UNIVERSITY OF CRETE

DOCTORAL THESIS

Aspects of the dynamics of the one-dimensional XXZ Heisenberg spin chain

Author:
Alexander Pavlis

Supervisor:
Prof. Xenophon Zotos

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Contents

Chapter 1

From Canal Waves to Quantum Magnetism

Edinburgh, August 1834.

I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel [1].

The weird effect that ship designer John Scott Russell described in his notes is what is now known as a *soliton*-a localized non-linear wave that maintains its shape while traveling at a constant velocity.[1]

The corresponding wave equation which admits such solutions is the Korteweg-de Vries (KdV) equation, a non-linear non-dispersive partial differential equation. Many years after the discovery of the KdV equation it was realized by R.M. Miura C.S. Gardner and M.D. Kruskal [2] that this equation has infinitely many integrals of motion which can be given explicitly. This important result was the first connection between the well known Liouville integrability in Hamiltonian systems and classical non-linear field theories. Shortly after this discovery, many advances like the Lax Pair developed

[1] Solitons have played a crucial role to the development of modern physics, from particle physics and cosmology with the prediction of magnetic monopoles and the skyrme model to mesoscopic phenomena in magnetic films and superconductors.

FIGURE 1.1: In vivo experiment demonstrating a soliton wave. It was conducted at Herriot-Watt university in 1995.

by P. Lax [3] and the solution of the non-linear Schrödinger equation [4] contributed to the development of what is known as classical inverse scattering as a method to solve classical integrable field theories. Almost immediately with the development of the classical inverse scattering the Leningrand school developed the quantum inverse scattering method, practically what is nowadays known as *Algebraic Bethe Ansatz* (ABA). ABA elegantly exploits the infinite symmetries of the system in order to derive the spectrum of the Hamiltonian and serves as an alternative and if applicable, equivalent method to the one that H. Bethe developed based on symmetry arguments in his effort to derive the spectrum of the one-dimensional Heisenberg spin chain. However, although the two methods are meant to do the same job the ABA gained considerable attention when V. Korepin was able to prove Gaudin's conjecture [5] about the normalization of the Bethe wavefunctions and N. Kitanine, J.M. Maillet, V. Terras where able to calculate matrix elements for relatively large spin chains [6] bypassing the exact diagonalization method in which calculations where restricted for very small number of spin sites approximately $N \simeq 12$. Indeed, this method illuminated the path towards many advances in the field of integrable systems and their connection with experiments [7, 8, 9, 10, 11, 12, 13, 14, 15].

Amazingly, the structure of Integrability is inherently connected with progress in the field of strongly correlated systems and specifically with the development of the theory of quantum magnetism. Quantum magnetism was intially developed by E. Ising [16] and H. Bethe [17] when they used one-dimensional models as toy models in order to simulate magnetic materials. In particular, the cornerstone of this class of models is the so-called Heisenberg model discovered by W. Heisenberg (and almost simultaneously by P.M. Dirac). The Heisenberg model can be described as an effective description of the Pauli exclusion principle and the electrostatic (Coulomb) interactions. As an example, one can think of the energy difference between the orthohelium and parahelium which is a dot product between the two electron spins of the atom. In general, the effective coulomb interaction for fermions must have the dot product form $\vec{S}_i \cdot \vec{S}_j$. Therefore, expanding this recipe to a chain of atoms we can obtain the Heisenberg model. Of particular interest is the one-dimensional $S = 1/2$ antifferomagnetic Heisenberg model which can be understood using the superexchange process proposed by P.W. Anderson [18]. To this end, let us consider a model of weakly overlapping electron wavefunctions where we have added the Coulomb repulsion between to electrons at the same site

$$H = -t \sum_{\sigma=\pm} \sum_{i=1}^{N} a^{\dagger}_{i\sigma} a_{i+1\sigma} + V \sum N_{i+} N_{i-}, \tag{1.1}$$

where t is the hopping parameter and V denotes the coulomb repulsion. The above model is known as Hubbard model. In the strongly correlated case, $V/t >> 1$ the model is half-filled, $\langle N_i \rangle = 1$ and the dominant process is effectively a spin-spin interaction. To be more specific, if the spins on adjacent sites are parallel then due to the Pauli uncertainty principle nothing happens since double occupancy is forbidden. On the other hand, when the spins are antiparallel they can occupy the same site for a short time (since it is energetically unfavorable) and then one of the two spins will hop to the empty site. Consequently, there are two possibilities: Either nothing is changed or a spin exchange process has taken place. The later case is the superexchange process which as P.W. Anderson described leads to the Heisenberg model.

$$H = J \sum_{j=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}, \quad J \sim t^2/V. \tag{1.2}$$

Additionally this was expanded by P.W. Kasteleijn. to include an anisotropy parameter Δ in the quantization axis [19] and this model is known as the XXZ spin chain model.

Regarding the spectrum of the XXZ spin chain, L.D. Faddeev and L.A. Takhtajan in their seminal work [20] revealed that the elementary excitations are domain wall-like particles carrying $S = 1/2$ spin, called *spinons*, which are a collective cooperative motion of the real particles that constitute the material. In addition, it was found that spinons are *fractional* excitations meaning that in generally they cannot appear as single particles but only in pairs. It is rather interesting that even though the dynamics and the thermodynamics of the XXZ model has been extensively studied, there is still a lot of mystery about the behavior of spinons and their explicit contribution in the transport and thermodynamic properties of these materials. Hence, the thesis main objective is to contribute to the fundamental understanding of spinons.

1.1 Overwiew of this Thesis

This thesis is devoted to the study of some fundamental aspects of the dynamics of the one-dimensional $S = 1/2$ XXZ model. In particular, we study the scattering of a spinon from local potentials aiming at a microscopic understanding of scattering processes by impurities, phonons and barriers, relevant to (far-out of equilibrium) quantum spin transport. Additionally, we address the theoretical question,*how does a quantum many-body topological excitation scatters from a potential?*. This question is also relevant in other systems with topological excitations of actual experimental and theoretical interest. Moreover, we study the thermodynamics of the aforementioned system, where aiming at a physical picture of the (thermo-) dynamics, we look at the low energy dispersions of the underlying string excitations where we find that they are simple expressions in terms of dressed momenta which however are temperature dependent. By reformulating the expressions of the specific heat and magnetic susceptibility we point out that, in contrast to field theoretic approaches, completely different string excitations correspondingly contribute. On the relaxation functions, a very interesting recent extension of TBA was proposed for space-time dependent densities under the name of Generalized Hydrodynamics approach [21, 22](GHD). By this novel method the spin and thermal Drude weights [23, 24, 25, 26] were recovered as asymptotic states of a quench from an initial thermal/magnetization step [27]. Here, using the GHD approach in the linear approximation, we analyze the relaxation of wavevector-q dependent thermal/magnetization profiles. As a byproduct we obtain the Drude weights as integrals over frequency of the wavector-q relaxation spectral function, of course closely related to linear response conductivities. This study provides theoretical background to present and feature experiments in 1D quantum magnets [28], e.g "dynamic heat transport" [29] and "transient grating spectroscopy" experiments [30], that probe the relaxation of magnetization/thermal density profiles.

The Organization of this thesis is as follows:

• In chapter 2 we introduce the reader to the basic concepts of integrable systems and more importantly to the method of Bethe Ansatz. In particular, we derive the

Bethe-equations and present the elementary excitations of the $S = 1/2$ XXZ spin chain.

• In chapter 3 we present the Algebraic Bethe Ansatz technique for the XXZ spin chain. As we already mentioned this is an elegant method to derive the spectrum of the Hamiltonian. Besides that, a novel and efficient method was recently presented based on ABA which allow us to efficiently calculate the matrix elements for longitudinal, transverse and spin-phonon potentials for relatively large spin chains, in contrast to previous methods like the exact diagonalization method where the spin chains were restricted to $N \simeq 12$ sites.

• Chapter 4 is concerned with the scattering of spinons by local and extended potentials of the aforementioned form. Specifically, using Bethe ansatz calculations and a T-matrix approach we calculate the transmission coefficients corresponding to the probability that a spinon will asymptotically remain to the same state, i.e. the probability that the spinon will pass the barrier. To this end, we include the whole 2-spinon continuum as intermediate states for an even spin chain and the one-spinon states for an odd spin chain.

• Chapter 5 is an introduction to the method of Thermodynamic Bethe Ansatz (TBA) developed by M. Takahashi, which is used to derive the thermodynamic equations for integrable systems. Besides that we present a short description to the peculiar and amazing properties of the transport properties of integrable systems.

• Chapter 6 is concerned with the thermodynamics of the XXZ spin chain. Specifically, assisted by the novel method of GHD we look at the low/high temperature dynamics aiming at a physical understanding of the string spectrum. Moreover, we analyze the relaxation of wavevector-q dependent thermal/magnetization profiles where as a byproduct we obtain the Drude weights as integrals over frequency of the wavector-q relaxation spectral function.

Chapter 2

The Basic Elements of Bethe Ansatz

This chapter is concerned with the demonstration of the basic elements of the Bethe ansatz method, especially using the coordinate Bethe ansatz, since this was the original method developed by H. Bethe in 1931 in order to calculate the exact spectrum of the isotropic Heisenberg spin chain. The coordinate Bethe Ansatz method can be applied to a certain class of integrable systems, using properties such as the symmetries of the system and the factorization of the S-matrix. The first section shortly introduces the reader to the Liouvillian definition of integrability, while we also present some recent features of quantum integrable system. In the second section, for pedagogical reasons we present in detail the coordinate Bethe Ansatz treatment for the one dimensional Bose gas model, where by imposing periodic boundary conditions we arrive at the well known Bethe equations, whose solutions completely describe the eigenvectors of the model. The techniques needed and also many of the derived results can be used as a guidance for the XXZ Heisenberg spin chain. In the next sections, we focus on the XXZ model and using the same steps introduced in the previous section, we discuss about the existence of bound states solutions called *strings* and the fundamental excitations for the ferromagnetic, paramagnetic and antiferromagnetic regime. In particular, we give emphasis to the understanding of spinon excitations that are the elementary excitations in the paramagnetic/antiferromagnetic regime. Finally, we introduce an interesting quantity called *The fractional charge* which plays a central role to the understanding of the scattering mechanism of spinon excitations.

2.1 Classical and Quantum Integrability

2.1.1 Integrability in classical Hamiltonian systems

Let us consider a classical Hamiltonian system of n point particles. If (q_i, p_i), $i = 1, ..., n$ decribe the canonical pair of position and momentum, the phase space is then a $2n$-dimensional manifold $\mathcal{M}$ which can be equipped with the Poisson brackets $\{.,.\}$. A constant of motion $\mathcal{K}_j(q,p)$ is defined as follows:

$$\frac{d\mathcal{K}_j}{dt} = \{\mathcal{K}_j, H\} = 0. \tag{2.1}$$

Furthermore, a set of n constant of motions $\{\mathcal{K}_j\}$ is said to be in involution if $\{\mathcal{K}_i, \mathcal{K}_j\} = 0$.

To this end, we state the Liouville's definition of integrability: A dynamical system (of 2n-dimensional phase space manifold $\mathcal{M}$) is said to be Liouville integrable if there exist n independent constants of motion in involution.

Furthermore, the term *integrable* becomes apparent if we use the well known Liouville's theorem, which states that the solution of the equations of motion of a Liouville integrable system is obtained by *quadrature*. Quadrature essentially means that the problem's complexity is reduced to algebraic equations and that the solution will have in integral representation. In fact, a canonical transformation can be constructed in terms of action-angle variables, i.e., $(q_i, p_i) \to (\theta_i, \mathcal{K}_i)$

$$\frac{d\mathcal{K}_i}{dt} = 0, \quad , \frac{d\theta_i}{dt} = f(\mathcal{K}) \tag{2.2}$$

Finally, we give a very simple example of a classical integrable system:

$$H(q,p) = \frac{p^2}{2m} + V(q), \tag{2.3}$$

where the solutions is given by:

$$t(q) = \int \frac{dq}{\sqrt{2(E - V(q))}}. \tag{2.4}$$

If we are able to perform the integral on the RHS, then we must simply invert the relation to obtain the desired result.

Our purpose was to state the integrability condition for a classical integrable system in order to collate it with those of a quantum integrable system. However, it is important to mention that integrability also extends to $1+1$ classical field theories. In particular, two major contributions played a significant role for the rapid advance of this field. The first one was from Clifford S. Gardner, John M. Greene, Martin D. Kruskal and Robert M. Miura where they used for the first time the method of classical inverse scattering [31] to solve the KdV model[1] and the second one was from Peter Lax who was studying non-linear partial differential equations and found that if a PDE can be reformulated in terms of two operators $\partial_t L = [L, M]$, then the system is integrable [3]. Subsequently, A. Zakharov and V. Shabat combined the two seemingly unrelated methods to solve the non-linear Schrödinger equation [4]. Therefore, they consolidated the *inverse scattering method* which is widely used to solve $1 + 1$ integrable field theories. From the previous analysis, it is clear that a classical field theory is integrable if there exists a set of infinitely many independent local conserved quantities in involution[2]

2.1.2 Quantum Integrable systems

Unlike classical integrability, Quantum integrability is far more enigmatic since we cannot promote Liouville's theorem in its quantum version. It is evident that the Heisenberg uncertainty principle prevent us from a valid definition of the phase space manifold, since position and momentum cannot be defined simultaneously. In addition, Liouville's theorem is associated with the notion of solvability(at least in an integral form), which is not easily applicable in the quantum case. To be more specific, in a finite-dimensional quantum system the size of the Hilbert space increases exponentially with the number of its constituents, say N. Therefore, it is not a simple and doable task to diagonalize the Hamiltonian and to this end complicated but elegant methods have been created in order to deal with this task. Of course, although the Liouville theorem could provide us with a simple "too many symmetries" argument one could also identify the notion of integrability with the algebraic structure of Yang-Baxter algebra [32, 33], which could be loosely seen as a statement of non-diffractive scattering. Let us mention that a very interesting discussion about the definition of quantum integrability can be found in the work of Caux and Mossel [34].

2.2 An Interesting Application: Thermalization of Quantum integrable systems

As a first application of quantum integrability we compare the relaxation process of a closed integrable system with a non-integrable one. To begin with, let us assume that we have a generic isolated[3] quantum system. Due to the fact that the observation of quantum states themselves is problematic, we instead consider a local observable

[1] One of the most famous example of an integrable system is the Korteweg-de Vries (KdV) equation model which describes waves in shallow waters

[2] The definition of an integrable field theory ultimately excludes non-trivial theories that live in higher dimensions

[3] The isolated system denotes the absence of any interaction with the environment

$\mathcal{A}$. The locality property allows the complementary region in which the operator acts non-trivially to become an effective "bath" relaxing the expectation value of $\mathcal{A}$ towards its equilibrium value. Specifically,

$$\lim_{t\to\infty}\lim_{N\to\infty}\langle\psi|\mathcal{A}(t)|\psi\rangle = \langle\mathcal{A}\rangle_\beta, \tag{2.5}$$

where $\langle\mathcal{A}\rangle_\beta \equiv \mathrm{tr}[\rho_G\mathcal{A}]$, with $\rho_G = \frac{e^{-\beta H}}{\mathcal{Z}}$ the Gibbs ensemble and the effective temperature β is determined through the expectation value with respect to the Hamiltonian $\beta = \langle\psi|H|\psi\rangle$[4]. The mechanism of thermalization is described by the *Eigenstate Thermalization Hypothesis* (ETH) [35, 36, 37]. According to ETH, the thermalization process occurs at the level of the discrete eigenstates of a given Hamiltonian due to the fact that each eigenstate contains implicitly a thermal state. The ETH is in fact a substitute to the classical picture where the thermal ensemble was a consequence of the ergodicity of trajectories constrained to move onto a fixed energy surface.

The case for an integrable systems is completely different and this becomes visible from the existence of an unbounded in the thermodynamic limit set of conserved charges $\{Q_k\}$ and thus we expect that in the maximization of entropy all these conserved charges should be taken into account[5]. To contrast with the non-integrable case, the Gibbs ensemble is given by maximizing the entropy under the constraint of fixed energy which is expressed via the Lagrange multiplier β. Therefore the resulting equilibrium ensemble which is known as *Generalized Gibbs Ensemble*(GGE) is given by

$$\rho_{GGE} = \frac{1}{\mathcal{Z}}\exp(-\sum_k \beta_k Q_k), \tag{2.6}$$

where $\beta_k = \langle\psi|Q_k|\psi\rangle$.

Additionally, recent work showed that the local charges alone cannot exhaust the GGE state [38, 39] and that a new type of charges, called *quasilocal charges* should be included in order to achieve completeness [40, 41].

Finally, recent advances in the field of (ultra)cold atoms have made possible the study of isolated systems due to their very weak interaction with the environment, mainly in the form of particle loss through heating and due to the controllability of the system's

[4] The well known concept of negative temperatures which is observed experimentally is just the simple fact where $\frac{1}{N}\mathrm{tr}[\rho_G H] > \frac{1}{N}\mathrm{tr}H$ when $N\to\infty$.

[5] Global operators do not take part to the equilibration process and therefore we simply define the corresponding Lagrange multiplier as $\beta_k \equiv 0$ if Q_k is a global operator

parameters. To this direct a novel experiment, known as the *Quantum Newton's Cradle* was performed by T. Kinoshita, T. Wenger and D. Weiss [42], where they confined ^{87}Rb atoms within a trap and were able to manipulate the effective dimensionality of the system. The experiment suggested that when the system was driven out of equilibrium the the two and three-dimensional Bose gases relaxed very quickly towards an equilibrium state while the equilibration process of the one-dimensional bose gas which is modeled by an integrable system was very different suggesting the absence of the usual Gibbs thermalization for this case. In addition to the unusual thermalization of integrable systems, chapter 5 gives an overview of the transport theory for the aforementioned class of systems which shows that the existence of conservation laws give rise to interesting and novel transport properties.

2.3 One Dimensional Bose Gas

Let us consider a one-dimensional system of N-bosons with repulsive two body contact interaction. This system was first studied by Lieb and Liniger [43] and is one of the simplest, albeit interesting, integrable quantum many body system.

The quantum field theory for such a system is described by

$$\mathcal{H} = \int dx \left[\Psi^\dagger(x) H^0 \Psi(x) + \frac{1}{2} \int dy \Psi^\dagger(x) \Psi^\dagger(y) V(x,y) \Psi(y) \Psi(x) \right] \tag{2.7}$$

$$[\Psi(x), \Psi^\dagger(y)] = \delta(x-y), \qquad [\Psi^\dagger(x), \Psi^\dagger(y)] = [\Psi(x), \Psi(y)] = 0. \tag{2.8}$$

Replacing $H_0 = -\partial_x^2$ and $V(x,y) = g\delta(x-y)$, where $g > 0$, we obtain :

$$\mathcal{H} = \int dx \left[-\Psi^\dagger(x) \partial_x^2 \Psi(x) + g \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) \right] \tag{2.9}$$

The equation of motion in the second quantized form is

$$i\partial_t \Psi = -\partial_x^2 \Psi + 2g \Psi^\dagger \Psi \Psi \tag{2.10}$$

Note that, if we treat $\Psi(x)$ as a semi-classical field we recover the non-linear Schrödinger equation.

Moreover, the number and momentum operators are given by:

$$\mathcal{N} = \int dx \Psi^\dagger(x) \Psi(x), \tag{2.11}$$

$$P = -i \int dx \Psi^\dagger(x) \partial_x \Psi(x). \tag{2.12}$$

These two quantities are two of the infinitely many integrals of motion. Using (2.8) we can check that:

$$[\mathcal{H}, P] = [\mathcal{H}, \mathcal{N}] = 0. \tag{2.13}$$

The above integral of motions allow us to exploit the number conservation and translation symmetry and seek for common eigenstates of the H, P, N operators in the Nth subspace of the Fock space:

$$|\Psi(k_1, ..., k_N)\rangle = \frac{1}{\sqrt{N!}} \int d^N \phi_N(x_1, ..., x_N | \lambda_1, \lambda_2, ..., \lambda_N) \Psi^\dagger(x_1) ... \Psi^\dagger(x_N)|0\rangle. \tag{2.14}$$

Moreover, it is useful to reduce the quantum field theory problem into a quantum mechanical one by rewriting its Hamiltonian as:

$$\mathcal{H}_N = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2g \sum_{1 \leq i \leq j \leq N} \delta(x_i - x_j). \tag{2.15}$$

Since our particles are bosons, we can choose a suitable domain in order to simplify our calculations in the coordinate space:

$$\mathcal{D} = \{\vec{x} \in \mathbb{R}^N : x_1 \leq x_2 \leq ... \leq x_N\}. \tag{2.16}$$

Therefore, our problem is to solve the eigenvalues problem:

$$\mathcal{H}_N^0 \phi_N = E_N^0 \phi_N \quad , \quad \mathcal{H}_N^0 \equiv -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2}, \tag{2.17}$$

constrained by the following boundary conditions induced by the δ- interaction[6]

$$\left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} - g \right) \phi_N = 0 \quad , \quad j = 1, 2, ..., N-1, \tag{2.18}$$

where $x_{j+1} = x_j + \varepsilon$.

Finally, before we proceed to the solution of the eigenvalues problem we impose periodic

[6] Since we have chosen this specific domain $\mathcal{D}$, the following boundary conditions are easily obtained by changing coordinates to a center of mass-like system $r_j = x_{j+1} - x_j$, $X_j = (x_{j+1} + x_j)/2$ and integrate over an arbitrarily small region $|r| < \varepsilon$, $\varepsilon \to 0$

boundary conditions, i.e. constraining our system into a ring of perimeter L:

$$\phi_N(x_1, ...x_j + L, ..., x_N|\lambda_1, \lambda_2, ..., \lambda_N) = \phi_N(x_1, ...x_j, ..., x_N|\lambda_1, \lambda_2, ..., \lambda_N). \quad (2.19)$$

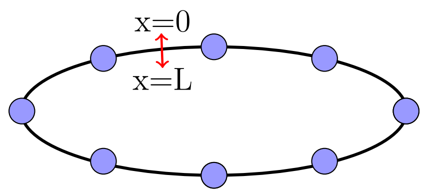

FIGURE 2.1: A cartoon of the Bose particles (blue balls) constrained to move in a ring of length L.

We proceed with an ansatz for the wavefunction ϕ_N in the given domain $\mathcal{D}$ of the form:

$$\phi_N(x_1, ...x_N|\lambda_1, ..., \lambda_N) = \sum_{\mathcal{P}\in\mathbb{S}_N} A_{\mathcal{P}} e^{i\sum_j \lambda_{\mathcal{P}_j} x_j}, \quad (2.20)$$

where $\mathcal{P} \in \mathbb{S}_N$ and denotes an N-cycle permutation of the particles momenta, which is produced by interchanging neighbor particles.

Let us take a step back and for the sake of simplicity counter the $N = 2$ body problem. The $N = 2$ wavefunction becomes:

$$\phi_2(x_1, x_2|k_1, k_2) = A_{12}e^{i(\lambda_1 x_1+\lambda_2 x_2)} + A_{21}e^{i(\lambda_2 x_1+\lambda_1 x_2)} \quad (2.21)$$

by substituting to equation (2.18) we deduce a relation between A_{12} and A_{21}, specifically:

$$\frac{A_{12}}{A_{21}} = \frac{i(\lambda_1 - \lambda_2) - g}{i(\lambda_1 - \lambda_2) + g} = -e^{i\theta(\lambda_1-\lambda_2)}, \quad (2.22)$$

$$\theta(\lambda) \equiv -2 \arctan \frac{\lambda}{g}. \quad (2.23)$$

Additionally, one can naturally determine the S-matrix between two rapidities

$$S(\lambda_1, \lambda_2) = S(\lambda_1 - \lambda_2) = \frac{\lambda_1 - \lambda_2 - ig}{\lambda_1 - \lambda_2 + ig} \quad (2.24)$$

The above results are interesting consequences of integrability, i.e. that when two particles collide they only acquire a phase shift described by the phase shift function

$\theta(k)$. In fact every integrable model is characterized by a specific phase shift function. Moreover having described the two body problem it is straightforward to repeat this calculation for the N body problem, since the S matrix is factorisable into two-body parts[7].

Additionally, using eq.(2.17) we find that the energy and momentum of state eq.(2.21) are given by:

$$E = \lambda_1^2 + \lambda_2^2 \quad , \quad P = \lambda_1 + \lambda_2. \tag{2.25}$$

Repeating the above calculations for the N body problem using eq.(2.18) we get that

$$\frac{A_{\mathcal{P}}}{A_{\mathcal{Q}}} = \frac{i(\lambda_{\mathcal{P}_j} - \lambda_{\mathcal{P}_{j+1}}) - g}{i(\lambda_{\mathcal{Q}_j} - \lambda_{\mathcal{Q}_{j+1}}) + g} = -e^{i\theta(\lambda_1 - \lambda_2)}, \tag{2.26}$$

where $\mathcal{Q}$ is defined through $\mathcal{P}$ by exchanging $\mathcal{P}_j$ and $\mathcal{P}_{j+1}$.

Therefore, we find that the eigenstate ϕ_N can be described by:

$$A_{\mathcal{P}} = C_N \prod_{j<k} (\lambda_{\mathcal{P}_j} - \lambda_{\mathcal{P}_k} + ig) \tag{2.27}$$

The energy and momentum of our eigenstate are given by:

$$E = \sum_{j=1}^{N} \lambda_j^2 \quad , \quad P = \sum_{j=1}^{N} \lambda_j \tag{2.28}$$

Note that, even though we found the exact eigenstates and eigenvalues of the system, they are described through a set of unknown quasi-momenta parameters $\{\lambda_j\}$. Therefore, our last step is to calculate these unknown numbers, that fully characterize the quantum state, via the quantization that is provided from the periodic boundary conditions. Since we have chosen a specific domain $\mathcal{D}$ the periodic boundary conditions are equivalent of taking the particle in the x_j position and move it trough the ring via two-cycle permutations of $\mathbb{S}_N$. This means that the particle will scatter with all the $N-1$ particles in the ring.

Hence, we arrive the following set of algebraic equations called the Bethe equations

$$e^{i\lambda_j L} = \prod_{l \neq j}^{N} \frac{\lambda_j - \lambda_l + ig}{\lambda_j - \lambda_l - ig} = (-1)^{N-1} \prod_{l \neq j}^{N} e^{i\theta(\lambda_j - \lambda_l)}, \quad j = 1, ..., N. \tag{2.29}$$

[7]This is a magnificent property of integrable systems, which is not generally true. For example a general three-body problem can be an intractable problem due to the highly increased complexity

Using the S-matrix we arrive at the following interesting form:

$$e^{i\lambda_j L}\prod_{l\neq j} S(\lambda_j,\lambda_l)=1. \tag{2.30}$$

The above result is a straightforward presentation of the previous statement, that if we move a particle of rapidity λ_j through the ring, it will scatter consecutively with all the other particles in the ring.

The logarithmic form of the Bethe equations is

$$\lambda_j=\frac{2\pi}{L}I_j+\frac{1}{L}\sum_{i=1}^{N}\theta(\lambda_j-\lambda_l), \tag{2.31}$$

where I_j are analogs of the quantum numbers in the sense that they completely characterize our quantum state, and take integer values if the number of particles N is odd and half integer values if N is even. Additionally, since $\theta(-\lambda)=-\theta(\lambda)$ the momentum of the state is $P=\frac{2\pi}{L}\sum_{j=1}^{N} I_j$, which implies that it is quantized and does not depend on the coupling constant g. Note that, there is a critical question concerned with the existence and uniqueness of solutions of the Bethe equations: For a specific set of $\{I_j\}$ does a unique solution $\{\lambda_j\}$ of the Bethe equations exist?

The answer is provided by a theorem of Yang and Yang [44] which states that:

Theorem 1. *The solutions of the Bethe Equations exist and can be uniquely parameterized by a set of integer (half-integer) numbers I_j.*

Proof. : Let us write an action S_{BE} from which the Bethe equations can be derived

$$S_{BE}=\frac{1}{2}L\sum_{j=1}^{N}\lambda_j^2-2\pi\sum_{j=1}^{N}I_j\lambda_j+\frac{1}{2}\sum_{j,k}\int_0^{\lambda_j-\lambda_k}\theta(\mu)d\mu \tag{2.32}$$

Bethe equations are derived from a variational principle (extremum conditions) of equation (2.31). In order to prove that the solution exists and that for each I_j is unique, it is sufficient to prove that the Hessian matrix $\frac{\partial^2 S}{\partial\lambda_j\partial\lambda_k}$ is positive definite

$$\frac{\partial^2 S_{BE}}{\partial\lambda_j\partial\lambda_k}=\delta_{jk}\left[L+\sum_{m=1}^{N}\frac{2g}{g^2+(\lambda_j-\lambda_m)^2}\right]-\frac{2g}{g^2+(\lambda_j-\lambda_k)^2} \tag{2.33}$$

Therefore if for any real vector $\mathbf{w}$, the product $\mathbf{w}^T\frac{\partial^2 S_{BE}}{\partial\lambda_j\partial\lambda_k}\mathbf{w}\geq\mathbf{0}$ then we have proved our statement

$$\sum_{j,k} w_j w_k \frac{\partial^2 S_{BE}}{\partial \lambda_j \partial \lambda_k} = \sum_{j=1}^{N} L w_j^2 + \sum_{j>k=1}^{N} \frac{2g}{g^2 + (\lambda_j - \lambda_m)^2}(u_j - u_k)^2 \geq 0 \tag{2.34}$$

□

Note that although we have proved that a solution $\{\lambda_j\}$ exists for the Bethe equation and in fact describes the exact solution of the system, it cannot be found analytically and should be calculated via numerical methods

Another interesting question to ask is, to think that we have an increasing monotonic sequence of $\{I_j\}$, i.e. $I_1 < I_2 < ... < I_N$. Is it true that also $\lambda_1 < \lambda_2 < ... < \lambda_N$?. The answer is given by the following statement which can be found in [45]:

Theorem 2. *If $I_j > I_k$ then $\lambda_j > \lambda_k$, if $I_j = I_k$ then $\lambda_j = \lambda_k$.*

The proof of the above theorem can be found in [45]

These two theorems are going to serve as guidance for the properties of the Bethe roots in more complex models such as the XXZ spin chain model.

Finally, the set of quantum numbers $\{I_j\}$ that characterize the ground state must be described. For this purpose, we take a special limit $g \to \infty$ (Tonks-Girardeau case) in which the problem is simplified substantially. In this limit we find that bosons become effectively fermions[8], known as hard core bosons, since from the boundary conditions we get that $\phi_N|_{x_i=x_j} = 0$ which implies that if $\lambda_i = \lambda_j$ the wavefunction vanishes. Moreover, $\theta(\lambda) \to 0$ which means that $\lambda_j = \frac{2\pi}{L}$. Therefore, the ground state for the Tonks-Girardeau gas is given by a symmetric configuration of quantum numbers without holes

$$I_j = -\frac{N+1}{2} + j \quad , \quad j = 1, ..., N, \tag{2.35}$$

where excited states can be in principle constructed from different choices of $\{I_j\}$.

