Heisenberg Spin Chains: from Quantum Groups to Neutron Scattering Experiments

Jean Michel Maillet Laboratoire de Physique ENS Lyon et CNRS 46, allée d'Italie 69364 Lyon, France

Abstract. Heisenberg spin-1/2 chains are the archetype of quantum integrable one dimensional models describing magnetic properties of a vide range of compounds, (like the $KCuF_3$ crystal) which can be probed experimentally through neutron scattering experiments, while being at the same time at the root of the invention of Bethe ansatz and Yang-Baxter structures that led in turn to quantum groups discovery. The aim of this lecture is to describe these algebraic ingredients and to show how to obtain from them (using combined analytical and numerical analysis) dynamical correlation functions of integrable Heisenberg spin-1/2 chain, the Fourier transform of which, the so called dynamical structure factors, being directly measured in inelastic neutron scattering experiments. Our method is based on the the algebraic Bethe ansatz and the resolution of the quantum inverse scattering problem. It leads to recent progress in the computation of integrable Heisenberg spin-1/2 chains correlation functions that we review here.

1 Introduction

One of the main tasks of statistical mechanics is to understand macroscopic quantities such as specific heat, susceptibility, or transport properties for a fluid or a crystal in terms of microscopic elementary interactions between the constituents which are for example molecules, or ions. A fundamental theoretical quantity for this study is the so called dynamical structure factor (the Fourier transform of the dynamical two-point correlation function). The importance of these functions originates from the following facts: (i) They can be measured directly via scattering of neutrons or photons at the material to be studied [1, 2, 3, 4, 5, 7, 6], so that if we are able to compute these functions within a model given by some Hamiltonian describing microscopic interactions, we can compare this model with the reality. (ii) From these quantities it is possible to compute other fundamental macroscopic quantities of statistical mechanics for systems in thermodynamical equilibrium and close to this equilibrium, like in particular transport coefficients (see e.g., [7]).

Thus if one is interested in understanding, for example, magnetic properties of crystals one should find models describing the microscopic interactions between the spins of the constituent ions and develop methods to calculate within such models the dynamical spin-spin correlation functions. This is for a generically interacting quantum Hamiltonian a very involved problem, quite often out of reach of any treatment by perturbation theory. Hence, the strategy to attack this difficult task has been first to construct simple enough but representative models encoding the main features of magnetic properties of crystals. A serious but not senseless simplification in this process is the reduction of the dimensionality of the problem leading in particular to

consider models defined in one dimension. Although drastic at first sight, this strategy proved to be quite successful. In fact there exists today an impressive list of magnetic materials where the interaction between the different constituents is mainly along one dimensional chains whereas the energy exchange between the different chains is negligible [8]. Strong one dimensional magnetic character is most usually produced by separating the chains carrying the dominant magnetic interaction by large non magnetic complex ions, like in $CuCl_2.2NC_5H_5$. Note however that in these systems, the three dimensional character is usually recovered at sufficiently low temperature.

A very interesting example of such a compound is provided by the (rather exotic) $KCuF_3$ crystal which displays properties characteristic of one dimensional antiferromagnets [9, 8, 10, 11, 12]. Although the $KCuF_3$ crystal is fully three dimensional, its one dimensional magnetic properties are attributed to the distortion of the octahedral environment of the Cu^{2+} ions due to the Jahn-Teller effect [13]. It leads to a spatial alignment of the 3d orbitals in Cu^{2+} resulting in a strong exchange interaction along one axis of the crystal (the chain axis) while in the perpendicular direction the exchange interaction is very small due to poor overlap of the corresponding orbitals. The ratio between the two interaction constants has been evaluated to be of the order 0.027 [9], making the magnetic behavior of the KCuF3 compound effectively one dimensional. Further, the Cu^{2+} ions provide [8] effective spin-1/2 dynamical variables in interaction which is well represented by the Heisenberg spin chain Hamiltonian [14]. The XXZ spin- $\frac{1}{2}$ Heisenberg chain in an external magnetic field h is a quantum interacting model defined on a one-dimensional lattice with Hamiltonian,

$$H = H^{(0)} - hS_z, (1)$$

$$H^{(0)} = \sum_{m=1}^{M} \left\{ \sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y + \Delta(\sigma_m^z \sigma_{m+1}^z - 1) \right\}, \tag{2}$$

$$S_z = \frac{1}{2} \sum_{m=1}^{M} \sigma_m^z, \qquad [H^{(0)}, S_z] = 0.$$
 (3)

Here Δ is the anisotropy parameter (essentially equal to one for $KCuF_3$), M is the number of sites of the chain (and here we assume for simplicity periodic boundary conditions), h denotes the uniform external magnetic field, and $\sigma_m^{x,y,z}$ are the local spin operators (here in the spin- $\frac{1}{2}$ representation) associated with each site m of the chain. The quantum space of states is $\mathcal{H} = \bigotimes_{m=1}^{M} \mathcal{H}_m$, where $\mathcal{H}_m \sim \mathbb{C}^2$ is called local quantum space, with $\dim \mathcal{H} = 2^M$. The operators $\sigma_m^{x,y,z}$ act as the corresponding Pauli matrices in the space \mathcal{H}_m and as the identity operator elsewhere.

Following our above discussion, to be able to compare predictions of such a one-dimensional model to actual magnetic compounds such as $KCuF_3$, we need to compute various physical observable quantities such as the dynamical structure factors; they are the Fourier transform of the dynamical spin-spin correlation functions which at non zero temperature T, lattice distance m and time difference t, are given as traces over the space of states,

$$S^{\alpha\beta}(m,t) = \frac{tr(\sigma_1^{\alpha} e^{iHt} \sigma_{m+1}^{\beta} e^{-iHt} e^{-\frac{H}{kT}})}{tr(e^{-\frac{H}{kT}})}.$$
 (4)

At zero temperature, this expression reduces to an average value of the product of Heisenberg spin operators taken in the ground state $|\psi_g\rangle$, the normalized (non degenerated in the disordered regime) state with lowest energy level of the Heisenberg chain ,

$$S^{\alpha\beta}(m,t) = \langle \psi_g | \sigma_1^{\alpha} e^{iHt} \sigma_{m+1}^{\beta} e^{-iHt} | \psi_g \rangle.$$
 (5)

The Fourier transform (in space and time) $S^{\alpha\beta}(q,\omega)$ of this dynamical correlation functions is related, at first order in the neutron-crystal interaction, to the differential magnetic cross sections for the inelastic scattering of unpolarized neutrons off a crystal (like $KCuF_3$), with energy transfer ω and momentum transfer q through the following formula [5]:

$$\frac{d\sigma}{d\Omega d\omega} \sim (\delta_{\alpha\beta} - \frac{q_{\alpha}q_{\beta}}{q^2}) S^{\alpha\beta}(q,\omega)$$
 (6)

Hence, to compare the Heisenberg model to experimental measurements of the neutron scattering cross sections, we need to compute the dynamical spin-spin correlation functions (4) or (5).

This amounts first to determine the spectrum of the Heisenberg Hamiltonian. Further, we need to identify the action of the local spin operators in the corresponding eigenstate basis and obtain their matrix elements to be summed up to perform the trace, and the scalar products, necessary in the actual computation of (4) or (5).

The solution to these different steps turns out to be a fantastic challenge involving deep algebraic structures hidden in the original Bethe ansatz solution [15] of the Heisenberg Hamiltonian spectrum and unraveled along its extensions [16, 17, 18, 19, 20] in particular through the associated Yang-Baxter structures [21, 22, 23, 24, 25, 26, 27]; these led, in the search of an algebraic way to construct new integrable models [28, 29, 30, 31], to the discovery of quantum groups [32, 33, 34, 35]; it was latter realized that the underlying the symmetry algebra of the Heisenberg model in the infinite lattice limit is the quantum affine algebra $U_q(\hat{s}l_2)$ [36, 37].

The aim of this lecture is to describe the methods used towards the solution of these successive steps. Some of them are already 75 years old and go back to H. Bethe [15], while others have been developed only in the last ten years. But before going into the historical developments and technical details about these tools, and as a motivation to eventually spend some time learning about them, I would like to give here one of the result that we obtained rather recently [38, 39, 40]: the graphical plot (as a function of q and ω) of the total dynamical structure factor at zero temperature $S(q,\omega)$ and its successful comparison to experimental neutron scattering measurements on the $KCuF_3$ crystal (the colors encode here the value of the function in the (q,ω) plane, from blue corresponding to zero value to dark red in the highest contributions), see Fig. 1.

This computation involves both analytical (exact) results about the spectrum of the Heisenberg Hamiltonian, the matrix elements of the local spin operators between eigenstates using Bethe ansatz techniques and numerical analysis used to perform the sums over these matrix elements to obtain the dynamical structure factor $S(q,\omega)$ (see section 3).

What makes these results at all possible is the integrable nature of the Heisenberg Hamiltonian, namely in particular the possibility to determine its exact spectrum. This model, introduced by Heisenberg in 1928 [14], can in fact be considered as the archetype of a large class of integrable (called also exactly solvable) models in low dimensions in classical and quantum statistical mechanics and field theory. They

142 J.-M. Maillet Séminaire Poincaré

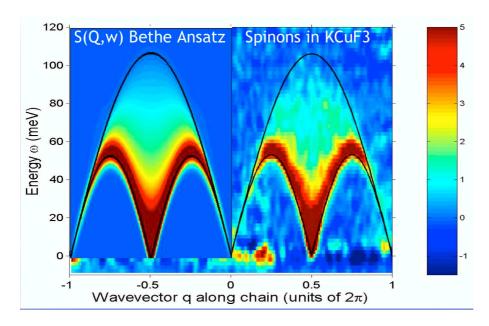


Figure 1: The dynamical structure factor $S(q, \omega)$, on the right computed using Bethe ansatz techniques and on the left from inelastic neutron scattering experiment on $KCuF_3$ [11] (experimental data and picture, courtesy A. Tennant)

already found many applications ranging from condensed matter physics (see e.g., [26, 41, 42, 43]) to high energy physics (see e.g., [44, 45, 46]).

The history of these integrable models of statistical physics started in fact a bit before the Heisenberg spin chain, with the proposal by Lenz and by Ising [47, 48]) of the Ising model to investigate ferromagnetic properties of solids. Ising first solved the one dimensional case where there is no phase transition at any finite temperature to a ferromagnetic ordered state. It is rather unfortunate that Ising did not realize at that time that this failure was a peculiarity of the one dimensional situation. However, this was taken by Heisenberg as a motivation to propose his own model in 1928 [14], based on a more sophisticated treatment of the interactions between the spins (using in particular their full quantum operator nature which was simplified drastically in the Ising case). In this way, the more complicated Heisenberg model was exploited (successfully) first, and only after did theoretical physicists (and chemists!) return to the somehow simpler Ising model [49, 50, 51, 52, 53].

The Bethe solution of the Heisenberg spin chain in 1931 gave the starting point for the development of the field of quantum integrable models in one-dimensional statistical mechanics, using his now famous Bethe ansatz and its further extensions [15, 17, 18, 20, 21]. The Ising model generated also fantastic line of research, starting with the Onsager solution of the two-dimensional case in 1942 [51]. It had a major impact on the theory of critical phenomena and launches a series of study of two-dimensional exactly solvable models of classical statistical mechanics (in fact related through their transfer matrices to the above quantum one-dimensional spin chains) culminating in the works of Baxter in the 70's on the 6-vertex (related to the XXZ chain) and 8-vertex (related to the XYZ chain) models (see the book [26] and references therein). These remarkable success (also with the works of Gaudin, Yang and

many others) (see [26, 25, 27] and references therein) led to apply these techniques to a quite interesting continuum model, the Non Linear Schroedinger model, which was also classically solvable through the inverse scattering methods using its Lax pair structure, see e.g. [54, 55] and references therein. This led to the discovery of an algebraic version of the Bethe ansatz by Faddeev, Sklyanin and Taktadjan [23, 24]. The algebraic structure at work in this method has been coined since this pioneering work, the Yang-Baxter algebra. It is written as a quadratic algebra of quantum operators depending on a continuous parameter λ (the spectral parameter) and governed by an R-matrix which in the case of the Heisenberg XXZ chain is directly related to the Boltzman weights of the 6-vertex model. For that case, there is four operators, A, B, C, D that can be considered as forming the operator entries of a 2×2 matrix, the monodromy matrix,

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \tag{7}$$

This monodromy matrix is constructed from the R-matrix of the model as a specific ordered product all along the chain (see the next section). The quadratic commutation relations between the operators A, B, C, D can the be written in a compact way as,

$$R_{12}(\lambda, \mu) T_1(\lambda) T_2(\mu) = T_2(\mu) T_1(\lambda) R_{12}(\lambda, \mu),$$
 (8)

with the tensor notations $T_1(\lambda) = T(\lambda) \otimes \text{Id}$ and $T_2(\mu) = \text{Id} \otimes T(\mu)$. There the R-matrix appears as the structure constants of the Yang-Baxter algebra. It is is a linear operator in the tensor product $V_1 \otimes V_2$, where each V_i is isomorphic to \mathbb{C}^2 , and depends generically on two spectral parameters λ_1 and λ_2 associated to these two vector spaces. It is denoted by $R_{12}(\lambda_1, \lambda_2)$. Such an R-matrix satisfies the Yang-Baxter equation,

$$R_{12}(\lambda_1, \lambda_2) \ R_{13}(\lambda_1, \lambda_3) \ R_{23}(\lambda_2, \lambda_3) = R_{23}(\lambda_2, \lambda_3) \ R_{13}(\lambda_1, \lambda_3) \ R_{12}(\lambda_1, \lambda_2). \tag{9}$$

These commutation relations imply in particular that the transfer matrices, defined as

$$T(\lambda) = \operatorname{tr} T(\lambda) = A(\lambda) + D(\lambda), \tag{10}$$

commute for different values of the spectral parameter $[\mathcal{T}(\lambda), \mathcal{T}(\mu)] = 0$ and also with S_z , $[\mathcal{T}(\lambda), S_z]$

= 0. The Hamiltonian (2) at h = 0 is related to $\mathcal{T}(\lambda)$ by the 'trace identity'

$$H^{(0)} = 2\sinh\eta \frac{d\mathcal{T}(\lambda)}{d\lambda}\mathcal{T}^{-1}(\lambda)\Big|_{\lambda = \frac{\eta}{2}} - 2M\cosh\eta.$$
 (11)

Therefore, the spectrum of the Hamiltonian (1) is given by the common eigenvectors of the transfer matrices and of S_z . They can be constructed by the successive action of operator $B(\lambda_i)$ (or equivalently by the $C(\lambda_i)$) on a reference state provided the spectral parameters λ_i satisfy the original Bethe equations. The analysis of these equations leads to the determination of the Hamiltonian spectrum, and to the determination of the groundstate, in particular in the limit of infinite chains.

It is interesting to mention that the above algebraic structures have nice classical limits that are related to Lie-Poisson structures (see [54, 55] and references therein). It enables to construct the corresponding classical integrable models purely from the knowledge of a Lie algebra and its representations. The similar question for the quantum case was of great importance in constructing new quantum integrable models, not only on the lattice but also in the continuum [28, 29, 30, 31]. In turn, the full solution of this problem led to the discovery of quantum groups [32, 33, 34, 35].

