilde{\eta}_m)$ as the density of the ground state energy at the degenerate point $\tilde{\eta}_m$ and $\epsilon_h(\tilde{\eta}_m)$ as the energy carried by the holes in the real axis. This means that the ground state energy is only related to the real Bethe roots and corresponding holes. Notice that, since e_0 only depends on the real roots, we have that the ground state energy is only related to the real Bethe roots and the corresponding holes. Although the strings could in principle affect the density of states, their contribution to the energies is zero.

This phenomenon derives from the *rearrangement of Fermi sea*.

3.4.4 Distinction between N odd and N even

Notice that no restriction on N has been done until now. We used the ODBA technique and the string hypothesis, but the proceeding is completely valid for both the odd and the even case. This is relevant because we can use the obtained results to compare the two cases directly and as fruits of the same technique. In this subsection will be shown how the strings affect the distribution of holes, and how they together determine different ground state energy in the two cases. Thus, first of all, let us analyze in general the string solutions satisfying (3.95). Suppose that, there are M_r r-strings (with $r \geq 2$). From the definition of the q's (3.102), we know that $-1 \leq q_r \leq \frac{N}{2m} - 1$ for $r = 2, ..., z_l + 1$. Since we have shifted all the variables into one periodicity to compute the values of elliptic functions, these strings should also be moved to the same periodicity. In order to minimize the energy, we need to reduce as much as possible the number of holes (since they contribute with positive energy). This can be expressed in the requirement

$$-1 < \sum_{r\neq 1}^{z_l+1} M_r q_r < \frac{N}{2m} - 1. \tag{3.122}$$

Then, using the parametrization of the q's in terms of the ω's as written in eq.(3.105)-(3.106), we have

$$\left\lfloor \left(\sum_{r\neq 1}^{z_l+1} M_r n_r - 1 \right) \frac{2m}{N} \right\rfloor + 1 = \sum_{r\neq 1}^{z_l+1} M_r \omega_r, \tag{3.123}$$

where

$$\sum_{r\neq 1}^{z_l+1} M_r n_r \tag{3.124}$$

constitutes the total number of string solutions. Substituting eq.(3.123) into the definition of the ω's (3.106), we end up with

$$\sum_{r\neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\sum_{r\neq 1}^{z_l+1} M_r n_r - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \sum_{r\neq 1}^{z_l+1} M_r n_r. \tag{3.125}$$

From this expression, it is clear that the contribution of the strings depends sensibly on the parity of N.

First, consider the case N **odd**. Since the real Bethe roots correspond to 1-strings, the number of real Bethe roots is $M_1 = \frac{N-1}{2}$, while the number of string solutions, i.e. all the other roots out of the real axis, is

$$\sum_{r\neq 1}^{z_l+1} M_r n_r = \frac{N+1}{2}, \tag{3.126}$$

and substituting (3.126) into (3.125), we get

$$\sum_{r\neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\sum_{r\neq 1}^{z_l+1} M_r n_r - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \frac{N+1}{2} = -\frac{1}{2}. \tag{3.127}$$

Now we can use the number of real Bethe roots $M_1 = \frac{N-1}{2}$ and our knowledge of the number of holes in the ground state as constraints to fix the density of roots and holes.

$$\tilde{\rho}_1(0) = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \rho_1(x)dx = \frac{M_1}{N} = \frac{N-1}{2N} = \frac{1}{2} - \frac{1}{2N}. \tag{3.128}$$

Then, using the expression for the density of states at the ground state (3.116), we obtain the values of $\tilde{\rho}_1(0)$ as

$$\tilde{\rho}_1(0) = \frac{1}{2} - \frac{\tilde{\rho}_1^h(0)}{2(1-\tilde{\eta}_m)} + \frac{\tilde{\eta}_m}{2M(1-\tilde{\eta}_m)}. \tag{3.129}$$

Consequently, substituting this expression into (3.128), we get the FT of the distribution of the holes at the ground state for $k = 0$.

$$\tilde{\rho}_1^h(0) = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \rho_1^h(x)dx = \frac{1}{N}. \tag{3.130}$$

Comparing this result with the definition of counting function, we know that such a configuration gives that there is only one hole in the real axis at the ground state. In particular, the density of holes $\rho_1^h(x)$ can be expressed by the δ-function centered in the position x^h of the single hole:

$$\rho_1^h(x) = \frac{1}{N}\delta(x - x^h), \quad \longleftrightarrow \quad \tilde{\rho}_1^h(k) = \frac{1}{N} e^{\frac{k\pi}{\tau} x^h}. \tag{3.131}$$

Now, this expression can be plugged in (3.120) to obtain the energy carried by the single hole

$$\epsilon_h(x^h, \tilde{\eta}_m) = \frac{i\pi}{\tau} \frac{\sigma(\tilde{\eta}_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{e^{\frac{k\pi}{\tau}x^h}}{\cosh(\frac{i}{\tau}k\pi\tilde{\eta}_m)}. \tag{3.132}$$

It remains to be determined the position of the hole. For this problem, some considerations on the thermodynamic limit come to the rescue. Indeed, in the thermodynamic limit, its position x^h can take continuous values in the interval $\left[-\frac{\tau}{i}, \frac{\tau}{i}\right]$. And it should be noted that the function $\epsilon_h(x^h, \tilde{\eta}_m)$ takes the minimum value at $x^h = \frac{\tau}{i}$. Then, since we are selecting the ground state, we are going to choose this point to minimize the positive energy brought by the hole.
Finally, the ground state energy reads

$$E^{\text{odd}}_{g,PBC}(\tilde{\eta}_m) = e_0(\tilde{\eta}_m)N + \epsilon_h\left(\frac{\tau}{i}, \tilde{\eta}_m\right). \tag{3.133}$$

Instead, if the system size N is even, at the ground state there exist $M_1 = \frac{N}{2}$ real Bethe roots (again, we take the maximum number to minimize the energy) and $\frac{N}{2}$ string solutions

$$\sum_{r\neq 1}^{z_l+1} M_r n_r = \frac{N}{2}; \tag{3.134}$$

plugging it into (3.125), we have

$$\sum_{r\neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\frac{N}{2} - 1\right)\frac{2m}{N}\right\rfloor + 1\right)\frac{N}{2m} - \frac{N}{2} = 0. \tag{3.135}$$

Performing the same procedure as before, namely using eq.s (3.116),(3.134) and (3.135), we have

$$\frac{M_1}{N} = \frac{1}{2} = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \bar{\rho}_1(x)dx = \tilde{\bar{\rho}}_1(0) = \frac{1}{2} - \frac{\tilde{\bar{\rho}}^h_1(0)}{2(1-\tilde{\eta}_m)}, \tag{3.136}$$

where $\bar{\rho}_1(x)$ is the density of real Bethe roots, $\tilde{\bar{\rho}}_1(x)$ is its FT and $\tilde{\bar{\rho}}^h_1(0)$ is the FT of the density of the holes. Such a configuration gives that there is no hole at the ground state, i.e. $\bar{\rho}^h_1(x) = 0$. Finally, the ground state energy for N even is

$$E^{\text{even}}_g(\tilde{\eta}_m) = e_0(\tilde{\eta}_m)N, \tag{3.137}$$

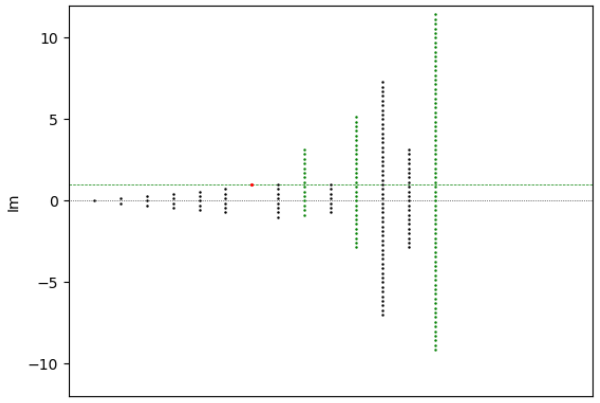


Figure 3.2: Disposition of the Bethe roots as strings on the complex plane for $N = 73$, $\tau = i$, and $\frac{2m}{N} = \frac{10}{73}$. The strings are vertical since the choice $l_1 = 0$ makes the crossing parameter independent from τ and then keeps η real. Notice that the centers of strings (3.91) with positive parity ($v_j = 1$) lay on the real axis, while the ones of strings with negative parity ($v_j = -1$) are on the shifted horizontal green line. The red point constitutes the whole 1-string for $j = 7$ and it represents a hole among the real roots.

which is lower than the one obtained in the odd N case, since lacking of the positive contribution coming from the hole.

The proceeding that brought us here was conducted using the imaginary crossing parameter $\tilde{\eta} = \frac{\tau}{N} + \frac{2m}{N}$. Now, it is interesting but non-trivial to note that these results for the ground state can be extended to the real η case just by substituting $\tilde{\eta}$ with

$$\bar{\eta}_m = \frac{2m}{N} \qquad m \in \mathbb{Z}. \tag{3.138}$$

This spectral parameter no longer depends on τ, and corresponds to the choice $l_1 = 0$ in eq.(3.82). The arrangement of the roots is no longer oblique, but vertical, and it shown in fig.(3.2). The reality of the spectral parameter is physically relevant because now it belongs to the region $\eta \in \left(0, \frac{1}{2}\right]$. This guarantees that we are selecting an AFM regime, that makes the frustration effects emerge.

3.4.5 Elementary excitations

So, consider the roots' scheme of the odd N ground state and move the hole from $x^h = \frac{\tau}{i}$ to another position in the real axis. This is called *hole excitation* and it is a typical elementary excitation of the system. The energy we are adding to the system is given by the difference between the energy of the new excited state and the one of the ground state (3.133). Since we are not touching the ground state energy density (3.119), the expression

of the excitation is

$$\Delta E^{\text{odd}}(x^h, \bar{\eta}_m) = E_e^{\text{odd}}(\bar{\eta}_m) - E_g^{\text{odd}}(\bar{\eta}_m) = \epsilon_h(x^h, \bar{\eta}_m) - \epsilon_h\left(\frac{\tau}{i}, \bar{\eta}_m\right). \tag{3.139}$$

This quantity is positive since we have seen that $\epsilon_h(x^h, \bar{\eta}_m)$ is minimal when the hole is placed at $x^h = \frac{\tau}{i}$. Therefore, any other position of the hole implies a higher value for the energy. An interesting aspect of the expression above is that, in the thermodynamic limit, the position of the hole x^h can tend to $\frac{\tau}{i}$ infinitely. Thus,

$$\lim_{x^h \to \frac{\tau}{i}} \Delta E^{\text{odd}}(x^h) \to 0 \tag{3.140}$$

and we conclude that the excitation spectrum is continuous.