In fact, this is also the ground state in the finite g case, since by an analytical continuation argument for the wavefunction, we expect that it should be also true in the finite case. Furthermore it is interesting that in the case of a repulsive one-dimensional Bose

[8] This weird situation should not estrange us since we have seen that one-dimensional interacting bosons cannot acquire the same quasi-momenta. In fact It is known that systems in 1+1 dimensions do not obey the usual spin-statistics theory, i.e the fundamental group is different, which is another remarkable property of one-dimensional interacting systems

gas, $g > 0$ all solutions of the Bethe equations, $\{\lambda\}$ are real, while the attractive case $g < 0$, as the Heisenberg model, contains also complex solutions, called *strings* [46, 47], which denote bound states of real excitations. Finally, it is very interesting that if we were to generalize the bosonic fields $\Psi(x)$, $\Psi^{\dagger}(x)$, to *anyonic* fields [48] parameterized by a parameter q, i.e. $\Psi_q(x)$, $\Psi_q^{\dagger}(x)$, the Bethe-Ansatz mechanism would perfectly work and the Bethe equations would become [49]:

$$e^{i\lambda_j L} = e^{i\pi q(N-1)} \prod_{l\neq j}^{N} \frac{\lambda_j - \lambda_l + ig'}{\lambda_j - \lambda_l - ig'} \quad , \quad g' = \frac{g}{\cos(\pi q/2)}. \tag{2.36}$$

The above result can be perceived as a nice demonstration of the flexibility and strength of the Bethe Ansatz formalism.

2.4 The Anisotropic Heisenberg Spin Chain

The discussion of the Lieb-Liniger was a useful prelude and a guidance, since we will use the same methodology for a more sophisticated and widely used one-dimensional model, namely the anisotropic Heisenberg spin chain.

The basic ingredients of the model are the spin matrices satisfying the $\mathfrak{su}(2)$ Lie algebra $[S_j^{\alpha}, S_k^{\beta}] = i\delta_{jk}\epsilon^{\alpha\beta\gamma}S_k^{\gamma}$

The Hamiltonian of the system with N sites, given the boundary conditions $\mathbf{S}_{N+j} = \mathbf{S}_j$ is

$$\mathcal{H} = J\sum_{n=1}^{N}[S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta(S_n^z S_{n+1}^z - \frac{1}{4})] - h\sum_{j=1} S_j^z, \tag{2.37}$$

where $S_n^a = \frac{\hbar}{2}\sigma_n^a$, with σ_n^a the Pauli matrices, J is the interaction strength between neighbor spins and Δ is an anisotropy parameter in the z $SU(2)$-space direction. The $\Delta = 1$ case is simply called *Heisenberg spin chain*. Finally note that the term $\frac{-J\Delta N}{4}$ is physically insignificant and is only added in this section in order to simplify our calculations

By introducing the spin flip operators $S_n^{\pm} \equiv S_n^x \pm iS_n^y$ we can rewrite the Hamiltonian

$$\mathcal{H} = J\sum_{n=1}^{N}\left[\frac{1}{2}(S_n^+ S_{n+1}^- + S_n^- S_{n-1}^+) + \Delta S_n^z S_{n+1}^z\right] - h\sum_{j=1} S_j^z, \tag{2.38}$$

where the $S_j^{\pm}$ operators satisfy the following commutation relations

$$[S_j^+, S_k^-] = 2\delta_{jk} S_j^z \quad , \quad [S_j^z, S_k^-] = \pm \delta_{jk} S_j^{\pm}. \tag{2.39}$$

The Hilbert space is spanned by the basis vectors $|\sigma_1, ...\sigma_N\rangle$ and is of dimension $\dim \mathcal{H} = 2^N$. Additionally, $J > 0$ favors ferromagnetic alignment, while $J < 0$ an antiferromagnetic alignment.

In the case where $\Delta = 1$, the Heisenberg chain posses full $SU(2)$ rotational invariance since $[H, S^{\alpha}_{tot}] = 0,\ S^{\alpha}_{tot} = \sum_{j=1}^{N} S^{\alpha}_{tot}$, while for $\Delta \neq 1$ the symmetry breaks down to rotational symmetry around the z axis, i.e. $U(1)$ symmetry. For general h the z-axis symmetry allow us to partition the Hilbert space $\mathcal{H}$ into subspaces of

fixed magnetization M, determined from the number of reversed spins, $M \equiv \frac{N}{2} - \langle S^z_{tot} \rangle$.

Moreover, by imposing periodic boundary conditions the Hamiltonian is also invariant under translations $\mathcal{T} = \prod_{j=1}^{N-1} P_{j,j+1}$, where P_{ij} is a permutation of spins on site i and j. Indeed, on can prove that $[H, \mathcal{T}] = 0$ and therefore each eigenstate will be a superposition of plane waves.

In addition, we can also find symmetries related to Δ and h namely

$$\begin{aligned} UH(\Delta,h)U^{-1} &= H(-\Delta,h) \quad , \quad U = \prod_{j=1}^{M/2} 2S^z_{2j} \\ VH(\Delta,h)V^{-1} &= H(\Delta,-h) \quad , \quad V = \prod_{j=1}^{M/2} 2S^x_{2j} \end{aligned} \tag{2.40}$$

In conclusion, the full symmetry group is $G = \mathbb{Z}/N\mathbb{Z} \times SU(2)$ for the isotropic case and $G = \mathbb{Z}/N\mathbb{Z} \times U(1)_z$ for the anisotropic case.

A comment on the experimental realizations of spin chains

Finally, let us mention that the $S = 1/2$ XXZ spin chain accurately describes various magnetic materials with strong one dimensional crystallographic direction like the $KCuF_3$, the Sr_2CuO_3 or CaCu2O3, $SrCuO_2$, and SrCuO2 the $CuSO_4{\cdot}5D_2O$ [50, 51, 52, 28]. These types of materials are mainly being studied for their transport properties. For instance, heat transport properties provide information about the various kind of excitations that take part, i.e. phonons electrons and others and their scattering properties.

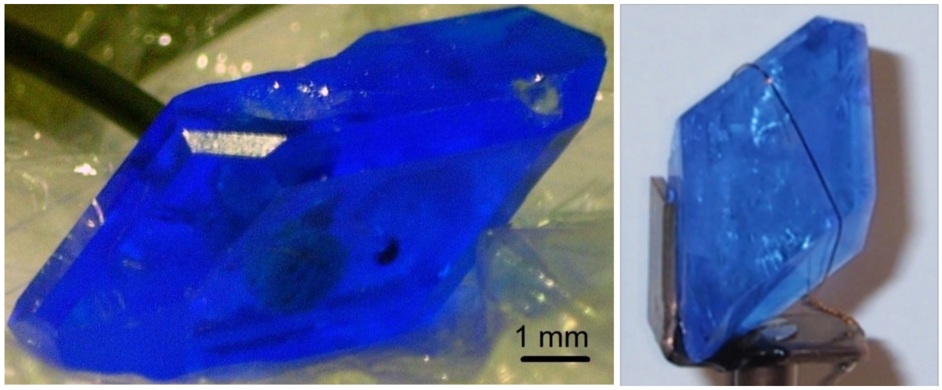

FIGURE 2.2: $CuSO_4{\cdot}5D_2O$ is an example of a material which is described by a one-dimensional $s = 1/2$ spin chain. In an elemntary unit cell there are two Cu^{2+} sites providing a localized $s = 1/2$ spin while the interchain interactions are found to be so small that the low dimensionality effectively applies. Figure taken from [52]

2.4.1 The Bethe Ansatz Solution

We start our analysis with a reference state $|0\rangle \equiv \otimes_{j=1}^{N} |\uparrow\rangle$, having energy $E_0 = JN/4 - hM$ and magnetization $M = N/2$.

If we define states that show us the location of the reversed spins in the chain, namely

$$|n_1, ..., n_M\rangle \equiv \prod_{l=1}^{M} S_{j_l}^{-}|0\rangle \quad , \quad 1 \leq n_k \leq N, \tag{2.41}$$

then a general eigenstate at $S_{tot}^{z} = N/2 - M$ sector can be written as follows:

$$|\psi\rangle = \sum_{1\leq n_1 \leq n_2 ... \leq n_M \leq N} \phi_M(n_1, n_2, ..., n_M)|n_1, n_2, ..., n_M\rangle, \tag{2.42}$$

The eigenvalue equation $H|\Psi\rangle = E|\Psi\rangle$ gives

$$\frac{J}{2}\sum_j (1 - \delta_{n_j+1,n_{j+1}})\Big\{\phi_M(n_1, ..., n_j + 1, n_{j+1}, ..., n_M) \tag{2.43}$$
$$+ \phi_M(n_1, ..., n_j, n_{j+1} - 1, ..., n_M)\Big\}$$
$$\left[E_0 - E - (J\Delta - 2h)M + J\Delta \sum_j \delta_{n_j+1,n_{j+1}}\right] \phi_M(n_1, ..., n_M) = 0$$

Next, let us make an ansatz for the wavefunction $\phi_M(n_1, ..., n_M)$ similar with the case of the Lieb Liniger model

$$\phi_M(n_1, n_2, ..., n_M) = \sum_{\mathcal{P} \in \mathbb{S}_M}^{M!} A_{\mathcal{P}} e^{i \sum_{j=1}^{M} \lambda_{\mathcal{P}_j} n_j} \tag{2.44}$$

The energy for the M particle state can be found form the $n_j + 1 < n_{j+1}$ case to be

$$E = E_0 + \sum_{j=1}^{M} [J(\cos k_j - \Delta) + h], \tag{2.45}$$

while the momentum of the state is $\mathcal{P} = \sum_{j=1}^{M} k_j$.

Moreover, if we consider the case $n_j + 1 = n_{j+1}$ we obtain

$$A_{\mathcal{P}}(e^{ik_{\mathcal{P}_j}} + e^{-ik_{\mathcal{P}_j}} - 2)e^{ik_{\mathcal{P}_{j+1}}} + A_{\mathcal{P}_{j+1}}(e^{ik_{\mathcal{P}_{j+1}}} + e^{-ik_{\mathcal{P}_j}} - 2)e^{ik_{\mathcal{P}_j}} = 0, \tag{2.46}$$

Similarly with the Lieb-Liniger model these $N!(N-1)/2$ equations can be satisfied if

$$A_{\mathcal{P}} = C(-1)^{[\mathcal{P}]} \prod_{l<j} (e^{i(k_{\mathcal{P}_l} + k_{\mathcal{P}_j})} + 1 - 2\Delta e^{ik_{\mathcal{P}_l}}) \tag{2.47}$$

where C is a normalization constant and $(-1)^{[\mathcal{P}]}$ was inserted to reflect the fermionic structure of the system

Therefore, we find that the scattering phase is defined as:

$$e^{\theta(k_i, k_j)} = -\frac{e^{i(k_i+k_j)} + 1 - 2\Delta e^{ik_i}}{e^{i(k_i+k_j)} + 1 - 2\Delta e^{ik_j}} \tag{2.48}$$

and the corresponding S-matrix is given by:

$$S(k_i, k_j) = S(k_i - k_j) = -\frac{e^{i(k_i+k_j)} + 1 - 2\Delta e^{ik_j}}{e^{i(k_i+k_j)} + 1 - 2\Delta e^{ik_i}} \tag{2.49}$$

The periodic boundary conditions are:

$$\phi_M(n_1, n_2, ..., n_M) = \phi_M(n_2, ..., n_M, n_1 + N), \tag{2.50}$$

where they can be thought as rotating the n_j down through the whole chain, thus acquiring a total phase $\sum_{l=1}^{M} \theta(k_j, k_l)$.

Hence for a term $A_{\mathcal{P}}$ the corresponding term will be $A_{\mathcal{Q}}$ where $\mathcal{Q} = (\mathcal{P}_2, ..., \mathcal{P}_M, \mathcal{P}_1)$.

Therefore we obtain the following Bethe equations:

$$e^{ik_{\mathcal{P}_1}N} = (-1)^{M-1}\frac{A_{\mathcal{P}}}{A_{\mathcal{Q}}}, \tag{2.51}$$

which by using eq.(2.49) and the fact that the above equation holds for every permutation $\mathcal{P}$ reduces to the following form:

$$e^{ik_jN} = (-1)^{M-1}\prod_{l\neq j}\frac{e^{i(k_j+k_l)} + 1 - 2\Delta e^{ik_j}}{e^{i(k_j+k_l)} + 1 - 2\Delta e^{ik_l}} \tag{2.52}$$

or in the equivalent form

$$e^{ik_jN}\prod_{l\neq j}S(k_j, k_l) = 1 \tag{2.53}$$

Although we have derived the Bethe equations for the XXZ spin chain, its current form is very difficult to handle and produce analytical or numerical solutions for the quasi-momenta $\{k_j\}$. In the following section we will cast another form for the Bethe equations using the Orbach Parametrization [43], which will be proved a useful tool not only for the numerical solution of the Bethe equations but also for calculating form factors and correlation functions which will appear in the next chapter.

2.4.2 Orbach Parametrization

In the previous section we derived the Bethe equations for the XXZ spin chain. The above form of the equations are not manageable and cannot be used for numerical calculations. Therefore, following the work of Orbach, we trade the set of quasi-momenta with another set of quantities, namely the rapidities $\{\lambda_j\}$. The set of rapidities have two main advantages, the first one is that they simplify the Bethe equations and the second one that they simplify the scattering phases. Unfortunately, the parametrization is not undivided, $\forall\Delta \in \mathbb{R}$, and thus, we have to consider different cases for different regions of Δ.

The main idea of this re-parametrization is to write Δ as a function of some parameter ζ and then write e^{ik_j} as follows:

$$e^{ik_j} = \frac{\varphi(\lambda_j + i\zeta/2)}{\varphi(\lambda_j - i\zeta/2)} \quad , \quad j = 1, ..., M \tag{2.54}$$

Taking the logarithm of eq.(2.54) :

$$k_j = -i \ln \left(\frac{\varphi(\lambda_j + i\zeta/2)}{\varphi(\lambda_j - i\zeta/2)} \right) \quad , \quad j = 1, ..., M \tag{2.55}$$

$$\theta_1(\lambda_j) \equiv i \ln \left(\frac{\varphi(\lambda_j + i\zeta/2)}{\varphi(\lambda_j - i\zeta/2)} \right) + \pi \tag{2.56}$$

$$\theta_2(\lambda_j - \lambda_k) \equiv i \ln \left(\frac{\varphi(\lambda_j - \lambda_k + i\zeta)}{\varphi(\lambda_j - \lambda_k - i\zeta)} \right) \tag{2.57}$$

Hence, we can bring the Bethe equations (2.51) in the following form:

$$\left(\frac{\varphi(\lambda_j + i\zeta/2)}{\varphi(\lambda_j - i\zeta/2)} \right)^N = \prod_{k \neq j} \frac{\varphi(\lambda_j - \lambda_k + i\zeta)}{\varphi(\lambda_j - \lambda_k - i\zeta)} \tag{2.58}$$

By taking the logarithm of eq.(2.58) we get:

$$\theta_1(\lambda_j) = \frac{2\pi}{N} I_j + \frac{1}{N} \sum_{k=1}^{M} \theta_2(\lambda_j - \lambda_k). \tag{2.59}$$

The momenta and total energy are given by:

$$P = \sum_{j=1}^{M} p(\lambda_j) = \pi M - \frac{2\pi}{N} \sum_{j=1}^{M} I_j, \tag{2.60}$$

$$E = J \sum_{j=1}^{M} \varepsilon(\lambda_j) - h(\frac{N}{2} - M), \tag{2.61}$$

where $p(\lambda_j) = k_j$, $\varepsilon(\lambda_j) = |\frac{\varphi(i\zeta)}{\zeta}| J \frac{dp(\lambda_j)}{d\lambda_j}$ and $P \equiv P \mod 2\pi$.

Gapless case $|\Delta| < 1$

In the gapless case we parametrize $\Delta = \cos\gamma$ and $\varphi(\lambda + i\gamma) = \sinh(\lambda + i\gamma)$. The resulting scattering phases θ_m are

$$\theta_m(\lambda) = 2 \frac{\tan^{-1}(\tanh \lambda)}{\tan m\gamma/2} \quad , \quad m = 1, 2 \tag{2.62}$$

Notice that in the gapless case $\Im(\lambda) \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.

Gapped case $|\Delta| > 1$

The gapped case can result from the gapless cases by performing the transformation $\gamma \to i\phi$ and $\lambda \to i\lambda$.

The Orbach parametrization is $\Delta = \cosh\phi$ and $\varphi(\lambda + i\phi) = \sin(\lambda + i\phi)$. The resulting θ_n are

$$\theta_m(\lambda) = 2\tan^{-1}\left[\frac{\tan\lambda}{\tanh n\phi/2}\right] + 2\pi\lfloor\frac{\lambda}{\pi} + \frac{1}{2}\rfloor \tag{2.63}$$

The introduction of the floor function $\lfloor x \rfloor = \{n \in \mathbb{Z} | n \leq x\}$ is necessary, since by making the transformation from the gapless case to gapped case we chose $\Re(\lambda) \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, which compel us to stay on the principal branch of the logarithm. Moreover, the generalization of θ_n to arbitrary n is useful for future reference.

Isotropic case $\Delta = 1$

The isotropic limit is easily obtained from the $\Delta > 1$ by taking the limit $\zeta \to 0$ and $\lambda \to \frac{\lambda}{\phi}$ is finite. In this case $\varphi(\lambda + i\phi) = \lambda + i$, while the resulting θ_n are

$$\theta_n(\lambda) = 2\tan^{-1}\frac{\lambda}{n} \tag{2.64}$$

2.5 Existence of complex solutions

The existence of complex solutions, called *strings* is discussed. Furthermore, we give a short presentation of the *string hypothesis* as well as the well known Gaudin-Bethe-Takahashi equations.

2.5.1 String solutions as bound states

For simplicity we analyze the Bethe equations for the XXX spin chain, and the other cases follow similarly. The simplest case, $M = 2$, we obtain the following the Bethe equations:

$$\left(\frac{\lambda_1 + i/2}{\lambda_1 - i/2}\right)^N = \frac{\lambda_1 - \lambda_2 + i}{\lambda_1 - \lambda_2 - i} \tag{2.65}$$

$$\left(\frac{\lambda_2 + i/2}{\lambda_2 - i/2}\right)^N = \frac{\lambda_2 - \lambda_1 + i}{\lambda_2 - \lambda_1 - i} \tag{2.66}$$

It is interesting to notice that when $N \to \infty$ and $\Im(\lambda_{1,2}) \neq 0$, the left hand side of eqs.(2.62,2.63) is either zero or diverging, therefore also the right hand side of the equations should behave in the same way. This lead to consider solutions of the form $\lambda_1 - \lambda_2 = \pm i$ or equivalently

$$\lambda_{1,2} = \lambda \pm \frac{i}{2} \tag{2.67}$$

If we calculate the energy of this state using eqs.(2.58,2.59) for $J < 0$ (ferromagnetic case) we get that $\varepsilon_s(p) = \frac{J}{2}(\cos p - 1)$, while the corresponding 1-magnon state energy is $\varepsilon_m(p) = J(\cos p - 1)$. Hence

$$\varepsilon_s(p) < \varepsilon_m(p - p') + \varepsilon_m(p') \quad , \quad p, p' \in [0, 2\pi). \tag{2.68}$$

The above equation clearly states that the string solution eq.(2.67) is a 2-magnon bound state, one could also see that the wavefunction amplitudes vanishes exponentially as the distance between the flipped spins grows larger, as expected for a bound state solution.

The above analysis demonstrates the existence of complex solutions for the XXX spin chain.

2.5.2 String hypothesis

A repetition of the argumentation used in the previous section and using the fact that every solution is self conjugate $\{\lambda_j\} = \{\bar{\lambda}_j\}$ [53] one can hypothesize a generalization for string solutions of length n [9]:

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \frac{i}{2}(n + 1 - 2j) \quad , \quad j = 1, ..., n \tag{2.69}$$

[9] The third chapter will provide an elegant and thorough argument for the form of string solutions. Moreover we will find out that they play a crucial role in the thermodynamics of integrable systems that admit string solutions

The conjecture that strings are arranged in such patterns is called *string hypothesis*. Note that it is remarkable that such solutions where already known to H. Bethe [17].

Due to the fact that in the $\Delta \geq 1$ case $\Im(\lambda) \in (-\infty, \infty)$ we can also treat the $\Delta > 1$ case in the same way :

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \frac{i\zeta}{2}(n+1-2j) \quad , \quad j = 1, ..., n \tag{2.70}$$

On the other hand the $\Delta < 1$ case is much more complex due to the restriction of the rapidities in the imaginary axis. In this case we have to manage the set $\{\lambda_\alpha^{n,j}\}$ to fulfill this condition, therefore the string hypothesis takes the form:

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \frac{i\zeta}{2}(n+1-2j) + i\frac{\pi}{4}(1-v_j) \quad , \quad j = 1, ..., n, \tag{2.71}$$

where $v_j = \pm 1$ and denotes the string parity.

Finally note the for finite spin chains we have a deviated form the above string hypothesis. Furthermore note that although the string hypothesis has been used to predict physical quantities there are cases where the hypothesis fails [54, 55, 56].

2.5.3 Bethe-Gaudin-Takahashi equations

Using the string hypothesis the Bethe equations take the form:

$$\left(\frac{\varphi(\lambda_\alpha^{n,j} + i\zeta/2)}{\varphi(\lambda_\alpha^{n,j} - i\zeta/2)}\right)^N = \prod_{(m,\beta)\neq(n,\alpha)} \prod_{k=1}^{m} \frac{\varphi(\lambda_\alpha^{n,j} - \lambda_\beta^{m,k} + i\zeta)}{\varphi(\lambda_\alpha^{n,j} - \lambda_\beta^{m,k} - i\zeta)} \prod_{l\neq j} \frac{\varphi(\lambda_\alpha^{n,j} - \lambda_\alpha^{n,l} + i\zeta)}{\varphi(\lambda_\alpha^{n,j} - \lambda_\alpha^{n,l} - i\zeta)} \tag{2.72}$$

Multiplying the equations of the n rapidities $\lambda_\alpha^{n,j}$ forming a string, we can remove the last product. Therefore the Bethe equations become

$$\left(\frac{\varphi(\lambda_\alpha^{n} + in\zeta/2)}{\varphi(\lambda_\alpha^{n} - in\zeta/2)}\right)^N = \prod_{(m,\beta)\neq(n,\alpha)} \prod_{j=1}^{n} \prod_{k=1}^{m} \frac{\varphi(\lambda_\alpha^{n,j} - \lambda_\beta^{m,k} + i\zeta)}{\varphi(\lambda_\alpha^{n,j} - \lambda_\beta^{m,k} - i\zeta)} \tag{2.73}$$

Hence, calculating the n, k-products we get

$$\left(\frac{\varphi_n(\lambda_\alpha^n)}{\varphi_{-n}(\lambda_\alpha^n)}\right)^N = \prod_{(m,\beta)\neq(n,\alpha)} \Phi_{nm}(\lambda_\alpha^n - \lambda_\beta^n), \tag{2.74}$$

where $\varphi_n \equiv \varphi(\lambda + in\zeta/2)$ and

$$\Phi_{nm} = \begin{cases} \frac{\varphi_{n+m}}{\varphi_{-(n+m)}} \frac{\varphi_{|n-m|}}{\varphi_{-(|n-m|)}} \left[\left(\frac{\varphi_{|n-m|+1}}{\varphi_{-(|n-m|+2)}} \right)^2 \left(\frac{\varphi_{|n-m|+4}}{\varphi_{-(|n-m|+4)}} \right)^2 \ldots \left(\frac{\varphi_{m+n-2}}{\varphi_{-(m+n-2)}} \right)^2 \right] & , \quad n \neq m, \\ \frac{\varphi_{2n}}{\varphi_{-2n}} \left[\left(\frac{\varphi_2}{\varphi_{-2}} \right) \ldots \left(\frac{\varphi_{2n-2}}{\varphi_{-(2n-2)}} \right)^2 \right] & , \quad n = m \end{cases} \tag{2.75}$$

Finally, by taking the logarithm of eq.(2.74) we obtain the Bethe-Takahashi equations

$$\theta_n(\lambda_\alpha^n) = \frac{2\pi}{N} I_\alpha^n + \frac{1}{N} \sum_{(m,\beta)\neq(n,\alpha)} \Theta_{nm}(\lambda_\alpha^n - \lambda_\beta^m), \tag{2.76}$$

$$\theta_n(\lambda) = 2\arctan\left(\frac{\tan\lambda}{\tanh\frac{n\phi}{2}} \right) + 2\pi \lfloor \frac{\lambda}{\pi} + \frac{1}{2} \rfloor \tag{2.77}$$

$$\Phi_{nm} = \begin{cases} \theta_{|n-m|}(\lambda) + 2\theta_{|n-m|+2}(\lambda) + \ldots + 2\theta_{n+m-2}(\lambda) + \theta_{n+m}(\lambda) & , \quad n \neq m, \\ 2\theta_2(\lambda) + 2\theta_4(\lambda) + \ldots + 2\theta_{2n-2}(\lambda) + \theta_{2n}(\lambda) & , \quad n = m \end{cases} \tag{2.78}$$

Note that we have assumed that $\Delta \geq 1$, where the string length n can be arbitrary. In the case $\Delta < 1$ we it will be proven in the next chapter that only a finite number of string lengths n are available. Nevertheless the present procedure is very useful since the derivation of the Bethe-Takahashi equations for the $\Delta < 1$ case is similar.

2.6 Elementary excitations of the XXZ anisotropic spin chain

In this section, the ground states configuration and the elementary excitations of the XXZ anisotropic spin chain are introduced. After the description of the ground state configuration, we calculate the ground state energy in the thermodynamic limit. Consequently, we construct the elementary excitations above the ground state.

2.6.1 The Ground State Configuration

In order to be able to describe excited states of the XXZ Heisenberg spin chain we should first describe the ground state of the XXZ spin chain model.

Gapless case $|\Delta| \leq 1$

For simplicity let us initiate our discussion with the XXX model on the grounds that it will simplify our reasoning. In the ferromagnetic case, $J < 0$, since alignment of neighbor spins is favorable the ground state is the completely polarized state $|FM\rangle = \prod_{j=1}^{N} \otimes|\uparrow\rangle$. The ground state can be perceived as a magnon-vacuum state and all excited states can be built by flipping spins, i.e. adding magnons to the system. We have already seen that excitations over this state $|G\rangle$ are magnons and bound states of magnons.

In the opposite case, namely the antiferromagnetic regime and the one that we will be interested throughout this thesis since this is the most relevant regime for physical applications, we intuitively expect that due to the antifferomagnetic couplings that tend to anti-align neighbor spins, the ground state of an even numbered spin chain will belong in the $S^z = 0$ magnetization sector while an odd numbered spin chain in the $S^z = \pm 1/2$ magnetization sector. In fact for finite spin chains it was proven by C.N. Yang and C.P. Yang that $\forall \Delta > 0$ and for each magnetization sector M the lowest energy state is given by the following set of quantum numbers [57]:

$$I_j = -\frac{M+1}{2} + j \quad , \quad j = 1, ..., M, \tag{2.79}$$

where we assumed an even numbered spin chain. As expected the ground state configuration is given for $M = N/2$.

In an odd numbered spin the lowest state is doubly degenerate and it can be obtained by choosing either:

$$I_j = -\frac{M}{2} + j \quad , \quad j = 1, ..., M \tag{2.80}$$

or

$$I_j = -\frac{M}{2} + j + 1 \quad , \quad j = 1, ..., M \tag{2.81}$$

This time the ground state is give by $M = \frac{N}{2} - 1$

Gapped case $\Delta > 1$

In this case the ground state is still given by eq.(2.79) for the even chain or by eq.(2.80) for the odd chain, but there exists another state that is slightly degenerate with all the quantum numbers I_j shifted by one to the right. The energy difference of the quasi-degenerate ground state and the true ground state reduces faster than exponentially with the number of spins N. Additionally in the Ising limit $\Delta \to \infty$ the two states are exactly degenerate, $|\uparrow\downarrow\uparrow\downarrow ...\rangle \pm |\downarrow\uparrow\downarrow\uparrow ...\rangle$.

2.6.2 Ground State Energy in the Thermodynamic Limit

The Bethe equations are a coupled system of M algebraic equations, making intractable the analytical calculation of the ground state energy or the excitation energies and momenta. To this end, rather than working with a finite lattice spin chain we work in the thermodynamic limit, $N \to \infty$, while keeping $\frac{M}{N}$ fixed. Additionally, in this case instead of working with a finite discrete set $\{\lambda_j\}$ we work with a continuous distribution of rapidities $\rho(\lambda)$ by taking the limit

$$\rho(\lambda) = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{M} \delta(\lambda - \lambda_k). \tag{2.82}$$

Moreover, we replace the summation with a Riemann integral along with the distribution $\rho(\lambda)$

$$\frac{1}{N} \sum_{k=1}^{M} \to \int_{-\Lambda}^{\Lambda} \rho(\mu) d\mu, \tag{2.83}$$

where Λ is the Fermi spectral parameter and depends on the magnetic field h.

Therefore in the thermodynamic limit the equation eq.(2.55) becomes

$$\theta_1(\lambda) - \int_{-\Lambda}^{\Lambda} d\mu \theta(\lambda - \mu)\rho(\mu) = 2\pi z(\lambda|\{\lambda_j\}), \tag{2.84}$$

where $z(\lambda|\{\lambda_j\}) \equiv \lim_{N\to\infty} \frac{I_j}{N}$ is called the counting function for the specific set of Bethe roots $\{\lambda\}$. For simplicity we denote it $z(\lambda)$.

By taking the derivative with respect to λ

$$\alpha_1(\lambda) - \int_{-\Lambda}^{\Lambda} d\mu \alpha_2(\lambda - \mu)\rho(\mu) = \frac{dz(\lambda)}{d\lambda}, \tag{2.85}$$

where $\alpha_m \equiv \frac{1}{2\pi} \frac{d\theta_m(\lambda)}{d\lambda}$. Furthermore one can define the density of holes, i.e. the absence of quantum numbers numbers by the following relation:

$$\rho(z(\lambda) + \rho_h(z(\lambda)) = 1 \Rightarrow \frac{dz(\lambda)}{d\lambda} = \rho(\lambda) + \rho_h(\lambda). \tag{2.86}$$

Using eq.(2.58) and eq.(2.59) we find the total energy and momentum in the thermodynamic limit:

$$E = -NJ\pi\phi(i\zeta)\int_{-\Lambda}^{\Lambda} d\lambda\alpha_1(\lambda)\rho(\lambda) \tag{2.87}$$

$$P = 2\pi\int_{-\infty}^{\infty} d\lambda N\left(z(\lambda) + \frac{1}{N}\sum_{1\leq k\leq card\{I_k^h\}} \vartheta(z(\lambda) - \frac{I_k^h}{N})\right), \tag{2.88}$$

where ϑ denotes the step function.