After determining the spectrum, the next task is to consider the computation of correlation functions such as (5). There is two main routes to compute dynamical two point correlation functions of this type, namely, depending on the lattice distance m and on the time variable t (we assume here translational invariance):

(i) Compute first the action of local operators on the ground state

$$\sigma_1^{\alpha} e^{iHt} \, \sigma_{m+1}^{\beta} e^{-iHt} \, | \, \psi_g \, \rangle = | \, \tilde{\psi}_g \, \rangle \tag{12}$$

and then calculate the resulting scalar product to get

$$S^{\alpha\beta}(m,t) = \langle \psi_a | \tilde{\psi_a} \rangle. \tag{13}$$

Note however that for dynamical correlation functions this amounts to evaluate the action of the exponential of the Hamiltonian operator not only on Hamiltonian eigenstates (which is easy) but also on general states resulting from the action of local operators on Hamiltonian eigenstates (which is rather complicated).

(ii) Insert the identity as a sum over a complete set of normalized states $|\psi_i\rangle$ (for instance, the basis constructed out of the eigenvectors of the Hamiltonian) between the local operators to obtain a representation for the correlation function as a sum over matrix elements of local operators,

$$S^{\alpha\beta}(m,t) = \sum_{i} \langle \psi_g | \sigma_1^{\alpha} | \psi_i \rangle \langle \psi_i | \sigma_1^{\alpha} | \psi_g \rangle e^{i(E_i - E_g)t} e^{im(P_i - P_g)}, \qquad (14)$$

where, E_i, P_i and E_g, P_g are the energy and momentum eigenvalues of the states $|\psi_i\rangle$ and of the groundstate $|\psi_g\rangle$ respectively. This amounts again to be able to act with local operators on eigenstates, to compute the resulting scalar products, and finally to perform the above sum containing in the XXZ spin- $\frac{1}{2}$ model case with M sites 2^M terms.

In both approaches, we need to obtain the action of local operators on Hamiltonian eigenstates in a compact and manageable form and then to evaluate the resulting scalar product. This problem turns out to be very involved due to the highly non local nature of the Bethe eigenstates. Indeed, the creation operators of Bethe eigenstates (the operators $B(\lambda)$) are extremely nonlocal in terms of local spin operators σ_i^{α} . In fact (see next section) they are the sum of 2^M terms (M is the number of lattice sites in the chain), each term being some product of spin operators σ_i^{α} from the site one to the site M. As a consequence, A, B, C, D operators do not have an priori simple commutation relations with the local spin operators, which is the ingredient we would need to compute the action of the latter on Bethe eigenstates. It is a major problem that prevents for very long the computation of correlation functions. In fact, the first case to be understood was the free fermion point $\Delta = 0$ (a computation essentially equivalent to the one for the two-dimensional Ising model). In that case, thanks to a Jordan-Wigner transformation, it is possible to rewrite the Hamiltonian as a quadratic expression in the fermionic operators and hence to use them as creation operators for its eigenstates while the local spin operators have also a simple expression in terms of them. It is this property, namely the fact that all relevant quantities can be embedded inside the same Clifford algebra, that finally opened the possibility to compute the correlation functions in that case. Nevertheless tremendous work was necessary to achieve full answers [51, 52, 53, 56, 57, 58, 59, 60].

Going beyond the free Fermion case has been a major challenge for the last thirty years.

For integrable quantum spin chains [61, 62, 63] and lattice models [26], the first attempts to go beyond free Fermion models relied on the Bethe ansatz techniques [23, 64] and was undertaken by A. G. Izergin and V. E. Korepin (see e.g. [61] and references therein). Their approach yields formulae for the correlation functions [61, 65, 66, 67] written as vacuum expectation values of some determinants depending on so-called "dual fields" which were introduced to overcome the huge combinatorial sums arising in particular from the action of local operators on Bethe states. However these formulae are not completely explicit, since these "dual fields" cannot be eliminated from the final result.

In the last fifteen years, two main approaches to a more explicit computation of form factors and correlation functions have been developed, mainly for lattice models.

One of these approaches was initiated by M. Jimbo, T. Miwa and their collaborators [68, 36, 37, 69] and enables, using some (rather well controlled) hypothesis, to compute form factors and correlation functions of quantum spin chains of infinite length (and in their massive regime) by expressing them in terms of traces of q-deformed vertex operators over an irreducible highest weight representation of the corresponding quantum affine algebra. This quantum affine algebra is conjectured to be the infinite dimensional symmetry algebra of the Heisenberg infinite chain, and all relevant quantities can be embedded in this algebra, making the computation of correlation functions possible. The vertex operators traces turn out to satisfy an axiomatic system of equations called q-deformed Knizhnik-Zamolodchikov (q-KZ) equations, the solutions of which can be expressed in terms of multiple integral formulae. Using these equations similar formulae can be conjectured in the massless regime. Recently, a more algebraic representation for the solution of these q-deformed Knizhnik-Zamolodchikov equations have been obtained for the XXX and XXZ (and conjectured for the XYZ) spin 1/2 chains; in these representations, all elementary blocks of the correlation functions can be expressed in terms of some transcendental functions [70, 71, 72]. A detailed review of the approach can be found in [62].

These results, their proofs, together with their extension to non-zero magnetic field have been obtained in 1999 [38, 73] using the algebraic Bethe ansatz framework [23, 24, 25] and the actual resolution of the so-called quantum inverse scattering problem [38, 74]. The main steps of this method are as follows. Let us first note that any *n*-point correlation function of the Heisenberg chain can be reconstructed as a sum of elementary building blocks defined in the following way:

$$F_m(\{\epsilon_j, \epsilon_j'\}) = \langle \psi_g | \prod_{j=1}^m E_j^{\epsilon_j', \epsilon_j} | \psi_g \rangle.$$
 (15)

Here $|\psi_g\rangle$ is the normalized ground state of the chain and $E_j^{\epsilon'_j,\epsilon_j}$ denotes the elementary operator acting on the quantum space \mathcal{H}_j at site j as the 2×2 matrix of elements $E_{lk}^{\epsilon',\epsilon}=\delta_{l,\epsilon'}\delta_{k,\epsilon}$.

A multiple integral representation for these building blocks was obtained for the first time in [68, 69]. We briefly recall how we derived them in the framework of algebraic Bethe Ansatz [38, 73] by solving the following successive problems:

- (i) determination of the ground state $\langle \psi_q |$,
- (ii) evaluation of the action the product of local operators on this ground state,

- (iii) computation of the scalar product of the resulting state with $|\psi_q\rangle$,
- (iv) thermodynamic limit.

The starting point of our method is to use in step (i) the description of the eigenstates obtained via algebraic Bethe Ansatz [23, 61]. They are constructed in this framework in terms of generalized creation and annihilation operators which are themselves highly non-local. Acting with local operators on such states in step (ii) is therefore a priori a non-trivial problem. One of the key-ingredient of our method, which enables us to compute this action explicitly, is the solution of the so-called quantum inverse scattering problem [38, 74]: local operators are reconstructed in terms of the generators of the so-called Yang-Baxter algebra, which contains in particular the creation/annihilation operators for the eigenstates. Hence, all computations can now be done in the Yang-Baxter algebra. In particular, the step (ii) is now completed using only the quadratic commutation relations satisfied by these generators [73]. The computation of the resulting scalar products in step (iii) may also present some technical difficulties. In the case of the XXZ Heisenberg chain, it has been solved using again the algebraic structure of the Yang-Baxter algebra [83, 38]. Finally, the step (iv) is obtained using the results of [19, 20].

Note that this procedure remains essentially the same in the case of the two-point correlation functions. The main difference is that, in step (ii), the reconstruction of the corresponding local operators from the solution of the inverse problem gives rise to a more complicated combination of the generators of the Yang-Baxter algebra, so that the use of their commutation relations to determine their action on the eigenstates involves a more complicated combinatoric.

At zero magnetic field our method gives a complete proof of the multiple integral representations obtained in [68, 69, 37] both for massive and massless regimes. Hence, together with the works [68, 69], it also gives a proof that correlation functions of the XXZ (inhomogeneous) chain indeed satisfy (reduced) q-deformed Knizhnik-Zamolodchikov equations. Moreover, time or temperature dependent correlation functions can also be computed [80, 63, 81] using such techniques.

This method allows also for the computation of the matrix elements of the local spin operators and the above elementary blocks of the correlation functions for the finite chain. Hence, thermodynamic limit can be considered separately. In particular, using both analytical results from Bethe ansatz for these matrix elements of the spin operators [84, 38, 73, 74] and numerical methods to take the summation over intermediate states it has been possible recently to compute [39, 40] dynamical structure factors (i.e., Fourier transform of the dynamical spin-spin correlation functions) for finite XXZ Heisenberg spin chain in a magnetic field (with for example 500 or 1000 sites) and to compare successfully these theoretical results with actual neutron scattering experiments, for example on KCuF3 as shown in Fig. 1.

This article is meant to be a rather brief review on the problem of correlation functions in quantum integrable models and more specifically in the XXZ Heisenberg model. More detailed account of the results sketched here together with their proofs can be found in the original articles [84, 38, 73, 74, 75, 76, 77, 78, 79, 63, 80, 85, 86] and in [39, 40, 87]. This lecture is organized as follows. The space of states of the Heisenberg spin chain will be described in the next section. It includes a brief introduction to the algebraic Bethe ansatz and to various tools of importance in the computation of correlation functions, like in particular the solution of the quantum inverse scattering problem and the determinant representations of the scalar products of states. Section 3 is devoted to the correlation functions of the finite chain and the description of

the method leading to Fig. 1. Correlation functions in the thermodynamic limit are studied in the section 4. In the section 5 we describe several exact and asymptotic results together with some open problems. Conclusions and some perspectives are given in the last section.

2 Heisenberg spin chain and algebraic Bethe ansatz

The space of states is of dimension 2^M as it follows from the definition of the Hamiltonian in (1). Apart from the completely ferromagnetic states with all spins up or down, the construction of the Hamiltonian eigenvectors is rather non trivial. The purpose of this section is to briefly explain the basics of the knowledge of the space of states in the framework of the algebraic Bethe ansatz, leading in particular to the determination of the spectrum of (1).

2.1 Algebraic Bethe ansatz

The algebraic Bethe ansatz originated from the fusion of the original (coordinate) Bethe ansatz and of the inverse scattering method in its Hamiltonian formulation [23, 24, 25]. At the root of the algebraic Bethe ansatz method is the construction of the quantum monodromy matrix. In the case of the XXZ chain (1) the monodromy matrix is a 2×2 matrix,

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \tag{16}$$

with operator-valued entries A, B, C and D which depend on a complex parameter λ (spectral parameter) and act in the quantum space of states \mathcal{H} of the chain. One of the main property of these operators is that the trace of T, namely A+D, commutes with the Hamiltonian H, while operators B and C can be used as creation operators of respectively eigenvectors and dual eigenvectors of A+D and hence of H itself. The monodromy matrix is defined as the following ordered product,

$$T(\lambda) = L_M(\lambda) \dots L_2(\lambda) L_1(\lambda), \tag{17}$$

where $L_n(\lambda)$ denotes the quantum L-operator at the site n of the chain:

$$L_n(\lambda) = \begin{pmatrix} \sinh(\lambda + \frac{\eta}{2} \sigma_n^z) & \sinh \eta \, \sigma_n^-\\ \sinh \eta \, \sigma_n^+ & \sinh(\lambda - \frac{\eta}{2} \sigma_n^z) \end{pmatrix}. \tag{18}$$

The parameter η is related to the anisotropy parameter as $\Delta = \cosh \eta$. It follows from this definition that the monodromy matrix is an highly non local operator in terms of the local spin operators $\sigma_n^{x,y,z}$. However, the commutation relations between the operators A,B,C,D can be computed in a simple way. They are given by the quantum R-matrix,

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & b(\lambda, \mu) & c(\lambda, \mu) & 0\\ 0 & c(\lambda, \mu) & b(\lambda, \mu) & 0\\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(19)

where

$$b(\lambda, \mu) = \frac{\sinh(\lambda - \mu)}{\sinh(\lambda - \mu + \eta)}, \ c(\lambda, \mu) = \frac{\sinh(\eta)}{\sinh(\lambda - \mu + \eta)}, \tag{20}$$

The R-matrix is a linear operator in the tensor product $V_1 \otimes V_2$, where each V_i is isomorphic to \mathbb{C}^2 , and depends generically on two spectral parameters λ_1 and λ_2 associated to these two vector spaces. It is denoted by $R_{12}(\lambda_1, \lambda_2)$. Such an R-matrix satisfies the Yang-Baxter equation,

$$R_{12}(\lambda_1, \lambda_2) R_{13}(\lambda_1, \lambda_3) R_{23}(\lambda_2, \lambda_3) = R_{23}(\lambda_2, \lambda_3) R_{13}(\lambda_1, \lambda_3) R_{12}(\lambda_1, \lambda_2).$$
 (21)

It gives the following commutation relations among the operators entries of the monodromy matrix,

$$R_{12}(\lambda, \mu) T_1(\lambda) T_2(\mu) = T_2(\mu) T_1(\lambda) R_{12}(\lambda, \mu),$$
 (22)

with the tensor notations $T_1(\lambda) = T(\lambda) \otimes \text{Id}$ and $T_2(\mu) = \text{Id} \otimes T(\mu)$. These commutation relations imply in particular that the transfer matrices, defined as

$$T(\lambda) = \operatorname{tr} T(\lambda) = A(\lambda) + D(\lambda), \tag{23}$$

commute for different values of the spectral parameter $[\mathcal{T}(\lambda), \mathcal{T}(\mu)] = 0$ and also with S_z , $[\mathcal{T}(\lambda), S_z]$

= 0. The Hamiltonian (2) at h = 0 is related to $\mathcal{T}(\lambda)$ by the 'trace identity' (11).

Therefore, the spectrum of the Hamiltonian (1) is given by the common eigenvectors of the transfer matrices and of S_z .

For technical reasons, it is actually convenient to introduce a slightly more general object, the twisted transfer matrix

$$\mathcal{T}_{\kappa}(\lambda) = A(\lambda) + \kappa D(\lambda), \tag{24}$$

where κ is a complex parameter. The particular case of $\mathcal{T}_{\kappa}(\lambda)$ at $\kappa = 1$ corresponds to the usual (untwisted) transfer matrix $\mathcal{T}(\lambda)$. It will be also convenient to consider an inhomogeneous version of the XXZ chain, for which

$$T_{1...M}(\lambda; \xi_1, ..., \xi_M) = L_M(\lambda - \xi_M + \eta/2) ... L_1(\lambda - \xi_1 + \eta/2).$$
 (25)

Here, ξ_1, \ldots, ξ_M are complex parameters (inhomogeneity parameters) attached to each site of the lattice. The homogeneous model (1) corresponds to the case where $\xi_j = \eta/2$ for $j = 1, \ldots, M$.