In the even N case, there were no holes in the ground state. So, the simplest hole excitation consists of replacing a real Bethe root of the ground state configuration with a z_1-string of length $n_{z_1} = 1$ and parity $v_{z_1} = -1$. The energy carried by this 1-string is positive. Intuitively, in this kind of excited state, there are $M_1 = \left(\frac{N}{2} - 1\right)$ real Bethe roots and $\left(\frac{N}{2} + 1\right)$ string solutions. Then, the real roots satisfies

$$\frac{M_1}{N} = \frac{1}{2} - \frac{1}{N} = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \rho_1'(x) = \tilde{\rho}_1'(0), \tag{3.141}$$

while the string solutions satisfy

$$\sum_{r \neq 1}^{z_l+1} M_r n_r = \frac{N}{2} + 1, \tag{3.142}$$

$$\sum_{r \neq 1}^{z_l+1} M_r q_r = \left(\left\lfloor \left(\frac{N}{2} - 1 \right) \frac{2m}{N} \right\rfloor + 1 \right) \frac{N}{2m} - \frac{N}{2} + q_{z_1} = -1. \tag{3.143}$$

Due to these two constraints on the string solutions, the density of states (3.116) with $k = 0$ becomes

$$\tilde{\rho}_1'(0) = \frac{1}{2} - \frac{\tilde{\rho}_1'^h(0)}{2 - (1 - \bar{\eta}_m)} - \frac{\bar{\eta}_m}{N(1 - \bar{\eta}_m))}. \tag{3.144}$$

Plugging this expression in the constraint for the real roots (3.141), we get

$$\tilde{\rho}_1'^h(0) = \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \rho_1'^h(x) dx = \frac{2}{N}. \tag{3.145}$$

This result for the FT of the density of holes tells us that there are two holes in the real axis, that will be placed in x_1^h and x_2^h respectively. Then, the Fourier anti-transform yields the density of holes

$$\rho_1'^h(x) = \frac{1}{N}\left[\delta(x - x_1^h) + \delta(x - x_2^h)\right]. \tag{3.146}$$

Summing up these results, the energy of this hole excitation is

$$\Delta E^{\text{even}}(x_1^h, x_2^h, \bar{\eta}_m) = E_{exc}^{\text{even}}(\bar{\eta}_m) - E_g^{\text{even}}(\bar{\eta}_m) = \epsilon_h(x_1^h, x_2^h, \bar{\eta}_m) + \epsilon_h(x_1^h, x_2^h, \bar{\eta}_m). \tag{3.147}$$

In the thermodynamic limit, we can put both the holes x_1^h and x_2^h on the point $\frac{\tau}{i}$, getting

$$\lim_{x_1^h, x_2^h \to \frac{\tau}{i}} \Delta E^{\text{even}}(x_1^h, x_2^h) \to 2\epsilon_h\left(\frac{\tau}{i}, \bar{\eta}_m\right). \tag{3.148}$$

This means that for even N, the excitation is gapped. These results are justified by both analytical and numerical (DMRG method) computations [11].

Chapter 4

Connection with the sine-Gordon model

In 1976, Alan Luther showed explicitly [34] the connection that exists between the spin-$\frac{1}{2}$ XYZ chain and the sine-Gordon model, with suitable relations between coupling constants. First of all, let us introduce the sine-Gordon model and its characteristics.

4.1 Introduction to the sine-Gordon model

In Chapter 1 we discussed the concept of integrability for classical and quantum systems. So far we have been dealing with discrete quantum models whose integrability did not have an unambiguous definition. Quantum Field Theories fit into this discussion in a very interesting way since, although they describe quantum systems, their integrability is well-defined. In fact, an integrable QFT is characterized by an infinite number of conserved charges, i.e., of conservation laws [35]. Therefore, for them, we can derive the exact mass spectrum of its excitations, the correlation functions, the thermodynamics, etc. Anyway, we still deal with only (1+1) dimensions, for which non-trivial integrable QFTs can occur. Many of these integrable Quantum Field Theories are associated with a Lagrangian density: one of them is the *sine-Gordon model*.

4.1.1 The Lagrangian

The (1+1)-dimensional Lagrangian density for the quantum sine-Gordon model [36] can be written as:

$$\mathcal{L}_{sG} = \frac{1}{2}\partial_\mu\phi\,\partial^\mu\phi + \frac{m^2}{\beta^2}(\cos\beta\phi - 1) \tag{4.1}$$

where ϕ is a scalar bosonic field while m and β are two parameters of the model: m^2 is the "squared mass" associated with the spectrum of small oscillations about the minimum, while β measures the strength of the interactions between these small oscillations. It is interesting to notice that, using the bosonization procedure, this Lagrangian can be transformed in the massive Thirring model's [37]:

$$\mathcal{L}_{Th} = i\bar{\Psi}\gamma^\mu\partial_\mu\Psi - M\bar{\Psi}\Psi - \frac{1}{2}g(\bar{\Psi}\gamma^\mu\Psi)(\bar{\Psi}\gamma_\mu\Psi) \tag{4.2}$$

where Ψ is instead a complex fermionic field, provided that the coupling constants are related by the identity

$$\frac{\beta^2}{4\pi} = \frac{1}{1+\frac{g}{\pi}}. \tag{4.3}$$

Note that $\beta^2 = 4\pi$ is equivalent to $g = 0$, i.e., a free fermionic model.

The first term in (4.1) is the kinetic one, while the second is the scalar potential

$$V(\phi) = \frac{m^2}{\beta^2}(\cos\beta\phi - 1). \tag{4.4}$$

This potential presents an infinite series of degenerate minima placed at $\phi = \frac{2\pi n}{\beta}$ ($n = 0, \pm1, ...$), that correspond to an infinite family of equivalent quantum vacua. Around each minimum, the potential has a quadratic concavity m^2 that can be seen as the mass of the scalar particle created out of the vacuum by the field ϕ. But this is not the only type of excitation of the model [38]. Indeed, the sine-Gordon hosts also *topological excitations* of finite energy, associated with the field configurations that interpolate between two degenerate vacua.

4.1.2 Topological excitations

Consider two vacua among the infinite family seen before: $\frac{2\pi n_1}{\beta}$ and $\frac{2\pi n_2}{\beta}$, labeled by two integers (n_1, n_2). The field $\phi(x)$ reaches the two vacua at $x \to \pm\infty$. This scheme is

associated with a *topological charge* defined by

$$\mathcal{T} = n_1 - n_2 = \frac{1}{2\pi\beta}\int_{-\infty}^{\infty} dx \frac{\partial\phi}{\partial x}. \tag{4.5}$$

A generic configuration $\phi(x,t)$ has energy given by the expression

$$E(\phi) = \int_{-\infty}^{\infty} dx \left[\frac{1}{2}\left(\frac{\partial^2\phi}{\partial t^2}\right)^2 + \left(\frac{\partial^2\phi}{\partial x^2}\right)^2 + V(\phi)\right], \tag{4.6}$$

and it obeys the equation of motion of the model

$$\frac{\partial^2\phi}{\partial t^2} - \frac{\partial^2\phi}{\partial x^2} = \frac{\partial V}{\partial\phi}. \tag{4.7}$$

Looking at the static solutions of the equation of motion, we are left with

$$\frac{\partial^2\phi}{\partial x^2} = -\frac{\partial V}{\partial\phi}. \tag{4.8}$$

These solutions of (4.8) are the classical expressions of the elementary topological configurations, i.e. those associated with $\mathcal{T} = \pm 1$. In practice, the expression (4.8) coincides with the equation of motion of classical mechanics of a fictitious particle with coordinate $\phi(x)$ and subjected to the potential $-V(\phi)$. We can also individuate its integral of motion, typical of a classical system under a conservative force. It is given by

$$W = \frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 - V(\phi). \tag{4.9}$$

which corresponds to its mechanical energy and it must not be confused $E(\phi)$. By the way, it must be identically zero, since at $x \to \pm\infty$ both $V(\phi)$ and $\frac{\partial\phi}{\partial x}$ must be zero to guarantee finite energy $E(\phi)$ in (4.6). The solution of eq.(4.8) can be recovered by quadrature from (4.9):

$$\frac{d\phi}{dx} = \sqrt{2V(\phi)} \quad \to \quad (x - x_0) = \pm\int_{\phi(x_0)}^{\phi(x)} \frac{d\bar{\phi}}{\sqrt{2V(\bar{\phi})}}, \tag{4.10}$$

where x_0 is an arbitrary constant of integration. Plugging V (4.4) in the expression above and integrating, we obtain the two solutions

$$\bar{\phi}(x) = \pm\frac{4}{\beta}\arctan[e^{m(x-x_0)}]. \tag{4.11}$$

The solution with positive sign corresponds to a *soliton*: it has topological charge $\mathcal{T} = 1$ and interpolates between the vacuum $\bar{\phi} = 0$ and the next one $\bar{\phi} = \frac{2\pi}{\beta}$ (or equivalently between a generic pair $\frac{2\pi n}{\beta}$ and $\frac{2\pi(n+1)}{\beta}$ since the theory is defined modulus $\frac{2\pi}{\beta}$). The other one, with the minus sign, is the *anti-soliton* with $\mathcal{T} = -1$ and interpolating between the vacuum $\frac{2\pi n}{\beta}$ and the previous one $\frac{2\pi(n-1)}{\beta}$.
We can consider the energy of the soliton static solution as the integral of an energy density:

$$E(\bar{\phi}) = \int_{-\infty}^{\infty} dx\, \epsilon(x), \qquad \text{with} \qquad \epsilon(x) = \frac{4m^2}{\beta^2} \frac{1}{\cosh^2 m(x - x_0)}. \tag{4.12}$$

Since $\epsilon(x)$ is strongly localized at x_0, the soliton can be interpreted as a particle excitation of the system with mass corresponding to the energy (4.12):

$$M_s = \frac{8m^2}{\beta^2}. \tag{4.13}$$

The soliton and the anti-soliton have the same mass M_s [39].