At zero magnetic field $h = 0$ $\Lambda = \infty$, we can fourier transform equation eq.(2.84) to obtain:

$$\alpha_1(\omega) = \alpha_2(\omega)\rho(\omega) + \rho(\omega) + \rho_h(\omega) \tag{2.89}$$

For the ground state the density of holes is $\rho_h = 0$. Therefore the ground state density is simply given by:

$$\rho_{GS}(\omega) = \frac{\alpha_1(\omega)}{1 + \alpha_2(\omega)} \tag{2.90}$$

The above relation makes clear the strategy that we have to follow: We find the Fourier transform for the α_m and then we perform the inverse Fourier transform to find the ground state density. Below, we explicitly perform the calculation for the ground state energy.

Ground state energy for the isotropic case

$$\alpha_m(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda e^{i\omega\lambda}\frac{m}{\lambda^2 + (m/2)^2} = e^{-|\omega|m/2} \tag{2.91}$$

Therefore the ground state density is

$$\rho_{GS}(\omega) = \frac{1}{2\cosh(\omega/2)} \tag{2.92}$$

Performing the inverse Fourier transform we get

$$\rho_{GS}(\lambda) = \frac{1}{\cosh\pi\lambda} \tag{2.93}$$

And thus the ground state energy is

$$E = \frac{NJ}{4} - NJ\ln 2, \tag{2.94}$$

while the total momentum is $P \equiv \pi M \mod 2\pi$. This result was originally derived by E. Hulthen in 1938 [58]

Ground state energy for the $\Delta < 1$ case

A similar calculation for the $|\Delta| < 1$ shows that the ground state energy is

$$E = E_0 - JN \sin\gamma \int_0^\infty \frac{\sinh[(\pi-\gamma)\omega]}{\sinh(\pi\omega)\cosh(\gamma\omega)} d\omega, \tag{2.95}$$

where we have used the fact that

$$\alpha_n(x) = \frac{1}{2\pi} \frac{\gamma \sin n\gamma}{\cosh\gamma x - \cos n\gamma}. \tag{2.96}$$

Ground state energy for the $\Delta > 1$ case

The $\Delta > 1$ case is more subtle since the ground state rapidities are confined in the $[-\pi/2, \pi/2]$ interval. Therefore, the corresponding Fourier transforms are

$$\rho_k = \int_{-\pi/2}^{\pi/2} d\lambda e^{-2ik\lambda} \rho(\lambda) \quad , \quad \rho(\lambda) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} d\lambda e^{2ik\lambda} \rho_k \tag{2.97}$$

Similarly with the previous cases $\rho_{GS}(\lambda)$ is given by eq.(2.89)

$$\rho_{GS}(k) = \frac{1}{2\cosh(2k\phi)} \tag{2.98}$$

Taking the inverse Fourier Transform

$$\rho_{GS}(\lambda) = \frac{1}{\pi} \sum_{k=-\infty}^{\infty} e^{ik\phi x} \rho_{GS}(k) \tag{2.99}$$

$$\rho_{GS}(\lambda) = \frac{1}{\pi} \sum_{k=-\infty}^{\infty} \cos(2k\lambda) \frac{e^{-|k|\phi]}}{1+e^{-2|k|\phi}} = \frac{1}{\pi} = \frac{K}{\pi^2} dn(\frac{2K\lambda}{\pi}, u) \tag{2.100}$$

Finally, the ground state energy is

$$E = \frac{J\Delta}{4} - JN\sinh(\phi) \sum_{k=-\infty}^{\infty} \frac{1}{e^{2k\phi}+1}. \tag{2.101}$$

Note that $dn(x, u)$ is the Jacobian elliptic function[59]

2.6.3 Elementary Excitations: *Spinons*

The elementary excitations of an antiferromagnetic system and a ferromagnetic one differ substantially. In the latter, we have seen that the elementary excitations are translationally invariant spin flips called magnons, collective excitations of the system that carry a fixed amount of energy and momentum, and are $S = 1$ particles. Initially, in 1962, J. des Cloizeaux and J.J. Pearson using a Bethe Ansatz approach calculated the lowest energy spectrum of an even antiferromagnetic Heisenberg chain [60], where they found that the elementary excitation was an $S = 1$ particle. Although Cloizeaux and Pearson calculated correctly the energy dispersion, they could not, at that time, understand that in reality what they had found was a pair of elementary excitations, each carrying $S = 1/2$, and not a single one. This was revealed by the novel work of L. Fadeev and L.A. Takhtajan [20], where they correctly described the spectrum of an antiferromagnetic spin chain-1/2 system. Furthermore, the acknowledgment that a spin flip, namely a process of changing the spin of the system by unit, creates a pair of two $S = 1/2$ particles, has an amazing consequence which is introduced by the concept of *fractionalization*[10]. Underneath, we explicitly construct these excitations, which are called *spinons*, and further discuss their physical properties.

Spinons in the $|\Delta| \leq 1$ case

Let us proceed to construct the elementary excitations over the ground state, where for simplicity we assume an even numbered spin chain. This is described by $\nu_0 = \frac{N}{2}$ and $\nu_M = 0, M \geq 1/2$. The simplest excited states are characterized by two holes in the ground state configuration. Assuming that the non-occupying quantum numbers are I_1^h and I_2^h the configuration is

$$z(\lambda) = z_{GS} + \frac{1}{N}\vartheta(z - \frac{I_1^h}{N}) + \frac{1}{N}\vartheta(z - \frac{I_2^h}{N}) \tag{2.102}$$

Therefore, the density configuration satisfies the following Fourier transformed equation

$$\rho_{exc}(\omega) = \frac{1}{1 + \alpha_2(\omega)}\Big(\alpha_1 + \frac{e^{i\omega\lambda_1^h}}{N} + \frac{e^{i\omega\lambda_2^h}}{N}\Big) \tag{2.103}$$

Hence,

$$\rho_{exc}(\lambda) = \rho_{GS}(\lambda) - \frac{1}{N}\rho_{sp}(\lambda - \lambda_1^h) - \frac{1}{N}\rho_{sp}(\lambda - \lambda_2^h) \tag{2.104}$$

[10] Interestingly, fractionalization is also depicted in the Hubbard model where the physical excitations carrying spin $S = 1/2$ and charge e can be rewritten in terms of uncharged spins and spinless charges

Therefore, the energy difference over the ground state, ΔE is given by:

$$\Delta E = \varepsilon(\lambda_1^h) + \varepsilon(\lambda_2^h), \tag{2.105}$$

where

$$\begin{aligned}\varepsilon(\lambda^h) =& J\pi \frac{\sin\gamma}{\gamma} \int_{-\infty}^{\infty} d\lambda \alpha_1(\lambda) \rho_{sp}(\lambda - \lambda^h) = \frac{J\pi \sin\gamma}{\gamma} \int_{-\infty}^{\infty} d\lambda \rho_{GS}(\omega) e^{-i\omega\lambda^h} = \\ & \frac{J\pi\sin\gamma}{2\gamma} \frac{1}{\cosh(\frac{\pi\lambda^h}{2})}\end{aligned} \tag{2.106}$$

Similarly the momentum difference is given by:

$$\Delta P = Q(\lambda_1^h) + Q(\lambda_2^h), \tag{2.107}$$

where

$$Q(\lambda^h) = 2\pi \int_{\lambda_1^h}^{\infty} d\lambda \rho(\lambda) = \frac{\pi}{2} - \arctan(\sinh\frac{\pi\lambda}{2}) \tag{2.108}$$

Therefore the spinon dispersion is

$$\varepsilon(Q) = \frac{J\pi\sin\gamma}{2\gamma} |\sin Q|, \quad Q \in [0, \pi] \tag{2.109}$$

Let us mention that in the odd case, instead of a pair of spinons we obtain a single spinon state with the same dispersion relation as eq.(2.109). In fact, there is no vacuum state (in the sense that there are no spinons), since all physical states contain an odd number of spinons (m-spinon states, $m = 2k + 1$). Therefore, the physical spectrum of the spin chain completely depends on the parity of the chain.

Additionally, let us comment on the dimension of the two-spinon states subspace, assuming a finite chain of even length N. Two-spinon states do not span the whole Hilbert space $\mathcal{H}$, having dimension $\dim \mathcal{H} = 2^N$, but only a small but physically significant part of it. Specifically, in accordance with L. Fadeev and L.A. Takhtajan [20], taking the limit $\lambda \to \infty$ in eq.(2.59), we find that the maximum allowed value of the quantum number $I_{max} = \frac{N}{2}$ and therefore, the number of vacancies is $2I_{max}+1 = \frac{N}{2}+1$, while the quantum numbers for a specific are $\frac{N}{2} - 1$. Hence,

$$\dim \mathcal{H}_{2sp}^{|\Delta|\leq 1} = \binom{N/2+1}{N/2-1} = \frac{N}{8}(N+2). \tag{2.110}$$

Let us make a comment for the construction of two-spinon states in the case of a finite chain of even length N. Since we work in the magnetization sector $M = \frac{N}{2} - 1$ and the number of vacancies is $\frac{N}{2}+1$, the construction of the two-spinon states in the finite is straightforward; The two holes in the distribution of possible Bethe quantum numbers are interpreted as spinons excited from the new physical vacuum. Therefore, by moving the two holes inside the possible number of vacancies and solving numerically the Bethe-equations eq.(2.59) we obtain all two-spinon solutions. It is interesting that all two-spinon solutions correspond to real sets of rapidities λ_j. Finally, let us mention that in general one can construct a m-spinon state by choosing an appropriate set of quantum numbers I_j and solving numerically eq.(2.59) for real rapidities or eq.(2.76) for complex rapidities (string solutions).

Spinons in the $\Delta > 1$ case

A similar calculation for the $\Delta > 1$ case gives:

$$\Delta E = \varepsilon_s(\lambda_1^h) + \varepsilon_s(\lambda_2^h), \tag{2.111}$$

where

$$\begin{aligned} \varepsilon &= J\sinh(\eta)\pi\int_{-\pi/2}^{\pi/2} d\lambda\alpha_1(\lambda)\rho_{sp} \\ &= J\pi\sinh(\eta)\rho_{GS}(\lambda^h) = \\ &\frac{J}{\pi}\sinh(\eta)K(u)dn(K2\lambda^h/\pi|u). \end{aligned} \tag{2.112}$$

$$\Delta P = Q(\lambda_1^h) + Q(\lambda_2^h), \tag{2.113}$$

where

$$Q(\lambda^h) = 2\pi\int_{\lambda_1^h}^{\pi/2}\rho_{GS}(\lambda)d\lambda = \frac{\pi}{2} - \arcsin dn(2\lambda^h\frac{K}{\pi}, u). \tag{2.114}$$

Therefore,

$$\epsilon(Q) = \frac{JK(u)\sinh(\eta)}{\pi}\sqrt{1-u^2\cos^2 Q}, \quad Q\in[0,\pi]. \tag{2.115}$$

In contrast with previous spinon states, gapped spinons have a more complex structure due to the fact that they can built by two almost degenerate ground states instead of one. This time the total number of two-spinon states are [61]:

$$\dim\mathcal{H}_{2sp}^{\Delta>1} = 2\binom{N/2+1}{N/2-1} - \frac{N}{2} = \frac{N^2}{4}, \tag{2.116}$$

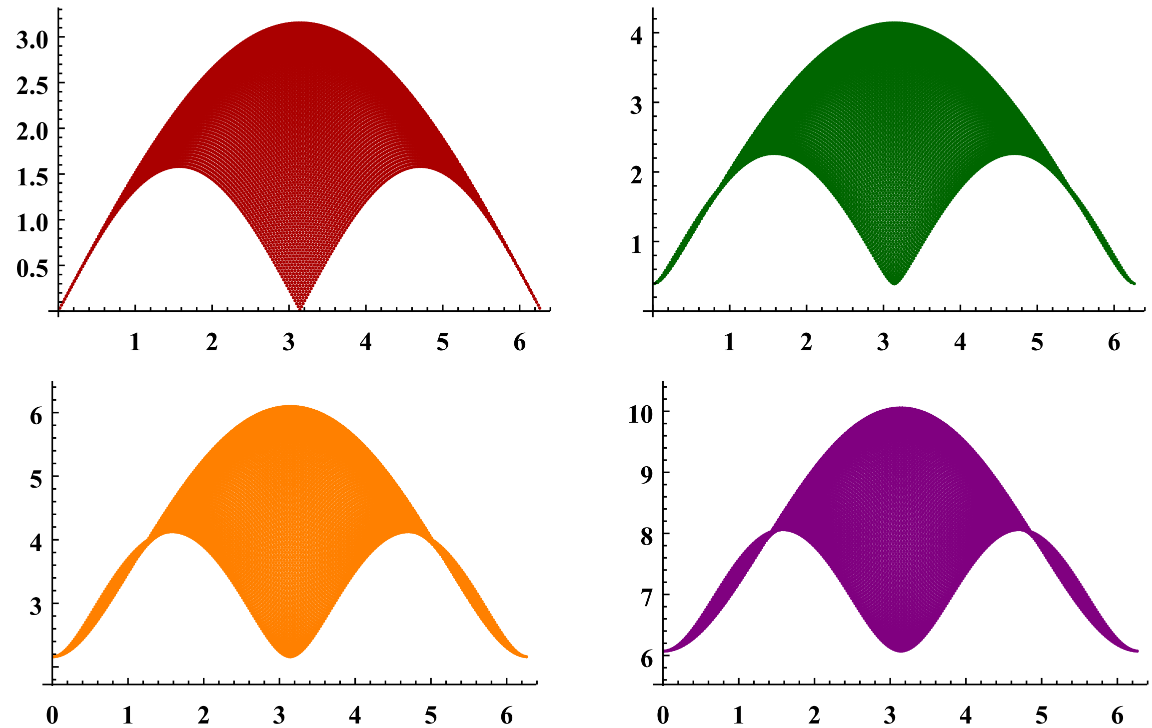

FIGURE 2.3: The Two spinon spectrum for a spin chain of length N=300 and Δ =1(top left),2(top right),4(bottom left),8(bottom right). For the $\Delta > 1$ there exists also another two spinon continuum excited from the quasi-ground state

where the $\frac{N}{2}$ are states that can be excited from both ground states.

The gapped case has also another importance distinction; Spinons are localized objects exhibiting solitonic behavior, i.e. propagating domain walls in the local antiferromagnetic ordering of the spins, while in the Ising limit $\Delta \to \infty$ they become exact classical domain walls [62].

2.6.4 A short note on spinon's remarkable nature

So far, we have derived the dispersion relation of the spinon excitation and described its basic properties. However, spinons have remarkable and exotic properties which are due to both the strongly correlated nature of the system and the low dimensionality. In particular, in the even case they cannot be created by a finite sequence of raising/lowering operators $S_n^{\pm}$ since this would cause a total change of $\Delta S = 1$, while

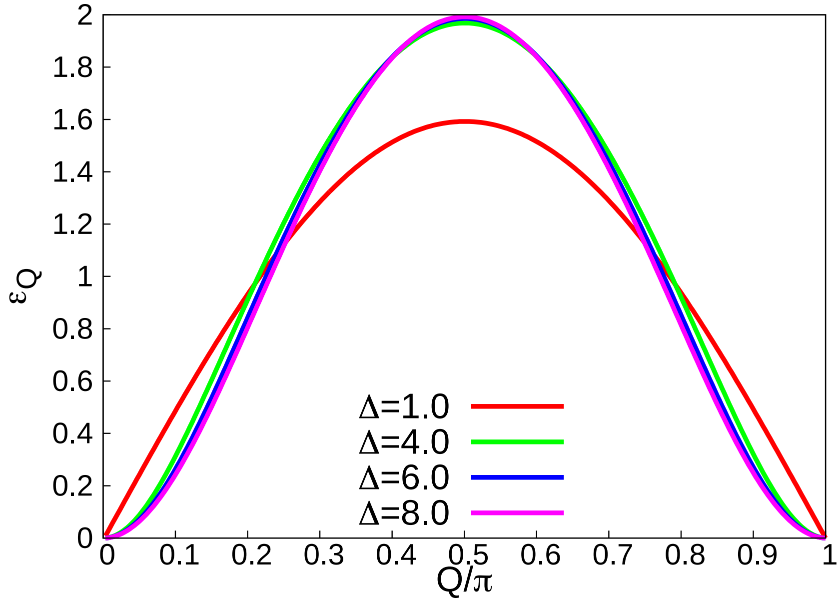

FIGURE 2.4: The spinon dispersion versus Q/π for various $\Delta \geq 1$. Note that as $\Delta \to \infty$, $\varepsilon_Q \to 2\sin^2 Q$

spinons[11] possess spin $S = 1/2$. Therefore, it is immediate that spinons cannot be created by a sequence local operators, and thus are another important example of *fractional excitations*. As we have already mention, the above are in principle a manifestation of one-dimensional systems, while in two-dimensional systems we have the well known charge fractionalization that occurs in the fractional hall effect. Moreover, the aforementioned property has another amazing consequence, the fact that they do not obey the usual spin statistics theorem. In particular, they are neither bosons or fermions, they are semions and they obey the fractional exclusion principle as discovered by F.D. Haldane [63]. The groundbreaking element of this generalization was the introduction of a parameter, let us call it g, which corresponds to the statistical interaction among the particle species. Specifically,let us assume a Hilbert space of finite and extensive dimension $\dim \mathcal{H} = d < \infty$[12] which is spanned by the single particle

[11]Note that in the literature the term *spinon* is widely used for a class of low dimensional excitations which are spin-1/2 particles while physical processes can only change the total spin of the system by an integer unit

[12]This is a plausible assumption for a condensed matter system due to the fact that the elementary excitations are constrained to live within the material region and cannot exist in the vacuum space where the the spectrum is unbounded

wavefunctions $\{\psi_\nu(r)\}_{\nu=1}^{d}$. If we take N identical particles and fix the coordinates of the $N-1$ then the ith particle wavefunction $\phi_\nu(r; r; \{r_j, j \neq i\})$, it generates a single particle Hilbert space of dimension d_N. In principle, d_N should change if a particle is added and consequently this makes necessary the introduction of a parameter g with the task to determine the change due to statistical constrains. Therefore, assuming that ΔN particles are added then the change of the dimension is quantified as $\Delta d_N = -g\Delta N$. For instance, if all the particles are Bosons then $g = 0$, while if all particles are fermions then $g = 1$ and $d_N = d-(N-1)$. On the contrary, F.D. Haldane proved that a spinon is neither a fermion or boson but something completely different which he called it semion. In particular, using a simple reasoning he concluded that the statistical interaction is given by $g_{\sigma,\sigma'} = \frac{1}{2}$ (note that spin up and spin down spinons are considered as different states) and that $d_\sigma = \frac{1}{2}(N+1) - \frac{1}{2}\sum_{\sigma'}(N_{\sigma'} - \delta_{\sigma,\sigma'})$. Finally, the total number of eigenstates, or equivalently the full size of the Hilbert space composed by (N_+, N_-) spinons, is simply given by $W(\{N_s\}) = \prod_\sigma \binom{d_\sigma+N_\sigma-1}{N_\sigma}$, while if we perform the summation over all spinon states we obtain, $\sum_{N_s} W(\{N_s\}) = 2^N$, verifying the above arguments.

2.7 Experimental probing of spinons

So far, it is of huge theoretical interest the ability to describe a complex quantum many body system in terms of spinons because it help us to encapsulate the many body dynamics within a quasiparticle and thus reduce the degrees of freedom. Hence, many physical quantities having an experimental relevance can be in principle calculated using the spinon basis. However, in order for this to be truly useful even as a theoretical concept we should be able to design an experiment telling us whether calculations in terms of spinons correspond to an actual physical and comprehensible picture. Fortunately, inelastic neutron scattering experiments proves to be a very good experimental method to excite a magnetic system where the charge neutrality of the scattered beam ensures that electric interactions do not occur allowing us to explore solely the magnetic dynamics. Specifically, neutrons can interact with a magnetic material via direct collisions with the nuclei or with spin dipole interactions. Inelastic neutron scattering is an efficient method because by measuring the scattering cross section we can obtain the dynamical structure factor as a function of k, $\hbar\omega$. In particular, for a one dimensional spin system the cross section[13] is given by [64]

$$\frac{d^2\sigma_{mag}}{d\omega d\Omega} = N\frac{k_f}{k_i}(r_m)^2|\frac{g_{ab}}{2}F(k)|^2\sum_{a,b}\left(\delta_{ab} - \frac{q_a q_b}{q^2}\right)S^{ab}(k,\omega), \tag{2.117}$$

[13]The calculation of the cross section is carried out using the Born approximation. Magnetic scattering has a weak coupled interaction and thus the Born approximation is very accurate

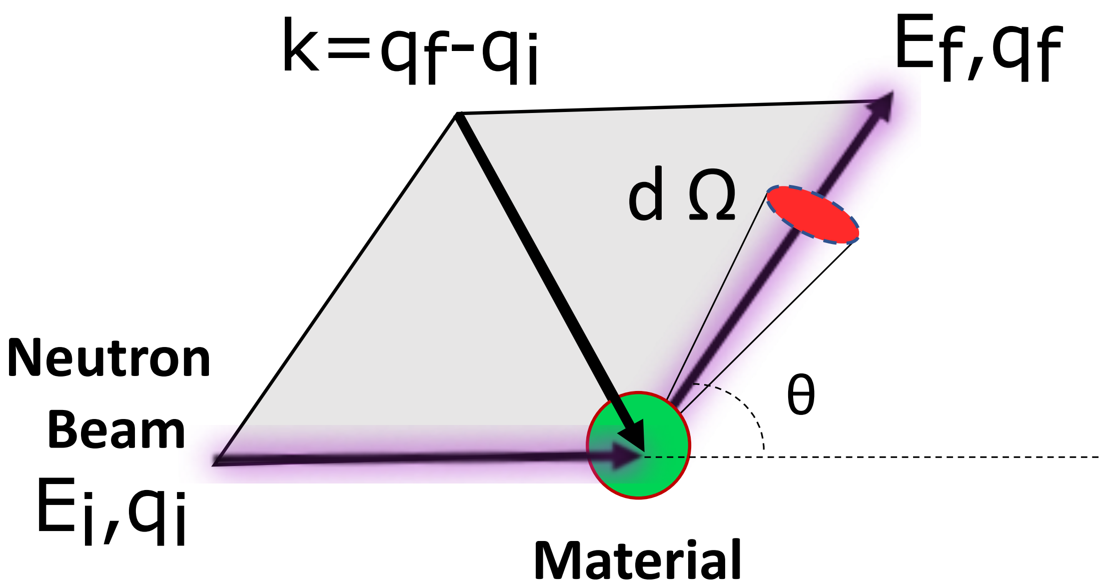

FIGURE 2.5: A cartoon of the inelastic neutron scattering experiment. The incident neutron beam "hits" the material and a detector measures the scattered beam energy and momentum, where $E_f < E_i$ since some of the energy converts to spinon excitations.

where N is the number of spin sites, k_i, k_f are the corresponding initial and final momentum of the neutron, r_m is the magnetic scattering length, g_{ab} is the magnetic g-factor, $F(k)$ is the Fourier transform of the magnetic electron density, $k = q_f - q_i$, $\hbar\omega = E_f - E_i$ and $S^{ab}(k,\omega)$ is a quantity called dynamical structure factor which is defined as

$$S^{ab}(k,\omega) = \frac{1}{N}\sum_{n,m=1}^{N} e^{-ik(n-m)} \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{i\omega t} \langle S_n^a(t) S_m^b(0)\rangle, \quad a,b = x,y,z. \tag{2.118}$$

The next step is to express eq.(2.119) in terms of a multispinon basis in the form of Bethe states and rewrite the operators in the Schödinger picture.

$$S^{ab}(k,\omega) = \frac{1}{N}\sum_{n,m=1}^{N} e^{-ik(n-m)} \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} \frac{e^{i\omega t - \beta E_\lambda}}{\mathcal{Z}} \langle \lambda | S_n^a(t) | \mu \rangle \langle \mu | S_m^b(0) | \mu \rangle. \tag{2.119}$$

The complexity of the problem reduces significantly if we use the fact that for a Hamiltonian which commutes with the total z component of S^z_{tot}, $S^{ab}(k,\omega) = 0$, when $b \neq a$ [65, 66]. Therefore, by performing the Fourier transform we obtain that

$$S^{a\bar{a}}(k,\omega) = \frac{2\pi}{\mathcal{Z}} \sum_{\lambda,\mu} |\langle\lambda|S^a_k|\mu\rangle|^2 e^{-\beta E_\lambda} \delta(\omega - E_\mu + E_\lambda), \tag{2.120}$$

where for convinience we re-evaluated the DSF in terms of $a = \pm, z$

Finally, at the limit of very low temperatures $\beta \to \infty$ the above expressions reduces to

$$S^{a\bar{a}}(k,\omega) = 2\pi \sum_{\mu} |\langle GS|S^a_k|\mu\rangle|^2 \delta(\omega - E_\mu + E_{GS}), \tag{2.121}$$

where the system is not thermally excited and thus the sum over all $|\lambda\rangle$ states is simply replaced by the ground state $|GS\rangle$. By restricting the state $|\mu\rangle$ to belong to the sets of m-spinon states we can understand quantitatively the spinon dynamics by measuring the effect they have in the scattering cross section of the neutron.

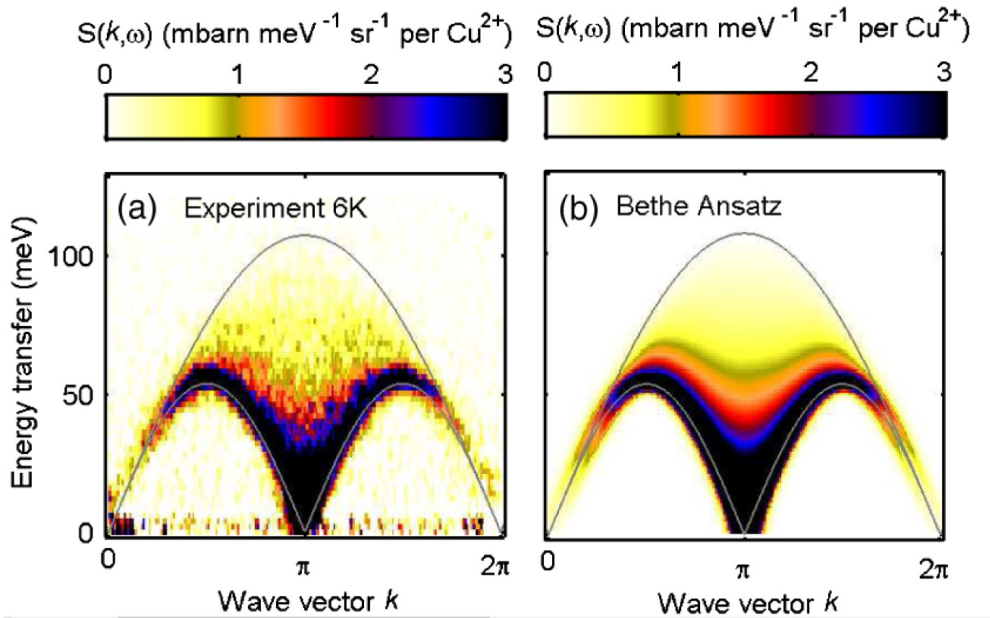

FIGURE 2.6: (a) Inelastic neutron scattering experiment data for $KCuF_3$ compared to (b) Bethe Ansatz calculations. Figure taken from [8]

In recent years, there are numerous experiments using inelastic neutron scattering to study extract the quantum magnetic correlations by evaluating the dynamical structure factor(DSF). This was motivated by the fact that many materials which exhibit interesting dynamics can be simulated by one dimensional systems [67, 68, 69]. For instance, the magnetic material $KCuF_3$ can be modeled as a quasi one-dimensional $s = 1/2$ isotropic Heisenberg antiferromagnet and one can calculate the magnetic correlations [65, 70]. To this end, a great deal of theoretical effort has concentrated in order to quantify the contribution of each of the m-spinon sectors in the presence or absence of magnetic fields [9, 71, 72, 73, 74]. while a comparison between Bethe Ansatz calculations and experimental data confirmed the validity of the spinon physical picture [8]. In particular, it is found that for the isotropic Heisenberg model the 2-spinon continuum exhaust the 71% [75] of the first frequency moment and with the addition of the 4-spinon sector this result rises to 98%[72] sum-rule which was supplemented with specially designed experiments with that were able to experimentally quantify the contribution of higher than 4-spinon and thus verify the existence of higher order spinon states [52].

2.8 Fractional Charge

We conclude this chapter with an important quantity called *fractional/dressed charge*. The term *fractional charge* comes from the fractionalization of the charge[14] that appears in the massive Thirring model [76, 45]. Moreover, the *dressed charge* appears as the simplest integral equation from a set of dressing equations

The dressed charge is defined as the simplest integral equation

$$Z(\lambda) - \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} K(\lambda, \mu) Z(\mu) d\mu = 1 \tag{2.122}$$

An important relation of the dressed charge that unveils its physical significance is the following:

$$Z(\lambda) = \frac{1}{2} \frac{\partial \varepsilon}{\partial h} \tag{2.123}$$

and therefore by relating $Z(\lambda)$ with the magnetization σ we find that:

$$\sigma = 1 - \frac{1}{\pi} \int_{-\Lambda}^{\Lambda} Z(\mu) \frac{dp(\lambda)}{d\lambda} d\lambda, \tag{2.124}$$

[14] In the excited states, some of the particles are repulsed beyond the ultraviolet cutoff Λ, leading to a fractional response, $\Delta\mathcal{N}$ to the number of the particles

which lead us to the conclustion that the $Z(\lambda)$ serves as the intrinsic magnetic moment of the elementary excitations.