In the framework of algebraic Bethe ansatz, an arbitrary quantum state can be obtained from the vectors generated by multiple action of operators $B(\lambda)$ on the reference vector $|0\rangle$ with all spins up (respectively by multiple action of operators $C(\lambda)$ on the dual reference vector $\langle 0|$),

$$|\psi\rangle = \prod_{j=1}^{N} B(\lambda_j)|0\rangle, \qquad \langle\psi| = \langle 0|\prod_{j=1}^{N} C(\lambda_j), \qquad N = 0, 1, \dots, M.$$
 (26)

2.2 Description of the spectrum

Let us consider here the subspace $\mathcal{H}^{(M/2-N)}$ of the space of states \mathcal{H} with a fixed number N of spins down. In this subspace, the eigenvectors $|\psi_{\kappa}(\{\lambda\})\rangle$ (respectively

 $\langle \psi_{\kappa}(\{\lambda\}) | \rangle$ of the twisted transfer matrix $\mathcal{T}_{\kappa}(\mu)$ can be constructed in the form (26), where the parameters $\lambda_1, \ldots, \lambda_N$ satisfy the system of twisted Bethe equations

$$\mathcal{Y}_{\kappa}(\lambda_j|\{\lambda\}) = 0, \qquad j = 1, \dots, N.$$
 (27)

Here, the function \mathcal{Y}_{κ} is defined as

$$\mathcal{Y}_{\kappa}(\mu|\{\lambda\}) = a(\mu) \prod_{k=1}^{N} \sinh(\lambda_k - \mu + \eta) + \kappa \, d(\mu) \prod_{k=1}^{N} \sinh(\lambda_k - \mu - \eta), \qquad (28)$$

and $a(\lambda)$, $d(\lambda)$ are the eigenvalues of the operators $A(\lambda)$ and $D(\lambda)$ on the reference state $|0\rangle$. In the normalization (18) and for the inhomogeneous model (25), we have

$$a(\lambda) = \prod_{a=1}^{M} \sinh(\lambda - \xi_a + \eta), \qquad d(\lambda) = \prod_{a=1}^{M} \sinh(\lambda - \xi_a).$$
 (29)

The corresponding eigenvalue of $\mathcal{T}_{\kappa}(\mu)$ on $|\psi_{\kappa}(\{\lambda\})\rangle$ (or on a dual eigenvector) is

$$\tau_{\kappa}(\mu|\{\lambda\}) = a(\mu) \prod_{k=1}^{N} \frac{\sinh(\lambda_k - \mu + \eta)}{\sinh(\lambda_k - \mu)} + \kappa d(\mu) \prod_{k=1}^{N} \frac{\sinh(\mu - \lambda_k + \eta)}{\sinh(\mu - \lambda_k)}.$$
 (30)

The solutions of the system of twisted Bethe equations (27) have been analyzed in [88]. In general, not all of these solutions correspond to eigenvectors of $\mathcal{T}_{\kappa}(\mu)$.

Definition 2.1 A solution $\{\lambda\}$ of the system (27) is called admissible if

$$d(\lambda_j) \prod_{\substack{k=1\\k\neq j}}^N \sinh(\lambda_j - \lambda_k + \eta) \neq 0, \qquad j = 1, \dots, N,$$
(31)

and un-admissible otherwise. A solution is called off-diagonal if the corresponding parameters $\lambda_1, \ldots, \lambda_N$ are pairwise distinct, and diagonal otherwise.

One of the main result of [88] is that, for generic parameters κ and $\{\xi\}$, the set of the eigenvectors corresponding to the admissible off-diagonal solutions of the system of twisted Bethe equations (27) form a basis in the subspace $\mathcal{H}^{(M/2-N)}$. It has been proven in [80] that this result is still valid in the homogeneous case $\xi_j = \eta/2$, $j = 1, \ldots, N$, at least if κ is in a punctured vicinity of the origin (i.e. $0 < |\kappa| < \kappa_0$ for κ_0 small enough). Note however that, for specific values of κ and $\{\xi\}$, the basis of the eigenvectors in $\mathcal{H}^{(M/2-N)}$ may include some states corresponding to un-admissible solutions of (27) (in particular in the homogeneous limit at $\kappa = 1$).

At $\kappa = 1$, it follows from the trace identity (11) that the eigenvectors of the transfer matrix coincide, in the homogeneous limit, with the ones of the Hamiltonian (1). The corresponding eigenvalues in the case of zero magnetic field can be obtained from (11), (30):

$$H^{(0)} | \psi(\{\lambda\}) \rangle = \left(\sum_{j=1}^{N} E(\lambda_j) \right) \cdot | \psi(\{\lambda\}) \rangle, \tag{32}$$

where the (bare) one-particle energy $E(\lambda)$ is equal to

$$E(\lambda) = \frac{2\sinh^2 \eta}{\sinh(\lambda + \frac{\eta}{2})\sinh(\lambda - \frac{\eta}{2})}.$$
 (33)

2.3 Drinfel'd twist and F-basis

As already noted, the operators A, B, C, D are highly non local in terms of local spin operators. There exists however an interesting description of these operators by means of a change of basis of the space of states. In particular, this basis will provide a direct access to the scalar products of states. The root of this new basis is provided by the notion of Drinfel'd twist [35] associated to the R-matrix of the XXZ chain. It leads to the notion of factorizing F-matrices. To be essentially self-contained we briefly recall here their main properties and refer to [84] for more details and proofs.

Definition 2.2 For inhomogeneity parameters ξ_j in generic positions and for any integer n one can associate to any element σ of the symmetric group S_n of order n a unique R-matrix $R_{1...n}^{\sigma}$ $(\xi_1, ..., \xi_n)$, denoted for simplicity $R_{1...n}^{\sigma}$, constructed as an ordered product (depending on σ) of the elementary R-matrices $R_{ij}(\xi_i, \xi_j)$.

We have the following property for arbitrary integer n:

Proposition 2.1

$$R_{1...n}^{\sigma} T_{1...n}(\lambda; \xi_1, \dots, \xi_n) = T_{\sigma(1)...\sigma(n)}(\lambda; \xi_{\sigma(1)}, \dots, \xi_{\sigma(n)}) R_{1...n}^{\sigma}.$$
(34)

We can now define the notion of factorizing F-matrix:

Definition 2.3 A factorizing F-matrix associated to a given elementary R matrix is an invertible matrix $F_{1...n}(\xi_1,...,\xi_n)$, defined for arbitrary integer n, satisfying the following relation for any element σ of S_n :

$$F_{\sigma(1)...\sigma(n)}(\xi_{\sigma(1)},\ldots,\xi_{\sigma(n)}) R_{1-n}^{\sigma}(\xi_1,\ldots,\xi_n) = F_{1...n}(\xi_1,\ldots,\xi_n).$$
 (35)

In other words, such an F-matrix factorizes the corresponding R-matrix for arbitrary integer n. Taking into account the fact that the parameters ξ_n are in one to one correspondence with the vector spaces \mathcal{H}_n , we can adopt simplified notations such that

$$F_{1...n}(\xi_1,\ldots,\xi_n) = F_{1...n},$$

$$F_{\sigma(1)...\sigma(n)}(\xi_{\sigma(1)},\ldots,\xi_{\sigma(n)}) = F_{\sigma(1)...\sigma(n)}.$$

Theorem 2.1 [84] For the XXZ model with inhomogeneity parameters ξ_n in generic positions, there exist a factorizing, triangular F-matrix. It is constructed explicitly from the R-matrix.

It has two important properties:

Proposition 2.2 [84] In the F-basis, the monodromy matrix \tilde{T}

$$\widetilde{T}_{1...M}(\lambda; \xi_1, ..., \xi_M) = F_{1...M} T_{1...M}(\lambda; \xi_1, ..., \xi_M) F_{1...M}^{-1},$$
(36)

is totally symmetric under any simultaneous permutations of the lattice sites i and of the corresponding inhomogeneity parameters ξ_i .

The second property gives the explicit expressions of the monodromy matrix in the F-basis. For the XXZ- $\frac{1}{2}$ model, the quantum monodromy operator is a 2×2 matrix with entries A, B, C, D which are obtained as sums of 2^{M-1} operators which themselves are products of M local spin operators on the quantum chain. As an example, the B operator is given as

$$B_{1...M}(\lambda) = \sum_{i=1}^{N} \sigma_i^- \Omega_i + \sum_{i \neq j \neq k} \sigma_i^- (\sigma_j^- \sigma_k^+) \Omega_{ijk} + higher terms, \quad (37)$$

where the matrices Ω_i , Ω_{ijk} , are diagonal operators acting respectively on all sites but i, on all sites but i, j, k, and the higher order terms involve more and more exchange spin terms like $\sigma_j^ \sigma_k^+$. It means that the B operator returns one spin somewhere on the chain, this operation being however dressed non-locally and with non-diagonal operators by multiple exchange terms of the type $\sigma_j^ \sigma_k^+$.

So, whereas these formulas in the original basis are quite involved, their expressions in the F-basis simplify drastically:

Proposition 2.3 [84] The operators D, B and C in the F-basis are given by the formulas

$$\widetilde{D}_{1...M}(\lambda;\xi_1,\ldots,\xi_M) = \underset{i=1}{\overset{M}{\otimes}} \left(\begin{array}{cc} b(\lambda,\xi_i) & 0\\ 0 & 1 \end{array} \right)_{[i]}.$$
(38)

$$\widetilde{B}_{1...M}(\lambda) = \sum_{i=1}^{M} \sigma_i^- c(\lambda, \xi_i) \underset{j \neq i}{\otimes} \begin{pmatrix} b(\lambda, \xi_j) & 0\\ 0 & b^{-1}(\xi_j, \xi_i) \end{pmatrix}_{[j]}.$$
 (39)

$$\widetilde{C}_{1...M}(\lambda) = \sum_{i=1}^{M} \sigma_i^+ c(\lambda, \xi_i) \underset{j \neq i}{\otimes} \left(\begin{array}{cc} b(\lambda, \xi_j) & b^{-1}(\xi_i, \xi_j) & 0\\ 0 & 1 \end{array} \right)_{[j]}, \tag{40}$$

and the operator \widetilde{A} can be obtained from quantum determinant relations.

We wish first to stress that while the operators \widetilde{A} , \widetilde{B} , \widetilde{C} , \widetilde{D} satisfy the same quadratic commutation relations as A, B, C, D, they are completely symmetric under simultaneous exchange of the inhomogeneity parameters and the of the spaces \mathcal{H}_n . It really means that the factorizing F-matrices we have constructed solve the combinatorial problem induced by the non-trivial action of the permutation group S_M given by the R-matrix. In the F-basis the action of the permutation group on the operators \widetilde{A} , \widetilde{B} , \widetilde{C} , \widetilde{D} is trivial.

Further, it can be shown that the pseudo-vacuum vector is left invariant, namely, it is an eigenvector of the total F-matrix with eigenvalue 1; in particular, the algebraic Bethe ansatz can be carried out also in the F-basis. Hence, a direct computation of Bethe eigenvectors and of their scalar products in this F-basis is made possible, while it was a priori very involved in the original basis. There, only commutation relations between the operators A, B, C, D can be used, leading (see [61]) to very intricate sums over partitions.

2.4 Solution of the quantum inverse problem

The very simple expressions of the monodromy matrix operators entries D, B, C in the F-basis suggests that any local operator $E_j^{\epsilon'_j, \epsilon_j}$, acting in a local quantum space

 \mathcal{H}_j at site j, can be expressed in terms of the entries of the monodromy matrix. This is the so-called quantum inverse scattering problem. The solution to this problem was found in [38, 74]:

Theorem 2.2

$$E_j^{\epsilon_j',\epsilon_j} = \prod_{\alpha=1}^{j-1} \mathcal{T}(\xi_\alpha) \cdot T_{\epsilon_j,\epsilon_j'}(\xi_j) \cdot \prod_{\alpha=1}^j \mathcal{T}^{-1}(\xi_\alpha). \tag{41}$$

The proof of this theorem is elementary (see [38, 74]) and hence it can be obtained for a large class of lattice integrable models. It relies essentially on the property that the R-matrix $R(\lambda, \mu)$ reduces to the permutation operator for $\lambda = \mu$. An immediate consequence of this theorem is that the operators A, B, C, and D generate the space of all operators acting in \mathcal{H} .

2.5 Scalar products

We give here the expressions for the scalar product of an eigenvector of the twisted transfer matrix with any arbitrary state of the form (26). These scalar products can be expressed as determinant of rather simple matrices. The root of all these determinants is in fact the determinant representation for the partition function of the 6-vertex model with domain wall boundary conditions [89]. Let us first define, for arbitrary positive integers n, n' ($n \le n'$) and arbitrary sets of variables $\lambda_1, \ldots, \lambda_n, \mu_1, \ldots, \mu_n$ and $\nu_1, \ldots, \nu_{n'}$ such that $\{\lambda\} \subset \{\nu\}$, the $n \times n$ matrix $\Omega_{\kappa}(\{\lambda\}, \{\mu\} | \{\nu\})$ as

$$(\Omega_{\kappa})_{jk}(\{\lambda\}, \{\mu\}|\{\nu\}) = a(\mu_k) t(\lambda_j, \mu_k) \prod_{a=1}^{n'} \sinh(\nu_a - \mu_k + \eta) - \kappa d(\mu_k) t(\mu_k, \lambda_j) \prod_{a=1}^{n'} \sinh(\nu_a - \mu_k - \eta), \quad (42)$$

with

$$t(\lambda, \mu) = \frac{\sinh \eta}{\sinh(\lambda - \mu) \sinh(\lambda - \mu + \eta)}.$$
 (43)

Proposition 2.4 [83, 38, 63] Let $\{\lambda_1, \ldots, \lambda_N\}$ be a solution of the system of twisted Bethe equations (27), and μ_1, \ldots, μ_N be generic complex numbers. Then,

$$\langle 0 | \prod_{j=1}^{N} C(\mu_{j}) | \psi_{\kappa}(\{\lambda\}) \rangle = \langle \psi_{\kappa}(\{\lambda\}) | \prod_{j=1}^{N} B(\mu_{j}) | 0 \rangle$$

$$= \frac{\prod_{a=1}^{N} d(\lambda_{a}) \prod_{a,b=1}^{N} \sinh(\mu_{b} - \lambda_{a})}{\prod_{a>b}^{N} \sinh(\lambda_{a} - \lambda_{b}) \sinh(\mu_{b} - \mu_{a})} \cdot \det_{N} \left(\frac{\partial}{\partial \lambda_{j}} \tau_{\kappa}(\mu_{k} | \{\lambda\}) \right)$$

$$= \frac{\prod_{a=1}^{N} d(\lambda_{a})}{\prod_{a>b}^{N} \sinh(\lambda_{a} - \lambda_{b}) \sinh(\mu_{b} - \mu_{a})} \cdot \det_{N} \Omega_{\kappa}(\{\lambda\}, \{\mu\} | \{\lambda\}).$$

$$(45)$$

These equations are valid for any arbitrary complex parameter κ , in particular at $\kappa = 1$. In this case we may omit the subscript κ and denote

$$(\psi, \tau, \mathcal{Y}, \Omega) = (\psi_{\kappa}, \tau_{\kappa}, \mathcal{Y}_{\kappa}, \Omega_{\kappa})|_{\kappa=1}.$$

If the sets $\{\lambda\}$ and $\{\mu\}$ are different, the eigenvector $|\psi_{\kappa}(\{\lambda\})\rangle$ is orthogonal to the dual eigenvector $\langle \psi_{\kappa}(\{\mu\})|$. Otherwise we obtain a formula for the norm of the corresponding vector [90, 82, 38],

$$\langle \psi_{\kappa}(\{\lambda\}) | \psi_{\kappa}(\{\lambda\}) \rangle = \frac{\prod_{a=1}^{N} d(\lambda_{a})}{\prod_{\substack{a,b=1\\a\neq b}}^{N} \sinh(\lambda_{a} - \lambda_{b})} \cdot \det_{N} \Omega_{\kappa}(\{\lambda\}, \{\lambda\} | \{\lambda\})$$

$$= (-1)^{N} \frac{\prod_{\substack{a=1\\a\neq b}}^{N} d(\lambda_{a})}{\prod_{\substack{a,b=1\\a\neq b}}^{N} \sinh(\lambda_{a} - \lambda_{b})} \cdot \det_{N} \left(\frac{\partial}{\partial \lambda_{k}} \mathcal{Y}_{\kappa}(\lambda_{j} | \{\lambda\})\right).$$