4.2 Connection between sine-Gordon and XYZ spin chain

The interesting work by Luther [34] was initially devoted to obtaining the eigenvalues of the sine-Gordon making use of its mapping on the discrete XYZ spin-$\frac{1}{2}$ chain, that allows us to work on a lattice. Anyway, in describing this bilateral mapping, he took the most intuitive route, consisting of the continuum limit of the lattice theory. His work has been taken up and expanded upon by Ercolessi, Evangelisti, and Ravanini in [40]. First of all, take again the Hamiltonian of the XYZ model defined in eq.(2.1) (keep in mind that Cao's H does not have the minus sign present in ERE's and Luther's paper). We have seen in subsection (2.2.2) how the couplings can be written in terms of the eight-vertex model parameters. In eq.(3.33) we reported the parametrization adopted by Cao et al., but there actually exist many ways of doing that. Following Baxter [24], for example, the relations that make $\mathbf{T}$ commute with H are

$$J_x^{\mathrm{A}} \,:\, J_y^{\mathrm{A}} \,:\, J_z^{\mathrm{A}} = 1 \,:\, \Gamma \,:\, \Delta, \tag{4.14}$$

where the constants Δ and Γ are parametrized in terms of elliptic functions

$$\Gamma = \frac{1 + k^2 \mathrm{sn}^2(i\lambda)}{1 - k\,\mathrm{sn}^2(i\lambda)}, \qquad \Delta = \frac{\mathrm{cn}(i\lambda)\,\mathrm{dn}(i\lambda)}{1 - k\,\mathrm{sn}^2(i\lambda)}. \tag{4.15}$$

Notice that we introduced the superscript L to remark that these are the couplings used by Luther in his work. The distinction is relevant since they are opposite in sign with respect to the J's used by Cao et al. The Jacobian elliptic functions $\mathrm{cn}(x)$, $\mathrm{dn}(x)$, $\mathrm{sn}(x)$ are described in Appendix (A) and the parameters λ and k have specific domains:

$$0 < k < 1, \qquad 0 < \lambda < I(k'), \tag{4.16}$$

where $I(k')$ is the complete elliptic integral of the first kind of argument $k' = \sqrt{i - k^2}$. This parametrization is particularly suitable to describe the antiferromagnetic phase. Notice that we are keeping $J_x = 1$ in the following, without any way affecting the generality of the approach.

The first step in the method proposed by Luther consists of using the Jordan-Wigner transformation to fermion operators, $\sigma_i^+ = a_i^+ \exp(i\pi \sum_0^{i-1} n_j)$, etc., where $\sigma_i^+ = \sigma_i^x + \sigma_i^y$, a_i is a Fermi operator, and $n_j = a_j^+ a_j$. This transforms the XYZ chain Hamiltonian into a simple Fermi one, written in terms of fermionic construction and annihilation operators. Under the further transformation $a_n \to (i)^n a_n$, the result is

$$\mathcal{H} = \sum_i \mathcal{H}(i) \tag{4.17}$$

with

$$\mathcal{H} = -\frac{1}{2} iv(a_i^+ a_{i+1} + a_{i+1}^+ a_i) + \frac{1}{2} J_\perp (a_i^+ a_{i+1}^+ + a_i a_{i+1})(-1)^i + J_z a_i^+ a_i a_{i+1}^+ a_{i+1}, \tag{4.18}$$

with

$$v \equiv \frac{J_x^{\mathrm{A}} + J_y^{\mathrm{A}}}{2} \qquad \text{and} \qquad J_\perp \equiv \frac{J_x^{\mathrm{A}} + J_y^{\mathrm{A}}}{2}, \tag{4.19}$$

where the apex A stands for Alan Luther's notation. Then, he converts the chain of N discrete fermion states, one at each site, to a string of length L involving an infinite number of fermion states. This is done by considering the Fourier-series transformation for the operators at the lattice sites. In this set-up, the lattice constant is $a = \frac{L}{N}$; as it tends to zero for fixed L, while $N \to \infty$, the discrete sum of the Fourier series becomes an integral with cut-off. Calculations are performed with the equations of motion involving

the Fourier transform of the fermionic operators, depending on the k-vectors inside the Brillouin zone $-\frac{\pi}{2a} < k < \frac{\pi}{2a}$. The limit $a \to 0$ has to be taken afterward. This limit also defines the cut-off prescription, strictly related to the renormalizability of the theory. It has to be read in the renormalization of the parameters in the lattice theory that follows from the requirement that observable quantities must be finite in the final limit $a \to 0$. In particular, the cut-off at a^{-1} arises from the restriction of k to the first Brillouin zone. We remark, anyway, that these Fourier transforms are defined as sums in n, an even integer that is summed up to $\frac{N}{2}$, that assumes an even N number of sites. The next step consists of determining the Hamiltonian density $\mathcal{H}_c(x)$ from the lattice Hamiltonian $\mathcal{H}(i)$:

$$\sum_{i=1}^{N} \mathcal{H}(i) \to \int_0^L dx\, \mathcal{H}_c(x), \tag{4.20}$$

where $x = si$ is a fixed distance in the continuum, and $\mathcal{H}_c(x) = a^{-1}\mathcal{H}(i)$. What becomes relevant in performing the continuum limit is that, as $a \to 0$, i has to tend to ∞. This is crucial to keep the distance $x = si$ fixed in the ratio $\frac{i}{N} = \frac{x}{L}$. Then, Luther recognized that the equations of motion involving the fermionic fields are very similar to the ones of the massive Thirring model. They become equal if we identify $\beta^2 = 8\pi\theta$, where $\theta = \frac{1}{2}[(\pi v_0 - 2J_z^{\mathrm{A}})(\pi v_0 - 2J_z^{\mathrm{A}})]^{-\frac{1}{2}}$, with $v_0 = v - \frac{J_z^{\mathrm{A}}}{2\pi}$. Moreover, these equations provide the basis for calculating the excitation spectrum of the XYZ in the continuum limit. To do that, he took the results obtained by Baxter [24] for the excitation spectrum in the discrete case and analyzed its extension to the continuum. Let us consider the quantity l defined by

$$l^2 = \frac{(J_x^{\mathrm{A}})^2 - (J_y^{\mathrm{A}})^2}{(J_x^{\mathrm{A}})^2 - (J_z^{\mathrm{A}})^2}; \tag{4.21}$$

It is clear that its value sets the anisotropy of the chain. The crucial step to perform the continuum limit is to select a small x-y anisotropy ($J_x^{\mathrm{A}} \sim J_y^{\mathrm{A}}$), namely $l \sim 0$. Indeed, this limit of weak anisotropy allows us to obtain a well-defined value Δ^{gap} of the "free"-state solution at zero momentum among the excitation spectrum of the spin chain in terms of the parameters of the model:

$$\Delta^{gap} = 8\pi \left(\frac{\sin\mu}{\mu}\right) |J_x^{\mathrm{A}}| \left(\frac{l}{4}\right)^{\frac{\pi}{\mu}}, \tag{4.22}$$

where

$$\mu = \pi(1-\theta) \equiv \pi\left(1 - \frac{\beta^2}{8\pi}\right) = \arccos(-J_z^{\mathrm{A}}) = \arccos(J_z). \tag{4.23}$$

It may appear curious that we wrote J_x^{A} in this expression even if it was put $= 1$ in the beginning. Actually, it is useful in order to make more clear the justification of the weak anisotropy regime: all the computations performed until now were still for finite L; to take the $L \to \infty$ limit, the J_x^{A} coupling constant in (4.22) becomes replaced by $(J_x^{\mathrm{A}} a^{-1})$, and Δ^{gap} would clearly diverge as $a \to 0$, unless the anisotropy parameter l is renormalized to 0. This requires the introduction of the renormalized coupling constant

$$l_r = l a^{-\frac{\mu}{\pi}}. \tag{4.24}$$

At this point, we can write the renormalized mass gap of the theory that, provided the previous relations on the parameters, coincides with the solitonic mass of the sine-Gordon model:

$$M = \Delta_r^{gap} = 8\pi \left(\frac{\sin \mu}{\mu} \right) \left(\frac{l_r}{4} \right)^{\frac{\pi}{\mu}} \tag{4.25}$$

From these identities, we know how the coupling constant J_z^{A} is connected with the parameter β of the sine-Gordon model. This parameter needs to be limited in the domain $0 < \beta^2 < 8\pi$ in order to identify correctly the physical regimes of the XYZ chain. For example, for $\beta^2 > 8\pi$, the continuum theory has some problems since the ground state of the massive Thirring model is unbounded from below; this means that for these values of β^2, the theory can only be studied on lattice. A similar instability occurs for $\beta^2 = 0$. Actually, Luther showed how to circumvent this issue with some tricks but, for our aims, it is sufficient to stay in the standard domain $0 < \beta^2 < 8\pi$. The point $\beta^2 = 0$ is seen to correspond to $J_z^{\mathrm{A}} = J_x^{\mathrm{A}} \, (= J_y^{\mathrm{A}})$, i.e. the ferromagnetic point, $\beta^2 = 8\pi$ is the antiferromagnetic one, and $\beta^2 = 4\pi$ give the isotropic XY model, known to be a Dirac fermion free-field theory.
Anyway, for our aims, it is convenient to stay in the interval $0 < \beta^2 < 8\pi$, which corresponds to the antiferromagnetic regime $-1 < J_z^{\mathrm{A}} < 0$, i.e., $0 < J_z < 1$.

4.3 Continuum limit of the XYZ with N odd: analysis in terms of sine-Gordon

Thermodynamic limit and continuum limit do not coincide. The former is a limit on the dimension of the system, that has to be sent to infinite. The latter is way more tricky: it consists of sending the lattice spacing to zero after doing the thermodynamic limit itself.

In practice, the continuum limit ends up being a limit on the parameters of the XYZ chain (J_x, J_y, J_z), or equivalently, of the eight-vertex model (Γ, Δ). Consider Δ to be in the interval $[-1, 1]$, i.e. the repulsive regime. If we take Γ finite, we end up with a massive theory, i.e. gapped. Statistical field theory tells us that, to close the gap, we have to approach a critical point of the spin chain model. Even without actually reaching it, moving toward it allows us to isolate the contribution coming from the critical point only, which gives a massless theory. This point lives in the space of the couplings, so we have to calibrate them to organize the flow that generates the continuum limit. This is exactly what we did in section (4.2) if we recognize $l = 0$ as our critical point, or better, our critical line. Indeed, substituting $l = 0$ in (4.22), we obtain a gapless, i.e. massless, theory that can be successfully read as a field theory. Luther described this proceeding by starting from a finite number of sites, while Ravanini et al. start from results already in the thermodynamic limit. Our idea is to make use of their works to derive the continuum limit of the results obtained by Cao et al. for the frustrated XYZ in the TD limit.