The most important property of the fractional charge is the relation with the critical XXZ spin chain model, where it is defined as the critical exponent of the ground state's correlation function dominant oscillatory part, as predicted by CFT and Bethe Ansatz calculations [77, 78]. Finally, we should mention that in chapter 5 we will discuss its relation with the scattering matrix elements and the dominant scattering mechanism of spinon excitations by potentials.

$$\theta = 2\mathcal{Z}^2 \quad , \quad \mathcal{Z} \equiv Z(\Lambda) \tag{2.125}$$

Moreover, one can prove [45] that in the case $h = 0$ or equivalently $\Lambda = \infty$, $Z(0) = \frac{\pi}{\pi - 2\gamma}$

$$\lim_{\Lambda\to\infty} \mathcal{Z} = \sqrt{\frac{\pi}{\pi - 2\gamma}}. \tag{2.126}$$

Chapter 3

Algebraic Treatment of Quantum Integrable Systems

3.1 The invisible hand of Quantum Integrable Systems: Yang-Baxter Algebra

In 1776, Adam Smith, in his book "the wealth of the nations", came out with an analysis of market trends of production and consumption, where he concluded that the markets have a tendency of equilibration without any intervention, only by means of self interest and competition. He called this unseen force that moves the economy "*the invsible hand*". Metaphorically speaking one could say that there exists an algebraic structure that plays the role of the invisible hand behind all integrable systems, the well known *Yang-Baxter algebra*, introduced by C.N. Yang [32] and R. Baxter [33]. In fact, every integrable system must obey the Yang-Baxter equation and on the opposite direction every solution of the Yang-Baxter equation corresponds to an integrable system. To be more specific, we consider a quantum system and a matrix $\mathcal{R}(\lambda_1, \lambda_2)$, where $\lambda_1, \lambda_2 \in \mathbb{C}$ acting on a space $\mathcal{V}_1 \otimes \mathcal{V}_2$. Introducing a space $\mathcal{V}_1 \otimes \mathcal{V}_2 \otimes \mathcal{V}_3$ and the matrices $\mathcal{R}_{12}(\lambda_1, \lambda_2)$,$\mathcal{R}_{13}(\lambda_1, \lambda_3)$,$\mathcal{R}_{23}(\lambda_2, \lambda_3)$ the Yang-Baxter equation is

$$\mathcal{R}_{12}(\lambda_1, \lambda_2)\mathcal{R}_{13}(\lambda_1, \lambda_3)\mathcal{R}_{23}(\lambda_2, \lambda_3) = \mathcal{R}_{23}(\lambda_2, \lambda_3)\mathcal{R}_{13}(\lambda_1, \lambda_3)\mathcal{R}_{12}(\lambda_1, \lambda_2), \tag{3.1}$$

or equivalently in a more compact notation:

$$\begin{aligned}(\mathcal{R}(\lambda_1, \lambda_2) \otimes I)(I \otimes \mathcal{R}(\lambda_1, \lambda_3))(\mathcal{R}(\lambda_2, \lambda_3) \otimes I) = \\ (\mathcal{R}(\lambda_2, \lambda_3) \otimes I)(I \otimes \mathcal{R}(\lambda_1, \lambda_3))(\mathcal{R}(\lambda_1, \lambda_2) \otimes I).\end{aligned} \tag{3.2}$$

Each particular solution of eq.(3.1) generates a family of closely related integrable models.

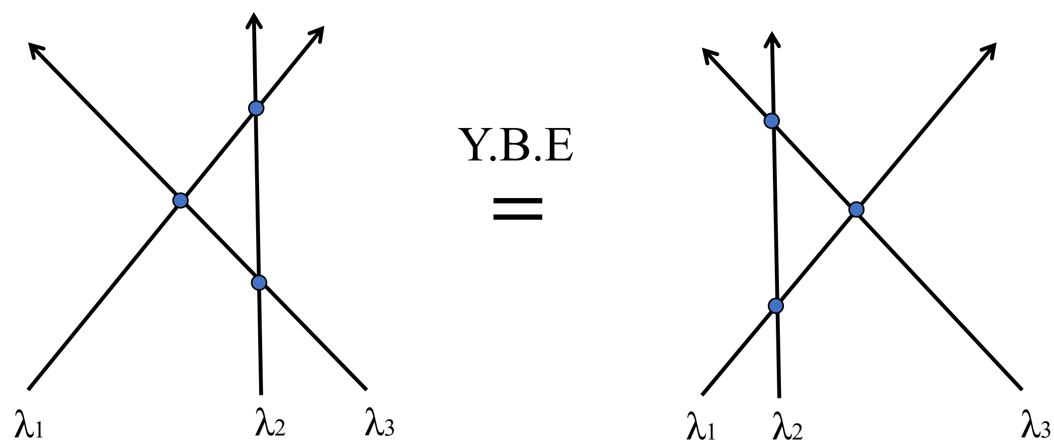

FIGURE 3.1: An illustration of the Yang-Baxter equation.

To give a specific example, a simple solution of the Yang-Baxter equation is

$$\mathcal{R}(\lambda,\mu) = f(\lambda,\mu)\Big[(\lambda-\mu)I + c\mathcal{P}\Big], \tag{3.3}$$

where $\mathcal{P} \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is the permutation matrix, $c \in \mathbb{C}$ is a constant and $f(\lambda_1,\lambda_2) : \mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C}$ is an arbitrary function.

The next step is to consider a physical Hilbert space $\mathcal{H}$ and enlarge it by introducing an auxiliary space $\mathcal{V}_a$. This will allow us to obtain an exact solution for the enlarged system and afterwards we will trace out the unwanted degrees of freedom. To this direction, to relate with integrable spin chains we assume a lattice system partitioned in N sites $\mathcal{H} = \bigotimes_{j=1}^{N} \mathcal{H}_j$ and introduce an operator called the *Lax operator* $\mathcal{L}_{ja} : \mathcal{H}_j \otimes \mathcal{V}_a$, which satisfies an equivalent of the Yang-Baxter relation

$$R(\lambda,\mu)\mathcal{L}_{j1}(\lambda)\mathcal{L}_{j2}(\mu) = \mathcal{L}_{j2}(\mu)\mathcal{L}_{j1}(\lambda)R(\lambda,\mu). \tag{3.4}$$

The above relation can be extended to the whole Hilbert space by introducing the *monodromy matrix* $\mathcal{T}_a(\lambda) = \prod_{j=1}^{N} \mathcal{L}_{ja}(\lambda) : \mathcal{H} \otimes \mathcal{V}_a \to \mathcal{H} \otimes \mathcal{V}_a$. Monodromy matrices give us another representation of the Yang-Baxter equation

$$R(\lambda,\mu)\mathcal{T}_1(\lambda)\mathcal{T}_2(\mu) = \mathcal{T}_2(\mu)\mathcal{T}_1(\lambda)R(\lambda,\mu), \tag{3.5}$$

and in fact can be thought as functions of the generators of the Yang-Baxter Algebra.

However, the monodromy matrix carries the unwanted auxiliary space, and thus a more appropriate quantity is the *transfer matrix* $\tau(\lambda) \equiv tr_a \mathcal{T}_a(\lambda) : \mathcal{H} \to \mathcal{H}$. The transfer matrix by definition obeys the commutation relation

$$[\tau(\lambda), \tau(\mu)] = 0, \quad \forall \lambda, \mu \in \mathbb{C} \tag{3.6}$$

Besides the obvious mathematical interest of eq.(3.6) and the fact that allow it us to simultaneously construct the spectrum of the system, it ensures that an infinite set of independent and in involution conservation charges can be constructed via the following expansion around a convenient point, λ_0 of the spectral parameter λ[1]

$$\ln \tau(\lambda) = \sum_{n=0}^{\infty} Q_n (\lambda - \lambda_0)^n, \quad Q_n = \frac{1}{n!} \frac{d^n}{d\lambda^n} \ln \tau(\lambda)|_{\lambda=\lambda_0}, \quad \lambda_0 \in \mathbb{C}. \tag{3.7}$$

S-matrix interpretation of the Yang-Baxter equation

Yang-Baxter equation can have a simple interpretation in terms of scattering matrices. To this end, let us take a detour and turn to a 1+1 integrable relativistic field theory. Massive particles of mass m_a, energy ϵ_a and momentum p_a in 1+1 dimensions can be parametrized as $\epsilon_a = m_a \cosh \theta_a$ and $p_a = m_a \sinh \theta_a$. The two particle elastic S-matrix is given by

$$|\theta_1, \theta_2\rangle^{in}_{\alpha\beta} = S^{\gamma\delta}_{\alpha\beta}(\theta_1 - \theta_2) |\theta_1, \theta_2\rangle^{out}_{\gamma\delta}, \tag{3.8}$$

where the momentum difference is due to the fact that we demand S to be a Lorentz invariant.

integrability is directly related to the existence of an infinite set of independent conserved charges $\{Q_n\}$ that are in involution. Using this condition A. Zamolodchikov and A. Zamolodchikov proved [79, 80] that for an integrable relativistic field theory: 1) there is no particle production, 2) the initial and final set of momenta are the same and 3) the S-matrix is factorisable. Notice that the first two conditions is the definition of *elastic* scattering.

Now, let us consider without loss of generality a three-body scattering[2] of particles with rapidities $\theta_1, \theta_2, \theta_3$. We are going to use the same idea for deriving the Bethe

[1] The point of expansion λ_0 is arbitrary and although different choices will end up with different sets of $\{Q_n\}$, all these are connected via linear transformations

[2] The three body scattering can be considered without any loss of generality, since any N-body scattering is a straightforward extension of the three-body scattering

equations by changing the order of the particles and demanding the possible routes to be equivalent. As an example, let us try the following permutation $(123) \to (321)$, which can be done via two two routes A and B:

$$\begin{aligned} A: &\quad (123) \to (132) \to (312) \to (321) \\ B: &\quad (123) \to (213) \to (231) \to (321) \end{aligned} \tag{3.9}$$

Since every permutation is associated with the act of the corresponding two-body S-matrix we obtain the Yang-Baxter equation

$$S_{12}(\theta_1 - \theta_2)S_{13}(\theta_1 - \theta_3)S_{23}(\theta_2 - \theta_3) = S_{23}(\theta_2 - \theta_3)S_{13}(\theta_1 - \theta_3)S_{12}(\theta_1 - \theta_2). \tag{3.10}$$

Equivalently, in explicit notation

$$\sum_{\gamma_1,\gamma_2,\gamma_3} S^{\alpha_1\alpha_2}_{\gamma_1\gamma_2}(\theta_{12})S^{\gamma_1\alpha_3}_{\beta_1\gamma_3}(\theta_{13})S^{\alpha_1\alpha_2}_{\gamma_1\gamma_2}(\theta_{23}) = \sum_{\gamma_1,\gamma_2,\gamma_3} S^{\alpha_2\alpha_3}_{\gamma_2\gamma_3}(\theta_{12})S^{\alpha_1\gamma_3}_{\gamma_1\beta_3}(\theta_{13})S^{\gamma_1\gamma_2}_{\beta_1\beta_2}(\theta_{23}), \tag{3.11}$$

where $\theta_{ij} \equiv \theta_i - \theta_j$.

At this point an interesting interpretation of the Yang-Baxter equation in term of scattering matrices arises. It expresses the condition that the three-particle scattering is determined by the two-particle scattering and is independent of which particles interact first. In this connection the Yang-Baxter equation is also called the factorization equation. A graphical representation is given in Fig.(3.2).

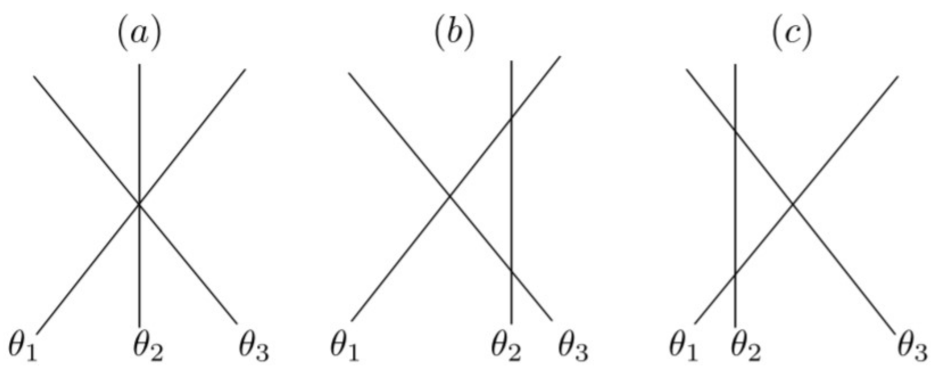

FIGURE 3.2: An illustration of three equivalent sacattering processes. Note the equivalence with the Yang-Baxter graphical representation.

3.2 The Algebraic Bethe Ansatz for the XXZ spin chain

The spin-1/2 model live in a Hilbert space

$$\mathcal{H} = \bigotimes_{k=1}^{N} H_k, \quad H_k \cong \mathbb{C}^2, \quad \dim \mathcal{H} = 2^N \tag{3.12}$$

The monodromy matrix can be written as a 2×2 matrix

$$\mathcal{T}(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda), \end{pmatrix} \tag{3.13}$$

where $A(\lambda), B(\lambda), C(\lambda), D(\lambda)$ are non-local operators acting on the Hilbert space $\mathcal{H}$

The corresponding $\mathcal{R}$ matrix is

$$\mathcal{R}(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda-\mu) & c(\lambda-\mu) & 0 \\ 0 & c(\lambda-\mu) & b(\lambda-\mu) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.14}$$

where

$$b(\lambda-\mu) = \frac{\varphi(\lambda-\mu)}{\varphi(\lambda-\mu+i\eta)}, \quad c(\lambda-\mu) = \frac{\varphi(i\eta)}{\varphi(\lambda-\mu+i\eta)}. \tag{3.15}$$

Using the $\mathcal{R}$-matrix it is possible to construct the quantum Lax-operator $\mathcal{L}$ of the model at site j as

$$\mathcal{L}_{ja}(\lambda-\xi_j) = \mathcal{R}_{ja}(\lambda-\xi_j) \tag{3.16}$$

The rapidities $\xi_j \in \mathbb{C}$ are arbitrary complex parameters called inhomogeneities. Their usefulness comes from the fact that they technically allow us to distinguish different sites of the spin chain. Moreover, they have a physical interpretation as being some kind of mathematically induced *impurities* with the property of preserving the integrable structure of the model.

In terms of spin operators

$$\mathcal{L}_{ja}(\lambda) = \frac{1}{\sin\gamma} \begin{pmatrix} \sinh\gamma(\lambda + iS_j^z) & \sin\gamma S_j^- \\ \sin\gamma S_j^+ & \sinh\gamma(\lambda - iS_j^z), \end{pmatrix} \tag{3.17}$$

where $S_j^z = \frac{1}{2}\sigma_j^z, \; S^{\pm} = \sigma^{\pm}$

An interesting interpretation of the Lax operator $\mathcal{L}_{ja}$ and the monodromy matrix $\mathcal{T}_a$ is given by [46], rewriting the operators as

$$\mathcal{L}_{ja}(\lambda) = \frac{1+\sigma_j^z\tau_a^z}{2} + t(\lambda)\frac{1-\sigma_j^z\tau_a^z}{2} + r(\lambda)(\sigma_j^+\tau_a^- + s_j^-\tau_a^+), \tag{3.18}$$

$$\mathcal{T}_a(\lambda) = \frac{1}{2}\tau(\lambda)I_a + \frac{1}{2}[A(\lambda)-B(\lambda)]\tau_a^z + B(\lambda)\tau_a^+ + C(\lambda)\tau_a^-, \tag{3.19}$$

where $\tau_a^{\pm}$ and τ_a^z are the Pauli matrices in the auxiliary space $\mathcal{V}_a$. The $r(\lambda) \equiv b(\lambda),\ t(\lambda) \equiv c(\lambda)$ are analogs of the reflection coefficient and transmission coefficients respectively in spin exchange process between the local spin in the physical space $\mathcal{H}_j$ and the spin in the auxiliary space $\mathcal{V}_a$. Therefore, the Lax-operator is a scattering matrix which describes the interaction of the physical and auxiliary spins, while the monodromy matrix describes the interaction of the auxiliary spin with the whole spin chain, with $C(\lambda)$ the global-spin raising operator in the physical space and $B(\lambda)$ the corresponding global-spin lowering operator.

If we substitute eq.(3.19) into the RTT Yang-Baxter equation eq.(3.5) we obtain the following commutation relations for the non-local operators A, B, C, D:

$$[A(\lambda), A(\mu)] = [B(\lambda), B(\mu)] = [C(\lambda), C(\mu)] = [D(\lambda), D(\mu)] = 0, \tag{3.20}$$
$$[A(\lambda), D(\mu)] = g(\lambda-\mu)\big\{C(\lambda)B(\mu) - C(\mu)B(\lambda)\big\}, \tag{3.21}$$
$$[D(\lambda), A(\mu)] = g(\lambda-\mu)\big\{B(\lambda)C(\mu) - B(\mu)C(\lambda)\big\}, \tag{3.22}$$
$$[B(\lambda), C(\mu)] = g(\lambda-\mu)\big\{D(\lambda)A(\mu) - D(\mu)A(\lambda)\big\}, \tag{3.23}$$
$$[C(\lambda), B(\mu)] = g(\lambda-\mu)\big\{A(\lambda)D(\mu) - A(\mu)D(\lambda)\big\}, \tag{3.24}$$
$$A(\lambda)B(\mu) = f(\mu-\lambda)B(\mu)A(\lambda) + g(\lambda-\mu)B(\lambda)A(\mu), \tag{3.25}$$
$$B(\lambda)A(\mu) = f(\mu-\lambda)A(\mu)B(\lambda) + g(\lambda-\mu)A(\lambda)B(\mu), \tag{3.26}$$
$$A(\lambda)C(\mu) = f(\lambda-\mu)C(\mu)A(\lambda) + g(\mu-\lambda)C(\lambda)A(\mu), \tag{3.27}$$
$$C(\lambda)A(\mu) = f(\lambda-\mu)A(\mu)C(\lambda) + g(\mu-\lambda)A(\lambda)C(\mu), \tag{3.28}$$
$$D(\lambda)B(\mu) = f(\lambda-\mu)B(\mu)D(\lambda) + g(\mu-\lambda)B(\lambda)D(\mu), \tag{3.29}$$
$$B(\lambda)D(\mu) = f(\lambda-\mu)D(\mu)B(\lambda) + g(\mu-\lambda)D(\lambda)B(\mu), \tag{3.30}$$
$$D(\lambda)C(\mu) = f(\mu-\lambda)C(\mu)D(\lambda) + g(\lambda-\mu)C(\lambda)D(\mu), \tag{3.31}$$
$$C(\lambda)D(\mu) = f(\mu-\lambda)D(\mu)C(\lambda) + g(\lambda-\mu)D(\lambda)C(\mu). \tag{3.32}$$

Furthermore, it is immediate from eq.(3.7) that the Hamiltonian is directly related to the transfer matrix τ. Specifically evaluating the derivative of the $\ln\tau$ at $\lambda = i\eta/2$ we obtain

$$H = \sin(i\eta)\frac{1}{2}\frac{d}{d\lambda}\ln\tau(\lambda)_{\lambda=i\eta/2}, \tag{3.33}$$

which leads to the conclusion that an arbitrary Bethe-eigenstate, $|\lambda_1, ..., \lambda_M\rangle$, is an eigenvector of the transfer matrix $\tau(\lambda) = A(\lambda) + D(\lambda)$.

In otder to be functional, the algebraic Bethe Ansatz technique needs one last ingredient. It requires the assumption that there exists a pseudo-vacuum state $|\Omega\rangle$ (not necessarily the true vacuum vector of the system) which serves as a reference in order to construct all Bethe states. For the XXZ model such a reference state exists[3] and as expected is the one where all the spin are up :

$$|\Omega\rangle = \bigotimes_{j=1}^{N} |\uparrow_j\rangle. \tag{3.34}$$

Since,

$$\mathcal{L}_{ja}(\lambda - \xi_j)|\uparrow_j\rangle = \begin{pmatrix} |\uparrow_j\rangle & c(\lambda-\xi_j)|\downarrow_j\rangle \\ 0 & b(\lambda-\xi_j)|\uparrow_j\rangle, \end{pmatrix} \tag{3.35}$$

we obtain that

$$\mathcal{T}_a = \begin{pmatrix} 1 & * \\ 0 & \prod_{j=1}^{N} b(\lambda-\xi_j) \end{pmatrix} |\Omega\rangle \tag{3.36}$$

Therefore,

$$A(\lambda)|\Omega\rangle = a(\lambda)|\Omega\rangle \quad , \quad \langle\Omega|B(\lambda) = 0 \tag{3.37}$$

$$C(\lambda)|\Omega\rangle = 0 \quad , \quad D(\lambda)|\Omega\rangle = d(\lambda)|\Omega\rangle, \tag{3.38}$$

$$\tag{3.39}$$

where

$$a(\lambda) = 1 \tag{3.40}$$

$$d(\lambda) = \prod_{j=1}^{N} b(\lambda - \xi_j). \tag{3.41}$$

Since the global-spin raising operator is $B(\lambda)$ every Bethe vector can be represented as

$$|\Psi_M\rangle \equiv \prod_{j=1}^{M} B(\lambda_j)|\Omega\rangle \tag{3.42}$$

[3] It is important to be mentioned that not all integrable models have reference state. For example

$$A(\mu)\prod_{j=1}^{M}B(\lambda_j)=\Lambda(\{\lambda_j\},\mu)\Big[\prod_{j=1}^{B}(\lambda_j)\Big]A(\mu)+B(\mu)\sum_{k=1}^{M}\Lambda_k(\{\lambda_j\},\mu)\Big[\prod_{j\neq k}^{M}B(\lambda_j)\Big]A(\lambda_k) \tag{3.43}$$

$$D(\mu)\prod_{j=1}^{M}B(\lambda_j)=W(\{\lambda_j\},\mu)\Big[\prod_{j=1}^{M}D(\lambda_j)\Big]A(\mu)+B(\mu)\sum_{k=1}^{M}W_k(\{\lambda_j\},\mu)\Big[\prod_{j\neq k}^{M}D(\lambda_j)\Big]A(\lambda_k) \tag{3.44}$$

$$\Lambda(\{\lambda_j\},\mu)=\prod_{j=1}^{M}\frac{1}{b(\lambda_j-\mu)},\quad \Lambda_k(\{\lambda_j\},\mu)=-\frac{c(\lambda_k-\mu)}{b(\lambda_k-\mu)}\prod_{j\neq k}^{M}\frac{1}{b(\lambda_j-\lambda_k)} \tag{3.45}$$

$$W(\{\lambda_j\},\mu)=\prod_{j=1}^{M}\frac{1}{b(\lambda_j-\mu)},\quad \Lambda_k(\{\lambda_j\},\mu)=-\frac{c(\lambda_k-\mu)}{b(\lambda_k-\mu)}\prod_{j\neq k}^{M}\frac{1}{b(\lambda_j-\lambda_k)} \tag{3.46}$$

Hence,

$$\begin{aligned}\tau(\mu)|\Psi_M\rangle=&\Big[a(\mu)\Lambda(\{\lambda_j\},\mu)+d(\mu)W(\{\lambda_j\},\mu)\Big]|\Psi_M\rangle+\\ &B(\mu)\sum_{k=1}^{M}\Big\{a(\lambda_k)\Lambda_k(\{\lambda_j\},\mu)+d(\lambda_k)W_k(\{\lambda_j\},\mu)\Big\}\Big[\prod_{j\neq k}^{M}D(\lambda_j)\Big]|\Omega\rangle\end{aligned} \tag{3.47}$$

So far we have assumed an arbitrary set of complex numbers $\{\lambda_j\}$, which does not diagonalize the transfer matrix $\tau(\mu)$. If we constrain this set such that :

$$a(\lambda_k)\Lambda_k(\{\lambda_j\},\mu)+d(\lambda_k)W_k(\{\lambda_j\},\mu)=0, \tag{3.48}$$

the transfer matrix is diagonalized and the rapidities satisfy the following equation

$$\frac{a(\lambda_k)}{d(\lambda_k)}\prod_{j\neq k}\frac{b(\lambda_k-\lambda_j)}{b(\lambda_j-\lambda_k)}=1 \tag{3.49}$$

or equivalently

$$\left(\frac{\varphi(\lambda_k+i\zeta/2)}{\varphi(\lambda_k-i\zeta/2)}\right)^N=\prod_{j\neq k}\frac{\varphi(\lambda_k-\lambda_j+i\zeta)}{\varphi(\lambda_k-\lambda_j-i\zeta)}, \tag{3.50}$$

giving us the Bethe equations which were derived using the coordinate Bethe-Ansatz in Chapter II.

3.3 Quantum Inverse scattering Method

In the previous sections we have used the non-local operators A, B, C, D in order to find the eigenvalues and eigenfunctions of the XXZ spin chain model. The next step would be to obtain expressions for local operators, which will allow us to have mathematical control over certain areas of our system. Although this may seems as an impossible task, since the auxiliary and the physical degrees of freedom are somewhat tangled(as matter of fact it is a very hard problem in general situations), we will derive elegant expressions for the XXZ spin chain model which relate local operators such as $\sigma_j^z, \sigma_j^-, \sigma_j^+\sigma_{j+1}^-$ with the non-local operators A, B, C, D. The general method for writing local degrees of freedom in terms of non-local degrees of freedom is called *the quantum inverse scattering method* developed by the Leningrad school [81, 82, 83]. The peculiar name "quantum inverse scattering" was given in order to relate with its classical analog called *inverse scattering method* a general method for solving classical 1+1 dimensional integrable systems as first described in a primitive form by C.S. Gardner, J. M. Greene, M D. Kruskal, and R M. Miura [31] and further developed by P. Lax [3]. The main idea of the inverse scattering method is to obtain the solution of an integrable non-linear partial differential equation, say $u(x,t)$ by associating it with a linear ordinary differential equation, where the solution $u(x,t)$ appears as a scattering potential of a Schrödinger-like equation [4, 84, 85, 86, 87, 88] . Therefore, by obtaining the asymptotic scattering-like data we can recover the scattering potential, which the desired solution of our initial problem.

To start with we consider an *inhomogeneous* XXZ spin chain, with inhomogeneities ξ_j. Our main goal is to associate an arbitrary local operator $\mathcal{F}_n$ acting non-trivially in the space $\mathcal{H}_m$ in terms of a global operator $\mathcal{F}_a$ acting in the auxiliary space $\mathcal{V}_a$. This can be done using the following identity proven in [89]

$$\mathcal{F}_n = \Big(\prod_{k=1}^{n-1} \tau(\xi_k)\Big) \mathrm{tr}_a[\mathcal{F}_a \mathcal{T}_a(\xi_n)] \Big(\prod_{k=1}^{n} \tau^{-1}(\xi_k)\Big) \tag{3.51}$$

To consider local operators of the usual XXZ spin chain with set $\xi_j = \xi$. Therefore

$$\mathcal{T}_a(\xi_k) = \mathcal{T}_a(\xi) = \mathcal{P}_{1a}\mathcal{W} \tag{3.52}$$

$$\mathcal{W} = \prod_{j=0}^{N-2} \mathcal{P}_{1N-k} = \mathcal{P}_{123\ldots N} = \mathcal{T} \tag{3.53}$$

This solution was first given by N Kitanine,V Teras and JM Maillet [6] with the help of a complex algebraic structure, the *F-basis*.

Note that $\mathcal{P}_{1,a}$ can be written as

$$\mathcal{P}_{a1} = \frac{1 + \vec{\sigma}_1 \cdot \vec{\tau}_a}{2} \tag{3.54}$$

$$\mathcal{T}_a(\xi) = \frac{1 + \vec{\sigma}_1 \cdot \vec{\tau}_a}{2} \mathcal{W}, \tag{3.55}$$

where $\mathcal{T}_a$ is given by eq.(3.19)

Therefore, the local operators $\mathcal{I}, \sigma_1^z, \sigma_1^{\pm}$ are given by

$$\mathcal{I} = [A(\xi) + D(\xi)]\mathcal{W}^{-1} \tag{3.56}$$

$$\sigma_1^z = [A(\xi) - D(\xi)]\mathcal{W}^{-1} \tag{3.57}$$

$$\sigma_1^+ = C(\xi)\mathcal{W}^{-1} \tag{3.58}$$

$$\sigma_1^- = B(\xi)\mathcal{W}^{-1} \tag{3.59}$$

Using the above relations we find that the local operators acting non-trivially in the subspace $\mathcal{H}_n$ are given by:

$$\sigma_n^z = \tau(\xi)^{n-1}\Big(A(\xi) - D(\xi)\Big)\tau(\xi)^{N-n} \tag{3.60}$$

$$\sigma_n^- = \tau(\xi)^{n-1}B(\xi)\ \tau(\xi)^{N-n} \tag{3.61}$$

$$\sigma_n^+ = \tau(\xi)^{n-1}C(\xi)\ \tau(\xi)^{N-n} \tag{3.62}$$

$$\tag{3.63}$$

The general inhomogeneous case is:

$$\sigma_n^z = \prod_{k=1}^{n-1} \tau(\xi_k)\Big(A(\xi_n) - D(\xi_n)\Big) \prod_{k=n+1}^{N} \tau(\xi_k) \tag{3.64}$$

$$\sigma_n^- = \prod_{k=1}^{n-1} \tau(\xi_k)\ B(\xi_n) \prod_{k=n+1}^{N} \tau(\xi_k) \tag{3.65}$$

$$\sigma_n^+ = \prod_{k=1}^{n-1} \tau(\xi_k)\ C(\xi_n) \prod_{k=n+1}^{N} \tau(\xi_k), \tag{3.66}$$

where we have used the fact that the propagator through the whole chain gives the identity $\prod_{k=1}^{N} \tau(\xi_k) = I$.

3.4 Inner products and matrix elements

The present section is devoted to the study of scalar/inner products and matrix elements. Firstly, we begin with the presentation of the scalar products and the norm of a Bethe state and thereafter we proceed to a sketch of proof regarding the derivation of the Matrix elements for a longitudinal, transverse and a spin-phonon potential.