2.6 Action of operators A, B, C, D on a general state

An important step of the computation of correlation function is to express the action of any product of local operators on any Bethe eigenvector. From the solution of the quantum inverse scattering problem, this is given by the successive action of A, B, C, D operators on a vector constructed by action of C operators on the reference vector. Action of A, B, C, D on such a vector are well known (see for example [61]). They can be written in the following form:

$$\langle 0 | \prod_{k=1}^{N} C(\lambda_{k}) A(\lambda_{N+1}) = \sum_{a'=1}^{N+1} a(\lambda_{a'}) \frac{\prod_{k=1}^{N} \sinh(\lambda_{k} - \lambda_{a'} + \eta)}{\prod_{\substack{k=1\\k \neq a'}}^{N+1} \sinh(\lambda_{k} - \lambda_{a'})} \langle 0 | \prod_{\substack{k=1\\k \neq a'}}^{N+1} C(\lambda_{k}); \quad (46)$$

$$\langle 0 \mid \prod_{k=1}^{N} C(\lambda_k) D(\lambda_{N+1}) = \sum_{a=1}^{N+1} d(\lambda_a) \frac{\prod_{k=1}^{N} \sinh(\lambda_a - \lambda_k + \eta)}{\prod_{\substack{k=1\\k \neq a}}^{N+1} \sinh(\lambda_a - \lambda_k)} \langle 0 \mid \prod_{\substack{k=1\\k \neq a}}^{N+1} C(\lambda_k).$$
 (47)

The action of the operator $B(\lambda)$ can be obtained similarly,

$$\langle 0 | \prod_{k=1}^{N} C(\lambda_k) B(\lambda_{N+1}) = \sum_{a=1}^{N+1} d(\lambda_a) \frac{\prod_{k=1}^{N} \sinh(\lambda_a - \lambda_k + \eta)}{\prod_{\substack{k=1\\k \neq a}}^{N+1} \sinh(\lambda_a - \lambda_k)} \times \sum_{\substack{a'=1\\a' \neq a}}^{N+1} \frac{a(\lambda_{a'})}{\sinh(\lambda_{N+1} - \lambda_{a'} + \eta)} \frac{\prod_{\substack{j=1\\j \neq a}}^{N+1} \sinh(\lambda_j - \lambda_{a'} + \eta)}{\prod_{\substack{j=1\\j \neq a}}^{N+1} \sinh(\lambda_j - \lambda_{a'})} \langle 0 | \prod_{\substack{k=1\\k \neq a,a'}}^{N+1} C(\lambda_k),$$
(48)

and the action of C is obvious.

3 Correlation functions: finite chain

To compute correlation functions of some product of local operators, the following successive problems have to be addressed: (i) determination of the ground state $\langle \psi_g |$, (ii) evaluation of the action of the product of the local operators on it, and (iii) computation of the scalar product of the resulting state with $|\psi_g\rangle$. Using the solution of the quantum inverse scattering problem together with the explicit determinant formulas for the scalar products and the norm of the Bethe state, one sees that matrix elements of local spin operators and correlation functions can be expressed as (multiple) sums of determinants [73]. It should be stressed that this result is purely algebraic and is valid for finite chains of arbitrary length M.

3.1 Matrix elements of local operators

We begin with the calculation of the one-point functions. These results follow directly from the solution of the quantum inverse scattering problem, the above action of operators A, B, C and D, and the determinant representation of the scalar products. We consider,

$$F_N^-(m, \{\mu_j\}, \{\lambda_k\}) = \langle 0 \mid \prod_{j=1}^{N+1} C(\mu_j) \ \sigma_m^- \prod_{k=1}^N B(\lambda_k) \mid 0 \rangle, \tag{49}$$

and

$$F_N^+(m, \{\lambda_k\}, \{\mu_j\}) = \langle 0 \mid \prod_{k=1}^N C(\lambda_k) \ \sigma_m^+ \ \prod_{j=1}^{N+1} B(\mu_j) \ | \ 0 \rangle, \tag{50}$$

where $\{\lambda_k\}_n$ and $\{\mu_j\}_{n+1}$ are solutions of Bethe equations.

Proposition 3.1 For two Bethe states with spectral parameters $\{\lambda_k\}_N$ and $\{\mu_j\}_{N+1}$,

the matrix element of the operator σ_m^- can be represented as a determinant,

$$F_{N}^{-}(m, \{\mu_{j}\}, \{\lambda_{k}\}) = \frac{\phi_{m-1}(\{\mu_{j}\})}{\phi_{m-1}(\{\lambda_{k}\})} \frac{\prod_{j=1}^{N+1} \sinh(\mu_{j} - \xi_{m} + \eta)}{\prod_{k=1}^{N} \sinh(\lambda_{k} - \xi_{m} + \eta)} \cdot \frac{\det_{N+1} H^{-}(m, \{\mu_{j}\}, \{\lambda_{k}\})}{\prod_{N+1 \ge k > j \ge 1} \sinh(\mu_{k} - \mu_{j}) \prod_{1 \le \beta < \alpha \le N} \sinh(\lambda_{\beta} - \lambda_{\alpha})},$$
(51)

$$\phi_m(\{\lambda_k\}) = \prod_{k=1}^{N} \prod_{j=1}^{m} b^{-1}(\lambda_k, \xi_j),$$
 (52)

and the $(N+1) \times (N+1)$ matrix H^- is defined as

$$H_{ab}^{-}(m) = \frac{\varphi(\eta)}{\varphi(\mu_a - \lambda_b)} \left(a(\lambda_b) \prod_{\substack{j=1\\j \neq a}}^{N+1} \varphi(\mu_j - \lambda_b + \eta) - d(\lambda_b) \prod_{\substack{j=1\\j \neq a}}^{N+1} \varphi(\mu_j - \lambda_b - \eta) \right)$$
(53)

for b < N + 1,

$$H_{aN+1}^{-}(m) = \frac{\varphi(\eta)}{\varphi(\mu_a - \xi_m + \eta)\varphi(\mu_a - \xi_m)}.$$
(54)

The matrix element $F_N^+(m, \{\lambda_k\}, \{\mu_j\})$ we get,

$$F_N^+(m,\{\lambda_k\},\{\mu_j\}) = \frac{\phi_m(\lambda_k)\,\phi_{m-1}(\lambda_k)}{\phi_{m-1}(\mu_j)\,\phi_m(\mu_j)} F_N^-(m,\{\mu_j\},\{\lambda_k\}). \tag{55}$$

The matrix elements of the operator σ_m^z between two Bethe states have been obtained similarly [38].

3.2 Elementary blocks of correlation functions

In this section we consider a more general case of correlation functions: the ground state mean value of any product of the local elementary 2×2 matrices $E_{lk}^{\epsilon',\epsilon} = \delta_{l,\epsilon'} \delta_{k,\epsilon}$:

$$F_m(\{\epsilon_j, \epsilon_j'\}) = \frac{\langle \psi_g \mid \prod_{j=1}^m E_j^{\epsilon_j', \epsilon_j} \mid \psi_g \rangle}{\langle \psi_g \mid \psi_g \rangle}.$$
 (56)

An arbitrary *n*-point correlation function can be obtained as a sum of such mean values. Using the solution of the quantum inverse scattering problem, we reduce this problem to the computation of the ground state mean value of an arbitrary ordered product of monodromy matrix elements,

$$F_m(\{\epsilon_j, \epsilon_j'\}) = \phi_m^{-1}(\{\lambda\}) \frac{\langle \psi_g | T_{\epsilon_1, \epsilon_1'}(\xi_1) \dots T_{\epsilon_m, \epsilon_m'}(\xi_m) | \psi_g \rangle}{\langle \psi_g | \psi_g \rangle}, \tag{57}$$

To calculate these mean values we first describe generically the product of the monodromy matrix elements. For that purpose, one should consider the two following sets of indices, $\alpha^+ = \{j : 1 \le j \le m, \epsilon_j = 1\}$, $\operatorname{card}(\alpha^+) = s'$, $\max_{j \in \alpha^+}(j) \equiv j'_{\max}$,

 $\min_{j\in\alpha^+}(j)\equiv j'_{\min}$, and similarly $\alpha^-=\{j:1\leq j\leq m,\,\epsilon'_j=2\}$, $\operatorname{card}(\alpha^-)=s$, $\max_{j\in\alpha^-}(j)\equiv j_{\max},\,\min_{j\in\alpha^-}(j)\equiv j_{\min}$. The intersection of these two sets is not empty and corresponds to the operators $B(\xi_j)$. Consider now the action,

$$\langle 0 | \prod_{k=1}^{N} C(\lambda_k) T_{\epsilon_1, \epsilon'_1}(\lambda_{N+1}) \dots T_{\epsilon_m, \epsilon'_m}(\lambda_{N+m}),$$
 (58)

applying one by one the formulae (46)-(48). For all the indices j from the sets α^+ and α^- one obtains a summation on the corresponding indices a'_j (for $j \in \alpha^+$, corresponding to the action of the operators $A(\lambda)$ or $B(\lambda)$) or a_j (for $j \in \alpha^-$, corresponding to the action of the operators $D(\lambda)$ or $B(\lambda)$). As the product of the monodromy matrix elements is ordered these summations are also ordered and the corresponding indices should be taken from the following sets, $\mathbf{A}_j = \{b : 1 \leq b \leq N + m, \ b \neq a_k, a'_k, \ k < j\}$ and $\mathbf{A}'_j = \{b : 1 \leq b \leq N + m, \ b \neq a'_k, \ k < j, \ b \neq a_k, \ k \leq j\}$. Thus,

$$\langle 0 \mid \prod_{k=1}^{N} C(\lambda_k) T_{\epsilon_1, \epsilon'_1}(\lambda_{N+1}) \dots T_{\epsilon_m, \epsilon'_m}(\lambda_{N+m}) =$$

$$= \sum_{\{a_j, a'_j\}} G_{\{a_j, a'_j\}}(\lambda_1, \dots, \lambda_{N+m}) \langle 0 \mid \prod_{b \in \mathbf{A}_{m+1}} C(\lambda_b)$$
(59)

The summation is taken over the indices a_j for $j \in \alpha^-$ and a'_j for $j \in \alpha^+$ such that $1 \leq a_j \leq N+j, \ a_j \in \mathbf{A}_j, \ 1 \leq a'_j \leq N+j, \ a'_j \in \mathbf{A}'_j$. The functions $G_{\{a_j,a'_j\}}(\lambda_1,\ldots\lambda_{N+m})$ can then be easily obtained from the formulae (46)-(48) taking into account that $\lambda_a = \xi_{a-N}$ for a > N:

$$G_{\{a_{j},a'_{j}\}}(\lambda_{1},\ldots,\lambda_{N+m}) = \prod_{j \in \alpha^{-}} d(\lambda_{a_{j}}) \frac{\prod_{\substack{b=1\\b \in \mathbf{A}_{j}}}^{N+j-1} \sinh(\lambda_{a_{j}} - \lambda_{b} + \eta)}{\prod_{\substack{b=1\\b \in \mathbf{A}'_{j}}}^{N+j} \sinh(\lambda_{a_{j}} - \lambda_{b})} \times \prod_{j \in \alpha^{+}} a(\lambda_{a'_{j}}) \frac{\prod_{\substack{b=1\\b \in \mathbf{A}'_{j}}}^{N+j-1} \sinh(\lambda_{b} - \lambda_{a'_{j}} + \eta)}{\prod_{\substack{b=1\\b \in \mathbf{A}_{j}}}^{N+j} \sinh(\lambda_{b} - \lambda_{a'_{j}})}.$$
(60)

Now to calculate the normalized mean value (57) we apply the determinant representation for the scalar product. It should be mentioned that the number of operators $C(\lambda)$ has to be equal to the number of the operators $B(\lambda)$, as otherwise the mean value is zero, and hence the total number of elements in the sets α^+ and α^- is s + s' = m. Taking into account that in (57), for b > N, $\lambda_b = \xi_{b-N}$ one has to consider the following scalar products,

$$\frac{\langle 0 \mid \prod_{b \in \mathbf{A}_{m+1}} C(\lambda_b) \prod_{k=1}^N B(\lambda_k) \mid 0 \rangle}{\langle 0 \mid \prod_{k=1}^N C(\lambda_k) \prod_{k=1}^N B(\lambda_k) \mid 0 \rangle},$$

for all the permitted values of a_i, a'_i . Finally we obtain:

$$F_m(\{\epsilon_j, \epsilon_j'\}) = \frac{1}{\prod_{k < l} \sinh(\xi_k - \xi_l)} \sum_{\{a_j, a_j'\}} H_{\{a_j, a_j'\}}(\lambda_1, \dots, \lambda_{N+m}), \tag{61}$$

the sum being taken on the same set of indices a_j, a'_j as in (59). The functions $H_{\{a_j, a'_j\}}(\{\lambda\})$ can be obtained using (60) and the determinant representations for the scalar products.

3.3 Two-point functions

The method presented in the last section is quite straightforward and gives formally the possibility to compute any correlation function. However, it has been developed for the computation of the average values of monomials in the monodromy matrix operators entries, leading to the elementary building blocks, whereas the study of the two-point functions involves big sums of such blocks. Indeed, let us consider for example the correlation function $\langle \sigma_1^z \sigma_{m+1}^z \rangle$. Then, according to the solution of the inverse scattering problem (41), we need to calculate the expectation value

$$\langle \psi(\{\lambda\}) | (A-D)(\xi_1) \cdot \prod_{a=2}^{m} \mathcal{T}(\xi_a) \cdot (A-D)(\xi_{m+1}) \cdot \prod_{b=1}^{m+1} \mathcal{T}^{-1}(\xi_b) | \psi(\{\lambda\}) \rangle.$$
 (62)

Since $|\psi(\{\lambda\})\rangle$ is an eigenvector, the action of $\prod_{b=1}^{m+1} \mathcal{T}^{-1}(\xi_b)$ on this state merely produces a numerical factor. However, it is much more complicated to evaluate the action of $\prod_{a=2}^m \mathcal{T}(\xi_a)$. Indeed, we have to act first with $(A-D)(\xi_1)$ on $\langle \psi(\{\lambda\}) |$ (or with $(A-D)(\xi_{m+1})$ on $|\psi(\{\lambda\})\rangle$), which gives a sum of states which are no longer eigenvectors of the transfer matrix, and on which the multiple action of \mathcal{T} is not simple. In fact, the product $\prod_{a=2}^m (A+D)(\xi_a)$ would lead to a sum of 2^{m-1} elementary blocks. This is not very convenient, in particular at large distance m. Therefore, to obtain manageable expressions for such correlation functions, it is of great importance to develop an alternative and compact way to express the multiple action of the transfer matrix on arbitrary states or, in other words, to make an effective re-summation of the corresponding sum of the 2^{m-1} terms. This can be achieved in the following way.

Proposition 3.2 Let κ , x_1, \ldots, x_m and μ_1, \ldots, μ_N be generic parameters. Then the action $\prod_{a=1}^m \mathcal{T}_{\kappa}(x_a) \text{ on a state of the form } \langle 0 | \prod_{j=1}^N C(\mu_j) \text{ can be formally written as}$

$$\langle 0 | \prod_{j=1}^{N} C(\mu_{j}) \prod_{a=1}^{m} \mathcal{T}_{\kappa}(x_{a}) = \frac{1}{N!} \oint_{\Gamma\{x\} \cup \Gamma\{\mu\}} \prod_{j=1}^{N} \frac{dz_{j}}{2\pi i} \cdot \prod_{a=1}^{m} \mathcal{T}_{\kappa}(x_{a} | \{z\}) \cdot \prod_{a=1}^{N} \frac{1}{\mathcal{Y}_{\kappa}(z_{a} | \{z\})} \times \prod_{\substack{j,k=1\\j < k}}^{N} \frac{\sinh(z_{j} - z_{k})}{\sinh(\mu_{j} - \mu_{k})} \cdot \det_{N} \Omega_{\kappa}(\{z\}, \{\mu\} | \{z\}) \cdot \langle 0 | \prod_{j=1}^{N} C(z_{j}), \quad (63)$$

where the integration contour $\Gamma\{x\} \cup \Gamma\{\mu\}$ surrounds the points¹ x_1, \ldots, x_m and μ_1, \ldots, μ_N and does not contain any other pole of the integrand.