Before doing it, we have to spend some lines discussing the physical meaning of the Δ^{gap} introduced in the previous section. That gap is crucial to identifying our lattice theory with the continuous one. It physically emerges from the fact that while performing the continuum limit, we are keeping away from the critical line $l = 0$. If we actually reach that line, the mass gap vanishes. To sum up, the modus operandi to get the correct continuum limit of the XYZ chain consists of approaching the critical line without touching it, sending the lattice spacing to zero but providing the correct renormalization of the parameters. This last step makes the Δ^{gap} not diverge as $a \to 0$; it then remains finite as long as $l \neq 0$.

4.3.1 Why N odd could give us something new?

Investigating the low-lying excitations of the XYZ chain for even N, an interesting question arises. These excitations are given by spin-$\frac{1}{2}$ flips, implying that, the global excitation can only have an integer spin. This situation can be described in the continuum limit of the XYZ by the emergence of couples of sine-Gordon solitons, but never of a single one. Indeed, we can recognize the correspondence between these excitations and an even number of solitons of the sine-Gordon theory. Thus, our idea consists of analyzing the continuum limit of the N odd case and looking for the plausible emergence of the single soliton. From this perspective, the difference between the energy of the odd N ground

state and the one for N even

$$E^{\text{odd}}_{g,PBC} - E^{\text{even}}_{g,PBC}, \tag{4.26}$$

has a crucial role. In the continuum limit, we are looking forward to finding in it the energy of the single soliton $\epsilon_{sol}(y)$; where y stands for the rapidity of the soliton, which would be connected to the position of the hole x^h. In fact, we can get from eq.s (3.118) and (3.137) that, in the TD limit, the difference (4.26) is given by

$$E^{\text{odd}}_{g,PBC} - E^{\text{even}}_{g,PBC} = e_0(\bar{\eta}_m)(N^{\text{odd}} - N^{\text{even}}) + \epsilon_h(x^h, \bar{\eta}_m), \tag{4.27}$$

where we did not choose the position of the hole, leaving it as a variable. The expression on the r.h.s. is composed of two non-trivial terms. The first one depends on the difference between the number of sites that we consider in the two different parities. Even though we are already in the thermodynamic limit, this term is macroscopic and non-vanishing. If we assume $N^{\text{odd}} = N^{\text{even}} + 1$, we can rewrite the expression above as

$$E^{\text{odd}}_{g,PBC} - E^{\text{even}}_{g,PBC} = e_0(\bar{\eta}_m) + \epsilon_h(x^h, \bar{\eta}_m). \tag{4.28}$$

In any case, the first is independent of the position of the hole, and then also of any rapidity variable possibly connected with it, but is a finite term that ineluctably separates the two sectors. It is connected to the intrinsic extensive character of energy. We rewrite here the two expressions (3.132) and (3.119) here for convenience:

$$\epsilon_h(x^h, \bar{\eta}_m) = \frac{i\pi}{\tau}\frac{\sigma(\bar{\eta}_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{e^{\frac{k\pi}{\tau}x^h}}{\cosh(\frac{i}{\tau}k\pi\bar{\eta}_m)}. \tag{4.29}$$

$$e_0(\bar{\eta}_m) = -\frac{i\pi}{\tau}\frac{\sigma(\bar{\eta}_m)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{\sinh[\frac{i}{\tau}k\pi(1-\bar{\eta}_m)]}{\sinh(\frac{i}{\tau}k\pi)\,\cosh(\frac{i}{\tau}k\pi\bar{\eta}_m)} + \frac{1}{2}\frac{\sigma'(\bar{\eta}_m)}{\sigma'(0)} \tag{4.30}$$

Now, to analyze the physical implications of these two terms, let us focus on the x-y isotropic limit of our XYZ chain: the XXZ model. For example, according to the results obtained by Karbach in [41] in the TD limit, working directly with the XXZ chain with an odd number of sites, its ground state has the quantum numbers of an excited state. Thus, also the limit to the XXZ from the XYZ should be coherent with this evidence. First of all, we are going to describe such a limit.

4.3.2 Limit to the XXZ model

We have seen in [34] and [40] that the continuum limit goes along with the weak x-y anisotropy one. So, let us analyze the difference between the latter and the limit that gives the XXZ chain. In order to do this, let us rewrite here the parametrization of the couplings of the XYZ in terms of the elliptic functions depending on η and τ:

$$J_x = e^{i\pi\eta}\frac{\sigma(\eta+\frac{\tau}{2})}{\sigma(\frac{\tau}{2})}, \quad J_y = e^{i\pi\eta}\frac{\sigma(\eta+\frac{1+\tau}{2})}{\sigma(\frac{1+\tau}{2})}, \quad J_z = \frac{\sigma(\eta+\frac{1}{2})}{\sigma(\frac{1}{2})}. \tag{4.31}$$

Due to the properties of the elliptic function $\sigma(x)$, we see that, by sending $\tau \to i\infty$, we obtain

$$\lim_{\tau\to i\infty} J_x(\eta,\tau) \to 1, \qquad \lim_{\tau\to i\infty} J_y(\eta,\tau) \to 1, \qquad \lim_{\tau\to i\infty} J_z(\eta,\tau) \to \cos(\pi\eta). \tag{4.32}$$

This means that if we apply the same limit to the quantities obtained for the XYZ model in Chapter 3, we could extract their values for vanishing anisotropy, provided that such a limit exists also in those cases. In particular, we are interested in the behavior of the ground state energy, for both N odd and N even. In doing this, we need to keep in mind the constraints imposed during the proceedings: first of all $0 < \eta \leq \frac{1}{2}$, introduced for convenience before performing the TD limit in section (3.4). Then, we remember that we are still working with discrete degenerate values of the crossing parameter $\bar{\eta}_m = \frac{2m}{N}$, required to remove the inhomogeneous term from the TQ relation. But this time, we need to work with real values of η. Thus, in their work, Cao et al. generalized the results obtained for degenerate points η_m to an arbitrary real η in the interval $\left(0, \frac{1}{2}\right]$. They did it in [11] working with Taylor expansions of the physical quantities up to order $O(N^{-2})$. The equality of the results for generic η and for its degenerate values have been also proven numerically. Then, we can assume that the limit $\tau \to i\infty$ can be taken continuously. Finally, note that the constraint $0 < \eta \leq \frac{1}{2}$ implies that the related results are valid in the region $0 < J_z(\eta, i\infty) = \cos(\pi\eta) \leq 1$. This region corresponds correctly to the antiferromagnetic selected before.

Also Luther prepared the system in the anti-ferromagnetic regime in order to perform the continuum limit. All could seem the correct preliminary step needed. Actually, sending $\tau \to i\infty$ is too drastic. By doing this we have no longer a weak anisotropy, but we finish directly in the total x-y isotropy. This is exactly equivalent to touching the critical line

$l = 0$.

To see this explicitly, we report here the expression for the energy carried by the hole after the $\tau \to i\infty$ limit:

$$\bar{\epsilon}_h(x^h, \eta) = \lim_{\tau \to i\infty} \epsilon_h(x^h, \eta) = \frac{\sin \eta}{\eta} \frac{1}{\cosh(\frac{\pi x^h}{2\eta})}. \tag{4.33}$$

The very ground state still has to be selected by choosing the position of the hole x^h. In the XYZ model, we placed it at the boundary of its domain $\left[-\frac{\tau}{i}, \frac{\tau}{i}\right]$. This time we do the same, but the interval has expanded to $(-\infty, \infty)$. Thus, putting the hole at infinity, eq.(4.33) yields that the minimum energy carried by the hole is zero, namely $\bar{\epsilon}_h(\infty, \eta) = 0$. This is in agreement with the continuum limit theory, because we are practically placing the system exactly on the critical point, in fact obtaining a massless theory.

Thus, the only term that still separates the ground states with different parities is $\bar{e}_0(\eta)$, see eq.(4.28). In the $\tau \to i\infty$ limit, that term becomes

$$\bar{e}_0(\eta) = \lim_{\tau \to i\infty} e_0(\eta) = -\frac{\sin(\pi\eta)}{\pi} \int_{-\infty}^{\infty} \frac{\sinh[w(1-\eta)]}{\sinh(w)\cosh(w\eta)} dw + \frac{1}{2}\cos(\pi\eta). \tag{4.34}$$

This qualitatively shows the effective equality of Cao's and Karbach's [41] results, where a discrepancy between the odd and the even cases is present, but without any connection with a field theory.