3.4.1 Scalar product of an eigenstate with an arbitrary state

Let $\{\lambda_k\}_{k=1}^{M}$ be a solution of the Bethe equations and $\{\mu_j\}_{j=1}^{M}$ be an arbitrary set of parameters. Then the scalar product between these two states can be represented via the following formula [45]

$$S_M(\{\mu_j\},\{\lambda_j\}) = \frac{\det H(\{\mu_j\},\{\lambda_j\})}{\prod_{j>k}\varphi(\mu_k-\mu_j)\prod_{j<k}\varphi(\lambda_k-\lambda_j)}, \tag{3.67}$$

where

$$H_{\alpha\beta} = \frac{\varphi(i\eta)}{\varphi(\lambda_a-\lambda_b)}\left(r(\mu_b)\prod_{l\neq\alpha}\varphi(\lambda_l-\mu_b+i\eta) - \prod_{l\neq\alpha}\varphi(\lambda_l-\mu_b-i\eta)\right). \tag{3.68}$$

Gaudin's Formula for the Norm of eigenstates

Taking the limit $\mu_j \to \lambda_j$ one can prove the Gaudin formula for the square of the norm of the Bethe wavefunction.

$$\mathcal{N}_M = \langle 0|\prod_{j=1}^{M}\mathbb{C}(\mu_j)\prod_{k=1}^{M}\mathbb{C}(\lambda_k)|0\rangle\Big|_{\{\lambda_j^C\},\{\lambda_k^B\}}. \tag{3.69}$$

Taking the limit $\mu_j \to \lambda_j + \varepsilon$ we can Taylor expand $r(\mu)$

$$r(\mu) = r(\lambda)\left(1+\varepsilon\frac{\partial}{\partial\mu}\ln r(\mu)\right)_{\mu\to\lambda} \tag{3.70}$$

Inserting this relation to the scalar product S_N we get

$$\mathcal{N}_M = \varphi(\eta)^M \prod_{j\neq k}\frac{\varphi(\lambda_j-\lambda_k+\eta)}{\varphi(\lambda_j-\lambda_k)}\det\Phi(\{\lambda_j\}), \tag{3.71}$$

where Φ is the Gaudin matrix and is defined as

$$\Phi_{ab} \equiv -\frac{\partial}{\partial \lambda_b} \ln \left(r(\lambda_\alpha) \prod_{k \neq \alpha}^{M} \frac{b(\lambda_k, \lambda_\alpha)}{b(\lambda_\alpha, \lambda_k)} \right). \tag{3.72}$$

Finally using the fact that from the Bethe equations follows that $\prod_{i=1}^{M} d(\lambda_i) = 1$ we find the norm in the following form:

$$N_M = \varphi(\eta)^M \prod_{j \neq k} \frac{\varphi(\lambda_j - \lambda_k + \eta)}{\varphi(\lambda_j - \lambda_k)} \det \Phi(\{\lambda_j\}). \tag{3.73}$$

3.4.2 Matrix Elements

The present section is a short presentation regarding the calculation of *form factors* and subsequently the matrix elements. In particular, we derive expressions for the form factors of the local spin operators for the XXZ spin chains. The novel work of N. Kitanine, J.M Mailet and V. Terras [6] opened a new era for the calculation of correlations functions and matrix elements due to the fact that it sharply decreased the complexity needed in order to calculate matrix elements. In particular, before the appearance of the algebraic calculation of matrix elements, one would need either to diagonalize the Hamiltonian with complexity $\mathcal{O}(2^N)$ or by evaluating the summation in the wavefunction over the $M!$ magnon permutations, having complexity of at least $\mathcal{O}((M!)^2)$. In contrast, the algebraic treatment of the matrix elements reduces the complexity for each matrix element to approximately $\mathcal{O}(M^2)$, thus, making it technically feasible to calculate matrix elements for relatively large spin chains with $N \sim 1000$ spin sites. Let us mention that the Kitanine, Mailet and Terras formulas allowed for an accurate theoretical study of low temperature neutron scattering experiments due to the fact that they allowed the calculation of ground state transitions elements for large spin chains. For the interested reader we cite a small sample of relevant research that has been conducted in this area [9, 61, 90, 91, 74, 92, 93].

Transverse form factor

Firstly, we begin by introducing the form factors

$$F_n^-(\{\lambda_k\}, \{\mu_j\}) \equiv \langle 0| \prod_{j=1}^{M+1} C(\mu_j) \sigma_n^- \prod_{k=1}^{M} B(\lambda_k) |0\rangle, \tag{3.74}$$

$$F_n^+(\{\mu_j\}, \{\lambda_k\}) \equiv \langle 0| \prod_{j=1}^{M} C(\lambda_k) \sigma_n^+ \prod_{k=1}^{M+1} B(\mu_j) |0\rangle, \tag{3.75}$$

where both sets $\{\mu_j\}, \{\lambda_j\}$ are solutions of the Bethe equations.

The corresponding matrix elements is then simply expressed as

$$\langle\{\mu\}|\sigma_n^{\pm}|\{\lambda\}\rangle = \frac{F_n^{\pm}(\{\lambda_k\},\{\mu_j\})}{\sqrt{\mathcal{N}(\{\lambda_j\})\cdot\mathcal{N}(\{\mu_j\})}}. \tag{3.76}$$

To calculate the first form factor we recall that the σ_n^- operator is expressed as

$$\sigma_n^- = \prod_{j=1}^{n-1}\tau(\xi_j)B(\xi_n)\prod_{j=n+1}^{N}\tau(\xi_j) \tag{3.77}$$

and the fact that

$$\tau(\xi_j)\prod_{k=1}^{M}B(\lambda_k)|0\rangle = \left(a(\xi_j)\prod_{i=1}^{M}b^{-1}(\lambda_i,\xi_j) + d(\xi_j)\prod_{i=1}^{M}b^{-1}(\xi_j,\lambda_i)\right)\prod_{k=1}^{M}B(\lambda_k)|0\rangle. \tag{3.78}$$

Moreover, note that $d(\xi_j)=0$ and that for $\{\lambda_j\}$ satisfying the Bethe equations it holds that $\prod_{k=1}^{M}\prod_{j=1}^{N}b^{-1}(\lambda_k,\xi_j)=1$.

The act of σ_n^- operator results in a scalar product between a Bethe eigenstate characterized by the set $\langle\mu_j\}_{j=1}^{M}$ and a non-eigenstate characterized by the set $\{\lambda_j\}_{j=1}^{M}$ accompanied by the inhomogeneity $\{\xi_j\}$. Hence,

$$\begin{aligned} F_n^-(\{\lambda_k\},\{\mu_j\}) = &\left(\prod_{j=1}^{M+1}\prod_{k=1}^{n-1}b^{-1}(\lambda_j,\xi_k)\right)\times\left(\prod_{j=1}^{M+1}\prod_{k=n+1}^{N}b^{-1}(\lambda_j,\xi_k)\right)\\ &\times\langle 0|\prod_{j=1}^{M+1}C(\mu_j)B(\xi_n)\prod_{k=1}^{M}B(\lambda_k)|0\rangle \end{aligned} \tag{3.79}$$

Or equivalently using eq.(3.67)

$$F_n^-(\{\lambda_k\},\{\mu_j\}) = \phi_m^{-1}(\{\lambda_k\})\phi_{m-1}(\{\mu_j\})S_{M+1}(\{\mu_j\},\{\xi_m,\lambda_1,...,\lambda_n\}), \tag{3.80}$$

where

$$\phi_n(\{\lambda_k\}) \equiv \prod_{k=1}^{M}\prod_{j=1}^{n}b^{-1}(\lambda_k,\xi_j) \tag{3.81}$$

Note that, in the homogeneous limit $\xi_j = 0, j = 1, ..., N$. The coefficients $\phi_n(\{\lambda_k\})$ are expressed in terms of the total momentum P

$$\phi_n(\{\lambda_k\}) = e^{-iPn} \tag{3.82}$$

$$P = \frac{i}{N} \sum_{k=1}^{n} \ln r(\lambda_k). \tag{3.83}$$

Finally, the form factor $F_n^-(\{\lambda_k\}, \{\mu_j\})$ is expressed as follows

$$F_n^-(\{\mu_j\}, \{\lambda_k\}) = \frac{\phi_{n-1}(\{\mu_j\})}{\phi_{n-1}(\{\lambda_k\})} \frac{\prod_{k=1}^{M+1} \varphi(\mu_k - \xi_j + i\eta)}{\prod_{k=1}^{M} \varphi(\lambda_k - \xi_j + i\eta)} \frac{\det H^-(\{\mu_j\}, \{\lambda_k\})}{\prod_{l>m} \varphi(\mu_l - \mu_m) \prod_{l<m}^{M} \varphi(\lambda_l - \lambda_m)}, \tag{3.84}$$

$$H_{\alpha b}^- = \frac{\varphi(i\eta)}{\varphi(\mu_\alpha - \lambda_b)} \left(\alpha(\lambda_b) \prod_{j \neq \alpha}^{M+1} \varphi(\mu_j - \lambda_b + i\eta) - d(\lambda_b) \prod_{j \neq \alpha}^{M+1} \varphi(\mu_j - \lambda_b - i\eta) \right), \quad b < M+1$$
$$H_{\alpha M+1}^- = \frac{\varphi(i\eta)}{\varphi(\mu_\alpha - \xi_j + i\eta)\varphi(\mu_\alpha - \xi_j)}. \tag{3.85}$$

We should mention that the H^- matrix is derived from H by using the fact that $\lambda_{M+1} = \xi_j$

Longitudinal form factor

We continue with the calculation of the longitudinal matrix element. The corresponding form factor is defined as

$$F_n^z(\{\mu_j\}, \{\lambda_k\}) = \langle 0| \prod_{j=1}^{M} C(\mu_j) \sigma_n^z \prod_{k=1}^{M} B(\lambda_k) |0\rangle, \tag{3.86}$$

while similar to the previous case the matrix elements are expressed as

$$\langle \{\lambda\} | \sigma_n^z | \{\lambda\} \rangle = \frac{F_n^z(\{\mu_j\}, \{\lambda_k\})}{\sqrt{\mathcal{N}(\{\lambda\}) \mathcal{N}(\{\mu\})}}. \tag{3.87}$$

To begin with, we use that σ_n^z is expressed in terms of the non-local operators as follows

$$\sigma_n^z = \prod_{k=1}^{n-1} \tau(\xi_k) \Big(A(\xi_n) - D(\xi_n) \Big) \prod_{k=n+1}^{N} \tau(\xi_k) \tag{3.88}$$

Using that $\prod_{k=1}^{N} \tau(\xi_k) = I$ we obtain the following form for σ_n^z

$$\sigma_n^z = 2 \prod_{\alpha=1}^{n-1} \tau(\xi_\alpha) A(\xi_n) \prod_{\alpha=n+1}^{N} \tau(\xi_\alpha) - I. \tag{3.89}$$

Therefore, the form factor will have the form

$$F_n^z(\{\mu_j\},\{\lambda_k\}) = 2\phi_n^{-1}(\{\lambda_k\})\phi_{n-1}(\{\mu_j\})P_1(\xi_n,\{\mu_j\},\{\lambda_k\}) - S_M(\{\mu_j\},\{\lambda_k\}) \tag{3.90}$$

To calculate the form of the function P_1, we shall make use of the action of the A operator on an arbitrary state

$$\begin{aligned} A(\xi_n) \prod_{k=1}^{M} B(\lambda_k)|0\rangle =& \prod_{k=1}^{M} b^{-1}(\lambda_k,\xi_m) \prod_{k=1}^{n} B(\lambda_k)|0\rangle \\ & - \sum_{\alpha=1}^{N} \frac{\phi(i\eta)}{\phi(\lambda_\alpha - \xi_n)} \prod_{k\neq\alpha} b^{-1}(\lambda_k - \lambda_a) B(\xi_n) \prod_{k\neq\alpha}^{M} B(\lambda_k)|0\rangle \end{aligned} \tag{3.91}$$

Taking the assumption that $\{\lambda_j\} \neq \{\mu_k\}$, i.e. that the two Bethe states are orthogonal we are left with

$$\begin{aligned} F_n^z(\{\mu_j\},\{\lambda_k\}) = -2\phi_n^{-1}(\{\lambda_k\})\phi_{n-1}(\{\mu_j\}) \sum_{\alpha=1}^{N} \frac{\phi(i\eta)}{\phi(\lambda_\alpha - \xi_n)} \left(\prod_{k\neq\alpha}^{M} \frac{\phi(\lambda_k - \lambda_\alpha + i\eta)}{\phi(\lambda_k - \lambda_\alpha)} \right) \\ \times \langle 0| \prod_{j=1}^{M} C(\mu_j) B(\xi_n) \prod_{k\neq\alpha}^{M} B(\lambda_k)|0\rangle \end{aligned} \tag{3.92}$$

each scalar product can be written according to (**??**) as

$$\langle 0| \prod_{j=1}^{M} C(\mu_j) B(\xi_n) \prod_{k\neq\alpha}^{M} B(\lambda_k)|0\rangle = \frac{\det H(\{\mu_j\},\{\lambda_k\})}{\prod_{j>k} \phi(\mu_j - \mu_k) \prod_{j<k} \phi(\lambda_j - \lambda_k)} \quad , \quad \lambda_a = \xi_n \tag{3.93}$$

Extracting the n-th product factor from $\phi_n(\{\mu_j\})$, i.e.

$$\phi_n(\{\lambda_k\}) = \phi_{n-1}(\{\lambda_k\}) \prod_{k=1}^{M} \frac{\varphi(\lambda_k - \xi_n + i\eta)}{\varphi(\lambda_k - \xi_n)}, \tag{3.94}$$

multiplying the α-th column with the factor $-2\prod_{k=1}^{M}\varphi(\lambda_k-\lambda_\alpha+i\eta)$ and dividing the α-th column by the factor $\prod_{k=1}^{M}\varphi(\mu_k-\xi_n+i\eta)$

We get the following result

$$F_n^z(\{\mu_j\},\{\lambda_k\}) = \frac{\phi_{n-1}(\{\mu_j\})}{\phi_{n-1}(\{\lambda_k\})}\prod_{j=1}^{M}\frac{\varphi(\mu_j-\xi_n+i\eta)}{\varphi(\lambda_j-\xi_n+i\eta)}\frac{\det H^\alpha}{\prod_{j>k}\varphi(\mu_k-\mu_j)\prod_{\alpha<\beta}\varphi(\lambda_\beta-\lambda_\alpha)}, \tag{3.95}$$

where

$$\begin{aligned} H^\alpha_{ln} &= \frac{\varphi(i\eta)}{\varphi(\mu_l-\lambda_n)}\left(\alpha(\lambda_n)\prod_{j\neq l}^{n}\varphi(\mu_j-\lambda_n+i\eta)-d(\lambda_n)\prod_{j\neq m}^{n}\varphi(\mu_j-\lambda_n-i\eta)\right),\\ H^\alpha_{l\alpha} &= -2P_{l\alpha}, \end{aligned} \tag{3.96}$$

where

$$P_{ln} = \frac{\varphi(i\eta)}{\varphi(\mu_l-\xi_n)\varphi(\mu_l-\xi_n+i\eta)}\prod_{k=1}^{n}\varphi(\lambda_k-\lambda_n+i\eta). \tag{3.97}$$

One can immediately see that the P matrix is a matrix of rank $r(P)=1$. Note that the final formula is as of scalar products. In fact, it can be simplified using the fact that if $\mathcal{A}$ is an arbitrary $n\times n$ matrix and $\mathcal{B}$ a rank one $n\times n$ matrix, the determinant of the sum $\mathcal{A}+\mathcal{B}$ is

$$\det(\mathcal{A}+\mathcal{B}) = \det\mathcal{A}+\sum_{k=1}^{n}\det\mathcal{A}^{(k)}, \tag{3.98}$$

where

$$\mathcal{A}^{(k)}_{ab} = \mathcal{A}_{ab}, \quad b\neq k \tag{3.99}$$

$$\mathcal{A}^{(k)}_{ak} = \mathcal{B}_{ak} \tag{3.100}$$

Finally using that $\det(P)=0$, we obtain the following formula

$$F_n^z(\{\mu_j\},\{\lambda_k\}) = \frac{\phi_{n-1}(\{\mu_j\})}{\phi_{n-1}(\{\lambda_k\})}\prod_{j=1}^{M}\frac{\varphi(\mu_j-\xi_n+i\eta)}{\varphi(\lambda_j-\xi_n+i\eta)}\frac{\det_M\left[H(\{\mu_j\},\{\lambda_k\})-2P(\{\mu_j\},\{\lambda_k\})\right]}{\prod_{j>k}\varphi(\mu_k-\mu_j)\prod_{\alpha<\beta}\varphi(\lambda_\beta-\lambda_\alpha)}, \tag{3.101}$$

Form factor of spins at adjacent sites

Finally, we wish to compute the $\langle\{\lambda\}\rangle|\sigma_n^-\sigma_{n+1}^+|\{\mu\}\rangle$ matrix element. The corresponding form factor is

$$F_n^{-+}(\{\mu_j\},\{\lambda_k\}) \equiv \langle 0|\prod_{j=1}^{M} C(\mu_j)\sigma_n^-\sigma_{n+1}^+\prod_{k=1}^{M} B(\lambda_k)|0\rangle \tag{3.102}$$

Similarly with the previous cases we use that the propagator over the whole chain equals to the identity matrix, which gives that

$$F_n^{-+}(\{\mu_j\},\{\lambda_k\}) = \phi_{n-1}(\{\mu_j\})\phi_{n+1}^{-1}(\{\lambda_k\})\langle 0|\prod_{j=1}^{M} C(\mu_j)B(\xi_n)C(\xi_{n+1})\prod_{k=1}^{M} B(\lambda_k)|0\rangle \tag{3.103}$$

Recall that the action of the operator $C(\xi_{m+1})$ on a Bethe eigenvector is

$$C(\xi_{m+1})\prod_{k=1}^{n} B(\lambda_k)|0\rangle = \sum_{l=1}^{n} M_l \prod_{j\neq l}^{n} B(\lambda_l)|0\rangle + \sum_{l>m}^{n} M_{l,m}B(\xi_{m+1})\prod_{k\neq l,m} B(\lambda_k)|0\rangle, \tag{3.104}$$

where

$$M_l = \frac{\varphi(\eta)}{\varphi(\lambda_l-\xi_{m+1})d(\lambda_l)}\prod_{k\neq l}^{n}\big(b^{-1}(\lambda_k,\xi_{m+1})b^{-1}(\lambda_\alpha,\lambda_k)\big) \tag{3.105}$$

and

$$\begin{aligned} M_{lb} = &-\frac{\varphi^2(\eta)}{\varphi(\lambda_l-\xi_{m+1})\varphi(\lambda_b-\xi_{m+1})}d(\lambda_l)b^{-1}(\lambda_l,\lambda_b) \\ &\times\prod_{k\neq l,b}^{n}\big(b^{-1}(\lambda_k,\lambda_b)b^{-1}(\lambda_l,\lambda_k)\big) \end{aligned} \tag{3.106}$$

Therefore we obtain

$$\begin{aligned} F_n^{-+}(\{\mu_j\},\{\lambda_k\}) &= \phi_{n-1}(\{\mu_j\})\phi_{n+1}^{-1}(\{\lambda_k\}) \\ &\times\left(\sum_{l=1}^{M} M_l S_n(\{\mu_j\},\{\xi_n,\lambda_1,...,\hat{\lambda}_l,...,\lambda_M\})\right. \\ &\left.\quad+\sum_{l\neq b} M_{lb}S_M(\{\mu_j\},\{\xi_n,\xi_{n+1},\lambda_1,...,\hat{\lambda}_l,\hat{\lambda}_b,...,\lambda_M\})\right) \end{aligned} \tag{3.107}$$

Chapter 4

Scattering of Spinon excitations by Potentials

In this chapter using a semi-analytical Bethe ansatz method and a T-matrix approach we study the scattering of a spinon, the elementary quantum many-body topological excitation in the 1D Heisenberg model, by local and phonon potentials. In particular, we compare the scattering of a spinon to that of a free spinless fermion in the XY model to highlight the effect of strong correlations. For the one spinon scattering in an odd-site chain, we find a regular behavior of the scattering coefficients. In contrast, in an even-site chain there is a transfer of transmission probability between the two spinon branches that grows exponentially with system size. We link the exponent of the exponential behavior to the dressed charge that characterizes the critical properties of the 1D Heisenberg model, an interplay of topological and critical properties. The aim of this study is a microscopic understanding of spinon scattering by impurities, barriers or phonons, modeled as prototype potentials, an input in the analysis of quantum spin transport experiments. More abstractly, we approach and point out the fundamental question of "*how does a quantum many-body topological excitation scatters from a potential?*". The first section is a very brief introduction to the basic tools of scattering theory. The next section are devoted to the spinon scattering.

4.1 Introduction: Motivation for this work

The novel mode of thermal transport by magnetic excitations in quasi-one dimensional quantum magnets has been over the last few years the focus of extensive experimental [94] and theoretical studies [26, 95, 25, 96, 97, 98]. It was promoted by the fortuitous coincidence of synthesis of excellent quality compounds very well described by prototype integrable spin chain models and the proposal of unconventional -ballistic- spin and thermal transport in these systems [95]. Of course the purely ballistic thermal transport predicted by theory is not observed in thermal conduction experiments as the, albeit very high, thermal conductivity is limited by the scattering of the magnetic excitations from impurities and phonons [94].

In parallel, in the field of spintronics (spin caloritronics) there is renewed interest in the transport of magnetization, with the (inverse) spin Hall and spin Seebeck effect employed for the generation and detection of spin currents [99, 100]. So far mostly metallic, semiconducting and magnetically ordered (ferro, antiferro, ferri) magnetic materials have been studied. Only very recently the spin Seebeck effect was studied in the quasi-one dimensional quantum magnet Sr_2CuO_3 accurately described by a spin-1/2 Heisenberg chain [51].

Regarding quasi-one dimensional quantum magnets, a lot is known on their bulk thermodynamic [101] and magnetothermal transport properties [102, 103, 104]. The prototype model for these systems is the well studied 1D Heisenberg model that is analytically solvable by the Bethe ansatz (BA) method. The elementary excitations in this strongly correlated system are topological in nature- the spinons [20] - and most of thermodynamic and transport experiments are discussed in terms of these low energy excitations [94, 96, 105].

In this work, we study the scattering of a spinon from local potentials aiming at a microscopic understanding of scattering processes by impurities, phonons and barriers, relevant to (far-out of equilibrium) quantum spin transport. At the moment, we do not address any particular experiment, we only present background work on the theoretical question, *how does a quantum many-body topological excitation scatters from a potential ?*[106]. This question is also relevant in other systems with topological excitations of actual experimental and theoretical interest.

To this end, we first use a recently developed semi-analytical Bethe ansatz method [6, 7] to evaluate scattering matrix elements by prototype potentials and then to evaluate scattering coefficients by a T-matrix method. We should emphasize that although it is an elementary exercise to evaluate the quantum mechanical scattering coefficients (reflection, transmission) of a free particle from a potential barrier, little is known on the scattering of a quantum many-body quasi-particle excitation even more so for a topological one. The Bethe ansatz solvable models offer exactly such a framework for the study of this fundamental problem.

Defining the Basic Quantities

The model which is considered is the XXZ gapless/easy-plane anisotropic Heisenberg Hamiltonian for a chain of N sites with periodic boundary conditions $S^a_{N+1} = S^a_1$ and in the presence of a local potential V of strength g, given by:

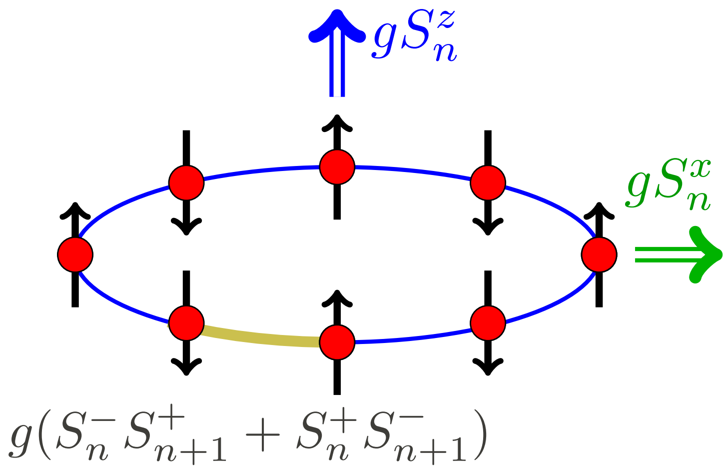

FIGURE 4.1: Schematic figure of the spin chain and the type of potentials in consideration.

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

where h is the magnetic field, $\Delta = \cos\gamma$. Moreover, note that throught this chapter we take $J = 1$.

Additionally, let us mention that we study chains with odd as well as even number N of spins. In odd chains, for each total $S^z = \pm 1/2$, as described in chapter 2, the ground state is doubly degenerate containing one spinon with dispersion given by the one-branch $\varepsilon_Q = v_s|\sin Q|, \quad 0 < Q < \pi$. For even N the lowest excitations involve at least two spinons, the dispersion of each spinon given by $\varepsilon_Q = v_s|\sin Q|$ i.e. states of the Cloizeaux-Pearson spinon spectrum [?, ?]. We will study states belonging to the lowest energy branch of the $M = N/2 - 1$ magnetization sector and obtained from the $S^z = 1$ states by keeping the one spinon momentum fixed at zero and considering the dispersion of the second. In the spinon dispersion, $v_s = \frac{\pi}{2}\frac{\sin\gamma}{\gamma}$ and Q is defined as the spinon momentum above the ground state. The matrix elements between two Bethe states describe a scattering process. Moreover we define the spinon group velocity as $u_Q = d\varepsilon_Q/dQ$.

4.2 Description of scattering matrix elements

In this section we evaluate the scattering matrix elements $|\mathcal{M}|^2 = |\langle Q'|V|Q\rangle|^2$ of a spinon from a state of momentum Q to a state of momentum Q' on finite size lattices using the Kitanine-Maillet-Terras formulas described in chapter 3. In particular, we consider three different types of potential interactions, namely, a longitudinal potential, a transverse potential and a spin-phonon lattice distortion known as ”weak link”. Note that, throughout this process we only depict the matrix between the lowest lying excitations due to the fact that they are of most importance for the scattering procedure. Nevertheless, the computation of scattering coefficients includes matrix elements between arbitrary two-spinon states in the even case, while in the odd case we are restricted to one-spinon states. In addition, we describe two classes of matrix elements, namely $Q \to \pi + Q$ and $Q \to \pi - Q$ transitions, since they have the most important impact in the system and for this reason we call them Dominant matrix elements.

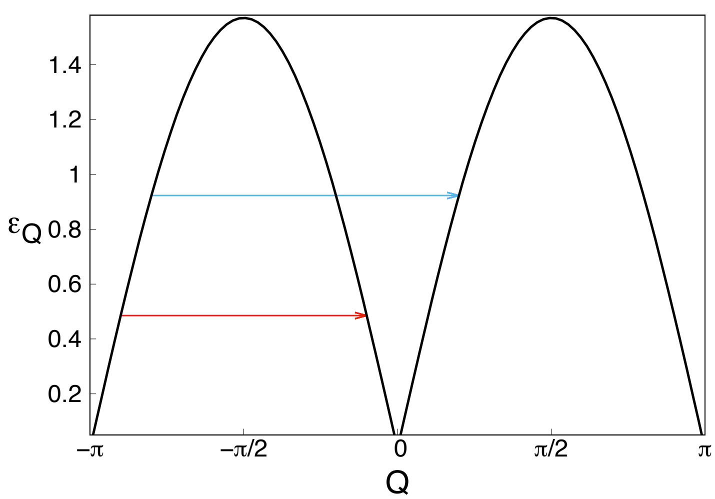

FIGURE 4.2: Schematic description of the $Q \to \pi + Q$ transition (blue) and $Q \to \pi - Q$ same branch velocity flipping transition (red).

4.2.1 Longitudinal potential

To start with the one site longitudinal potential is modeled by the interaction term

$$V = gS_n^z \tag{4.1}$$

The corresponding matrix element is given by

$$|\mathcal{M}_q^z(Q)|^2 = | < Q + q|S_q^z|Q > |^2, \tag{4.2}$$

where $S_n^z = \frac{1}{\sqrt{N}} \sum_q e^{-iqn} S_q^z$.

In the simple $\Delta = 0$ case (XY model) by a Jordan-Wigner transformation the spectrum corresponds to that of free spinless fermions, $|M_q^z|^2 = 1/N$ and the potential moves only one fermion to a different state [107].

In sharp contrast, in the isotropic Heisenberg model ($\Delta = 1$), due to strong anti-ferromagnetic fluctuations, the scattering matrix elements are drastically enhanced as shown in Fig.4.3. $|\mathcal{M}_q^z(Q = 0)|^2$ scales in overall as $1/\sqrt{N}$ and as indicated in the inset of Fig.4.3 in the region not close to $q = 0, \pi$ the matrix element behaves approximately as

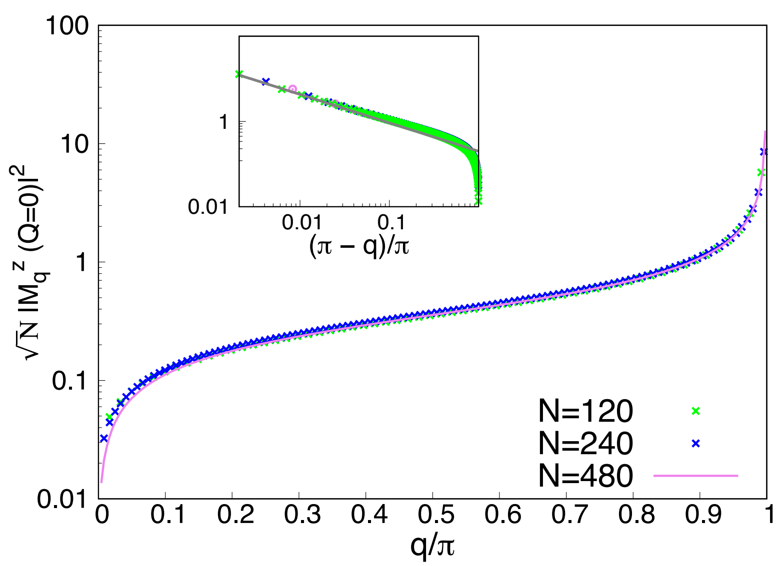

FIGURE 4.3: Scaled $\sqrt{N}|\mathcal{M}_q^z(Q = 0)|^2$ as a function of q/π for $N = 120, 240, 360, 480$, $\Delta = 1$. In the inset the asymptotic scaling of $|\mathcal{M}_q^z(Q = 0)|^2$ with a solid line indicating the asymptote $(\pi - q)^{2/3}$.

$$|\mathcal{M}_q^z(Q = 0)|^2 \sim \frac{1}{\sqrt{N}} \frac{1}{(\pi - q)^{2/3}}. \tag{4.3}$$

Note that this behavior does not describe the $q = \pi$, which should not be diverging and scales differently with N, as will be discussed below.

The most interesting part in Fig.4.3 and relation (4.3) is that the matrix elements scale in a non-trivial fashion with N. In the XY model and for a S_n^z potential all matrix elements scale as $1/N$ which is the usual case in lattice scattering. On the contrary for all $\Delta \neq 0$ the matrix elements have a non trivial relation with respect to the spinon momentum and a particular scaling with respect to the number of spin sites, which is crucial to the spinon scattering.

Furthermore, for the sake of convenience we introduce the concept *dominant matrix elements*, corresponding to two specific types [1] of on-shell transitions. The aforementioned transitions dominate the scattering process and as we will see further down, they are sufficient to give us an analytical approximation for the scattering coefficients. Specifically, the first one is the $q = \pi$ transition

$$|\langle Q+\pi|S_\pi^z|Q\rangle|^2 \simeq \frac{f^z(Q)}{N^{2\mathcal{Z}^2-1}}, \tag{4.4}$$

while the second is the same branch flipping velocity transition

$$|\langle \pi-Q|S_{\pi-2Q}^z|Q\rangle|^2 \simeq \frac{h^z(Q)}{N}, \tag{4.5}$$

where $\mathcal{Z}$ is the dressed charge introduced in chapter 2. The identification has been done numerically, which is depicted in fig.4.4 using the analysis in [108], since for small magnetic fields the dressed charge is $\mathcal{Z} \simeq \sqrt{\frac{\pi}{2(\pi-\gamma)}}$. In particular, $\mathcal{Z}^2 = 1$ for $\Delta = 0$ and $\mathcal{Z}^2 = 1/2$ for $\Delta = 1$. This particular scaling of the matrix elements is also valid in the $h = 0$ case, since by an analytical continuation the critical exponent $2\mathcal{Z}^2$ remains the same. Furthermore, $f^z(Q)$ is an almost constant function, while $h^z(Q)$ as illustrated in fig.4.5 is a rapidly decreasing one to a constant value . These types of matrix elements have been extensively studied in [109, 110] and the correspondence between the dressed charge and the scaling of the matrix elements has been proven analytically.