One of the simplest applications concerns the generating function of the two-point correlation function of the third components of spin, which is defined as the normalized expectation value $\langle Q_{l,m}^{\kappa} \rangle$ of the operator

$$Q_{l,m}^{\kappa} = \prod_{n=l}^{m} \left(\frac{1+\kappa}{2} + \frac{1-\kappa}{2} \cdot \sigma_n^z \right) = \prod_{j=1}^{l-1} \mathcal{T}(\xi_j) \cdot \prod_{j=l}^{m} \mathcal{T}_{\kappa}(\xi_j) \cdot \prod_{j=1}^{m} \mathcal{T}^{-1}(\xi_j), \tag{64}$$

where $|\psi(\{\lambda\})\rangle$ is an eigenvector of $\mathcal{T}(\mu)$ in the subspace $\mathcal{H}^{(M/2-N)}$. The two-point correlation function of the third components of local spins in the eigenvector $|\psi(\{\lambda\})\rangle$ can be obtained in terms of the second 'lattice derivative' and the second derivative with respect to κ of the generating function $\langle Q_{l,m}^{\kappa} \rangle$ at $\kappa = 1$:

$$\langle \sigma_l^z \sigma_{l+m}^z \rangle = \langle \sigma_l^z \rangle + \langle \sigma_{l+m}^z \rangle - 1 + 2 \frac{\partial^2}{\partial \kappa^2} \langle Q_{l,l+m}^{\kappa} - Q_{l,l+m-1}^{\kappa} - Q_{l+1,l+m}^{\kappa} + Q_{l+1,l+m-1}^{\kappa} \rangle_{\kappa=1}.$$
 (65)

Due to the translational invariance of the correlation functions in the homogeneous model, we will simply consider the expectation value $\langle Q_{1,m}^{\kappa} \rangle$. For any given eigenvector, we obtain the following result:

Theorem 3.1 Let $\{\lambda\}$ be an admissible off-diagonal solution of the system of untwisted Bethe equations, and let us consider the corresponding expectation value $\langle Q_{1,m}^{\kappa} \rangle$ in the inhomogeneous finite XXZ chain. Then there exists $\kappa_0 > 0$ such that, for $|\kappa| < \kappa_0$, the following representations hold:

$$\langle Q_{1,m}^{\kappa} \rangle = \frac{1}{N!} \oint_{\Gamma\{\xi\} \cup \Gamma\{\lambda\}} \prod_{j=1}^{N} \frac{dz_j}{2\pi i} \cdot \prod_{a=1}^{m} \frac{\tau_{\kappa}(\xi_a | \{z\})}{\tau(\xi_a | \{\lambda\})} \cdot \prod_{a=1}^{N} \frac{1}{\mathcal{Y}_{\kappa}(z_a | \{z\})} \times \det_{N} \Omega_{\kappa}(\{z\}, \{\lambda\} | \{z\}) \cdot \frac{\det_{N} \Omega(\{\lambda\}, \{z\} | \{\lambda\})}{\det_{N} \Omega(\{\lambda\}, \{\lambda\} | \{\lambda\})}, \quad (66)$$

The integration contours are such that the only singularities of the integrand which contribute to the integral are the points ξ_1, \ldots, ξ_m and $\lambda_1, \ldots, \lambda_N$.

From this result, we can extract a compact representation for the two-point function of σ^z [79]. Similar expressions exists for other correlation functions of the spin operators, and in particular for the time dependent case [79, 63]. Moreover, this multiple contour integral representation permits to relate two very different ways to compute two point correlation functions of the type, $g_{12} = \langle \omega | \theta_1 \theta_2 | \omega \rangle$, namely,

- (i) to compute the action of local operators on the ground state $\theta_1\theta_2|\omega\rangle = |\tilde{\omega}\rangle$ and then to calculate the resulting scalar product $g_{12} = \langle \omega | \tilde{\omega} \rangle$ as was explain in the previous sections
- (ii) to insert a sum over a complete set of states $|\omega_i\rangle$ (for instance, a complete set of

¹More precisely, for a set of complex variables $\{\nu_1,\ldots,\nu_l\}$, the notation $\Gamma\{\nu\}$ should be understood in the following way: $\Gamma\{\nu\}$ is the boundary of a set of poly-disks $\mathcal{D}_a(r)$ in \mathbb{C}^N , i.e. $\Gamma\{\nu\} = \cup_{a=1}^l \bar{\mathcal{D}}_a(r)$ with $\bar{\mathcal{D}}_a(r) = \{z \in \mathbb{C}^N : |z_k - \nu_a| = r, \quad k = 1,\ldots,N\}$.

eigenvectors of the Hamiltonian) between the local operators θ_1 and θ_2 and to obtain the representation for the correlation function as a sum over matrix elements of local operators,

$$g_{12} = \sum_{i} \langle \omega | \theta_1 | \omega_i \rangle \cdot \langle \omega_i | \theta_2 | \omega \rangle. \tag{67}$$

In fact the above representation as multiple contour integrals contains both expansions. Indeed there is two ways to evaluate the corresponding integrals : either to compute the residues in the poles inside Γ , or to compute the residues in the poles within strips of the width $i\pi$ outside Γ .

The first way leads to a representation of the correlation function $\langle \sigma_1^z \sigma_{m+1}^z \rangle$ in terms of the previously obtained [75] m-multiple sums. Evaluation of the above contour integral in terms of the poles outside the contour Γ gives us the expansion (ii) of the correlation function (i.e. an expansion in terms of matrix elements of σ^z between the ground state and all excited states). This relation holds also for the time dependent case [79, 63].

3.4 Towards the comparison with neutron scattering experiments

In this section, we first briefly review all elements necessary for the computation of the dynamical spin-spin correlation functions of the anisotropic Heisenberg model, following [39, 40] and leading in particular to the successful comparison with neutron scattering experiments, see Fig. 1. We start by giving our notations and discussing the eigenstates in some details. The reference state is taken to be the state with all spins up, $|0\rangle = \bigotimes_{i=1}^{M} |\uparrow\rangle_i$. Since the total magnetization commutes with the Hamiltonian, the Hilbert space separates into subspaces of fixed magnetization, determined from the number of reversed spins N. We take the number of sites M to be even, and $2N \leq M$, the other sector being accessible through a change in the reference state.

Eigenstates in each subspace are completely characterized for $2N \leq M$ by a set of rapidities $\{\lambda_j\}, j=1,...,N$, solution to the Bethe equations

$$\left[\frac{\sinh(\lambda_j + i\zeta/2)}{\sinh(\lambda_j - i\zeta/2)}\right]^M = \prod_{k \neq j}^N \frac{\sinh(\lambda_j - \lambda_k + i\zeta)}{\sinh(\lambda_j - \lambda_k - i\zeta)}, \qquad j = 1, ..., N$$
 (68)

where $\Delta=\cos\zeta$. In view of the periodicity of the sinh function in the complex plane, we can restrict the possible values that the rapidities can take to the strip $-\pi/2 < \mathrm{Im}\lambda \le \pi/2$, or alternately define an extended zone scheme in which λ and $\lambda + i\pi\mathbb{Z}$ are identified.

A more practical version of the Bethe equations is obtained by writing them in logarithmic form,

$$\operatorname{atan}\left[\frac{\tanh(\lambda_j)}{\tan(\zeta/2)}\right] - \frac{1}{M} \sum_{k=1}^{N} \operatorname{atan}\left[\frac{\tanh(\lambda_j - \lambda_k)}{\tan\zeta}\right] = \pi \frac{I_j}{M}.$$
(69)

Here, I_j are distinct half-integers which can be viewed as quantum numbers: each choice of a set $\{I_j\}$, j=1,...,N (with I_j defined $\operatorname{mod}(M)$) uniquely specifies a set of rapidities, and therefore an eigenstate. The energy of a state is given as a function of the rapidities by

$$E = J \sum_{i=1}^{N} \frac{-\sin^2 \zeta}{\cosh 2\lambda_j - \cos \zeta} - h(\frac{M}{2} - N), \tag{70}$$

whereas the momentum has a simple representation in terms of the quantum numbers,

$$q = \sum_{j=1}^{N} i \ln \left[\frac{\sinh(\lambda_j + i\zeta/2)}{\sinh(\lambda_j - i\zeta/2)} \right] = \pi N + \frac{2\pi}{M} \sum_{j=1}^{N} I_j \mod 2\pi.$$
 (71)

The ground state is given by $I_j^0 = -\frac{N+1}{2} + j$, j = 1, ..., N, and all excited states are in principle obtained from the different choices of sets $\{I_j\}$.

To study dynamics, some ingredients have to be added to the Bethe Ansatz: the matrix elements of spin operators between eigenstates (form factors). In terms of form factors for the Fourier-transformed spin operators $S_q^a = \frac{1}{\sqrt{M}} \sum_{j=1}^M e^{iqj} S_j^a$, the structure factor can be written as a sum

$$S^{a\bar{a}}(q,\omega) = 2\pi \sum_{\alpha \neq GS} |\langle GS|S_q^a |\alpha\rangle|^2 \delta(\omega - \omega_\alpha)$$
 (72)

over the whole set of intermediate eigenstates $|\alpha\rangle$ (distinct from the ground state $|GS\rangle$) in a fixed magnetization subspace. Each term in (72) can be obtained [38] as a product of determinants of specific matrices, which are fully determined for given bra and ket eigenstates by a knowledge of the corresponding sets of rapidities. The analytical summation of this series remains for the moment out of reach, but numerically, for chains of length a few hundred sites, quite feasible. Moreover, we know that the correlation functions of the finite chain approach their thermodynamic limit with errors of order $\frac{1}{M}$, hence if M=200 for example the error is usually quite acceptable to make comparison with experiments.

The strategy to follow is now clear. We compute the S^{zz} and S^{-+} structure factors by directly summing the terms on the right-hand side of equation (72) over a judiciously chosen subset of eigenstates. The momentum delta functions are broadened to width $\epsilon \sim 1/M$ using $\delta_{\epsilon}(x) = \frac{1}{\sqrt{\pi}\epsilon}e^{-x^2/\epsilon^2}$ in order to obtain smooth curves. We scan through the eigenstates in the following order. First, we observe that the form factors of the spin operators between the ground state and an eigenstate $\{\lambda\}$ are extremely rapidly decreasing functions of the number of holes that need to be inserted in the configuration of the lowest-energy state (in the same base) in order to obtain the configuration $\{I\}$ corresponding to $\{\lambda\}$. We therefore scan through all bases and configurations for increasing number of holes, starting from one-hole states for S^{zz} , and zero-hole states for S^{-+} . Although the number of possible configurations for fixed base and number of holes is a rapidly increasing function of the number of holes, we find that the total contributions for fixed bases also rapidly decrease for increasing hole numbers. We therefore limit ourselves to states with up to three holes, corresponding to up to six-particle excitations. We can quantify the quality of the present computational method by evaluating the sum rules for the longitudinal and transverse form factors. Namely, by integrating over momentum and frequency, we should saturate the values

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{M} \sum_{q} S^{zz}(q,\omega) = \frac{1}{4} - \langle S^z \rangle^2 = \frac{1}{4} \left[1 - (1 - \frac{2N}{M})^2 \right]$$
 (73)

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{M} \sum_{q} S^{-+}(q,\omega) = \frac{1}{2} - \langle S^z \rangle = \frac{N}{M}.$$
 (74)

In Fig. 2, we plot the longitudinal structure factor as a function of momentum and frequency for anisotropy $\Delta = 0.75$, for four values of the magnetization. Fig. 3 contains the transverse structure factor for the same anisotropy and magnetizations.

For all intermediate states involving strings, we explicitly check that the deviations from the string hypothesis are small. We find in general that states involving strings of length higher that two are admissible solutions to the Bethe equations for high enough magnetizations. At zero field, only two-string states have exponentially small deviations δ , and all higher-string states must be discarded.

The relative contributions to the structure factors from different bases is very much dependent on the system size, the anisotropy, and the magnetization. In general, we find that two- and four-particle contributions are sufficient to saturate well over 90% of the sum rules in all cases, for system sizes up to M=200. Interestingly,

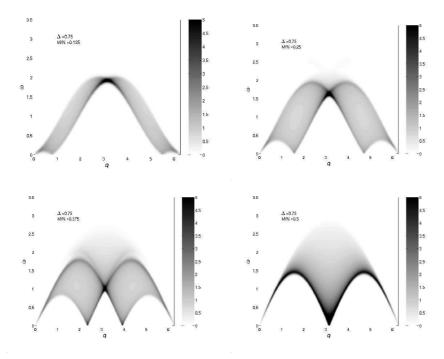


Figure 2: Longitudinal structure factor as a function of momentum q and frequency ω , for $\Delta=0.75$, and N=M/8,M/4,3M/8, and M/2. Here, M=200 and all contributions up to two holes are taken into account. The sum rule is thereby saturated to $98.6\%,\,97.0\%,\,95.4\%$ and 97.8%.

however, we find that string states also contribute noticeably in many cases. For example, in Fig. 4, we plot the zero-field transverse structure factor contributions coming from intermediate states with one string of length two and up to three holes. Around six or seven percent of the weight is accounted for by these states, and similar or somewhat lower figures are found in other cases. Strings of length higher than two do not contribute significantly. For example, we find only around 5.7e-8 % of the sum rule from states with one string of length three, for the longitudinal structure factor for $\Delta=0.25$ at M=N/4 with N=128. For $\Delta=0.75$, we find 6.3e-7 %. For the transverse correlators, the figures are 2.3e-12 % and 3.1e-12 %. Even though these

numbers would increase if we could go to larger system sizes, we do not expect them to ever become numerically significant.

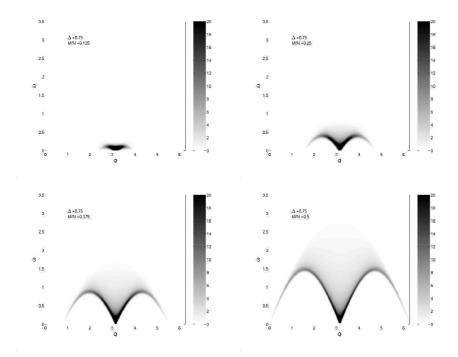


Figure 3: Transverse structure factor as a function of momentum q and frequency ω , for $\Delta=0.75$, and N=M/8, M/4, 3M/8, and M/2. Here, M=200 and all contributions up to two holes are taken into account. The sum rule is thereby saturated to 99.3%, 97.8%, 96.5% and 98.8%.