4.3.3 Aprroach to continuum limit

In the previous subsection, we saw how, in their work, Cao et al. generalized the results obtained for degenerate points η_m to an arbitrary real η in the interval $\left(0, \frac{1}{2}\right]$. So, let us consider the energy coming from the hole (3.132) for η continuous and real:

$$\epsilon_h(x^h, \eta) = \frac{i\pi}{\tau} \frac{\sigma(\eta)}{\sigma'(0)} \sum_{k=-\infty}^{\infty} \frac{e^{\frac{k\pi}{\tau} x^h}}{\cosh(\frac{i}{\tau} k\pi\eta)}, \tag{4.35}$$

and in particular the series over k. This can be rewritten as

$$\begin{aligned}\sum_{k=-\infty}^{\infty} \frac{e^{\frac{k\pi}{\tau}x^h}}{\cosh(\frac{i}{\tau}k\pi\eta)} &= 1 + \sum_{k=1}^{\infty} \frac{e^{\frac{-k\pi}{\tau}x^h}}{\cosh(\frac{i}{\tau}k\pi\eta)} + \sum_{k=1}^{\infty} \frac{e^{\frac{k\pi}{\tau}x^h}}{\cosh(\frac{i}{\tau}k\pi\eta)} \\ &= 1 + 2\sum_{k=1}^{\infty} \frac{\cosh(\frac{k\pi x^h}{\tau})}{\cosh(\frac{k\pi\eta i}{\tau})}\end{aligned} \tag{4.36}$$

Now, we recall that τ is purely imaginary. So, we define t as the imaginary part of τ, namely $\tau \equiv it$, and rewrite the series above as

$$1 + 2\sum_{k=1}^{\infty} \frac{\cos(\frac{k\pi x^h}{t})}{\cosh(\frac{k\pi\eta}{t})}. \tag{4.37}$$

and plug it back into (4.35), obtaining

$$\epsilon_h(x^h, \eta) = \frac{\pi}{t}\frac{\sigma(\eta)}{\sigma'(0)}\left(1 + 2\sum_{k=1}^{\infty} \frac{\cos(\frac{k\pi x^h}{t})}{\cosh(\frac{k\pi\eta}{t})}\right). \tag{4.38}$$

Now, let us investigate if this quantity may be the candidate for the role of sine-Gordon soliton energy in the continuum limit. The first idea is to realize this limit à la Luther; however, we run into an obstacle. In fact, as we saw in section (4.2), Luther's preliminary steps involve a connection between the XYZ chain and the Thirring model. This mapping is implemented using Fourier transforms that rely on the presence of an even number of sites in the original spin chain. It is not yet entirely clear to us whether the corresponding version in the odd case can be achieved by clever extension. Thus, we found an alternative approach based on matching the low-energy dispersion relation of the chain and of the sine-Gordon model. However, before presenting this, let us comment on a possible connection with another integrable model.

4.3.4 Hubbard spinon parallelism

Anyway, in order to look a the physics that could emerge, let us try to go on with the computation. We are interested to see if some relevant insights can emerge to accompany future research. Hence, let us focus on the fact that k is, for the moment a discrete variable $\in \mathbb{Z}$. This constraint comes from the FT of a periodic function. If the extremes of the integration domain $\frac{\tau}{i} = t \to \infty$, then we can just take a simple (continuous) FT passing from a discrete index k to the continuous w, obtaining, for the whole expression

of ϵ_h:

$$\epsilon_h(x^h,\eta) = \lim_{t\to\infty, b\to 0} \pi \frac{\sigma(\eta)}{\sigma'(0)} \left(\frac{1}{t} + 2\int_b^\infty \frac{dw}{bt} \frac{\cos(\frac{w\pi x^h}{bt})}{\cosh(\frac{w\pi\eta}{bt})} \right) \tag{4.39}$$

where, in principle, $b = \frac{1}{t}$ due to FT rule. The quotient of the two elliptic functions has been verified to tend, for big t, to $\frac{\sin(\pi\eta)}{\pi}$. So we end up with

$$\epsilon_h(x^h,\eta) \simeq 2\sin(\pi\eta) \int_0^\infty \frac{\cos(w\pi x^h)}{\cosh(w\pi\eta)} dw. \tag{4.40}$$

Notice that this expression is very similar to the one for the spectrum of the spinon s ($S^z = \frac{1}{2}$) emerging as elementary excitation in the Hubbard model [42]:

$$\mathcal{E}_s(\Lambda) = \mathcal{E}_{\bar{s}}(\Lambda) = 2\int_0^\infty \frac{J_1(w)}{w} \frac{\cos(w\Lambda)}{\cosh(w\omega)} dw. \tag{4.41}$$

The two expressions would coincide, unless irrelevant multiplicative constants if, the Bessel function $J_1(w)$ was reduced, in our case, to a linear function of w. This actually happens for $0 < w < \sqrt{2}$, where $J_1(w) \sim w$. In the integral (4.41) the domain of w is extended from 0 to ∞, but the argument of the integral has $\cosh(w\omega)$ in the denominator, which diverges rapidly as w increases. The Bessel $J_1(w)$, instead, is a limited oscillating function. Thus, the dominant part of the integral actually emerges from the small values of w.
We know that the Hubbard model, in the strong coupling regime, maps into the AFM Heisenberg chain. Although the XXX model can be seen as a specific limit of the XYZ one, in the transition we lose the cherished anisotropy between the couplings. Hence, this speculation is certainly a bit audacious, but it suggests that the search for spinon in the difference between the two sectors is reasonable. We remark that the spectrum above is a result obtained in the TD limit with TBA eq.s, but the continuum limit, according to their method, is still to be done. In [42], they performed their own scaling limit, working with the parameters of the Hubbard model. Anyway, a mapping between those parameters and the XYZ couplings would be very complex and certainly reckless. What is relevant is that the scaling limit of the Hubbard model is equivalent to the SU(2), which is, as its U(1) version, integrable with Bethe ansatz techniques. We firmly know that our model does not have U(1) symmetry, let alone SU(2), but it is quite interesting that we recover similar expressions. This aims to be the subject of future discussions.

4.3.5 Expansion for big t in the vicinity of the minimum

An alternative idea is to manipulate the expression (4.35) to look for the additional terms that separate it from the purely XXZ case. That is, given the obstacles to the formal realization of Luther's limit, we try to extract information about the system from the terms that might distance it from a massless theory. In order to do this, let us consider again the energy of the hole (4.35). To that expression, we can apply the *Poisson Sum Formula*:

$$\frac{1}{T}\sum_{m=-\infty}^{\infty}\hat{G}\left(\frac{2\pi m}{T}\right)\exp\left(\frac{2\pi i m x}{T}\right)=\sum_{m=-\infty}^{\infty}G(x+mT)=f(x), \tag{4.42}$$

valid for $G(x)$ admitting Fourier transform $\hat{G}(p)$. In our case, sending $k\to -k$, we can rewrite $\epsilon_h(x^h,\eta)$ as

$$\begin{aligned}\epsilon_h(x,\eta)&=\pi\frac{\sigma(\eta)}{\sigma'(0)}\frac{1}{t}\sum_{k=-\infty}^{\infty}\frac{1}{\cosh(\frac{k\pi\eta}{t})}e^{\frac{ik\pi\eta}{t}x}\\&=\pi\frac{\sigma(\eta)}{\sigma'(0)}f(x)\end{aligned} \tag{4.43}$$

where $x^h\equiv\eta x$. Now, identifying $T\equiv\frac{2t}{\eta}$, we can use (4.42) to get

$$\epsilon_h(x^h,\eta)=\pi\frac{\sigma(\eta)}{\sigma'(0)}\frac{1}{\eta}\sum_{k=-\infty}^{\infty}\frac{1}{\cosh\left(\frac{\pi}{2\eta}(x^h+2kt)\right)}. \tag{4.44}$$

If we separate the series, isolating the $k=0$ term, we obtain

$$\epsilon_h(x^h,\eta)=\pi\frac{\sigma(\eta)}{\sigma'(0)}\frac{1}{\eta}\left[\frac{1}{\cosh\left(\frac{\pi x^h}{2\eta}\right)}+\sum_{k=1}^{\infty}\frac{1}{\cosh\left(\frac{\pi}{2\eta}(x^h+2kt)\right)}+\sum_{k=1}^{\infty}\frac{1}{\cosh\left(\frac{\pi}{2\eta}(x^h-2kt)\right)}\right], \tag{4.45}$$

Manipulating a bit the two series for big t, we obtain, at first order:

$$\epsilon_h(x^h,\eta)=\pi\frac{\sigma(\eta)}{\sigma'(0)}\frac{1}{\eta}\left[\frac{1}{\cosh\left(\frac{\pi x^h}{2\eta}\right)}+4\cosh\left(\frac{\pi x^h}{2\eta}\right)e^{-\frac{\pi}{\eta}t}+\cdots\right]. \tag{4.46}$$

where the first term ($k=0$) reconnects to the XXZ model expression (4.33), while the second is its first correction, exponentially suppressed as $t\to\infty$. At this point, we can

expand this expression near the point of minimum energy, which, as we have seen, lies at the far end of the domain, i.e. in $x^h = \frac{\tau}{i} = t$. Hence, consider $x^h = t - \delta x$, and expand (4.46) at second order in δx, obtaining

$$\begin{aligned} \epsilon_h(\delta x, \eta) &= \pi \frac{\sigma(\eta)}{\sigma'(0)} \frac{1}{\eta} \left[2\, q \, \left(2 + \alpha (\delta x)^2 \right) \right] \qquad \text{where } \alpha \equiv \frac{\pi}{2\eta} \text{ and } q \equiv e^{-\alpha t} \\ &= \pi \frac{\sigma(\eta)}{\sigma'(0)} \frac{1}{\eta} \left[2\, e^{-\frac{\pi}{2\eta} t} \, \left(2 + \frac{\pi}{2\eta} (\delta x)^2 \right) \right]. \end{aligned} \tag{4.47}$$

The absence of a linear term in δx confirms that the energy of the hole finds its minimum (vanishing first derivative) in $x^h = \frac{\tau}{i} = t$. This leaves us with a quadratic dependence in δx, which gives a small positive correction above the ground state.