4.2.2 Transverse potential

Next, we consider a transverse magnetic potential, modeled by a potential of the form:

$$V = gS_n^x. \tag{4.6}$$

[1] and all equivalent transitions between the two spinon branches in the even case

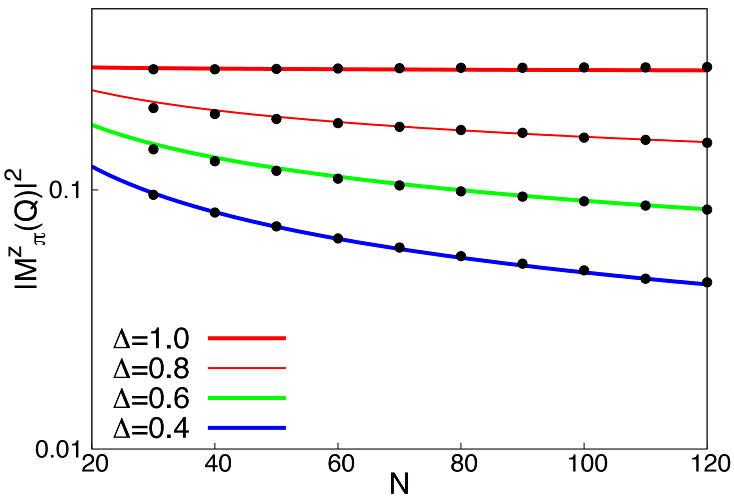

FIGURE 4.4: $|\langle Q+\pi|S^z_\pi|Q\rangle|^2$ versus N for $\Delta = 1, 0.8, 0.6, 0.4$, for $Q = 2\pi/10$. The solid lines correspond to the fitted curve of the form $|\langle Q + \pi|S^z_\pi|Q\rangle|^2 \simeq 1/N^{2\mathcal{Z}^2-1}$ while the dots are the numerical data

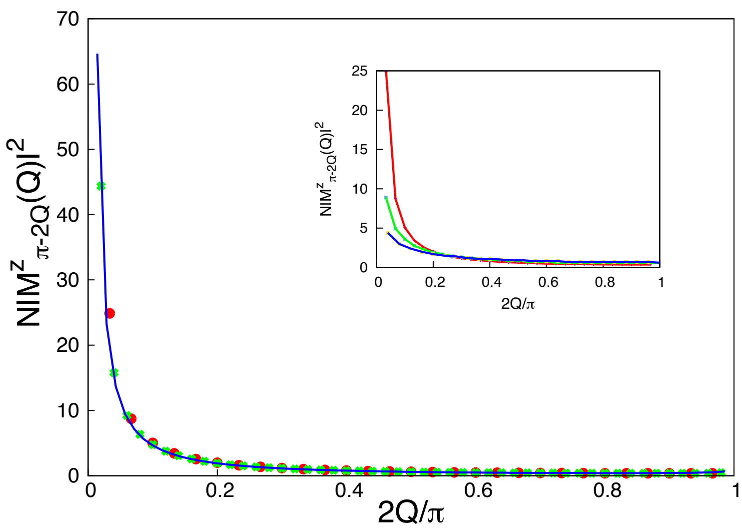

FIGURE 4.5: Scaled $N|\langle\pi - Q|S^z_{\pi-2Q}|Q\rangle|^2$ versus Q for $\Delta = 1$ and various N. The matrix elements are symmetric with respect to $Q = \pi/2$. The inset shows $N|\langle\pi - Q|S^z_{\pi-2Q}|Q\rangle|^2$ versus Q for $\Delta = 1, 0.6, 0.4$.

The main difference of this potential to the two previous ones is that it acts non-trivially only between states with $\Delta S^z = \pm 1$.

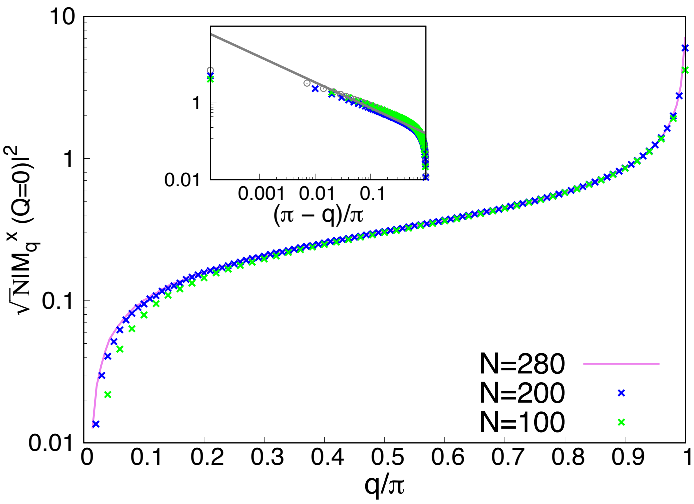

FIGURE 4.6: Scaled $|M_q^x(Q=0)|^2\sqrt{N}$ vs q for the isotropic model $\Delta = 1$ and various N. The solid line in the inset shows that the asymptote scales as $(\pi - q)^{2/3}$.

Similarly to the S_n^z potential, as shown in Fig.4.6, the asymptote behaves as,

$$|M_q^x(Q=0)|^2 \sim \frac{1}{\sqrt{N}}\frac{1}{(\pi - q)^{2/3}} \tag{4.7}$$

and the dominant matrix elements scale as,

$$|\langle Q+\pi|S_\pi^x|Q\rangle|^2 \simeq \frac{f^x(Q)}{N^{\frac{1}{2\mathcal{Z}^2}-1}}. \tag{4.8}$$

Note for values of Δ close to one, $f^x(Q)$ can be considered constant (inset Fig. 4.9), while for values of Δ close to zero it is a monotonically decreasing function.
This time, the XY model matrix elements behave non-trivially as they scale as $\sqrt{N}$ and in fact they imply a strongest scattering compared to the $0 < \Delta \leq 1$ case.

4.2.3 Spin-phonon potential

Next we consider the scattering of a spinon by a lattice distortion of wave-vector q,

$$h_q = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{iqn} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) \tag{4.9}$$

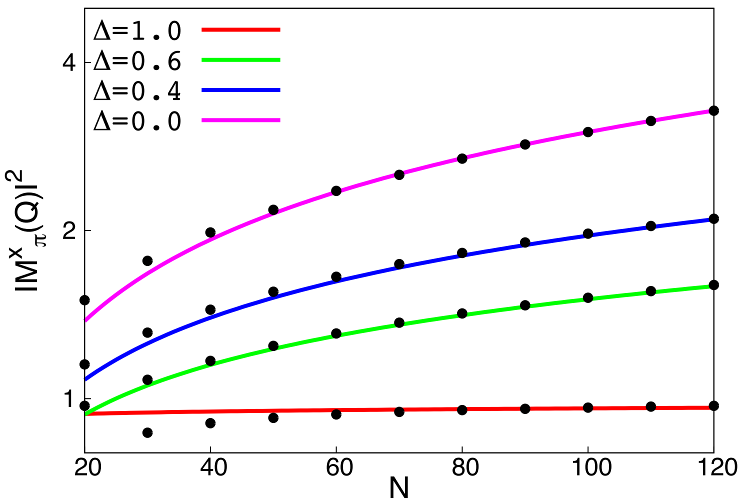

FIGURE 4.7: $|\langle Q+\pi|S^x_\pi|Q\rangle|^2$ versus N for $\Delta = 1, 0.6, 0.4, 0$ for $Q = 2\pi/10$. The solid lines are the fitted curve of the form $|\langle Q+\pi|S^x_\pi|Q\rangle|^2 \simeq 1/N^{\frac{1}{2Z^2}-1}$ while the dots are the numerical data.

from which we can deduce the scattering from a "weak link" $V = g(S^-_n S^+_{n+1} + S^+_n S^-_{n+1})$. Similarly to the previous case, the scaled scattering matrix element for $\Delta = 1$ and the asymptotic form

$$|\mathcal{M}^{ph}_q(Q=0)|^2 \sim N^{-2/3}\frac{1}{(\pi - q)^{1/2}}, \tag{4.10}$$

for $Q = 0$ are shown in Fig.4.8.

Finally we discuss a spin-phonon interaction. Similarly with the longitudinal magnetic potential, the dominant matrix elements are characterized by a π-transfer $|\langle Q+\pi|V_\pi|Q\rangle|^2$ and by a velocity-flipping $|\langle \pi - Q|V_{\pi-2Q}|Q\rangle|^2$ in the same branch of the one-spinon spectrum.

Similarly, we obtain that the π-transfer and the same branch velocity flipping matrix elements behave as,

$$\begin{aligned} |\langle Q+\pi|V_\pi|Q\rangle|^2 &\simeq \frac{f^{ph}(Q)}{N^\alpha} \\ |\langle \pi - Q|V_{\pi-2Q}|Q\rangle|^2 &\simeq \frac{h^{ph}(Q)}{N}, \end{aligned} \tag{4.11}$$

with $\alpha \simeq 0.4$ for $Q = 2\pi/10$ and small corrections with respect to Q. Note that similarly to the longitudinal potential, $h^{ph}(Q)$ is a rapidly decreasing function for $\Delta > 0$ while for $\Delta = 0$ is constant and equal to one. Moreover, $f^{ph}(Q)$ and $h^{ph}(Q)$ are symmetric with respect to $\pi/2$.

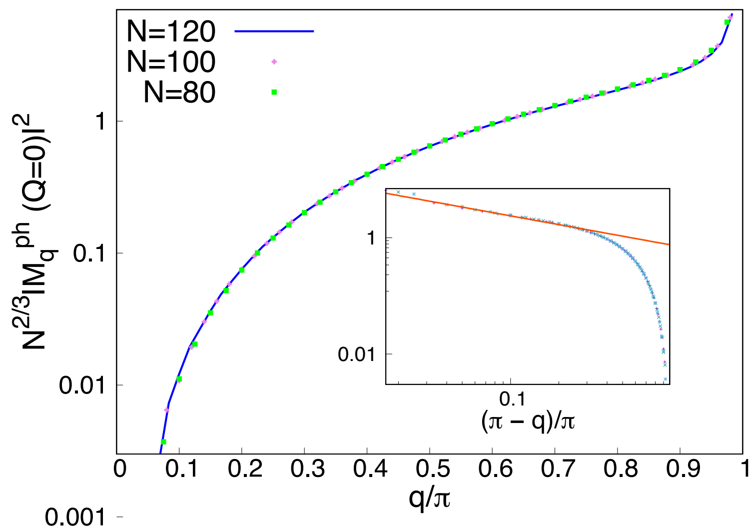

FIGURE 4.8: Scaled $N^{\frac{2}{3}}|\mathcal{M}_q^{ph}(Q=0)|^2$ as a function of q/π. The inset shows the asymptotic scaling of $|\mathcal{M}_q^{ph}(Q=0)|^2$ as a function of $(\pi-q)/\pi$. The solid line indicates the asymptote $(\pi-q)^{1/2}$.

4.2.4 Extended potentials

To close our discussion on the matrix elements, we consider an extended potential profile $V_{ext} = \sum_{n=1}^{N} g_n V_n$, where V_n represents one of the potentials we studied above and g_n is the potential profile

$$|\langle Q+q|V_{ext}|Q\rangle|^2 = \frac{1}{N}|\sum_{n=1}^{N} g_n e^{-iqn}|^2 |V_q|^2. \tag{4.12}$$

For example, for a segment of m-sites with a potential $V_m = \sum_{n=N/2}^{N/2+m-1} S_n^z$ the matrix element is given by,

$$| < Q+q|V_m|Q > |^2 = \frac{1}{N}\frac{\sin^2\frac{qm}{2}}{\sin^2\frac{q}{2}}|\mathcal{M}_q^z(Q)|^2. \tag{4.13}$$

This form of equation can be interpreted as a "diffraction"-like pattern modified by the scattering of the spinon. For the XY model it simply becomes,

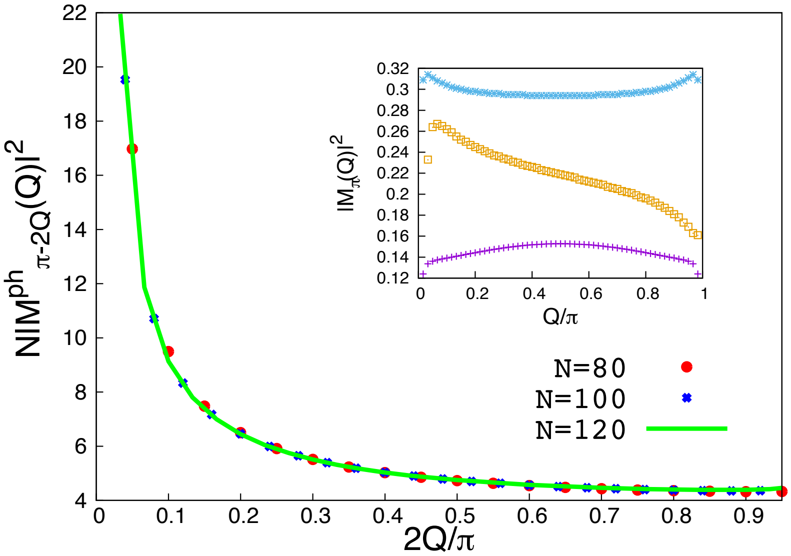

FIGURE 4.9: $N|\langle\pi - Q|V_{\pi-2Q}|Q\rangle|^2$ versus Q for $\Delta = 1$. The inset shows the π-transition versus Q for the longitudinal $|M^z_\pi(Q)|^2$ (light blue), transverse $|M^x_\pi(Q)|^2$ (orange) and spin-phonon interaction $|M^{ph}_\pi(Q)|^2$ (purple) for $N = 120$ and $\Delta = 1$.

$$| < Q + q|V_m|Q > |^2 = \frac{1}{N^2}\frac{\sin^2 \frac{qm}{2}}{\sin^2 \frac{q}{2}}. \tag{4.14}$$

4.3 Intermedio: A short introduction to scattering theory

First, we make a short presentation of rigorous scattering theory, in particular introducing the concepts of the Lippmann-Schwinger equation and the Green's function, the S matrix and the T-matrix approach, which are key ingredients for the development of a scattering theory for spinon excitations. Note that in some cases, we may use as a model Hamiltonian the usual non-relativistic free-particle one, in order to have more familiar expressions

The Lippmann-Schwinger equation

Let us consider a time-independent scattering problem.

$$H = H_0 + V, \tag{4.15}$$

where H_0 is the free from external interactions Hamiltonian and V denotes an external scatterer. We assume that we can solve the eigenvalue problem imposed by H_0,

$$H_0|\phi\rangle = E_0|\psi_0\rangle, \tag{4.16}$$

and our task is to look for solutions for the following scattering problem

$$(H_0 + V)|\psi\rangle = E|\psi\rangle, \tag{4.17}$$

constrained to reduce to the original solution when $V \to 0$, i.e. $|\psi\rangle \to |\psi_0\rangle$ and $E \to E_0$. The formal solution of this problem is:

$$|\psi\rangle = |\psi_0\rangle + \frac{1}{E - H_0 + i\varepsilon} V|\psi\rangle, \tag{4.18}$$

where $\epsilon \to 0^+$ and is introduced in order to avoid the singularity caused due the continuous spectrum of H_0. Eq.(4.18) is called Lippmann-Schwinger equation.

The Green's function, T-matrix and S-matrix

The next step is to define the Green's function

$$G_0(E) \equiv \lim_{\varepsilon \to 0^+} \frac{1}{E - H_0 + i\varepsilon} \tag{4.19}$$

The Lippmann-Schwinger equation takes the following form

$$|\psi\rangle = |\psi_0\rangle + G_0 V|\psi\rangle, \tag{4.20}$$

which gives the following formal solution

$$|\psi\rangle = (1 - G_0 V)^{-1}|\psi_0\rangle. \tag{4.21}$$

Expressing the operator $(1 - G_0 V)^{-1}$ as a series expansion, we obtain

$$|\psi\rangle = \sum_{k=0}^{\infty} (G_0 V)^k |\psi_0\rangle. \tag{4.22}$$

The above expansion is a powerful tool, known as *the Born series.*

Next, we define the T-matrix, a "black box" that contains all the relevant information about the scattering process

$$T = V(1 - G_0V)^{-1} = V\sum_{k=0}^{\infty}(G_0V)^k, \tag{4.23}$$

The usefulness of the above quantity becomes evident if we define the scattered part of the quantum state as $|\psi_s\rangle = |\psi\rangle - |\psi_0\rangle$, then

$$|\psi_s\rangle = G_0T|\psi_0\rangle. \tag{4.24}$$

Another important physical quantity is the so-called S-matrix already mentioned in chapter 2. The concept of S-matrix relates ingoing asymptotic states $|\psi\rangle_{in}$ with outgoing asymptotic states $|\psi\rangle_{out}$. In fact, if we assume that interactions have effect only in a small region of spacetime, then the S matrix is defined as

$$|\psi\rangle_{out} = S|\psi\rangle_{in}, \tag{4.25}$$

or more specifically

$$S = \mathcal{T}\exp\Big[-i\int_{-\infty}^{\infty}V(t)dt\Big] \tag{4.26}$$

In the case where V is a time independent potential, S reduces to

$$S = e^{-iV(t_{out}-t_{in})}, \tag{4.27}$$

where $t_{out} \to \infty$ and $t_{in} \to -\infty$.

It is very interesting that there exists an immediate connection between the S- matrix and the T-matrix, namely

$$S_{\alpha\beta} = \delta_{\alpha\beta} - 2\pi\delta(E_\beta - E_\alpha)T_{\alpha\alpha}, \tag{4.28}$$

which as expected the T matrix is a measure of the scattered part of the wavefunction, while the S matrix accounts for the whole wavefunction.

Transmission Probabilities

Using the aforementioned formalism, the "diagonal" transmission probability (probability to find the particle in the same state) of a particle in the state $|Q\rangle$ with energy ε_Q and group velocity $u_Q = d\varepsilon_Q/dQ$ can be found simply by integration of the diagonal part (4.28) around a region of Q

$$\mathcal{T}_{Q,Q} = \big(1 + \frac{N}{u_Q}\Im\langle Q|T|Q\rangle\big)^2 + \big(\frac{N}{u_Q}\Re\langle Q|T|Q\rangle\big)^2. \tag{4.29}$$

Moreover, in the case of an even spin chain, since it is impossible to physically distinguish between two spinon excitations that have the same energy and group velocity but live in different branches of the Cloiseaux-Pearson spectrum, we should also find the "non-diagonal" transmission probability which is calculated by integration of the $S_{Q,Q+\pi}$ part of the S-matrix

$$\mathcal{T}_{Q,Q+\pi} = (\frac{N}{u_Q}\Im\langle Q+\pi|T|Q\rangle)^2 + (\frac{N}{u_Q}\Re\langle Q+\pi|T|Q\rangle)^2. \quad (4.30)$$

The above relation evidently describes the probability of a spinon to be π-transfered on the other branch. Let us mention that in the odd site case, at least in the lower branch approximation this is not needed.

Finally, the total transmission probability is defined as $\mathcal{T}_{tot} = \mathcal{T}_{Q,Q} + \mathcal{T}_{Q,Q+\pi}$

4.4 Calculation of the spinon Scattering coefficients

We will analyze the transmission/reflection scattering coefficients of a spinon from a potential within the T-matrix approach by writing all quantities in the basis of Bethe ansatz eigenstates $|\{\lambda\}\rangle$,

$$\begin{aligned} T &= V\frac{1}{1-G_0V} \\ G_0(E) &= \lim_{\varepsilon\to 0}\sum_{\{\lambda\}}\frac{|\{\lambda\}\rangle\langle\{\lambda\}|}{E-E_{\{\lambda\}}+i\varepsilon} \\ V &= \sum_{\{\mu\},\{\lambda\}}\langle\{\lambda\}|V|\{\mu\}\rangle|\{\lambda\}\rangle\langle\{\mu\}|. \end{aligned} \quad (4.31)$$

$E_{\{\lambda\}}$ is the energy corresponding to the Bethe state $|\{\lambda\}\rangle$. Based on the discussion in the previous section for the particular scaling of the matrix elements with N, we write a typical matrix element in the form $\langle\{\lambda\}|V|\{\mu\}\rangle = gf_{\{\lambda\},\{\mu\}}/N^\alpha$ with g being the potential strength and $\alpha = \alpha(\{\lambda\},\{\mu\}) > 0$ a scaling factor. The potential matrix V belongs in a Hilbert space of dimension $\dim\mathcal{H} = 2^N$ which makes the problem intractable from a computational point of view. Therefore, in order to be able to calculate the scattering coefficients for relatively long spin chains, we restrict our numerical calculations to including only the two-spinon continuum i.e. a subspace of dimension $\dim\mathcal{H}_{2sp} = \frac{N}{8}(N+2)$. The calculation of the T-matrix is straightforward, we compute the matrix $1-G_0V$ and subsequently invert it and left multiply it by V. Note that for the evaluation of the Green's function G_0 we use the identity $\lim_{\varepsilon\to 0}\frac{1}{x+i\varepsilon} = P\frac{1}{x} - i\pi\delta(x)$, where P stands for the Cauchy principal value part.

4.4.1 "Free" spinon

It is instructive to consider the scattering of a free particle on a lattice with a spinon dispersion relation $\varepsilon_Q = v_s|\sin Q|$ by a one-site δ-like potential of strength g. In this case all the matrix elements are the same, $< Q'|V|Q >= g/N$ and the transmission coefficient $\mathcal{T}_{Q,Q}$ is a function of g/u_Q (Appendix), $u_Q = d\varepsilon_Q/dQ$.

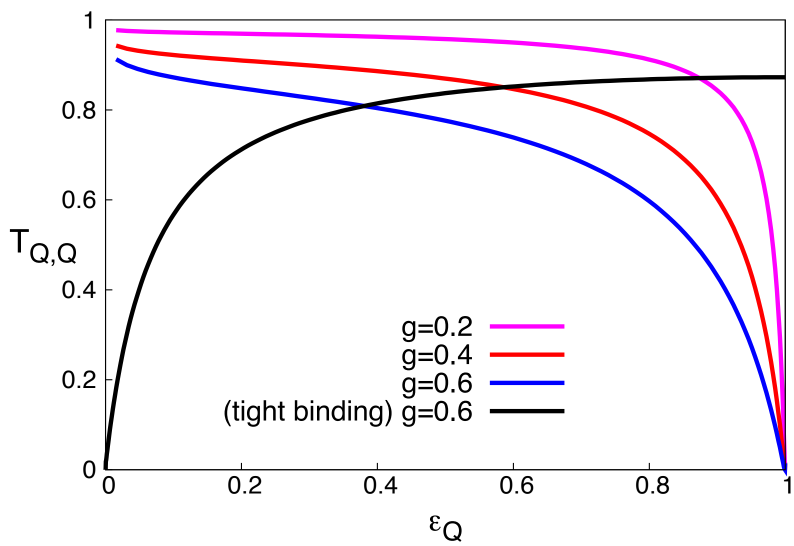

FIGURE 4.10: $\mathcal{T}_{Q,Q}$ vs ε_Q for a delta-like potential of strength g for a "free" spinon and a particle in a tight-binding model

In Fig.4.10 we show that the "free" spinon transmission probability and that of a particle in a tight-binding model with dispersion relation $\varepsilon_Q = v_s(1 - \cos Q)$ behave very differently. The "free" spinon transmission probability is generally a decreasing function of the energy, a property of the specific bounded spectrum. Moreover, we observe that in the linear part of the energy dispersion we have high transmission probability which is related to the fact that in a purely linear dispersion relation, i.e. a massless one dimensional Dirac equation only a phase is induced in the wavefunction and there is no reflection probability [111]. Additionally, from the specific form of the spinon dispersion relation we observe that when ε_Q decreases, u_Q increases, which implies that $\mathcal{T}_{Q,Q}$ is an increasing function of the spinon velocity. Thus a more sensible quantity for the description of the transmission coefficient is the spinon velocity and not the spinon energy as in usual scattering problems.

4.4.2 One-site longitudinal potential

We first consider the scattering of a spinon in an odd-site chain from a one-site potential $V = gS^z_n$. In the fermionic language of the $t-V$ model [112] this would indeed correspond to the scattering of a spinless fermion from a one-site potential. In our calculation of the transmission coefficient $\mathcal{T}_{Q,Q}$ as a function of spinon energy, Fig.4.11, we include only the lower one spinon branch as intermediate states. For $\Delta = 0$ we recover the free-spinon result of Fig.4.10, while for finite Δ we find a strong suppression of the transmission probability at low energies. Because of the finite size of the chain we cannot study the zero energy limit, however we expect the transmission to vanish at this limit as implied by comparing the $N = 121$ and $N = 301$ data at low energies. We should also note that the results are practically independent of system size, at least in this lowest branch approximation. Similar results are shown in Fig.4.12 for the isotropic model at different potential strengths g where, as expected, the transmission is suppressed with increasing potential strength. Furthermore, as in the free spinon case, note the vanishing of the transmission at high energies, related to the zero spinon velocity at the top of the energy dispersion. Furthermore, by taking a closer to look to the transmission probability at low energy we note that $0 < \Delta \leq 1$ spinons appear to behave as quadratic massive particles instead of "linear" ones in the $\Delta = 0$ case. The quadratic behavior of spinon could be produced by the emergence of an *induced effective mass* due to the breaking of criticality by the antiferromagnetic correlations.

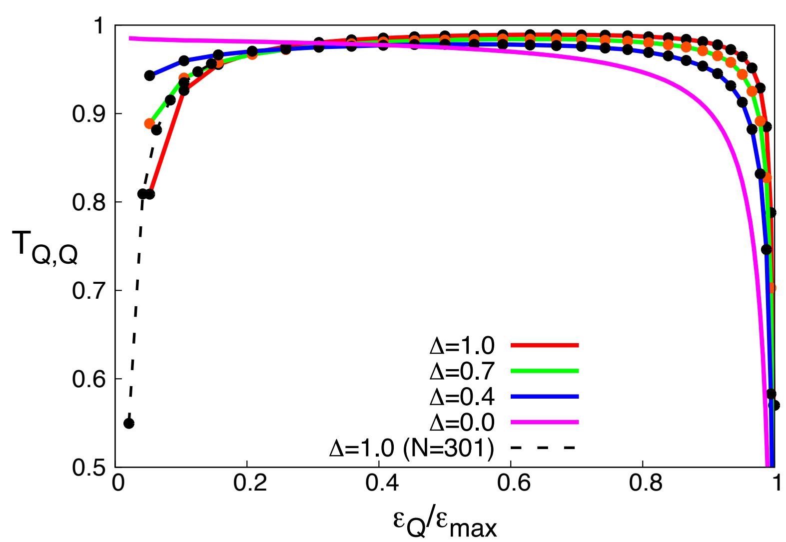

FIGURE 4.11: $\mathcal{T}_{Q,Q}$ vs ε_Q for various Δ, $g = 0.15$ for an odd spin chain, $N = 121$. The black dashed line indicates the $N = 301$ data. The solid lines are guides to the eye.

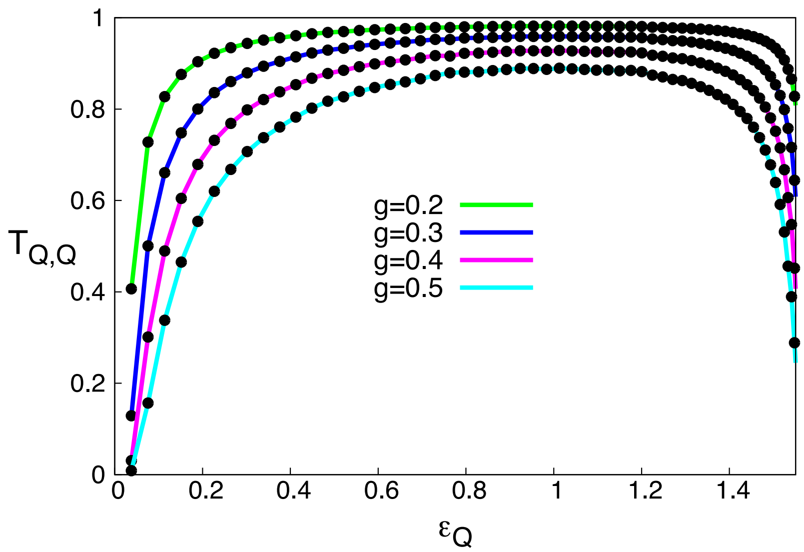

FIGURE 4.12: $\mathcal{T}_{Q,Q}$ vs ε_Q for an odd $N = 241$ isotropic model spin chain for various g. The solid lines are guides to the eye.

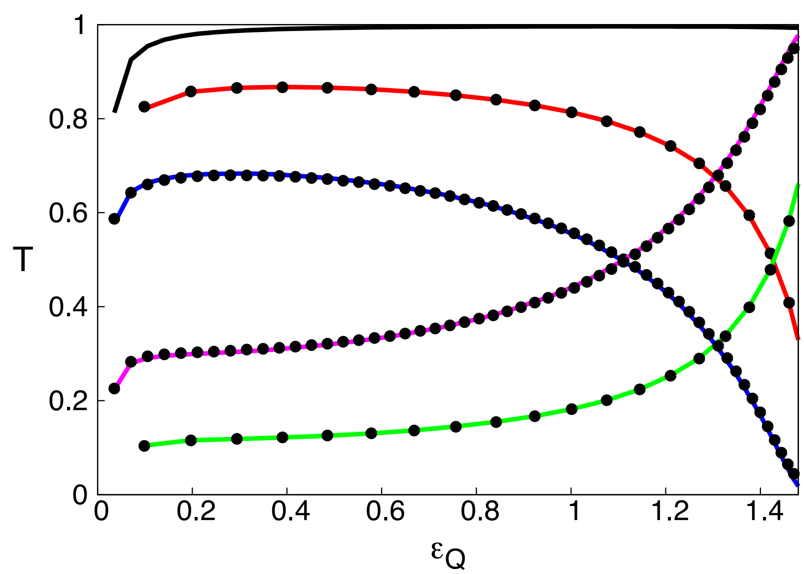

FIGURE 4.13: $\mathcal{T}_{Q,Q}$ (red $N = 100$, blue $N = 280$) and $\mathcal{T}_{Q,Q+\pi}$ (green $N = 100$, purple $N = 280$) vs ε_Q for $g = 0.15$ and $\Delta = 1$. The sum $\mathcal{T}_{tot} = \mathcal{T}_{Q,Q} + \mathcal{T}_{Q,Q+\pi}$ for $N = 280$ is indicated by a solid black line. The solid lines represent the analytical results while the dots the numerical data.