The imperfect saturation of the sum rules that we obtain in general can be ascribed either to higher states in the hierarchy which are not included in our partial summations, or states that are in principle included, but which are rejected in view of their deviations from the string hypothesis. As the proportion of excluded string states can be rather large (ranging anywhere from zero to fifty percent), we believe the latter explanation to be the correct one. In any case, these results are precise enough to be compared successfully to different data from neutron scattering experiments for several magnetic compounds. From our results covering the whole Brillouin zone and frequency space, it is straightforward to obtain space-time dependent correlation functions by inverse Fourier transform:

$$\langle S_{j+1}^a(t)S_1^{\bar{a}}(0)\rangle_c = \frac{1}{M} \sum_{\alpha \neq GS} |\langle GS|S_{q_\alpha}^a|\alpha\rangle|^2 e^{-iq_\alpha j - i\omega_\alpha t}.$$
 (75)

It is possible to compare these results to known exact results for equal-time correlators at short distance, and to the large-distance asymptotic form obtained from conformal field theory. This comparison can only be made at zero field, where both sets of results are known exactly. The comparison turns out to be extremely good, as can be expected from the high saturation of the sum rules [40].

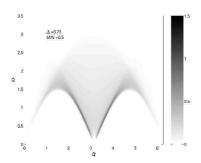


Figure 4: The two-string contributions to the transverse structure factor at zero magnetic field, as a function of momentum q and frequency ω , and for anisotropy 0.75. The density scale has been enhanced as compared to that used in the previous figures. Here, M=200 and contributions up to three holes are taken into account. The sum rule contributions from these states is 6.3 %.

4 Correlation functions: infinite chain

In the thermodynamic limit, $M \to \infty$ and at zero magnetic field, the model exhibits three different regimes depending on the value of Δ [26]. For $\Delta < -1$, the model is ferromagnetic, for $-1 < \Delta < 1$, the model has a non degenerated anti ferromagnetic ground state, and no gap in the spectrum (massless regime), while for $\Delta > 1$, the ground state is twice degenerated with a gap in the spectrum (massive regime). In both cases, the ground state has spin zero. Hence the number of parameters λ in the ground state vectors is equal to half the size M of the chain. For $M \to \infty$, these parameters will be distributed in some continuous interval according to a density function ρ .

4.1 The thermodynamic limit

In this limit, the Bethe equations for the ground state, written in their logarithmic form, become a linear integral equation for the density distribution of these λ 's,

$$\rho_{\text{tot}}(\alpha) + \int_{-\Lambda}^{\Lambda} K(\alpha - \beta) \rho_{\text{tot}}(\beta) \, d\beta = \frac{p'_{0_{\text{tot}}}(\alpha)}{2\pi},\tag{76}$$

where the new real variables α are defined in terms of general spectral parameters λ differently in the two domains. From now on, we only describe the massless regime (see [73] for the other case) $-1 < \Delta < 1$ where $\alpha = \lambda$. The density ρ is defined as the limit of the quantity $\frac{1}{M(\lambda_{j+1}-\lambda_j)}$, and the functions $K(\lambda)$ and $p'_{0_{\text{tot}}}(\lambda)$ are the

derivatives with respect to λ of the functions $-\frac{\theta(\lambda)}{2\pi}$ and $p_{0_{\text{tot}}}(\lambda)$:

$$K(\alpha) = \frac{\sin 2\zeta}{2\pi \sinh(\alpha + i\zeta) \sinh(\alpha - i\zeta)}$$

$$p'_{0}(\alpha) = \frac{\sin \zeta}{\sinh(\alpha + i\frac{\zeta}{2}) \sinh(\alpha - i\frac{\zeta}{2})}$$
for $-1 < \Delta < 1$, with $\zeta = i\eta$, (77)

with
$$p'_{0_{\text{tot}}}(\alpha) = \frac{1}{M} \sum_{i=1}^{M} p'_{0}(\alpha - \beta_{k} - i\frac{\zeta}{2}),$$
 (78)

where $\beta_k = \xi_k$. The integration limit Λ is equal to $+\infty$ for $-1 < \Delta < 1$. The solution for the equation (76) in the homogeneous model where all parameters ξ_k are equal to $\eta/2$, that is the density for the ground state of the Hamiltonian in the thermodynamic limit, is given by the following function [19]:

$$\rho(\alpha) = \frac{1}{2\zeta \cosh(\frac{\pi\alpha}{\zeta})}$$

For technical convenience, we will also use the function,

$$\rho_{\rm tot}(\alpha) = \frac{1}{M} \sum_{i=1}^{M} \rho(\alpha - \beta_k - i\frac{\zeta}{2}).$$

It will be also convenient to consider, without any loss of generality, that the inhomogeneity parameters are contained in the region $-\zeta < \text{Im}\beta_j < 0$. Using these results, for any \mathcal{C}^{∞} function f (π -periodic in the domain $\Delta > 1$), sums over all the values of f at the point α_j , $1 \leq j \leq N$, parameterizing the ground state, can be replaced in the thermodynamic limit by an integral:

$$\frac{1}{M} \sum_{i=1}^{N} f(\alpha_i) = \int_{-\Lambda}^{\Lambda} f(\alpha) \rho_{\text{tot}}(\alpha) d\alpha + O(M^{-1}).$$

Thus, multiple sums obtained in correlation functions will become multiple integrals. Similarly, it is possible to evaluate the behavior of the determinant formulas for the scalar products and the norm of Bethe vectors (and in particular their ratios) in the limit $M \to \infty$.

4.2 Elementary blocks

From the representations as multiple sums of these elementary blocks in the finite chain we can obtain their multiple integral representations in the thermodynamic limit. Let us now consider separately the two regimes of the XXZ model. In the massless regime $\eta = -i\zeta$ is imaginary, the ground state parameters λ are real and the limit of integration is infinity $\Lambda = \infty$. In this case we consider the inhomogeneity parameters ξ_j such that $0 > \text{Im}(\xi_j) > -\zeta$. For the correlation functions in the thermodynamic limit one obtains the following result in this regime:

Proposition 4.1

$$F_m(\{\epsilon_j, \epsilon_j'\}) = \prod_{k < l} \frac{\sinh \frac{\pi}{\zeta} (\xi_k - \xi_l)}{\sinh(\xi_k - \xi_l)} \prod_{j=1}^{s'} \int_{-\infty - i\zeta}^{\infty - i\zeta} \frac{d\lambda_j}{2i\zeta} \prod_{j=s'+1-\infty}^{m} i \frac{d\lambda_j}{2\zeta}$$

$$\prod_{a=1}^{m} \prod_{k=1}^{m} \frac{1}{\sinh \frac{\pi}{\zeta} (\lambda_a - \xi_k)} \prod_{j \in \alpha^-} \left(\prod_{k=1}^{j-1} \sinh(\mu_j - \xi_k - i\zeta) \prod_{k=j+1}^{m} \sinh(\mu_j - \xi_k) \right)$$

$$\prod_{j \in \alpha^+} \left(\prod_{k=1}^{j-1} \sinh(\mu_j' - \xi_k + i\zeta) \prod_{k=j+1}^{m} \sinh(\mu_j' - \xi_k) \right) \prod_{a > b} \frac{\sinh \frac{\pi}{\zeta} (\lambda_a - \lambda_b)}{\sinh(\lambda_a - \lambda_b - i\zeta)},$$

where the parameters of integration are ordered in the following way $\{\lambda_1, \ldots, \lambda_m\} = \{\mu'_{j'_{\max}}, \ldots, \mu'_{j'_{\min}}, \mu_{j_{\min}}, \ldots, \mu_{j_{\max}}\}.$

The homogeneous limit $(\xi_j = -i\zeta/2, \forall j)$ of the correlation function $F_m(\{\epsilon_j, \epsilon'_j\})$ can then be taken in an obvious way. We have obtained similar representations for the massive regime, and also in the presence of a non-zero magnetic field [73]. For zero magnetic field, these results agree exactly with the ones obtained by Jimbo and Miwa in [69], using in particular q-KZ equations. It means that for zero magnetic field, the elementary blocks of correlation functions indeed satisfy q-KZ equations. Recently, more algebraic representations of solutions of the q-KZ equations have been obtained that correspond to the above correlation functions [70, 71]. From the finite chain representation for the two-point function, it is also possible to obtain multiple integral representations for that case as well, in particular for their generating function [75, 76]. They correspond to different huge re-summations and symmetrization of the corresponding elementary blocks, as in the finite chain situation [75]. Moreover, the case of time dependent correlation functions as also been obtained [79, 63]. Finally, let us note that at the free fermion point, all the results presented here lead, in a very elementary way, to already know results [76, 80, 63].

5 Exact and asymptotic results

5.1 Exact results at $\Delta = 1/2$

Up to now, two exact results have been obtained for the case of anisotropy $\Delta=1/2$: the exact value of the emptiness formation probability for arbitrary distance m [77] and the two point function of the third component of spin [85]. These two results follow from the above multiple integral representations for which, due to the determinant structure of the integrand, the corresponding multiple integrals can be separated and hence explicitly computed for this special value of the anisotropy.

5.1.1 The emptiness formation probability

This correlation function $\tau(m)$ (the probability to find in the ground state a ferromagnetic string of length m) is defined as the following expectation value

$$\tau(m) = \langle \psi_g | \prod_{k=1}^m \frac{1 - \sigma_k^z}{2} | \psi_g \rangle, \tag{79}$$

where $|\psi_g\rangle$ denotes the normalized ground state. In the thermodynamic limit $(M \to \infty)$, this quantity can be expressed as a multiple integral with m integrations [68, 69, 37, 38, 73].

Proposition 5.1 For $\Delta = \cos \zeta$, $0 < \zeta < \pi$, $\tau(m) = \lim_{\xi_1, \dots \xi_m \to -\frac{i\zeta}{2}} \tau(m, \{\xi_j\})$, where

$$\tau(m, \{\xi_j\}) = \frac{1}{m!} \int_{-\infty}^{\infty} \frac{Z_m(\{\lambda\}, \{\xi\})}{\prod_{a < b}^{m} \sinh(\xi_a - \xi_b)} \det_m \left(\frac{i}{2\zeta \sinh\frac{\pi}{\zeta}(\lambda_j - \xi_k)}\right) d^m \lambda, \tag{80}$$

$$Z_{m}(\{\lambda\}, \{\xi\}) = \prod_{a=1}^{m} \prod_{b=1}^{m} \frac{\sinh(\lambda_{a} - \xi_{b}) \sinh(\lambda_{a} - \xi_{b} - i\zeta)}{\sinh(\lambda_{a} - \lambda_{b} - i\zeta)} \cdot \frac{\det_{m} \left(\frac{-i \sin \zeta}{\sinh(\lambda_{j} - \xi_{k}) \sinh(\lambda_{j} - \xi_{k} - i\zeta)}\right)}{\prod_{a>b}^{m} \sinh(\xi_{a} - \xi_{b})}.$$
(81)

The proof is given in [75]. Due to the determinant structure of the integrand, the integrals can be separated and computed for the special case $\Delta = \frac{1}{2} (\zeta = \pi/3)$:

Proposition 5.2 Let $\xi_k = \varepsilon_k - i\pi/6$ and $\varepsilon_{ab} = \varepsilon_a - \varepsilon_b$, we obtain,

$$\tau(m, \{\varepsilon_j\}) = \frac{(-1)^{\frac{m^2 - m}{2}}}{2^{m^2}} \prod_{a > b}^{m} \frac{\sinh 3\varepsilon_{ba}}{\sinh \varepsilon_{ba}} \prod_{\substack{a, b = 1 \\ a \neq b}}^{m} \frac{1}{\sinh \varepsilon_{ab}} \cdot \det_{m} \left(\frac{3 \sinh \frac{\varepsilon_{jk}}{2}}{\sinh \frac{3\varepsilon_{jk}}{2}} \right), \quad (82)$$

$$\tau(m) = \left(\frac{1}{2}\right)^{m^2} \prod_{k=0}^{m-1} \frac{(3k+1)!}{(m+k)!}.$$
 (83)

Observe that the quantity $A_m = \prod_{k=0}^{m-1} (3k+1)!/(m+k)!$ is the number of alternating sign matrices of size m. This result was conjectured in [91].

5.1.2 The two point function of σ^z

The two point functions can be obtained, as in the finite chain situation, from a generating function $\langle Q_{\kappa}(m) \rangle$; in the thermodynamic limit, we use the following multiple integral representation [79]:

$$\langle Q_{\kappa}(m) \rangle = \sum_{n=0}^{m} \frac{\kappa^{m-n}}{n!(m-n)!} \oint_{\Gamma\{-i\zeta/2\}} \frac{d^{m}z}{(2\pi i)^{m}} \int_{\mathbb{R}-i\zeta} d^{n}\lambda \int_{\mathbb{R}} d^{m-n}\lambda \cdot \prod_{j=1}^{m} \frac{\varphi^{m}(z_{j})}{\varphi^{m}(\lambda_{j})}$$

$$\prod_{j=1}^{n} \left\{ t(z_{j}, \lambda_{j}) \prod_{k=1}^{m} \frac{\sinh(z_{j} - \lambda_{k} - i\zeta)}{\sinh(z_{j} - z_{k} - i\zeta)} \right\} \prod_{j=n+1}^{m} \left\{ t(\lambda_{j}, z_{j}) \prod_{k=1}^{m} \frac{\sinh(\lambda_{k} - z_{j} - i\zeta)}{\sinh(z_{k} - z_{j} - i\zeta)} \right\}$$

$$\prod_{j=1}^{m} \prod_{k=1}^{m} \frac{\sinh(\lambda_{k} - z_{j} - i\zeta)}{\sinh(\lambda_{k} - \lambda_{j} - i\zeta)} \cdot \det_{m} \left(\frac{i}{2\zeta \sinh \frac{\pi}{\zeta}(\lambda - z)} \right). \tag{84}$$

Here,

$$\Delta = \cos \zeta, \qquad t(z, \lambda) = \frac{-i \sin \zeta}{\sinh(z - \lambda) \sinh(z - \lambda - i\zeta)}, \qquad \varphi(z) = \frac{\sinh(z - i\frac{\zeta}{2})}{\sinh(z + i\frac{\zeta}{2})}, \tag{85}$$

and the integrals over the variables z_j are taken with respect to a closed contour Γ which surrounds the point $-i\zeta/2$ and does not contain any other singularities of the integrand. The equation (84) is valid for the homogeneous XXZ chain with arbitrary $-1 < \Delta < 1$. If we consider the inhomogeneous XXZ model with inhomogeneities ξ_1, \ldots, ξ_m , then one should replace in the representation (84) the function φ^m in the following way:

$$\varphi^m(z) \to \prod_{b=1}^m \frac{\sinh(z - \xi_b - i\zeta)}{\sinh(z - \xi_b)}, \qquad \varphi^{-m}(\lambda) \to \prod_{b=1}^m \frac{\sinh(\lambda - \xi_b)}{\sinh(\lambda - \xi_b - i\zeta)}.$$
(86)

In order to come back to the homogeneous case, one should set $\xi_k = -i\zeta/2$, $k = 1, \ldots, m$ in (86). In the inhomogeneous model, the integration contour Γ surrounds the points ξ_1, \ldots, ξ_m , and the integrals over z_j are therefore equal to the sum of the residues of the integrand in these simple poles. It turns out that again for the special case $\Delta = \frac{1}{2}$ integrals can be separated and computed to give [85]:

Proposition 5.3

$$\langle Q_{\kappa}(m) \rangle = \frac{3^m}{2^{m^2}} \prod_{a>b}^m \frac{\sinh 3(\xi_a - \xi_b)}{\sinh^3(\xi_a - \xi_b)} \sum_{n=0}^m \kappa^{m-n} \sum_{\substack{\{\xi\} = \{\xi_{\gamma_+}\} \cup \{\xi_{\gamma_-}\}\\ |\gamma_+| = n}} \det \hat{\Phi}^{(n)}$$

$$\times \prod_{a \in \gamma_+} \prod_{b \in \gamma_-} \frac{\sinh(\xi_b - \xi_a - \frac{i\pi}{3}) \sinh(\xi_a - \xi_b)}{\sinh^2(\xi_b - \xi_a + \frac{i\pi}{3})},$$

$$\hat{\Phi}^{(n)}(\{\xi_{\gamma_{+}}\},\{\xi_{\gamma_{-}}\}) = \begin{pmatrix} \Phi(\xi_{j} - \xi_{k}) & \Phi(\xi_{j} - \xi_{k} - \frac{i\pi}{3}) \\ \hline \Phi(\xi_{j} - \xi_{k} + \frac{i\pi}{3}) & \Phi(\xi_{j} - \xi_{k}) \end{pmatrix}, \ \Phi(x) = \frac{\sinh\frac{x}{2}}{\sinh\frac{3x}{2}}.$$

Here the sum is taken with respect to all partitions of the set $\{\xi\}$ into two disjoint subsets $\{\xi_{\gamma_+}\}\cup\{\xi_{\gamma_-}\}$ of cardinality n and m-n respectively. The first n lines and columns of the matrix $\hat{\Phi}^{(n)}$ are associated with the parameters $\xi \in \{\xi_{\gamma_+}\}$. The remaining lines and columns are associated with $\xi \in \{\xi_{\gamma_-}\}$.