4.4 Momentum of the ground state

During the calculations realized to get the energy of the ground state, for both N odd and N even, we defined many new crucial functions in the thermodynamic limit. An analogous proceeding can be in principle used to obtain another interesting quantity of the system in the TD limit: the total momentum of the system. In fact, since the sine-Gordon soliton has its own energy and momentum, it could be useful to analyze both the corresponding quantities coming from the XYZ chain. Following [43], in addition to Cao's paper, we can derive, up to multiplicative constants, the expression for the total momentum at the ground state in the thermodynamic limit:

$$P = N \left\{ \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \vartheta_1(x) \rho_1(x) dx + \sum_{r \neq 1}^{z_l + 1} \int_{-\frac{\tau}{i}}^{\frac{\tau}{i}} \vartheta_r(x) \rho_r(x) dx \right\}, \tag{4.48}$$

where the function $\vartheta_j(x)$ has been defined in (3.100) as

$$\vartheta_j(x) \equiv \vartheta(x; n_j, v_j) = -i \ln[(-v_j)\, g(x; n_j, v_j)], \tag{4.49}$$

and all the other elements are the same as we encountered in Chapter 3. In particular, the densities of states are still the same. To perform the computation, we remember that

$$a_j(x) \equiv a(x; n_j, v_j) = \frac{1}{2\pi} \frac{d}{dx} \vartheta_j(x), \tag{4.50}$$

thus

$$\frac{d}{dx}\vartheta_j(x) = 2\pi a_j(x). \tag{4.51}$$

Then, for the Fourier transform for periodic functions in a limited domain $[-t, t]$, we have the following property: if $G(x) = \frac{dF(x)}{dx}$, then $\tilde{G}(k) = \frac{ik\pi}{t}\tilde{F}(k)$. Thus, we obtain that

$$\tilde{\vartheta}_1(k) = \frac{t}{ik\pi}\tilde{a}_1(k) = \frac{t}{ik\pi}\frac{\sinh\left[\frac{i}{\tau}k\pi(1-\eta_m)\right]}{\sinh(\frac{i}{\tau}k\pi)}. \tag{4.52}$$

Working in Fourier Transform, eq.(4.48) turns into

$$\begin{aligned} P_g(\eta_m) &= \frac{iN}{2\tau}\sum_{k=-\infty}^{\infty}\left\{\frac{\tilde{\vartheta}_1(k)}{2\cosh(\frac{i}{\tau}k\pi\eta_m)} - \frac{\frac{t}{ik\pi}\tilde{\rho}_1^h(k)}{2\cosh(\frac{i}{\tau}k\pi\eta_m)}\right\} \\ &= \frac{N}{2t}\sum_{k=-\infty}^{\infty}\frac{t}{ik\pi}\left\{\frac{\tilde{a}_1(k)}{2\cosh(\frac{i}{\tau}k\pi\eta_m)} - \frac{\tilde{\rho}_1^h(k)}{2\cosh(\frac{i}{\tau}k\pi\eta_m)}\right\} \\ &= \frac{N}{2\pi i}\sum_{k=-\infty}^{\infty}\frac{1}{k}\left\{\frac{\sinh[\frac{i}{\tau}k\pi(1-\eta_m)]}{2\sinh(\frac{i}{\tau}k\pi)\cosh(\frac{i}{\tau}k\pi\eta_m)} - \frac{\tilde{\rho}_1^h(k)}{2\cosh(\frac{i}{\tau}k\pi\eta_m)}\right\}. \end{aligned} \tag{4.53}$$

Also in this case, as for the energy, we can make the two separate contributions explicit, writing

$$\mathrm{p}_0(\eta_m) = \frac{1}{2\pi i}\sum_{k=-\infty}^{\infty}\frac{\frac{1}{k}\sinh[\frac{i}{\tau}k\pi(1-\eta_m)]}{\sinh(\frac{i}{\tau}k\pi)\cosh(\frac{i}{\tau}k\pi\eta_m)}, \tag{4.54}$$

$$p_h(\eta_m) = \frac{N}{2\pi i}\sum_{k=-\infty}^{\infty}\frac{\frac{1}{k}\tilde{\rho}_1^h(k)}{\cosh(\frac{i}{\tau}k\pi\eta_m)}. \tag{4.55}$$

The former comes from the Bethe roots while the latter from the corresponding holes. Thus, the total momentum of the ground state can be rewritten as

$$P_g(\eta_m) = N\mathrm{p}_0(\eta_m) + p_h(\eta_m). \tag{4.56}$$

This means that also for the momentum, there is no direct contribution coming from the strings, even though they could in principle affect the density of states.
To get the final value of the momentum, we still need to exploit the density of the holes $\tilde{\rho}_1^h(k)$. To do so, we have, also in this case, to treat separately the two possible parities of the system. Anyway, the considerations on the densities of states are the same realized for the energy.

So, if N is odd, we can consider eq.(3.131) and plug it into (4.55) obtaining

$$p_h(\eta_m, x^h) = \frac{1}{2\pi i} \sum_{k=-\infty}^{\infty} \frac{\frac{1}{k} e^{\frac{k\pi}{\tau} x^h}}{\cosh(\frac{i}{\tau} k\pi\eta_m)}. \tag{4.57}$$

The position of the hole $x^h = \frac{\tau}{i}$ is constrained by the minimization of the energy, giving us

$$P_g^{odd}(\eta_m) = N\mathrm{p}_0(\eta_m) + p_h\left(\frac{\tau}{i}, \eta_m\right). \tag{4.58}$$

If N is even, instead, the configuration of roots gives that there is no hole at the ground state, leaving us with the ground state energy

$$P_g^{even}(\eta_m) = N\mathrm{p}_0(\eta_m). \tag{4.59}$$

If we compute the difference between the momenta in the odd and even sectors, assuming η real and continuous, we get that the relevant term (dependent on the position of the hole) is

$$p_h(\eta, x^h) = \frac{1}{2\pi i} \sum_{k=-\infty}^{\infty} \frac{\frac{1}{k} e^{\frac{k\pi}{\tau} x^h}}{\cosh(\frac{i}{\tau} k\pi\eta)}. \tag{4.60}$$

Using the fact that $\frac{1}{k} e^{-i\frac{k\pi}{t} x^h} = -\frac{i\pi}{t} \int dx^h e^{-i\frac{k\pi}{t} x^h}$, we can use the same manipulation performed for hole energy and derive:

$$p_h(\eta, x^h) = -\frac{2}{\pi} \arctan\left[\tanh\left(\frac{\pi x^h}{4\eta}\right)\right] - \frac{4}{\pi} \sinh\left(\frac{\pi x^h}{2\eta}\right) e^{-\frac{\pi}{\eta} t} + \cdots \tag{4.61}$$

at first order. From the first term of this expression, the dominant one, we deduce that the hole momentum goes slowly to zero in the $t \to \infty$ limit. The second term is its first order correction that sees an exponential suppression.

As we did for the energy, we can perform the expansion of (4.61) in the proximity of the domain boundary, where the minimum of ϵ_h is placed. At first order in q, and keeping up

to quadratic terms of δx, we obtain

$$\begin{aligned} p_h(\eta, \delta x) &= -\frac{1}{2} + \frac{4\,q}{\pi}\alpha(\delta x) \\ &= -\frac{1}{2} + \frac{2}{\eta}e^{-\frac{\pi}{2\eta}t}\,(\delta x). \end{aligned} \tag{4.62}$$

The constant term represents the momentum carried by the hole in the ground state, while the second term is the exponentially dumped (as $t \to \infty$) correction emerging in proximity to the domain boundary: it is linear in δx and we can consider it as

$$\delta p = \frac{2}{\eta}e^{-\alpha t}\delta x. \tag{4.63}$$

4.4.1 Approximated dispersion relation for small momentum

If we invert this relation and plug it in (4.47), we obtain

$$\epsilon_h(\delta p, \eta) = \frac{\sigma(\eta)}{\sigma'(0)}\frac{\pi}{\eta}\left[4\,e^{-\alpha t} + \frac{\pi\eta}{8}e^{+\alpha t}(\delta p)^2\right], \tag{4.64}$$

and using $\frac{\sigma(\eta)}{\sigma'(0)} \simeq \frac{\sin(\pi\eta)}{\pi}$ for big t, we get

$$\epsilon_h(\delta p, \eta) \simeq \frac{\sin(\pi\eta)}{\eta}\left[4\,e^{-\alpha t} + \frac{\pi\eta}{8}e^{+\alpha t}(\delta p)^2\right]. \tag{4.65}$$

This expression can be read as a kind of dispersion relation for a massive quasi-particle at small momentum:

$$\epsilon = \sqrt{M^2 + \lambda p^2} \simeq M + \lambda\frac{p^2}{2M}. \tag{4.66}$$

Thus, we can identify the first term in (4.65) with the mass of the quasi-particle:

$$M = \frac{\sin(\pi\eta)}{\eta}\,4\,e^{-\alpha t}, \tag{4.67}$$

which vanishes exponentially in the $t \to \infty$ limit, as expected. In fact, if M is the mass of the soliton before the renormalization procedure, we want it to go to zero as we approach the critical isotropic point. The second term instead, depending on the momentum, can be used to recognize the parameter λ. In our case, we get:

$$\lambda = \frac{2\pi}{\eta}\sin^2(\pi\eta). \tag{4.68}$$

Let us focus on the mass term: working a bit with (4.67), we obtain

$$M = 4\pi \left(\frac{\sin \pi\eta}{\pi\eta} \right) \left(e^{-\frac{\pi}{2}t} \right)^{\frac{\pi}{\pi\eta}}. \tag{4.69}$$

Now compare this expression with the one obtained by Luther in [34] for the mass gap of the XYZ model

$$\Delta = 8\pi \left(\frac{\sin \mu}{\mu} \right) \left(\frac{l}{4} \right)^{\frac{\pi}{\mu}}. \tag{4.70}$$

First, notice that the factor two difference comes simply from the fact that our Hamiltonian (2.32) includes an overall $\frac{1}{2}$ that Luther does not insert (just a matter of definition). Then, we identify the correspondence

$$\mu = \pi\eta \tag{4.71}$$

and we can match the parameter l he uses to renormalize the theory in the continuum, to our $4\, e^{-\frac{\pi}{2}t}$:

$$l = 4\, e^{-\frac{\pi}{2}t} = 4\, e^{i\frac{\pi}{2}\tau}. \tag{4.72}$$

Luther uses μ as the parameter connected to the sine-Gordon $\frac{\beta^2}{8\pi}$ through

$$\frac{\beta^2}{8\pi} = \theta = 1 - \frac{\mu}{\pi}, \tag{4.73}$$

which also selects the regime of the system. The identification $\mu = \pi\eta$ gives us the mapping

$$\frac{\beta^2}{8\pi} = 1 - \eta. \tag{4.74}$$

Notice that $\eta = 0$ selects $J_z = 1$ in our chain (2.1), i.e. an AFM coupling. If we substitute $\eta = 0$ in (4.74), we get $\beta^2 = 8\pi$ that correctly identifies the AFM regime in Luther's description. More generally, $\eta \in \left(0, \frac{1}{2}\right]$, that is the domain we chose in our work, gives the repulsive regime $4\pi < \beta^2 < 8\pi$. And this, according to [40], is the regime in which the mass gap of the theory coincides with the soliton mass. We checked numerically the correspondence between our results and Luther's: going back to the definition of his parameters, μ was introduced as

$$\mu = \arccos\left(\frac{J_z}{J_x} \right). \tag{4.75}$$

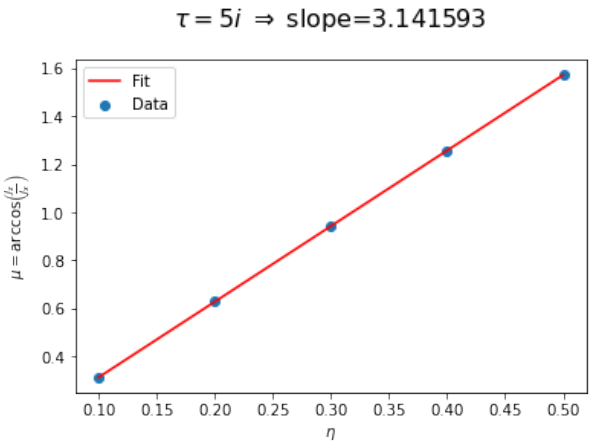


Figure 4.1: Plot and linear fit of μ vs η for $t = 5$. The resulting slope is π as expected.