As shown in Fig.4.6, in an even chain there are two low energy spinon branches. In Fig.4.13 we find that there is a complementarity in transmission, as when $\mathcal{T}_{Q,Q}$ decreases, $\mathcal{T}_{Q,Q+\pi}$ increases. The sum of the two closely resembles the transmission of the one spinon in a odd chain. Furthermore, there is a strong size dependence of $\mathcal{T}_{Q,Q}$ which can probably best be described as exponentially decreasing with N. This is argued in Appendix A and shown in Fig.4.15 where for comparison a power law dependence is also plotted (not shown, there is a corresponding exponential increase of $\mathcal{T}_{Q,Q+\pi}$). The exponential dependence increases with Δ as shown in Fig. 4.14 and with g, Fig.4.15. However, the sum $\mathcal{T}_{Q,Q} + \mathcal{T}_{Q,Q+\pi}$ of transmission probabilities shows a weak size dependence and of course in the $\Delta = 0$ case coincides with the one spinon in an odd chain with no size dependence. In other words, we conjecture that in the thermodynamic limit an incoming spinon from the one branch is fully transmitted/reflected in the other branch. In this calculation we have again included as intermediate states only the two lower spinon branches. As discussed below, including all the two-spinon states, only quantitatively changes this behavior. Another aspect of this transfer of transmission probability from the $\mathcal{T}_{Q,Q}$ to the $\mathcal{T}_{Q,Q+\pi}$ branch is shown in Fig.4.16 where we see that $\mathcal{T}_{Q,Q+\pi}$ increases with potential strength.

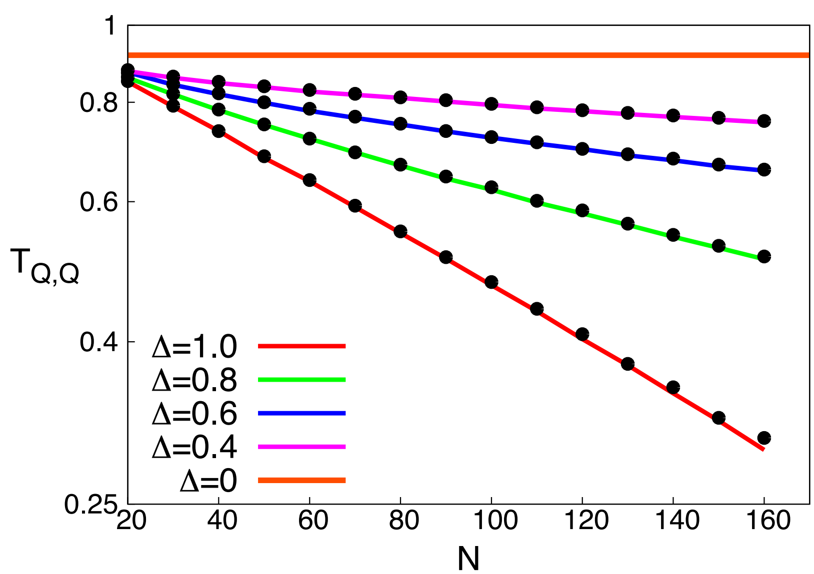

FIGURE 4.14: $\log \mathcal{T}_{Q,Q}$ vs N for $V = gS^z_n$, $g = 0.2$ for constant energy $\varepsilon_Q/v_s = \sin(2\pi/10)$ and $\Delta = 0.4, 0.6, 0.8, 1.0$ The solid lines represent the analytical approximation (appendix), while the dots represent the numerical data. The horizontal represents the $\Delta = 0$ case.

Based on the integrable structure of the Heisenberg model we can understand these results from first principles appendix. Re-summing to all orders the most important

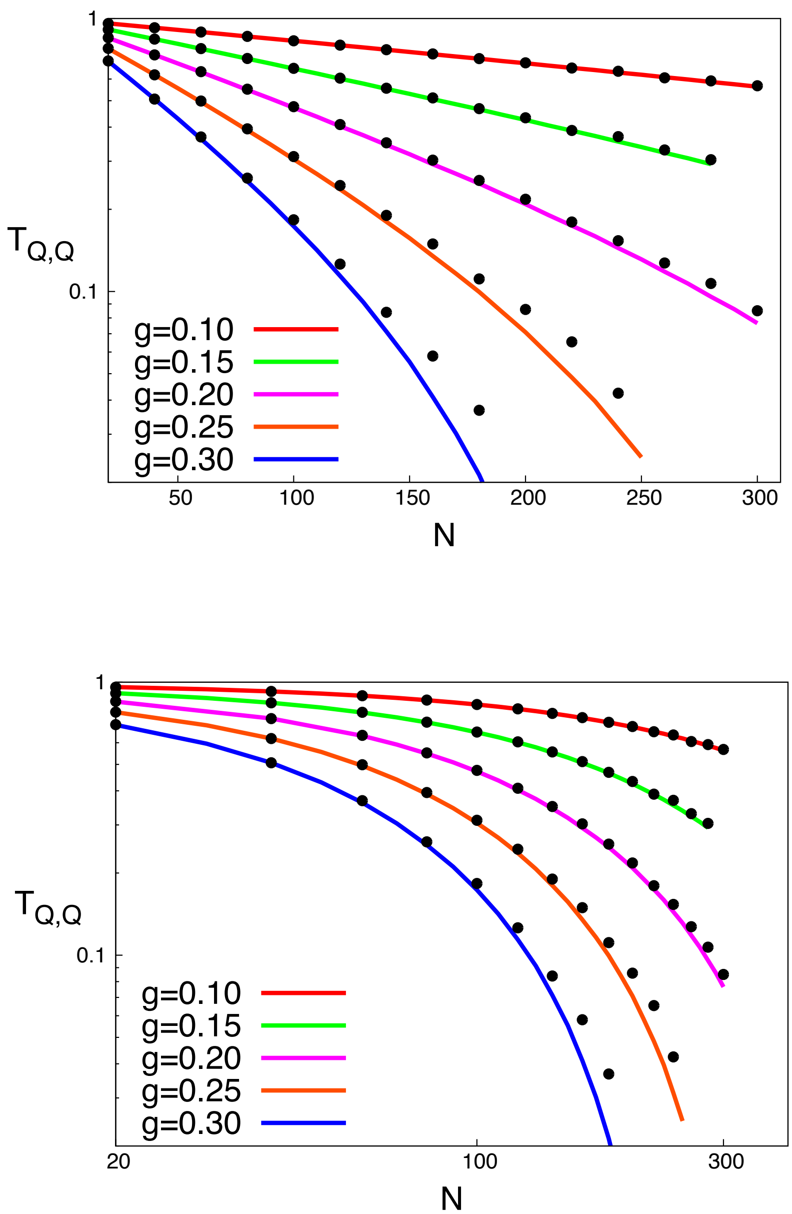

FIGURE 4.15: $\log \mathcal{T}_{Q,Q}$ vs N (top) and $\log \mathcal{T}_{Q,Q}$ vs $\log N$ (bottom) for $V = gS_n^z$ for the isotropic model $\Delta = 1$ and energy $\varepsilon_Q = \frac{\pi}{2}\sin(2\pi/10) \simeq 0.92$. The solid lines represent the analytical approximation (appendix), while the dots represent the numerical data.

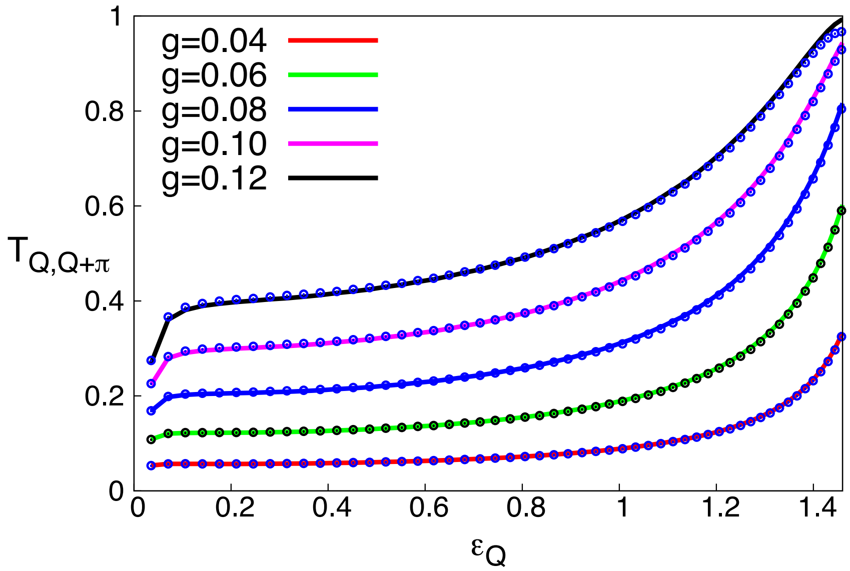

FIGURE 4.16: $\mathcal{T}_{Q,Q+\pi}$ vs ε_Q as a function of g for $N = 280$. The solid lines are guides to the eye.

on-shell matrix elements, $|Q\rangle \to |Q+\pi\rangle, |\pi - Q\rangle$ described in the previous section, we obtain a fairly good description of the transmission probabilities (even quantitative in the weak coupling limit). It is easily proved that these transitions result in a monotonically decreasing (increasing) transmission probability $\mathcal{T}_{Q,Q}(\mathcal{T}_{Q,\pi+Q})$ with spin chain length N. We expect this behavior to be generic in one dimensional spin chains, simply here, the integrability of the model allows us to explicitly evaluate the corresponding exponents.

By a numerical fit in Figs.4.14,4.15 we find that a useful quantity for the description of the scattering process is $g_{eff} = gN^{1-\mathcal{Z}^2}$ and that for ε_Q not close to zero the transmission coefficient behaves as

$$\mathcal{T}_{Q,Q} \simeq e^{-a(g_{eff}/u_Q)^2} \tag{4.32}$$

which holds for $g_{eff}/u_Q << 1$. Thus for the isotropic Heisenberg model ($\gamma = 0,\ \Delta = 1$) which is the most experimentally relevant $\mathcal{T}_{Q,Q} \simeq e^{-a(g/u_Q)^2 N}$. Although this approach does not offer an analytical solution of the scattering problem, using the framework of integrability we derived a connection between the transmission coefficients and $\theta_{zz} = 2\mathcal{Z}^2$, the critical exponent of the ground state's correlation function $\langle 0|s_1^z s_{n+1}^z|0\rangle$ dominant oscillatory part. Predicted by CFT and Bethe Ansatz calculations [?, ?], it offers a qualitative description of the scattering process.

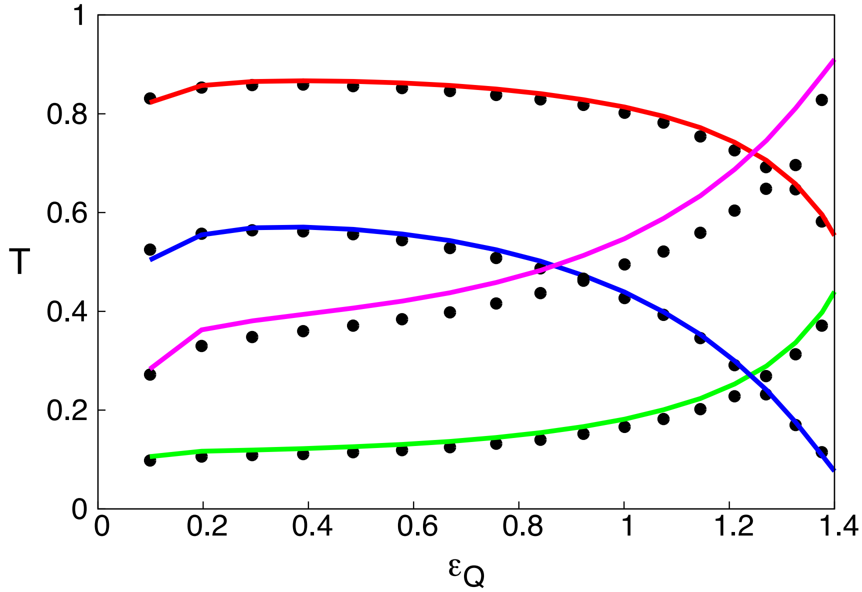

FIGURE 4.17: $\mathcal{T}_{Q,Q}$ (red $g = 0.1$, blue $g = 0.2$) and $\mathcal{T}_{Q,Q+\pi}$ (green $g = 0.1$, purple $g = 0.2$) vs ε_Q for $N = 100$ and $\Delta = 1$. The solid lines are produced by including only the lower branch while the dots represent the numerical data obtained by including the whole two-spinon continuum.

Note that this approximation gives reasonable results even though we have performed a rough elimination of most of the intermediate matrix elements. On the other hand from the specific form of the transmission probability of the "free" spinon model we observe that the dominant behavior is given by the on-shell matrix elements and the rest of the matrix V serves as a correction, which justifies the reasoning for the above approximation. Of course, as we see in Fig.4.15, it is a weak coupling approximation, albeit a very good one, that becomes increasingly unreliable in the strong g coupling limit. Even more, in the strong coupling $g/u_Q >> 1$ limit (e.g. $Q \to \pm\pi/2$) the numerical T-matrix approach we are using often does not converge at all.

Finally, to improve on the lower branch approximation we include all the two-spinon states which forces us however to study rather small size spin chains as the space of intermediate states increases as N^2. At this point it is important to mention that although there are not significant quantitative and qualitative differences in the scattering profile, As shown in Fig.4.17 there is a stabilizing effect which is shown in Fig. 4.18. To be more specific, the single particle image, i.e. the inclusion of only the lowest branch states do not provide a physical scattering picture regarding the number of spins N, since it appears that the finite size effects do not disappear as the system

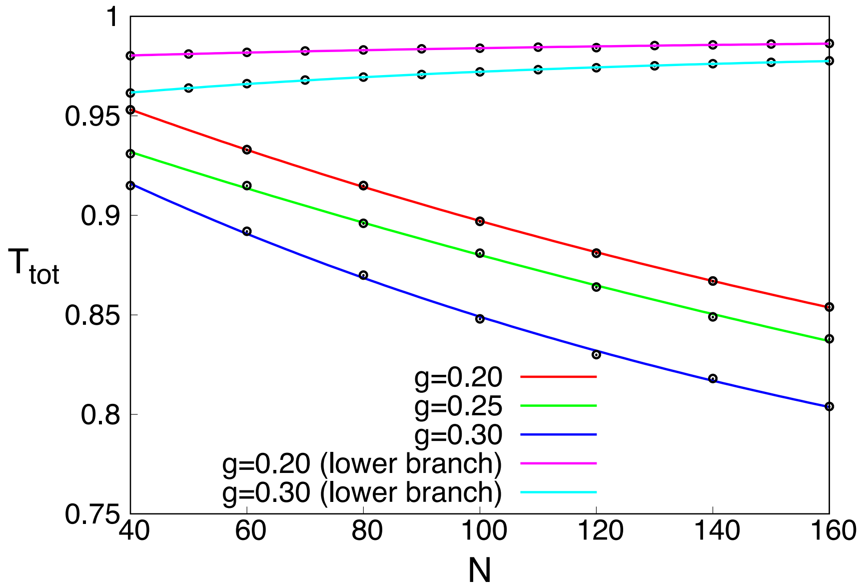

FIGURE 4.18: $\mathcal{T}_{tot}$ versus N for the $V = gS_n^z$ potential $\Delta = 1$ and $\varepsilon_Q \simeq 0.923$ including the two-spinon continuum along the lower branch data. The dots represent the numerical data, while the solid lines represent the fitted curve $\mathcal{T}_{tot} = A\exp(-Bf^z(Q)g^2N/u_Q^2) + C$.

grows. On the contrary, the two spinon continuum serves as an *intermediate states cloud* which stabilizes the spinon scattering and provides a regular particle scattering in the thermodynamic limit $N \to \infty$. The above claim is supported by the fact that $\mathcal{T}_{cal}(Q)$ is dependent only from the spinon energy ε_Q in the thermodynamic limit as depicted in Fig.4.18. Finally, Comparing the even and odd site case, we found an interesting topological effect. In the odd chains, in our one-spinon study where the spectrum is two-fold degenerate, we find a rather regular behavior of scattering coefficients. In the even chains, due to the topological two-spinon constraint, we have a four-fold degenerate spectrum that, together with the singular $\pi-$transition, implies a transfer of transmission probability between the two spinon branches. Thus, in the spinon scattering, we have an interplay of the topological character and the singular matrix elements of a critical system.

4.4.3 Spin-phonon potential

The spin-phonon interaction is described by a one-link potential of the form

$$V = g(S_n^- S_{n+1}^+ + S_n^+ S_{n+1}^-). \tag{4.33}$$

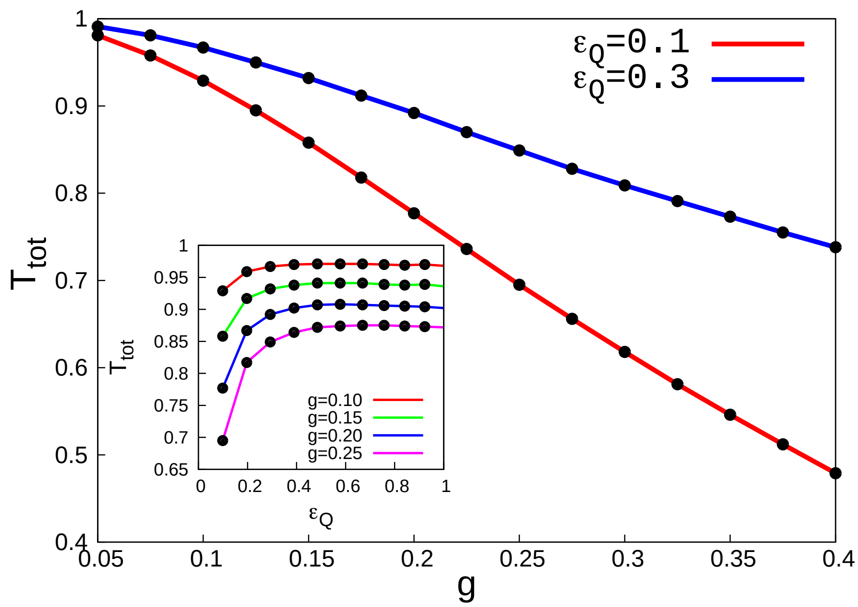

FIGURE 4.19: The total transmission coefficient $\mathcal{T}_{tot}$ vs g for $V = gS^z_n$, $N = 100$ and $\Delta = 1$. The lines are guide to the eye. The inset show the $\mathcal{T}_{tot}$ vs ε_Q for various g.

In Fig.4.20 the numerical calculation for an even-site chain shows that $\mathcal{T}_{Q,Q} \to 0$ as N increases. Similarly to the previous case, we obtain an approximate analytical result by using the dominant matrix elements that were described in the previous section. In particular, the monotonicity of the scaling factors implies that the transmission and reflection coefficients will be scale invariant for $\Delta = 0$ while on the contrary, for $0 < \Delta \leq 1$ $\mathcal{T}_{Q,Q} \to 0$ as N increases. Moreover, the relation of the scattering coefficients to the spinon energy ε_Q is very similar to that of a longitudinal magnetic potential as was depicted in Fig.4.13.

4.4.4 Transverse potential

We now turn to a transverse magnetic potential, $V = gS^x_n$. The main difference of this potential to the two previous ones we studied is that it acts non trivially only between states with $\Delta S^z = \pm 1$. We will restrict ourselves to transitions between the $S^z = 1$ and $S^z = 2$ magnetization sectors.

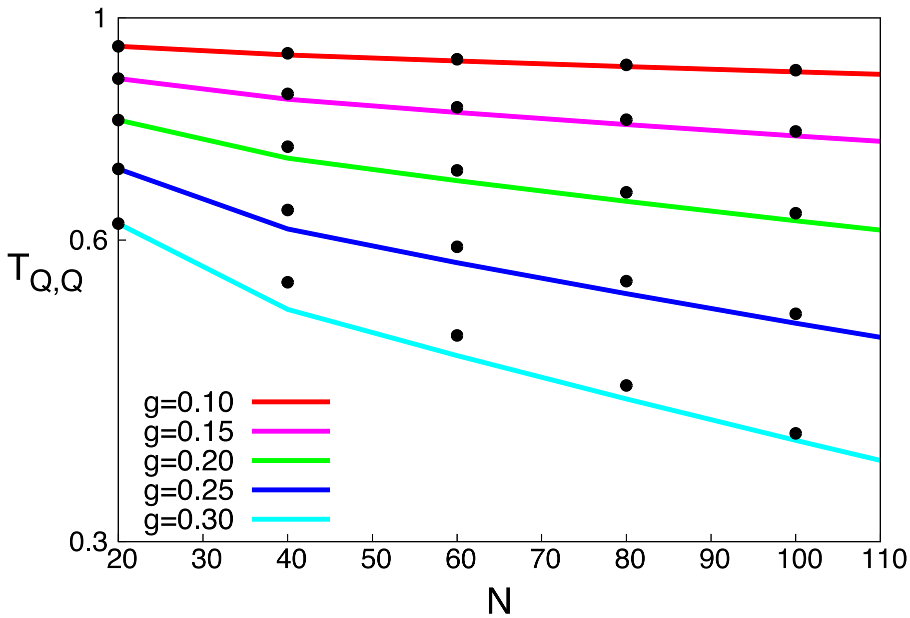

FIGURE 4.20: $\log \mathcal{T}_{Q,Q}$ vs N for a one-link spin-phonon potential V, $\varepsilon_Q \simeq 0.92$ and $g = 0.1, 0.15, 0.2, 0.25, 0.3$. Solid lines prediction based on the dominant matrix elements [?].

Fig.4.21 shows that similarly to the previous cases, for an even-site chain $\mathcal{T}_{Q,Q} \to 0$ as N increases. Again the dependence is probably best be described as exponential, as argued in [?] and by comparison with a power law one. However, this time we find that this holds also for $\Delta = 0$ and in fact the scattering increases as Δ decreases, which is the opposite to what happened in the previous cases. Again we can obtain a qualitative explanation of this behavior by using the fact [109, 110] that the dominant matrix element approximately scales as $\theta_{-+} = \frac{1}{2\mathcal{Z}^2} \simeq \frac{\pi-\gamma}{\pi}$ which is the dominant critical exponent of the ground state correlation $\langle 0|\sigma_1^- \sigma_{n+1}^+|0\rangle$. By re-summation [?] and the monotonicity of the critical exponents with respect to Δ one can argue that $\mathcal{T}_{Q,Q} \to 0$ for $0 < \Delta \leq 1$. Nevertheless, a full scale analysis of the matrix elements should be done in order to give a definite answer. Similarly to the previous cases, by defining $g_{eff} \equiv gN^{1-\frac{1}{4\mathcal{Z}^2}}$ implying $g_{eff} = g\sqrt{N}$ for $\Delta = 1$ (isotropic model) and $g_{eff} = gN^{3/4}$ for $\Delta = 0$ (XY model), we conclude that

$$\mathcal{T}_{Q,Q} \simeq e^{-f^x(Q)(g_{eff}/u_Q)^2} \tag{4.34}$$

in the region $g_{eff}/(4u_Q^2/f^x(Q)) << 1$, a behavior which agrees well with the numerical data.

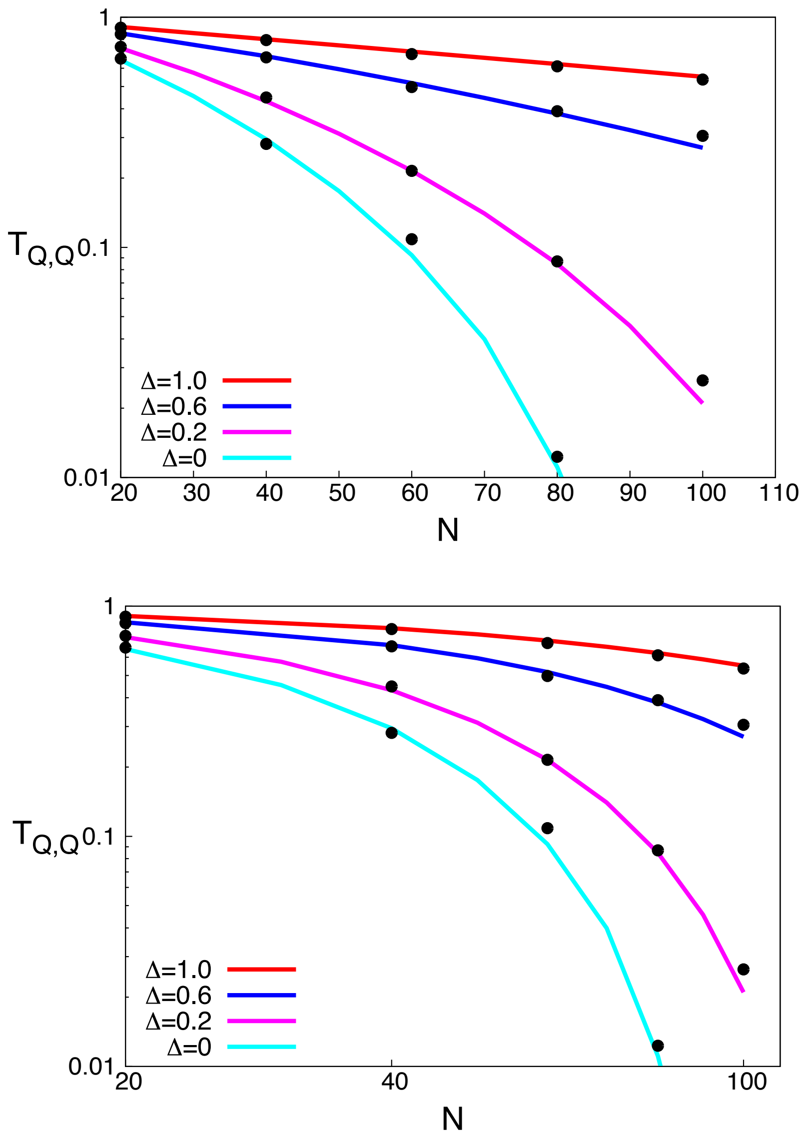

FIGURE 4.21: $\log \mathcal{T}_{Q,Q}$ vs system size N (top) and $\log \mathcal{T}_{Q,Q}$ vs system size $\log N$ for a one-site transverse potential $V = gS_n^x$, $g = 0.2$, $\varepsilon_Q = v_s \sin(\frac{2\pi}{10})$ and $\Delta = 1, 0.6, 0.2, 0.0$. Solid lines are the prediction considering the dominant matrix elements [**?**].

4.4.5 Extended potential

Finally, we consider the spinon scattering from an extended potential

$$V_{ext} = \sum_{n=1}^{m} g_n V_n. \tag{4.35}$$

By the numerical procedure presented earlier, we can calculate the transmission probability for an arbitrary potential profile $\{g_n\}$ in the two-spinon continuum approximation. We start with the scattering of a spinon in an odd chain by a two-site longitudinal potential, a case analogous to Fig.4.11 for a on-site potential. In Fig.4.22 we see a remarkable difference at low energies where there is complete transmission. This situation is consistent with the well known "cutting" and "healing" [113, 114, 115] effect in one dimensional correlated systems and spin chains, where one weak-link is cutting a chain at low energies while two weak-links are healed. This effect leads to a finite conductance with a power law dependence on the temperature due to thermal effects.

Here, we can understand the results of extended potentials by considering the "diffraction" relation (4.13). For an $m = 2$ longitudinal potential in an odd chain, at low energies $Q \to 0$, the $q = \pi - 2Q$ scattering matrix element vanishes leading to total transmission. Following the same argument, we also find that for an even chain with an $m = 2$ longitudinal potential the transfer of transmission probability from $\mathcal{T}_{Q,Q}$ to $\mathcal{T}_{Q,Q+\pi}$ found in Fig.4.11 is now totally suppressed as the $q = \pi$ matrix element vanishes. Following the same line of re-summation of dominant matrix elements and by taking into account the corresponding "diffraction" factor allows us to understand the transmission by extended potentials. Furthermore, it is important to mention that in this case the inclusion of the whole two spinon continuum induces negligible corrections and therefore the single particle picture is sufficient.

4.5 Extension to the massive case $\Delta > 1$

This section extends our study to the gapped case, $\Delta > 1$, for a longitudinal potential [116]. The main drive for this work is to understand the peculiar behavior of the spinon scattering. Specifically, there are three effects which characterize the spinon nature for the $\Delta \leq 1$ XXZ spin chain model. The criticality of the system $\Delta \leq 1$, the strongly correlated characteristics of the model and the topological nature of the quasiparticle induced by the boundary conditions. To this end, the extension of the previous analysis to the gapped model might help us distinguish which effect is responsible. In addition, spinons in the gapped case are localized objects which tend to become antiferromagnetic domain walls as $\Delta \to \infty$. Consequently, the scattering process becomes more apparent and approaches the usual localized particle picture while retaining the many

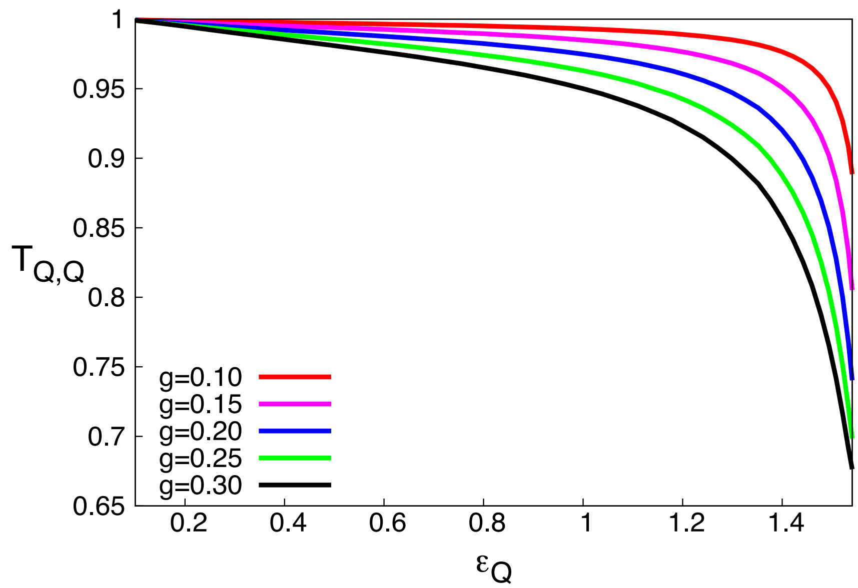

FIGURE 4.22: $\mathcal{T}_{Q,Q}$ vs spinon energy ε_Q for a potential $V = g(S^z_n + S^z_{n+1})$, $N = 201$.

body effects.

Similarly with the previous sections we start with a brief presentation of the matrix elements and subsequently an analysis of the scattering coefficients based on the same techniques used throughout this chapter.