Thus, we have obtained an explicit answer for the generating function $\langle Q_{\kappa}(m) \rangle$ of the inhomogeneous XXZ model. It is also possible to check that the above sum over partitions remains indeed finite in the homogeneous limit $\xi_k \to 0$. Finally, for small distances it is possible to compute the above expressions explicitly as polynomial functions of the variable κ of degree m. Interestingly, it turns out that all coefficients are integer numbers divided by 2^{m^2} [85], meaning a possible combinatorial interpretation of these numbers as for the emptiness formation probability computed in the previous section.

5.2 Asymptotic results

An important issue is the analysis of the multiple integral representations of correlation functions for large distances. There it means analyzing asymptotic behavior of m-fold integrals for m large. An interesting example to study in this respect is provided

by the emptiness formation probability. This correlation function reduces to a single elementary block. Moreover, we already described its exact value for an anisotropy $\Delta = \frac{1}{2}$ in the previous section. In fact, it is possible to obtain the asymptotic behavior of $\tau(m)$ using the saddle-point method for arbitrary values of the anisotropy $\Delta > -1$. This was performed for the first time in [76] in the case of free fermions ($\Delta = 0$), but it can be applied to the general case as well. We present here the results in the massless and massive regimes [78, 63].

To apply the saddle-point method to the emptiness formation probability, it is convenient to express its integral representation in the following form:

$$\tau(m) = \int_{\mathcal{D}} d^m \lambda \ G_m(\{\lambda\}) \ e^{m^2 S_m(\{\lambda\})}, \tag{87}$$

with

$$S_{m}(\{\lambda\}) = -\frac{1}{m^{2}} \sum_{a>b}^{m} \log[\sinh(\lambda_{a} - \lambda_{b} + \eta) \sinh(\lambda_{a} - \lambda_{b} - \eta)]$$

$$+ \frac{1}{m} \sum_{a=1}^{m} \log[\sinh(\lambda_{a} + \eta/2) \sinh(\lambda_{a} - \eta/2)]$$

$$+ \frac{1}{m^{2}} \lim_{\xi_{1} \dots \xi_{m} \to \eta/2} \log\left[\left(\frac{-2i\pi}{\sinh\eta}\right)^{m} \frac{\left(\det\rho(\lambda_{j}, \xi_{k})\right)^{2}}{\prod_{a \neq b} \sinh(\xi_{a} - \xi_{b})}\right]$$
(88)

and

$$G_m(\{\lambda\}) = \lim_{\xi_1 \dots \xi_m \to \eta/2} \frac{\det_m \left[\frac{i}{2\pi} t(\lambda_j, \xi_k) \right]}{\det_m \rho(\lambda_j, \xi_k)}.$$
 (89)

In (87), the integration domain \mathcal{D} is such that the variable of integration $\lambda_1, \ldots, \lambda_m$ are ordered in the interval $\mathcal{C} = [-\Lambda_h, \Lambda_h]$ (i.e. $-\Lambda_h < \lambda_1 < \cdots < \lambda_m < \Lambda_h$ in the massless case, and $-i\Lambda_h < i\lambda_1 < \cdots < i\lambda_m < i\Lambda_h$ in the massive case).

The main problem in the saddle point analysis is that, a priori, we do not know any asymptotic equivalent of the quantity $G_m(\lambda)$ when $m \to \infty$. Nevertheless, in the case of zero magnetic field, it is still possible to compute the asymptotic behavior of (87) in the leading order, provided we make the following hypothesis: we assume that the integrand of (87) admits a maximum for a certain value $\lambda'_1, \ldots, \lambda'_m$ of the integration variables $\lambda_1, \ldots, \lambda_m$, that, for large m, the distribution of these parameters $\lambda'_1, \ldots, \lambda'_m$ can be described by a density function $\rho_s(\lambda')$ of the form

$$\rho_s(\lambda_j') = \lim_{m \to \infty} \frac{1}{m(\lambda_{j+1}' - \lambda_j')},\tag{90}$$

on the symmetric interval $[-\Lambda, \Lambda]$ and that, at the leading order in m, we can replace the sums over the set of parameters $\{\lambda'\}$ by integrals weighted with the density $\rho_s(\lambda')$.

First, it is easy to determine the maximum of the function $S_m(\{\lambda\})$. Indeed, let $\{\tilde{\lambda}\}$ be solution of the system

$$\partial_{\lambda_j} S_m(\{\tilde{\lambda}\}) = 0, \qquad 1 \le j \le m. \tag{91}$$

In the limit $m \to \infty$, if we suppose again that the parameters $\tilde{\lambda}_1, \dots, \tilde{\lambda}_m$ become distributed according to a certain density $\tilde{\rho}_s(\lambda)$ and that sums over the $\tilde{\lambda}_j$ become

integrals over this density, the system (91) turns again into a single integral equation for $\tilde{\rho}_s$, that can be solved explicitly in the case of zero magnetic field. It gives the maximum of $S_m(\{\lambda\})$ when $m \to \infty^2$.

The second step is to show that the factor $G_m(\{\lambda\})$ gives always a negligible contribution compared to $S_m(\{\tilde{\lambda}\})$ at this order in m, at least for any distribution of the variables λ_j satisfying the previous hypothesis of regularity. We obtain,

$$\lim_{m \to \infty} \frac{1}{m^2} \log G_m(\{\lambda\}) = 0 \tag{92}$$

for any distribution of $\{\lambda\}$ with good properties of regularity, in particular for the saddle point. This means that, at the main order in m, the factor $G_m(\{\lambda\})$ does not contribute to the value of the maximum of the integrand.

Finally we obtain the following result concerning the asymptotic behaviour of $\tau(m)$ for $m \to \infty$ (see [78, 63]):

$$S^{(0)}(\Delta) = \lim_{m \to \infty} \frac{\log \tau(m)}{m^2},\tag{93}$$

$$= -\frac{\zeta}{2} - \sum_{n=1}^{\infty} \frac{e^{-n\zeta}}{n} \frac{\sinh(n\zeta)}{\cosh(2n\zeta)}, \qquad (\Delta = \cosh \zeta > 1), \qquad (94)$$

$$= \log \frac{\pi}{\zeta} + \frac{1}{2} \int_{\mathbb{R}-i0} \frac{d\omega}{\omega} \frac{\sinh \frac{\omega}{2} (\pi - \zeta) \cosh^2 \frac{\omega \zeta}{2}}{\sinh \frac{\pi \omega}{2} \sinh \frac{\omega \zeta}{2} \cosh \omega \zeta}, \quad (-1 < \Delta = \cos \zeta < 1). \quad (95)$$

It coincides with the exact known results obtained in [92, 76] at the free fermion point and in [91, 77] at $\Delta=1/2$, and is in agreement with the expected (infinite) value in the Ising limit. Similar techniques can be applied to the two point function. However, the result that has been extracted so far is only the absence of the gaussian term. Unfortunately, we do not know up to now how to extract the expected power law corrections to the gaussian behavior from this saddle point analysis. More powerful methods will certainly be needed to go further.

5.3 Asymptotic behavior of the two-point functions

The long-distance asymptotic behavior of physical correlation functions, such as the two-point functions, have attracted long-standing interest. In the case of the XXZ model, some predictions were made already a long time ago. These predictions are confirmed by the numerical sum over the exact form factors that we performed for the XXZ model in the disordered regime [40].

In the massive regime ($\Delta > 1$), spin-spin correlation functions are expected to decay exponentially with the distance and the exact value of the correlation length was proposed in [94]. For the XXZ chain in the massless regime ($-1 < \Delta \le 1$), zero temperature is a critical point and the correlation length becomes infinite in units of the lattice spacing. The leading long-distance effects can be predicted by conformal field theory and the correlation functions are expected to decay as a power of the

²At this main order in m, there exists a unique solution of the integral equation for $\tilde{\rho}_s$, and we know it corresponds to a maximum because $S_m(\{\lambda\}) \to -\infty$ on the boundary of \mathcal{D} .

distance. In particular, one expects that, at the leading order,

$$\langle \sigma_j^x \sigma_{j+n}^x \rangle = (-1)^n \frac{A}{n^{\pi-\zeta}} + \cdots,$$
 (96)

$$\langle \sigma_j^x \sigma_{j+n}^x \rangle = (-1)^n \frac{A}{n^{\pi-\zeta}} + \cdots,$$

$$\langle \sigma_j^z \sigma_{j+n}^z \rangle = -\frac{1}{\pi(\pi-\zeta)} \frac{1}{n^2} + (-1)^n \frac{A_z}{n^{\frac{\pi}{\pi-\zeta}}} + \cdots.$$

$$(96)$$

A conjecture for the non-universal correlation amplitudes A and A_z can be found in [95, 96, 97]. The exact value of the critical exponents in (96)-(97) was proposed for the first time in [98].

However, there does not exist at the moment any direct derivation of these predictions from the exact expressions of the correlation functions on the lattice. In the last subsection we have shown how to determine, at least in the main order, the asymptotic behavior of the emptiness formation probability using the saddle-point method. We could expect to be able to apply the same technique to the new multiple integral representation of the two-point function.

In particular, one can notice immediately that each term of the representation of the generating functional $\langle Q_{1,m}^{\kappa} \rangle$ has a structure very similar to the one for the emptiness formation probability. Indeed, it is possible to apply to the whole sum a slight modification of the saddle-point technique presented here. It shows that, as it should be, there is no contribution of order $\exp(\alpha m^2)$ when $m \to \infty$.

However, to obtain the precise asymptotic behavior of the two-point function, one should be able to analyze sub-leading corrections to this saddle-point method, which is technically quite difficult. It is not obvious in particular from these expressions that, in the massless regime, the leading asymptotic behavior of the two-point function is only of power-law order.

It is also quite interesting (and relevant experimentally) to consider other lattice models such as spin chains with magnetic or non magnetic impurities [99, 100, 101] or models with electrons (carrying both spin and charge) like the Hubbard model and to compute in particular their transport properties.

Conclusion and perspectives

In this article, we have reviewed recent results concerning the computation of correlation functions in the XXZ chain by the methods of the inverse scattering problem and the algebraic Bethe ansatz. In conclusion, we would like to discuss some perspectives and problems to be solved.

One of the most interesting open problems is to prove the conformal field theory predictions [98, 93] concerning the asymptotic behavior of the correlation functions. This is certainly a very important issue not only for physical applications but also from a theoretical view point. Moreover, it also would open the route towards the generalization of the methods presented here to quantum integrable models of field theory. We have seen that in particular cases, the multiple integral representations enable for a preliminary asymptotic analysis. Nevertheless, this problem remains one of the main challenges in the topics that have been described in this article.

A possible way to solve this problem would be to find the thermodynamic limit of the master equations (like the one obtained for the two point correlation functions). It is natural to expect that, in this limit, one should obtain a representation for these correlation functions in terms of a functional integral, which could eventually be estimated for large time and distance.

Note that the master equation shows a direct analytic relation between the multiple integral representations and the form factor expansions for the correlation functions. It seems likely that similar representations exist for other models solvable by algebraic Bethe ansatz. It would be in particular very interesting to obtain an analogue of this master equation in the case of the field theory models, which could provide an analytic link between short distance and long distance expansions of their correlation functions. Other models of interest include models with magnetic [99] or non magnetic impurities, meaning different integrable boundary conditions [100, 101], and also the Hubbard model the transport properties of which have high experimental interest, see e.g. [102] and references therein.

Acknowledgments

It is a great pleasure to thank N. Kitanine, N. A. Slavnov and V. Terras for their longstanding collaboration on the difficult but exiting topics presented here, and J.-S. Caux for his energy and skills that make our collaboration successful in comparing Bethe ansatz results to actual neutron scattering experiments.

References

- [1] F. Bloch, On the magnetic scattering of neutrons, Phys. Rev. **50** (1936), 259–260.
- [2] J. S. Schwinger, On the magnetic scattering of neutrons, Phys. Rev. 51 (1937), 544-552.
- [3] O. Halpern and M. H. Johnson, On the magnetic scattering of neutrons, Phys. Rev. 55 (1938), 898–923.
- [4] L. Van Hove, Correlations in space and time and Born approximation scattering in systems of interacting particles, Phys. Rev. 95 (1954), 249–262.
- [5] L. Van Hove, Time dependent correlations between spins and neutron scattering in ferromagnatic crystals, Phys. Rev. 95 (1954), 1374–1384.
- [6] W. Marshall and S. W. Lovesey, *Theory of thermal neutron scattering*, Academic Press, Oxford, 1971.
- [7] R. Balescu, Equilibrium and nonequilibrium statistical mechanics, J. Wiley, New York, 1975.
- [8] M. Steiner, J. Villain, and C. G. Windsor, Theoretical and experimental studies on one-dimensional magnetic systems, Adv. Phys. 25 (1976), 87–209.
- [9] S. K. Satija, J. D. Axe, G. Shirane, H. Yoshizawa, and K. Hirakawa, Neutron scattering study of spin waves in one-dimensional antiferromagnet KCuF3, Phys. Rev. B 21 (1980), 2001–2007.
- [10] S. E. Nagler, D. A. Tennant, R. A. Cowley, T. G. Perring, and S. K. Satija, Spin dynamics in the quantum antiferromagnetic chain compound KCuF3, Phys. Rev. B 44 (1991), 12361-12368.