In our model, J_z and J_x are functions of η and τ. We verified that choosing a big $t = \frac{\tau}{i}$ (e.g. $t > 5$) and a value for η in the domain $\left(0, \frac{1}{2}\right]$ for both, the result of $\mu = \arccos\left(\frac{J_z(\eta,\tau)}{J_x(\eta,\tau)}\right)$ gives exactly $\pi\eta$. As expected, the identity between the two values becomes less precise as τ decreases, since we are no longer in the weak-anisotropy ($l \sim 0$) regime. Figures (4.1)-(4.6) show how Luther's $\mu = \arccos\left(\frac{J_z}{J_x}\right)$ corresponds to our $\pi\eta$ for $t \gtrapprox 3$. For smaller values, the linear fit is no longer good and the match fails, as expected.
For completeness, we report also the numerical check of the correspondence between l and $4\,e^{-\frac{\pi}{2}t}$ in table (4.1). Luther's parameter l is computed using his definition

$$l = \sqrt{\frac{J_x^2 - J_y^2}{J_x^2 - J_z^2}}, \tag{4.76}$$

keeping $\eta = 0.2$ fixed and varying $t\,(= 5, 3, 1.5, 1, 0.8, 0.7)$. The same t is then used to calculate the value $4\,e^{-\frac{\pi}{2}t}$. The results show that two values coincide for $t \gtrapprox 3$, in agreement with theory and previous results for μ.

Now, having demonstrated the validity of the mapping, the corresponding parameters can be renormalized à la Luther, to obtain the actual scaling limit. In summary, since we could not realize Luther's mapping a priori, due to the constraint on the parity of N, we worked to identify its validity in our case, a posteriori. In doing so, we also obtained a dispersion relation that inevitably recalls that of a massive quasi-particle, that we identify with the single soliton.

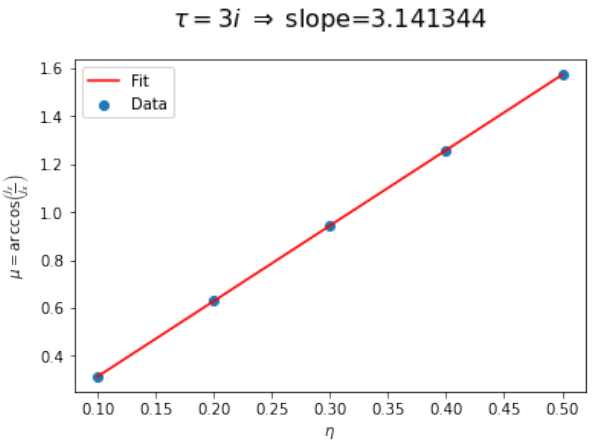


Figure 4.2: Plot and linear fit of μ vs η is repeated for $t = 3$. The purpose is to estimate approximately the tau threshold value below which the weak anisotropy regime is lost. The resulting slope is still π but with slightly less precision.

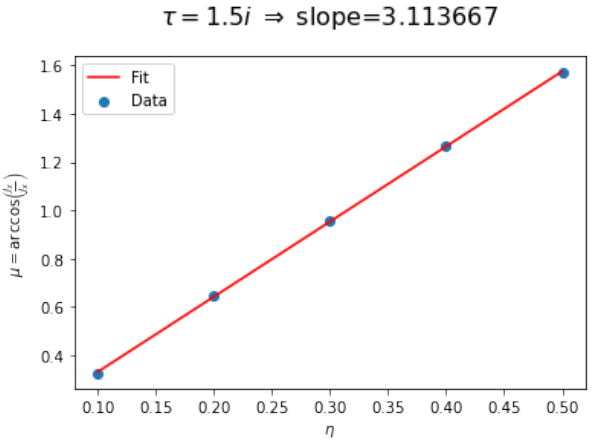


Figure 4.3: Plot and linear fit of μ vs η for $t = 1.5$. The resulting slope begins to deviate sensibly from the desired value π: the weak anisotropy regime is lost.

t	l	$4\,e^{-\frac{\pi}{2}t}$
0.7	0.913967	1.33207
0.8	0.854102	1.13844
1	0.707107	0.831518
1.5	0.365915	0.379121
3	0.0359216	0.0359332
5	0.00155281	0.00155281

Table 4.1: Comparison between values of Luther's parameter l and our $4\,e^{-\frac{\pi}{2}t}$ for $\eta = 0.2$ fixed. Since our description applies only to large t (small l), for small t the values differ from each other, as expected. As t grows, l tends to zero, the mapping gains validity and the values in the table actually coincide.

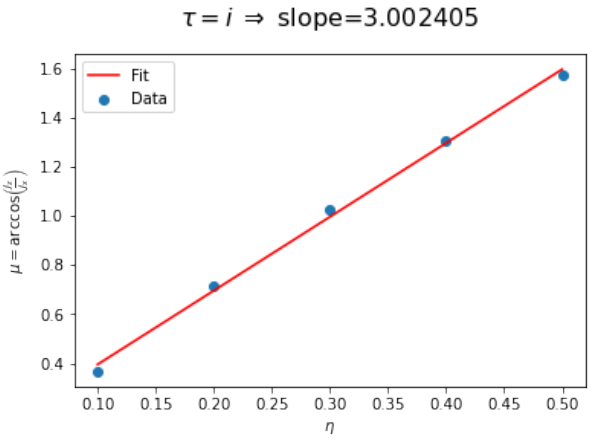


Figure 4.4: Plot and linear fit of μ vs η for $t = 3$. The resulting slope begins to deviate from the desired value π. The arrangement of the points suggests that the linear fit is no longer suitable.

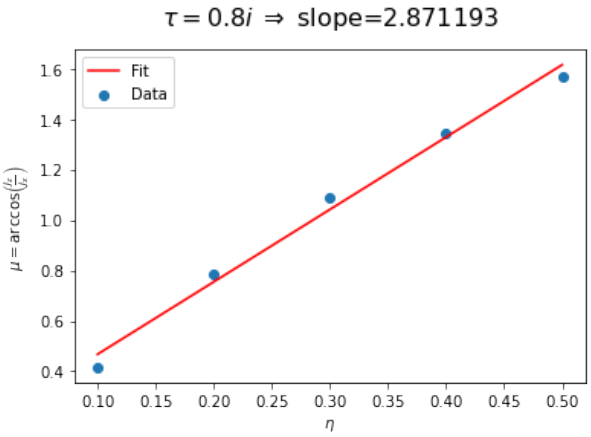


Figure 4.5: The linear fit is no longer appropriate.

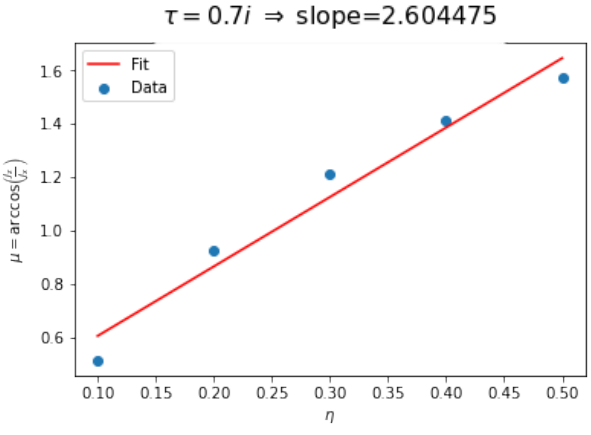


Figure 4.6: The linear fit is no longer appropriate.

Conclusions

The first objective of this dissertation has been to go over the most relevant integrability techniques, draw a thread through the intricate literature discussing them, and describe their extension to the XYZ chain with an odd number of sites. This last step required the treatment and use of a new recent technique, the off-diagonal Bethe ansatz. The second goal, pursuable using the solution obtained with ODBA, was to analyze the difference between the ground state with odd N and that with even N. The results in terms of the string hypothesis showed that the main difference lies in the presence of a hole in the ground state of the odd-numbered case, which is absent in the even-numbered one. This hole contributes to energy and momentum depending on its position. Our final aim was to interpret this particular contribution in terms of the well-known field theory counterpart of the XYZ spin chain, the sine-Gordon model. The limitation to even N in Luther's work was a formal obstacle we encountered. It forced us to take an alternative route to identify the match between the parameters. We computed the total momentum of the ground state and used our parameters to select the weak-anisotropy regime, required to perform the continuum limit. So, we worked in the proximity of the ground state to extract the quasi-particle content. In the approximated dispersion relation we recognized the nature of the massive solitonic quasi-particle. Essentially, we looked at the sine-Gordon sector with an odd number of solitons, unreachable for a chain with even N, confirming that the identification of the parameters remains correct. Thus, the mapping is still valid and allows us to identify the excitation carried by the hole in the odd-numbered chain with the single sine-Gordon massive soliton. The analytical calculation was supported by a numerical analysis that confirmed the equivalence between the examined parameters in the proper regime.

This work has shown that indeed the frustrated XYZ chain in the scaling limit flows to the sine-Gordon model in its sector with an odd number of topological excitations. It would

be interesting to reformulate Luther's procedure to eliminate the constraint on the parity of the system size or to find another approach that allows a direct mapping between the lattice model and the field theoretical one. In the literature, frustrated boundary conditions have been claimed to introduce "topological frustration" in the system. Indeed, the mapping we realized shows that only in this way one can excite a topological excitation in the system. For sure, a fascinating continuation could be to search for the spin chain equivalent of the sine-Gordon topological charge. Finally, having understood better the connection between the models, it would be interesting to study them both out of equilibrium, also by developing a proper Generalized Hydrodynamics description, which is yet lacking.

Appendix A

Elliptic functions

This Appendix aims to recap the properties and the notations of the elliptic function.

In particular, we made large use of the elliptic θ-functions [44]. We introduced the general expression for an elliptic θ-function:

$$\theta \begin{bmatrix} a \\ b \end{bmatrix} (u, \tau) = \sum_{m=-\infty}^{\infty} \exp\{i\pi[(m+a)^2\tau] + 2(m+a)(u+b)]\}, \tag{A.1}$$

where a and b are rational numbers called *characteristics*, and τ is a generic complex number called *parameter* with $\mathrm{Im}(\tau) > 0$. The four θ-functions we adopted are:

$$\theta \begin{bmatrix} 0 \\ 0 \end{bmatrix} (u, \tau), \qquad \theta \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} (u, \tau), \qquad \theta \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} (u, \tau), \qquad \theta \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} (u, \tau). \tag{A.2}$$

They are all doubly quasi-periodic functions of quasi-periods 1 and τ; so, keeping τ constant, they satisfy

$$\begin{aligned}
&\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+1) = -\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u), && \theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u+\tau) = -e^{-2i\pi(u+\frac{\tau}{2})}\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u)\\
&\theta\begin{bmatrix}\frac{1}{2}\\ 0\end{bmatrix}(u+1) = -\theta\begin{bmatrix}\frac{1}{2}\\ 0\end{bmatrix}(u), && \theta\begin{bmatrix}\frac{1}{2}\\ 0\end{bmatrix}(u+\tau) = e^{-2i\pi(u+\frac{\tau}{2})}\,\theta\begin{bmatrix}\frac{1}{2}\\ 0\end{bmatrix}(u)\\
&\theta\begin{bmatrix}0\\ 0\end{bmatrix}(u+1) = \theta\begin{bmatrix}0\\ 0\end{bmatrix}(u), && \theta\begin{bmatrix}0\\ 0\end{bmatrix}(u+\tau) = e^{-2i\pi(u+\frac{\tau}{2})}\,\theta\begin{bmatrix}0\\ 0\end{bmatrix}(u)\\
&\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u+1) = \theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u), && \theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u+\tau) = -e^{-2i\pi(u+\frac{\tau}{2})}\,\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u)
\end{aligned} \tag{A.3}$$

While $\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,\tau)$ is an odd function of u, the other three theta's are even functions of u. For simplicity, we can define two functions connected to the θ's:

$$\sigma(u) = \theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,\tau), \tag{A.4}$$

and

$$\zeta(u) = \frac{\partial}{\partial u}\{\ln\sigma(u)\}. \tag{A.5}$$

A more compact definition used frequently is

$$\begin{aligned}
\theta_1(z,q) &= -\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,q) = -i\sum_{n=-\infty}^{\infty}(-1)^n q^{(n+1/2)^2}e^{i\pi(2n+1)u},\\
\theta_2(z,q) &= \theta\begin{bmatrix}\frac{1}{2}\\ 0\end{bmatrix}(u,q) = \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}e^{i\pi(2n+1)u},\\
\theta_3(z,q) &= \theta\begin{bmatrix}0\\ 0\end{bmatrix}(u,q) = \sum_{n=-\infty}^{\infty} q^{n^2}e^{i\pi 2nu},\\
\theta_4(z,q) &= \theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,q) = \sum_{n=-\infty}^{\infty}(-1)^n q^{n^2}e^{i\pi 2nu},
\end{aligned} \tag{A.6}$$

where q is the *nome* of the functions ($|q| < 1$) and it is related to τ by $q = e^{i\pi\tau}$.
Notice that, in the limit $\tau \to i\infty$, they become:

$$\begin{aligned}
\theta_1(u,\tau) &= 2q^{\frac{1}{4}}\sin(\pi u) + O(q^{\frac{9}{4}}),\\
\theta_2(u,\tau) &= 2q^{\frac{1}{4}}\cos(\pi u) + O(q^{\frac{9}{4}}),\\
\theta_3(u,\tau) &= 1 + O(q),\\
\theta_4(u,\tau) &= 1 + O(q).
\end{aligned} \tag{A.7}$$

This represents *trigonometric limit*, coherent with the concept that the theory of θ-functions is a sort of "elliptically deformed" trigonometry.

Here we report some of the identities satisfied by the elliptic functions introduced in (A.2) and (A.4):

$$\begin{aligned}
&\sigma(u+x)\sigma(u-x)\sigma(v+y)\sigma(v-y) - \sigma(u+y)\sigma(u-y)\sigma(v+x)\sigma(v-x)\\
&= \sigma(u+v)\sigma(u-v)\sigma(x+y)\sigma(x-y),
\end{aligned} \tag{A.8}$$

$$\sigma(2u) = \frac{2\sigma(u)\sigma(u+\frac{1}{2})\sigma(u+\frac{\tau}{2})\sigma(u-\frac{1}{2}-\frac{\tau}{2})}{\sigma(\frac{1}{2})\sigma(\frac{\tau}{2})\sigma(-\frac{1}{2}-\frac{\tau}{2})}, \tag{A.9}$$

$$\frac{\sigma(u)}{\sigma(\frac{\tau}{2})} = \frac{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(u,2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(u,2\tau)}{\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(\frac{\tau}{2},2\tau)\,\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\frac{\tau}{2},2\tau)}, \tag{A.10}$$

$$\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(2u,2\tau) = \theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\tau,2\tau)\cdot\frac{\sigma(u)\sigma(u+\frac{1}{2})}{\sigma(\frac{\tau}{2})\sigma(\frac{\tau}{2}+\frac{1}{2})}, \tag{A.11}$$

$$\theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(2u,2\tau) = \theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\cdot\frac{\sigma(u-\frac{\tau}{2})\sigma(u+\frac{1}{2}+\frac{\tau}{2})}{\sigma(-\frac{\tau}{2})\sigma(\frac{\tau}{2}+\frac{1}{2})}. \tag{A.12}$$

Other notations for the elliptic θ-functions can be used depending on the situation. For example, Pozsgay in [12] uses the same form found in Wolfram Mathematica, just rewritten in a slightly different way. This makes his results more directly reproducible numerically.

Also in this case, they are defined as infinite sums:

$$\begin{aligned}
\theta_1(z,q) &= -i\sum_{n=-\infty}^{\infty}(-1)^n q^{(n+1/2)^2}e^{i(2n+1)z} = 2\sum_{n=-\infty}^{\infty}(-1)^{n+1}q^{(n+1/2)^2}\sin((2n-1)z),\\
\theta_2(z,q) &= \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}e^{i(2n+1)z} = 2\sum_{n=1}^{\infty} q^{(n+1/2)^2}\cos((2n-1)z),\\
\theta_3(z,q) &= \sum_{n=-\infty}^{\infty} q^{n^2}e^{i2nz} = 1+2\sum_{n=1}^{\infty} q^{n^2}\cos(2nz),\\
\theta_4(z,q) &= \sum_{n=-\infty}^{\infty}(-1)^n q^{n^2}e^{i2nz} = 1+2\sum_{n=1}^{\infty}(-1)^n q^{n^2}\cos(2nz).
\end{aligned} \tag{A.13}$$

where the only difference with respect (A.6) is a rescaling of the spectral parameter: the relation between the u adopted in our work and z is $z \equiv \pi u$. Keeping q (or equivalently τ) fixed, from their definitions, we extrapolate that $\theta_1(z)$ is an odd function of z, while $\theta_2(z)$, $\theta_3(z)$ and $\theta_4(z)$ are even. They are quasi-periodic functions with periods π and $\pi\tau$.

Baxter uses a definition with an infinite product instead of an infinite sum. Anyway it matches the one by Pozsgay, using the same spectral parameter and the same q (assumed fixed):

$$\begin{aligned}
H(z) &\equiv \theta_1(z),\\
H_1(z) &\equiv \theta_2(z),\\
\Theta_1(z) &\equiv \theta_3(z)\\
\Theta(z) &\equiv \theta_4(z).
\end{aligned} \tag{A.14}$$

Dealing with elliptic θ-functions, it can be useful to introduce the complete elliptic integral K:

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1-k^2\sin(\varphi)}}\partial\varphi, \tag{A.15}$$

of the first kind of modulus k, and the same integral K' of the complementary modulus $k' = \sqrt{1-k^2}$, i.e. $K'(k) = K(\sqrt{1-k^2})$. The nome q can be written in terms of these two quantities as $q = e^{-\pi\frac{K'(k)}{K(k)}}$. These elliptic integrals can be used to bring out other

properties of the elliptic theta's, such as

$$\begin{aligned}
&H(z+K) = H_1(z),\\
&\Theta(z+K) = \Theta_1(z),\\
\\
&H(z+2K) = -H(z),\\
&\Theta(z+2K) = \Theta(z),\\
\\
&\Theta(x \pm iK') = \pm q^{-\frac{1}{4}} e^{\mp \frac{i\pi z}{2K}} H(z)\\
&H(x \pm iK') = \pm q^{-\frac{1}{4}} e^{\mp \frac{i\pi z}{2K}} \Theta(z).
\end{aligned} \tag{A.16}$$

We conclude this addendum by reporting the expressions of the Jacobi elliptic functions in terms of the Theta functions $\theta_i(z,q)$:

$$\begin{aligned}
\mathrm{sn}(z;k) &= -\frac{\theta_3\left(0,q(k)\right)\,\theta_1\left(z \div \frac{2}{\pi}K(k), q(k)\right)}{\theta_2\left(0,q(k)\right)\,\theta_4\left(z \div \frac{2}{\pi}K(k), q(k)\right)}\\
\mathrm{cn}(z;k) &= \frac{\theta_4\left(0,q(k)\right)\,\theta_2\left(z \div \frac{2}{\pi}K(k), q(k)\right)}{\theta_2\left(0,q(k)\right)\,\theta_4\left(z \div \frac{2}{\pi}K(k), q(k)\right)}\\
\mathrm{dn}(z;k) &= \frac{\theta_4\left(0,q(k)\right)\,\theta_3\left(z \div \frac{2}{\pi}K(k), q(k)\right)}{\theta_3\left(0,q(k)\right)\,\theta_4\left(z \div \frac{2}{\pi}K(k), q(k)\right)}
\end{aligned} \tag{A.17}$$

As you can see, the notations for the θ-functions used in literature are of great variety. This can be a source of confusion. We hope that this Appendix may be helpful in shedding light on the multiple notations and how to move from one to the other.

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