- [11] D. A. Tennant, R. A. Cowley, S. E. Nagler, and A. M. Tsvelik, Measurement of the spin-excitation continuum in one-dimensional KCuF3 using neutron scattering, Phys. Rev. B 52 (1995), 13368–13380.
- [12] D. A. Tennant, S. E. Nagler D. Welz, G. Shirane, and K. Yamada, Effects of coupling between chains on the magnetic excitation spectrum of KCuF3, Phys. Rev. B 52 (1995), 13381–13389.
- [13] H. A. Jahn and E. Teller, Stability of polyatomic molecules in degenerate electronic states. I. Orbital degeneracy, Proc. Roy. Soc. London Ser. A 161 (1937), 220–235.
- [14] W. Heisenberg, Zur Theorie der Ferromagnetismus, Z. Phys. 49 (1928), 619.
- [15] H. Bethe, Zur Theorie der Metalle I. Eigenwerte und Eigenfunktionen Atomkete,Z. Phys. 71 (1931), 205.
- [16] L. Hulthen, Über das Austauschproblem eines Kristalls, Arkiv. Mat. Astron. Fys. 26 A(11) (1938), 1–106.
- [17] R. Orbach, Linear antiferromagnetic chain with anisotropic coupling, Phys. Rev. 112 (1958), 309.
- [18] L. R. Walker, Antiferromagnetic linear chain, Phys. Rev. 116 (1959), 1089.
- [19] C. N. Yang and C. P. Yang, One-dimensional chain of anisotropic spin-spin interactions. I. Proof of Bethe's hypothesis for ground state in a finite system, Phys. Rev. 150 (1966), 321.
- [20] C. N. Yang and C. P. Yang, One-dimensional chain of anisotropic spin-spin interactions. II. Properties of the ground state energy per lattice site for an infinite system, Phys. Rev. 150 (1966), 327.
- [21] C.-N. Yang, Some exact results for the many body problems in one dimension with repulsive delta function interaction, Phys. Rev. Lett. 19 (1967), 1312–1314.
- [22] E. H. Lieb and D. C. Mattis, Mathematical Physics in One Dimension (Academic Press, New-York, 1966).
- [23] L. D. Faddeev, E. K. Sklyanin, and L. A. Takhtajan, Quantum inverse problem method I, Theor. Math. Phys. 40 (1980), 688.
- [24] L. A. Takhtajan and L. D. Faddeev, The Quantum method of the inverse problem and the Heisenberg XYZ model, Russ. Math. Surveys 34 (1979), 11.
- [25] H. B. Thacker, Exact integrability in quantum field theory and statistical systems, Rev. Mod. Phys. 53 (1981), 253.
- [26] R. Baxter, Exactly solved models in statistical mechanics, Academic Press, London (1982).
- [27] M. Gaudin, La fonction d'onde de Bethe, Masson, 1983.
- [28] P. P. Kulish, N. Yu. Reshetikhin, and E. K. Sklyanin, Yang-Baxter equation and representation theory I, Lett. Math. Phys. 5 (1981), 393–403.

- [29] P. P. Kulish and N. Yu. Reshetikhin, Quantum linear problem for the sine-Gordon equation and higher representations, Zap. Nauch. Sem. LOMI 101 (1981), 101–110, Translation in J. Sov. Math. 23 (1983), 2435-41.
- [30] P. P. Kulish and N. Yu. Reshetikhin, Gl₃-invariant solutions of the Yang-Baxter equation and associated quantum systems, J. Sov. Math. 34 (1986), 1948–1971, translated from Zap. Nauch. Sem. LOMI 120 (1982), 92–121.
- [31] P. P. Kulish and E. K. Sklyanin, Quantum spectral transform method. Recent developments, Lectures Notes in Physics 151 (1982), 61–119.
- [32] M. Jimbo, A q-difference analogue of U(g) and the Yang-Baxter equation, Lett. Math. Phys. **10** (1985), 63–69.
- [33] M. Jimbo, A q-analogue of U(gl(N+1)), Hecke algebra, and the Yang-Baxter equation, Lett. Math. Phys. 11 (1986), 247–252.
- [34] V. G. Drinfeld, Hopf algebras and the quantum Yang-Baxter equation, Soviet Math. Dokl. **32(1)** (1985), 254–258.
- [35] V. G. Drinfel'd, Quantum groups, In the proceedings of the ICM 1986, Berkeley, USA, 1986, AMS, (1987).
- [36] O. Foda, M. Jimbo, T. Miwa, K. Miki, and A. Nakayashiki. Vertex operators in solvable lattice models, J. Math. Phys. 35 (1994), 1346.
- [37] M. Jimbo and T. Miwa, Algebraic analysis of solvable lattice models, AMS, Providence, RI (1995).
- [38] N. Kitanine, J. M. Maillet, and V. Terras, Form Factors of the XXZ Heisenberg spin-1/2 finite chain, Nucl. Phys. **B554** (1999), 647–678.
- [39] J.-S. Caux and J. M. Maillet, Computation of dynamical correlation functions of Heisenberg chains in a field, Phys. Rev. Lett. 95 (2005), 077201.
- [40] J.-S. Caux, R. Hagemans, and J. M. Maillet, Computation of dynamical correlation functions of Heisenberg chains: the gapless anysotropic regime, J. Stat. Mech., P09003 (2005).
- [41] N. Andrei, K. Furuya, and J. Lowenstein, Solution of the Kondo problem, Rev. Mod. Phys. 55 (1983), 331–402.
- [42] A. M. Tvselik and P. B. Wiegmann, Exact results in the theory of magnetic alloys, Adv. Phys. 32 (1983), 453–713.
- [43] I. Affleck, in "Fields, strings and critical phenomena", Les Houches Lectures 1988, North-Holland, (1990).
- [44] L. D. Faddeev and G. P. Korchemsky, High energy QCD as a completely integrable model, Phys. Lett. B 342 (1995), 311–322.
- [45] J. A. Minahan and K. Zarembo, The Bethe-ansatz for N=4 super Yang-Mills, JHEP, 013 (2003).
- [46] G. Arutyunov, S. Frolov, and M. Staudacher, Bethe ansatz for quantum strings, JHEP, 016 (2004).

- [47] W. Lenz, Beitrag zum Verständnis der magnetischen Erscheinungen in festen Körpern, Zeit. Phys. 21 (1920), 613–615.
- [48] E. Ising, Beitrag zur Theorie des Ferromagnetismus, Zeit. Phys. 31 (1925), 253–258.
- [49] H. A. Kramers and G. H. Wannier, Statistics of the Two-Dimensional Ferromagnet Part I, Phys. Rev. 60 (1941), 252–262.
- [50] H. A. Kramers and G. H. Wannier, Statistics of the Two-Dimensional Ferromagnet Part II, Phys. Rev. 60 (1941), 263–277.
- [51] L. Onsager, Crystal statistics I: A two-dimensional model with an orderdisorder transition, Phys. Rev. 65 (1944), 117–149.
- [52] B. Kaufman, Crystal Statistics. II. Partition Function Evaluated by Spinor Analysis, Phys. Rev. 76 (1949), 1232–1243.
- [53] C. N. Yang, The Spontaneous Magnetization of a Two-Dimensional Ising Model, Phys. Rev. 85 (1952), 808–816.
- [54] L. D. Faddeev and L. Takhtajan, *Hamiltonian methods in the theory of solitons*, Springer Verlag (1986).
- [55] O. Babelon, D. Bernard and M. Talon *Introduction to classical integrable systems*, Cambridge Univ. Press, (2003).
- [56] E. Lieb, T. Schultz, and D. Mattis, Two soluble models of an antiferromagnetic chain, Ann. Phys. 16 (1961), 407–466.
- [57] B. M. McCoy, Spin correlation functions of the XY model, Phys. Rev. 173 (1968), 531–541.
- [58] T. T. Wu, B. M. McCoy, C. A. Tracy, and E. Barouch, Spin-spin correlation functions of the two-dimensional Ising model: exact theory in the scaling region, Phys. Rev. B 13 (1976), 316–374.
- [59] B. M. McCoy, C. A. Tracy, and T. T. Wu, Two-Dimensional Ising Model as an Exactly Solvable Relativistic Quantum Field Theory: Explicit Formulas for n-Point Functions, Phys. Rev. Lett. 38 (1977), 793–796.
- [60] M. Sato, T. Miwa, and M. Jimbo, Holonomic quantum fields, IV Publ. Res. Inst. Math. Sci. IV Publ. Res. Inst. Math. Sci. 16 (1980), 531–584, 15 (1979), 871–972, 15 (1979), 577–629, 15 (1979), 201–278, 14(1978), 223–267.
- [61] V. E. Korepin, N. Bogoliugov, and A. G. Izergin, Quantum inverse scattering method and correlation functions, Cambridge University Press, Cambridge (1993).
- [62] H. Boos, M. Jimbo, T. Miwa, F. Smirnov, and Y. Takeyama, Algebraic representation of correlation functions in integrable spin chains, hep-th/0601132.
- [63] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, On the algebraic Bethe ansatz approach to the correlation functions of the XXZ spin-1/2 Heisenberg chain, in "Solvable Lattice Models 2004 - Recent Progress on Solvable Lattice Models", RIMS, Kyoto, Kokyuroku, No.1480 (2006) 14, hep-th/0505006.

- [64] L. D. Faddeev, How Algebraic Bethe Ansatz works for integrable model, Les Houches School of Physics: Relativistic gravitation and gravitational radiation (1995), 149–219.
- [65] A. G. Izergin and V. E. Korepin, The quantum inverse scattering method approach to correlation functions, Commun. Math. Phys. 94 (1984), 67–92.
- [66] A. G. Izergin and V. E. Korepin, Correlation functions for the Heisenberg XXZantiferromagnet, Commun. Math. Phys. 99 (1985), 271–302.
- [67] F. H. L. Eßler, H. Frahm, A. G. Izergin, and V. E. Korepin, Determinant representation for correlation functions of spin 1/2 XXX and XXZ Heisenberg magnets, Commun. Math. Phys. 174 (1995), 191–214.
- [68] M. Jimbo, K. Miki, T. Miwa, and A. Nakayashiki, Correlation functions of the XXZ model for $\Delta < -1$, Phys. Lett. A168 (1992), 256–263.
- [69] M. Jimbo and T. Miwa, Quantum KZ equation with |q| = 1 and correlation functions of the XXZ model in the gapless regime, J. Phys. **A29** (1996), 2923–2958.
- [70] H. Boos, M. Jimbo, T. Miwa, F. Smirnov, and Y. Takeyama, A recursion formula for the correlation functions of an inhomogeneous XXX model, Algebra and analysis 17 (2005), 115–159.
- [71] H. Boos, M. Jimbo, T. Miwa, F. Smirnov, and Y. Takeyama, *Reduced qKZ* equation and correlation functions of the XXZ model, Commun. Math. Phys. **261** (2006), 245–276.
- [72] H. Boos, M. Jimbo, T. Miwa, F. Smirnov, and Y. Takeyama, Traces on the Sklyanin algebra and correlation functions of the eight-vertex model, J. Phys. A38 (2005), 7629–7660.
- [73] N. Kitanine, J. M. Maillet, and V. Terras, Correlation functions of the XXZ Heisemberg spin-1/2 chain in a magnetic field, Nucl. Phys. B567 (2000), 554–582.
- [74] J. M. Maillet and V. Terras, On the quantum inverse scattering problem, Nucl. Phys. B575 (2000), 627–644.
- [75] N. Kitanine, J. M. Maillet, N. Slavnov and V. Terras, Spin-spin correlation functions of the XXZ-1/2 Heisenberg chain in a magnetic field, Nucl. Phys. B 641 (2002), 487–518.
- [76] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, Correlation functions of the XXZ spin-1/2 Heisenberg chain at the free Fermion point from their multiple integral representations, Nucl. Phys. B 642 (2002), 433–455.
- [77] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, *Emptiness formation probability of the XXZ spin-1/2 Heisenberg chain at Delta = 1/2*, J. Phys. A **35** (2002), L385.
- [78] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, Large distance asymptotic behaviour of the emptiness formation probability of the XXZ spin-1/2 Heisenberg chain, J.Phys. A **35** (2002), L753.

- [79] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, Master equation for spin-spin correlation functions of the XXZ chain, Nucl. Phys. B 712 [FS] (2005), 600.
- [80] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, *Dynamical correlation functions of the XXZ spin-1/2 chain*, Nucl. Phys. B **729** [FS] (2005), 558.
- [81] F. Göhmann, A. Klümper, and A. Seel, Integral representation of the density matrix of the XXZ chain at finite temperatures, J. Phys. A 38 (2005), 1833–1842.
- [82] V. E. Korepin, Calculation of norms of Bethe wave functions, Commun. Math. Phys. 86 (1982), 391–418.
- [83] N. A. Slavnov, Calculation of scalar products of wave functions and form factors in the framework of the algebraic Bethe Ansatz, Theor. Math. Phys. 79 (1989), 502.
- [84] J. M. Maillet and J. Sánchez de Santos, Drinfel'd twists and algebraic Bethe ansatz, Amer. Math. Soc. Transl. 201 (2000), 137–178.
- [85] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, Exact results for the sigma-z two-point function of the XXZ chain at Delta=1/2, J. Stat. Mech. (2005), L09002.
- [86] N. Kitanine, J. M. Maillet, N. A. Slavnov, and V. Terras, On the spin-spin correlation functions of the XXZ spin-1/2 infinite chain, J. Phys. A: Math. Gen. 38 (2005), 74417460.
- [87] R. G. Pereira, J. Sirker, J. -S. Caux, R. Hagemans, J. M. Maillet, S. R. White, and I. Affleck, Dynamical Spin Structure Factor for the Anisotropic Spin-1/2 Heisenberg Chain, Phys. Rev. Lett. 96 (2006), 257202.
- [88] V. Tarasov and A. Varchenko, Completeness of Bethe vectors and difference equations with regular singular points, Int.Math.Res.Notices 13 (1996), 637.
- [89] A. G. Izergin, Partition function of the six-vertex model in a finite volume, Sov. Phys. Dokl. 32 (1987), 878.
- [90] M. Gaudin, B. M. Mc Coy and T. T. Wu, Normalization sum for the Bethe's hypothesis wave functions of the Heisenberg-Ising model, Phys. Rev. D 23 (1981), 417.
- [91] A. V. Razumov and Y. G. Stroganov, Spin chains and combinatorics, J. Phys. A 34 (2001), 3185.
- [92] M. Shiroishi, M. Takahashi, and Y. Nishiyama, Emptiness Formation Probability for the One-Dimensional Isotropic XY Model, J. Phys. Soc. Jap. 70 (2001), 3535.
- [93] A. A. Belavin, A. M. Polyakov, and A. B. Zamolodchikov, Infinite conformal symmetry in two-dimensional quantum field theory, Nucl. Phys. B 241 (1984), 333.
- [94] J. D. Johnson, S. Krinsky, and B. M. McCoy, Vertical-Arrow Correlation Length in the Eight-Vertex Model and the Low-Lying Excitations of the XYZ Hamiltonian, Phys. Rev. A 8 (1973), 2526.

- [95] S. Lukyanov and A. Zamolodchikov, Exact expectation values of local fields in the quantum sine-Gordon model, Nucl. Phys. B 493 (1997), 571.
- [96] S. Lukyanov, Correlation amplitude for the XXZ spin chain in the disordered regime, Phys. Rev. B **59** (1999), 11163.
- [97] S. Lukyanov and V. Terras, Long-distance asymptotics of spin-spin correlation functions for the XXZ spin chain, Nucl. Phys. B **654** (2003), 323.
- [98] A. Luther and I. Peschel, Calculation of critical exponents in two dimensions from quantum field theory in one dimension, Phys. Rev. B 12 (1975), 3908.
- [99] O. Castro Alvaredo and J. M. Maillet Form factors of integrable Heisenberg (higher) spin chains, arXiv:hep-th/0702186.
- [100] N. Kitanine, K. Kozlowski, J. M. Maillet, G. Niccoli, N. A. Slavnov, and V. Terras, *Correlation functions of open Heisenberg chain I*, to appear.
- [101] N. Kitanine, K. Kozlowski, J. M. Maillet, G. Niccoli, N. A. Slavnov, and V. Terras, *Correlation functions of open Heisenberg chain II*, to appear.
- [102] F. H. L. Essler, H. Frahm, F. Goehmann, A. Klumper, and V. E. Korepin, *The One-Dimensional Hubbard Model*, Cambridge Univ. Press (2005).