Matrix Elements

The most important distinction from the gapless case is shown in Fig.4.24, where the $|\langle Q+\pi|S^z_\pi|Q\rangle|^2$ matrix elements for the longitudinal potential is depicted. As we clearly notice the matrix elements are linearly dependent, $|\langle Q+\pi|S^z_\pi|Q\rangle|^2 \simeq f(\Delta, Q)N + g(\Delta, Q)$, where the coefficients f, g are increasing functions which converge to a constant value with respect to Δ as we approach the Ising limit. Additionally, $|\langle Q+\pi|S^z_n|Q\rangle|^2 \simeq f(\Delta, Q) + g(\Delta, Q)/N$. The above results evidently will result to a strong π transfer of the spinon from the one branch to the other. Additionally, in (Fig2) we present the $Q = 0$ matrix element and in a similar fashion with the previous graph we find that the $q \to \pi$ scattering matrix elements increases as Δ increases up to the point where it effectively reaches the Ising limit $\Delta = \infty$. Additionally, we find that the same branch velocity flipping matrix elements have a similar form as in the gapless case, thus expecting that for an odd chain and within the 1-spinon approximation we

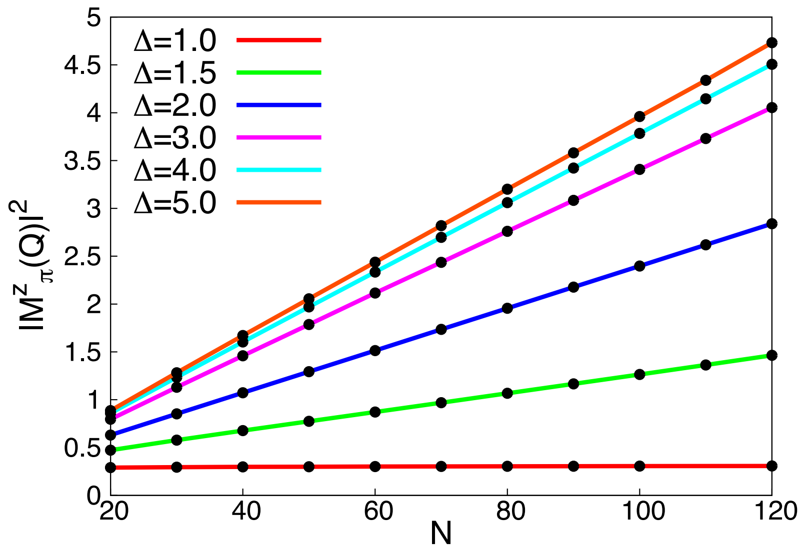

FIGURE 4.23: $|\langle Q+\pi|S^z_\pi|Q\rangle|^2$ versus N for $\Delta = 1, 1.5, 2, 3, 4, 5$ for $Q = 2\pi/10$.

will not have apparent differences with the $\Delta \le 1$ case apart from the strong scattering close to the $Q = 0$ point.

Scattering coefficients in the gapped case

Let us start our discussion of the gapped scattering coefficients by presenting the "free" spinon case, which will illustrate the transmission versus velocity relation. Specifically, Fig.6.4 shows that in the gapped case due to the fact that the dispersion relation is slowly becoming analogous to Q^2, the velocity becomes zero at Q close to zero. Note that although the results in Fig.6.4 are for the odd case, the results coincide with the total transmission $\mathcal{T}_{tot} = \mathcal{T}_{Q,Q} + \mathcal{T}_{Q,Q+\pi}$ of the corresponding even case.

The presentation of the dominant matrix elements for the gapped case $\Delta > 1$ and the arguments used throughout this chapter reveal that for the longitudinal potential and for an even spin chain $\mathcal{T}_{Q,Q} \sim \exp(-g^2N^2f^z(Q)/u_s^2)$, while all the other features remain qualitatively the same. Additionally, an interesting observation is that up to the two spinon continuum $\mathcal{T}_{tot}$ does not strongly depends on Δ, namely that within numerical error it appears constant, while it depends on N in a similar way as in the critical case, i.e. it decreases exponentially as long as finite-size corrections play a

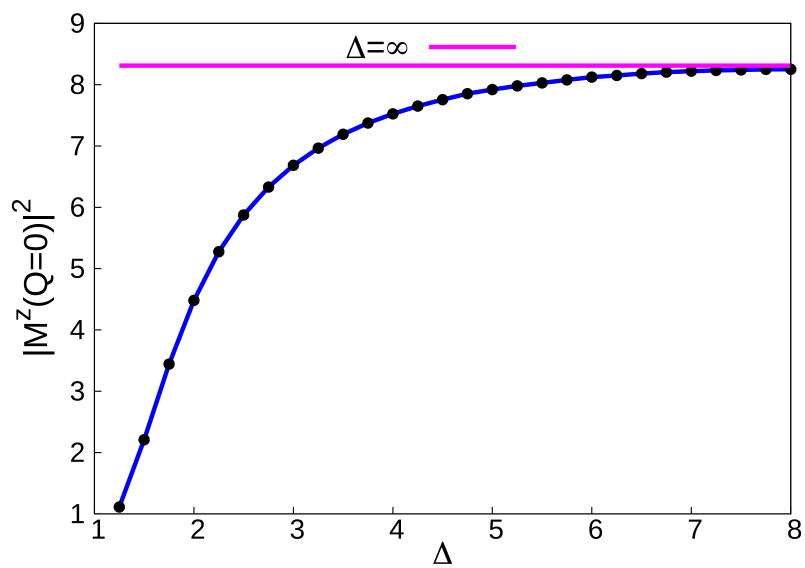

FIGURE 4.24: $|\langle q|S_q^z|0\rangle|^2$ versus Δ for $q = \pi - \frac{2\pi}{N}$ and $N = 120$. The black dots represent the numerical results while the blue line is a guide to the eye. The purple line representes the asymptotic value for $\Delta = \infty$ using extrapolation of the available numerical data

significant role, with exponent analogous to N^2. Moreover, similarly with the $\Delta < 1$ case the inclusion of the two spinon continuum makes the spinon behavior to be similar to that of a regular particle, since it is evident from the inset of the Fig.4.26 that the transmission coefficient increases as the energy increases. Again this behavior is due to the intermediate spinon states acting as an effective cloud which regularizes the scattering process.

extended potentials in the gapped case

Finally it is interesting that although the spinon velocity for $\Delta > 1$ becomes zero at $\varepsilon_Q \simeq 0$ as Δ increases again we have a healing effect in the case of $V = g(S_n^z + S_{n+1}^z)$ for every non zero energy ε_Q.

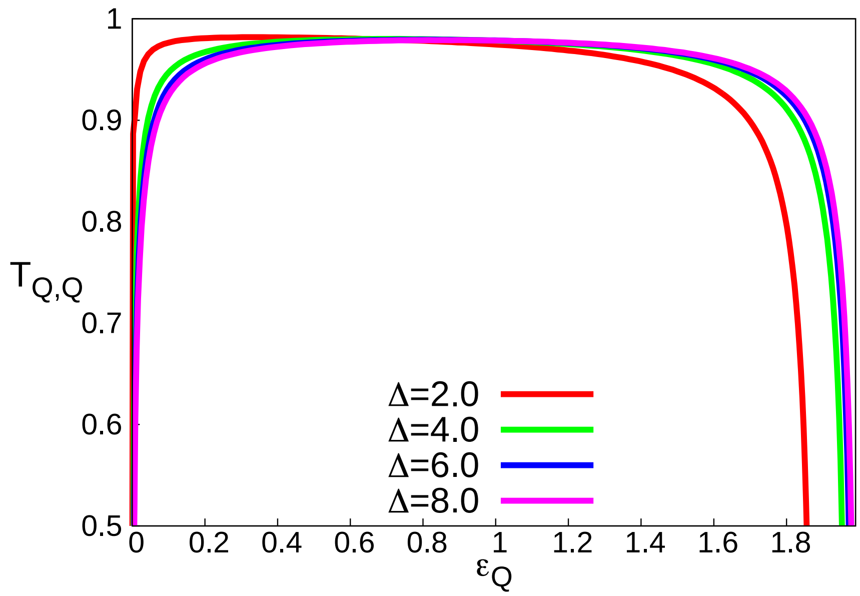

FIGURE 4.25: The transmission coefficient $\mathcal{T}_{Q,Q}$ vs ε_Q for the "free" spinon in the gapped case. The lines are for various Δ and $N = 601$.

4.6 Conclusions

Using the Bethe ansatz method and the T-matrix approach, we have studied the scattering of a spinon from prototype potentials. Three main features emerged from this study; first, we are considering a quantum many-body problem, so in principle outgoing states with creation of spinons or "electron-hole" pairs is possible although we expect from the scattering matrix elements that these processes have lower probability. We have limited our study to outgoing states with the same number of spinons as the incoming state. Second, we can qualitatively account for the transmission probabilities by re-summing the dominant scattering elements. Their dependence on the size of the spin chain is given by the critical exponents characterizing the anisotropic Heisenberg model. Thus, we linked the scattering to the critical properties of this integrable model and we evaluated them by the Bethe ansatz method. It is an open, technically very difficult, question whether including all intermediate states $O(2^N)$ would qualitatively change the present picture. Third, we have found an intriguing topological effect as, in an even chain there is complete transfer of the incoming spinon transmission probability from the one branch of the dispersion to the other branch. At the moment, in a

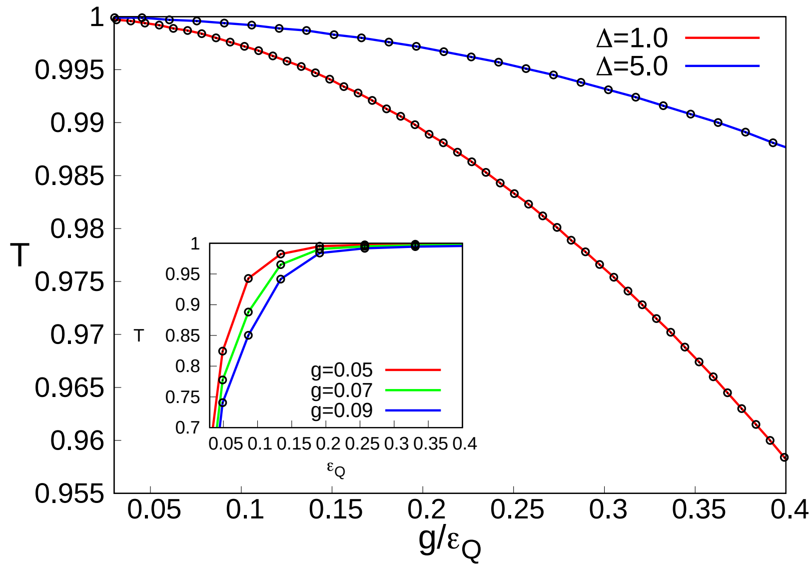

FIGURE 4.26: The total transmission coefficient $\mathcal{T}_{tot}(Q)$ vs ε_Q/g for $V = gS_n^z$ and $N = 100$. The inset shows that the total transmission actually is quite similar to that of an ordinary particle

macroscopic open chain the role of this odd-even effect is ambiguous. Further study is necessary to clarify it, presumably including further outgoing states, e.g. three-spinon states in odd chains. Note that, several experimental and theoretical studies [117] have addressed the physical effect of even vs. odd chain length in the thermodynamic properties of finite size chains.

Along the line of dominant matrix elements, we analyzed a basic difference in the scattering coefficients of longitudinal and weak link potentials to those of a transverse potential. We also discussed extended potentials where, a drastic dependence of scattering coefficients on the potential extent, we attributed it to a geometric "diffraction" factor and dominant scattering matrix elements. These results are consistent with previous studies on "cutting-healing" in 1D correlated systems [113, 114, 115, 118]. In addition, we have discovered that the interemediate states although they do not play a significant role in the functional form of the transmission probability with respect to the spinon energy, they are significant in the scattering procedure since only with their

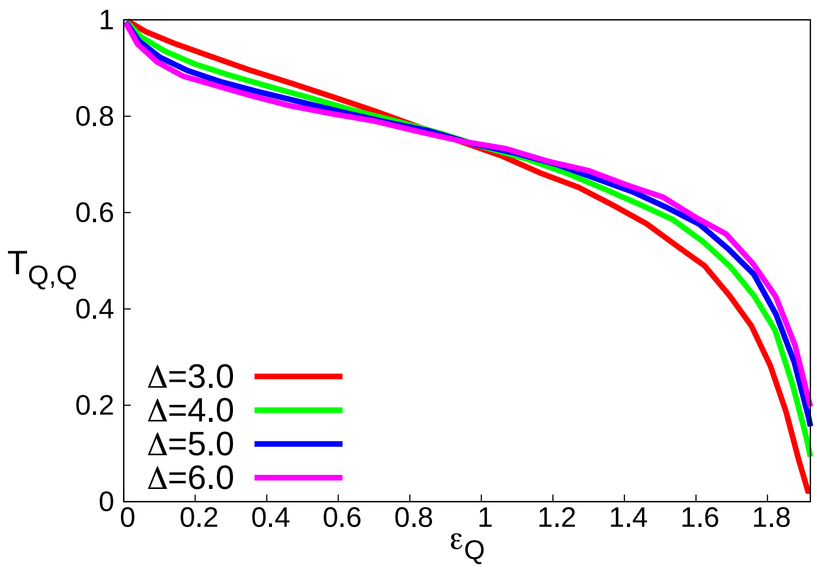

FIGURE 4.27: The transmission coefficient $\mathcal{T}_{Q,Q}$ vs ε_Q for $V = g(S^z_n + S^z_{n+1})$ and various $\Delta > 1$. The lines are for various Δ and $N = 100$. Similarly with the $|\Delta| < 1$ the healing property is apparent.

inclusion the spinon behaves regularly both in the finite N limit and the thermodynamic limit. Finally, we have seen a similar behavior in the $\Delta > 1$ region proving that the peculiar behavior of the spinon is not due to the criticality of the system but due to a combination of its topological nature and the strongly correlation of the underlying system.

Considering experiment, we studied the problem of a spinon excited above the ground state and scattering from a potential. Although we have not addressed any particular experiment, our study would provide key elements in the interpretation of far-out of equilibrium experiments as well as thermal transport ones. For instance zero temperature tunneling studied by a "Landauer" type approach or spinon transport probed e.g. by terahertz 2D coherent spectroscopy [119] experiments.

Appendix: Analytical approximation for the scattering coefficients

As yet, we have calculated numerically the transmission and reflection coefficients. Nevertheless, as we have already mentioned, there is an analytical approximation which is sufficient to qualitatively describe the spinon scattering coefficients $\mathcal{T}_{Q,Q}$, $\mathcal{T}_{Q,Q+\pi}$ and the corresponding factors for reflection. However, we should mention that the approximation gives an invalid result for the total transmission coefficient $\mathcal{T}_{Q,Q} + \mathcal{T}_{Q,Q+\pi}$.

To get started, In the case of the anisotropic Heisenberg the Green's function for the single spinon is

$$G_0(Q) = \lim_{\epsilon\to 0} \sum_{\{\lambda\}} \frac{|\{\lambda\}\rangle\langle\{\lambda\}|}{\varepsilon_Q - E_{\{\lambda\}} + i\epsilon}, \quad \varepsilon_Q = \frac{\pi}{2}\frac{\sin\gamma}{\gamma}|\sin Q|. \tag{4.36}$$

Analytical calculation for the "free" spinon

Let us analytically evaluate the transmission probability for a "free" spinon (including only one-spinon excitations) toy model in an odd site spin chain with a potential matrix

$$V = \frac{g}{N^\alpha}\sum_{Q,Q'} |Q\rangle\langle Q'|, \tag{4.37}$$

where $\alpha > 0$ and $|Q\rangle, |Q'\rangle$ are one-spinon states. Note that $\alpha = 1$ corresponds to the case of a δ-like potential which we presented in the main text. Using eqs.(4.23-4.30) we evaluate the T matrix and the transmission amplitude $\mathcal{T}$, a function of g_{eff}/u_Q, $g_{eff} \equiv gN^{1-\alpha}$

$$\begin{aligned} T(Q,Q') &= \frac{g}{N^\alpha}\frac{1}{1-(I_1+iI_2)}, \\ I_1 &= \frac{g_{eff}}{2\pi}P\int\frac{dq}{\varepsilon_Q-\varepsilon_q} = -\frac{g_{eff}}{2\pi|u_Q|}\log\left(\frac{1+|\cos Q|}{1-|\cos Q|}\right), \quad I_2 = -\frac{g_{eff}}{|u_Q|}, \\ \mathcal{T}_{Q,Q} &= t_1^2 + (1+t_2)^2, \\ t_1 &= \left(\frac{g_{eff}}{u_Q}\right)\frac{(1-I_1)}{(1-I_1)^2+(I_2)^2}, \quad t_2 = \left(\frac{g_{eff}}{u_Q}\right)\frac{I_2}{(1-I_1)^2+(I_2)^2}. \end{aligned} \tag{4.38}$$

This result holds for $I_1^2 + I_2^2 < 1$. An interesting observation is that if we include only the on-shell matrix elements, i.e. only the I_2 part, then we get the correct qualitative behavior in the dependence on N and the spinon energy ε_Q, with the rest of the matrix elements given by I_1 acting as corrections to the amplitude. Moreover, by repeating the same calculation for an even site spin chain, we can technically understand our results of the spinon transfer between the two branches, since for $\alpha < 1$ the transmission probability $\mathcal{T}_{Q,Q} \to 0$ as N increases while in the case $\alpha > 1$ the transmission probability $\mathcal{T}_{Q,Q} \to 1$ as N increases and $\mathcal{T}_{Q,Q}$ is scale invariant when $\alpha = 1$.

Analytical approximation for the spinon

In addition to the previous case, using only the dominant matrix elements we can obtain a qualitative expression for the transmission amplitudes of the potentials that we have previously discussed. Even though this picture is not consistent with the inherent many body character of spinons which is provided by the two-spinon continuum states it is enough to illustrate the quantitative significance of the dominant matrix elements in predicting the spinon's scattering behaviour with respect to the energy for finite size spin chains. In order to do so, we use the symmetry with respect to $Q = \pm\pi/2$, which holds for the longitudinal and the spin-phonon interaction, while for the transverse potential we notice that although this condition is not fulfilled, the same procedure gives essentially the correct result.

Let us we first apply the above for an even site spin chain. The diagonal element of the T-matrix is given by

$$
\begin{aligned}
T(Q,Q) &= i\frac{u_Q}{N}\sum_{n=1}^{\infty}(-1)^n\left(\frac{1}{2u_Q}\right)^{2n}(\mathcal{F}^n+\mathcal{G}^n), \\
\mathcal{F} &\equiv N(|\langle Q+\pi|V_\pi|Q\rangle| + |\langle \pi-Q|V_{\pi-2Q}|Q\rangle|)^2 \\
\mathcal{G} &\equiv N(|\langle Q+\pi|V_\pi|Q\rangle| - |\langle \pi-Q|V_{\pi-2Q}|Q\rangle|)^2,
\end{aligned}
\tag{4.39}
$$

where we have used that only the even terms contribute to the Born series and that

$$
\sum_{m=even}^{2n}\binom{2n}{m}|\langle Q+\pi|V_\pi|Q\rangle|^{2n-m}|\langle \pi-Q|V_{\pi-2Q}|Q\rangle|^m = \frac{1}{2N^n}(\mathcal{F}^n+\mathcal{G}^n). \tag{4.40}
$$

Summing up the series to obtain the diagonal T-matrix element,

$$
T(Q,Q) = -i\frac{u_Q}{N}\left[\frac{\mathcal{F}}{4u_Q^2+\mathcal{F}} + \frac{\mathcal{G}}{4u_Q^2+\mathcal{G}}\right] \tag{4.41}
$$

and the transmission amplitude,

$$\mathcal{T}_{Q,Q} = \left(\frac{16u_Q^4 - \mathcal{F}\mathcal{G}}{16u_Q^4 + \mathcal{F}\mathcal{G} + 4u_Q^2(\mathcal{F}+\mathcal{G})}\right)^2. \tag{4.42}$$

Additionally we calculate the probability that the spinon is transmitted through the second branch. Using a similar procedure we obtain the $T(Q, Q+\pi)$ T-matrix element

$$\begin{aligned} T(Q, Q+\pi) \quad &= 2u_Q^2 \left[\frac{|\langle Q+\pi|V_\pi|Q\rangle| + |\langle \pi - Q|V_{\pi-2Q}|Q\rangle|}{4u_Q^2 + \mathcal{F}}\right. \\ &+ \left.\frac{|\langle Q+\pi|V_\pi|Q\rangle| - |\langle \pi - Q|V_{\pi-2Q}|Q\rangle|}{4u_Q^2 + \mathcal{G}}\right], \end{aligned} \tag{4.43}$$

and $\mathcal{T}_{Q,Q+\pi} = (\frac{N}{u_Q})^2 T(Q, Q+\pi)^2$.

In the case of an odd site spin chain we have a much simpler situation, since the π-transfer matrix element and the second branch are non-existent.

Finall, note that when ε_Q is not close to zero, the quantity $N\langle \pi - Q|S^z_{\pi-2Q}|Q\rangle = f^z(Q)$ can be considered negligible. Therefore by taking the logarithm of the transmission coefficient and using the identity $\log(1-x) = x - x^2/2 + O(x^3)$, we obtain that for $(g_{eff}/u_Q)^2/4f^z(Q) << 1$,

$$\log \mathcal{T}_{Q,Q} \simeq -f^z(Q)(\frac{g_{eff}}{u_Q})^2 \Rightarrow \mathcal{T}_{Q,Q} \simeq e^{-f^z(Q)(\frac{g_{eff}}{u_Q})^2}, \quad g_{eff} \equiv gN^{1-\mathcal{Z}^2}. \tag{4.44}$$

Chapter 5

Elements of Thermodynamics and Transport Theory

This chapter serves as a brief introduction to the thermodynamics of integrable systems. In particular, for pedagocial reasons, we start with the Lieb-Liniger model and thereafter we continue with the XXZ spin chain, while the same method can be in principle extended for various models. In the first section by using the Yang-Yang method, the thermodynamics of the Lieb-Liniger model is described. In the following sections, using Takahashi's and Suzuki's method to extend the Yang-Yang method, we describe the thermodynamics of the XXZ spin chain. Furthermore, we present a brief description of transport theory and a new theory called generalized hydrodynamics (GHD) which is a valuable tool in our understanding of out of equilibrium physics in integrable and non-integrable systems.

5.1 Thermodynamics of the One Dimensional Bose Gas

The construction of a thermodynamic theory for the Lieb Liniger model eq.(2.15) means that we will be able to calculate various macroscopic quantities, an equivalent statement to the knowledge of the partition function. To this end, using the canonical ensemble we calculate the partition function $\mathcal{Z}$ and the free energy $\mathcal{F}$ of the model. The relation between the partition function and the free energy is given by:

$$\mathcal{Z} = tr(e^{-H/T}) = e^{-\mathcal{F}/T}, \tag{5.1}$$

where T is the temperature and H is the Hamiltonian of the model. The thermodynamic limit $N \to \infty$, $L \to \infty$, $N/L = D$, is assumed.

Consequently, we use a theory developed by C.N. Yang and C.P. Yang [44] that allow us to derive a non-linear integral equation which gives the free energy at a given temperature.

Additionally, as we have already described, in the thermodynamic limit the Bethe roots $\{\lambda_j\}$ are described by distribution densities $\rho(\lambda)$, $\rho_h(\lambda)$, $\rho_v(\lambda)$, where $\Delta\mathcal{N}_p = L\rho(\lambda)d\lambda$ is the number of λ's in $d\lambda$, $\Delta\mathcal{N}_h = L\rho_h(\lambda)d\lambda$ is the number of holes in $d\lambda$ and $\Delta\mathcal{N}_v = \rho_v(\lambda) = \rho(\lambda) + \rho_h(\lambda)$ is the number of available vacancies in the corresponding interval.

The definition for the densities of particles, holes and vacancies is given by:

$$\rho(\lambda_j) = \lim_{N,L\to\infty} \frac{1}{L(\lambda_{j+1} - \lambda_j)}, \tag{5.2}$$

$$\rho_h(\lambda_j) = \lim_{N,L\to\infty} \frac{1}{L(\lambda^h_{j+1} - \lambda^h_j)}, \tag{5.3}$$

$$\rho_v(\lambda_j) = \lim_{N,L\to\infty} \frac{1}{L(\lambda^v_{j+1} - \lambda^v_j)}. \tag{5.4}$$

Let us define

$$Lh(\lambda) \equiv pL - \sum_{\mu} \theta(\lambda - \mu), \tag{5.5}$$

where $h(\lambda_j) = \frac{2\pi}{L} I_j$ and $h(\lambda^v_j) = \frac{2\pi}{L} n$. The above equations clarify the interpretation of the various constituents $\{\lambda_j, \lambda^h_j, \lambda^v_j\}$. The vacancies correspond to the total available states, each quantum number n can be mapped to a λ^v_n, and thus the set $\{\lambda^v_j\}$ characterizes the set of available solutions for each state. Afterwards, each particle solution $\{\lambda_j\}$ corresponds to a subset of the total available solutions and finally the images of the omitted quantum numbers are defined as holes solutions $\{\lambda^h_j\}$.

In the thermodynamic limit $h(\lambda)$ is given by the following non-linear integral equation

$$h(\lambda) = \lambda - \int_{-\infty}^{\infty} \theta(\lambda - \mu)\rho(\mu)d\mu. \tag{5.6}$$

Taking the derivative of equation eq.(5.5) we obtain:

$$\frac{dh(\lambda)}{d\lambda} = 2\pi(\rho + \rho_h) \equiv 2\pi\rho_v(\lambda) \tag{5.7}$$

Differentiation of eq.(5.6) with respect to λ gives:

$$2\pi h(\lambda) = 2\pi(\rho + \rho_h) = 1 + \int_{-\infty}^{\infty} \mathcal{K}(\lambda - \mu)\rho(\mu)d\mu. \tag{5.8}$$

The entropy of the ”state” is not zero since the existence of the omitted quantum numbers allows many wavefunctions of approximately the same energy to be described by the same ρ and ρ_h. The number of ways of distributing $\Delta\mathcal{N}_p$ into $\Delta\mathcal{N}_v$ vacancies is

$$\mathcal{N} = \binom{\Delta\mathcal{N}_v}{\Delta\mathcal{N}_p} = \frac{[L(\rho + \rho_h)d\lambda]!}{[L\rho d\lambda]![L\rho_h d\lambda]!} \tag{5.9}$$

The logarithm of $\mathcal{N}$ gives the entropy for a $d\lambda$ interval. Therefore, the total entropy per unit length $\mathcal{S}$ is:

$$\mathcal{S} = \int_{-\infty}^{\infty} \left[(\rho + \rho_h)\ln(\rho + \rho_h) - L\rho \ln \rho - \rho_h \ln \rho_h\right] d\lambda \tag{5.10}$$

Let us write the partition function in the canonical ensemble

$$\mathcal{Z} = \frac{1}{N!} \sum_{n_1, n_2, n_3, \ldots n_N} e^{-E/T} = \sum_{n_1 < n_2 < n_3 < \ldots < n_N} e^{-E/T}, \tag{5.11}$$

where $E = \sum_{j=1}^{N} \lambda_j^2$, with λ_j being the solution of the Bethe equation.

Introducing new variables $n_{j+1,j} = I_{j+1} - I_j$ we can rewrite

$$\mathcal{Z} = \sum_{n_{21}=1}^{\infty} \sum_{n_{32}=1}^{\infty} \ldots \sum_{n_{NN-1}}^{\infty} e^{-E/T} \tag{5.12}$$

The next step is to estimate the integration measure for the partition function eq.(5.12) when the thermodynamic limit is taken

$$\begin{aligned} n_{j+1,j} =& I_{j+1} - I_j = \frac{L}{2\pi}\Big[h(\lambda_{j+1}) - h(\lambda_j)\Big] \\ =& \frac{L}{2\pi} \int_{\lambda_j}^{\lambda_j + \frac{1}{L\rho(\lambda_j)}} \rho_v(\mu)d\mu \simeq \frac{\rho_v(\lambda)}{\rho(\lambda)}, \end{aligned} \tag{5.13}$$

where following eq.(5.2) we have used that $\lambda_{j+1} = \lambda_j + \frac{1}{L\rho(\lambda_j)}$, when $N, L \to \infty$ and the assumption that ρ_v is approximately constant in the interval $[\lambda_j, \lambda_j + \frac{1}{L\rho(\lambda_j)}]$

Therefore, in the thermodynamic limit the functional representation of the partition function is given by:

$$\mathcal{Z} = \text{constant} \int \mathcal{D}\left(\frac{\rho_v(\lambda)}{\rho(\lambda)}\right) \delta\left(L \int \rho(\lambda) d\lambda - DL\right) e^{S-\frac{E}{T}}, \tag{5.14}$$

where

$$\mathcal{S} - \frac{E}{T} = -\frac{L}{T} \int d\lambda \left\{\lambda^2 f(\lambda) - T[f(\lambda) \ln f(\lambda) - \rho(\lambda) \ln \rho(\lambda) - \rho_h \ln \rho_h(\lambda)]\right\} \tag{5.15}$$

The fixed number of particles in the canonical ensemble lead to the appearance of a δ function with the introduction of a chemical potential A

$$\delta(x) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{iAx} dA \tag{5.16}$$

Hence the partition function becomes

$$\mathcal{Z} = \text{constant} \int dA \int \mathcal{D}\left(\frac{\rho_v(\lambda)}{\rho(\lambda)}\right) \exp\left[S - \frac{E}{T} + A\frac{L}{T}\left(\int \rho(\lambda) d\lambda - DL\right)\right]. \tag{5.17}$$

In the equilibrium phase the exponent of the partition function should be maximized[1]

$$\varepsilon(\lambda) = -A + \lambda^2 - \frac{T}{2\pi} \int_{-\infty}^{\infty} \mathcal{K}(\lambda - \mu) \ln(1 + e^{-\varepsilon(\mu)/T}) d\mu \tag{5.18}$$

$$\int_{-\infty}^{\infty} \rho(\mu) d\mu = D \tag{5.19}$$

The first equation is known as the *Yang-Yang equation*, were we defined

$$\frac{\rho_h}{\rho} = e^{\varepsilon/T} \quad , \quad \frac{\rho}{\rho + \rho_h} = \frac{1}{1 + e^{\varepsilon/T}}. \tag{5.20}$$

[1]Using a more formal approach we have recovered the well known fact that in the thermodynamic equilibrium the free energy per unit length $\mathcal{F} = E - T\mathcal{S}$ should be minimized under the condition that density D is constant. Therefore, the quantity $\mathcal{F} - AD$ should be minimized, where the parameter A is the corresponding Lagrange multiplier

5.2 Thermodynamics of the XXZ critical Heisenberg chain

Takahashi and Suzuki (TS), along the lines of C.N. Yang and C.P. Yang, obtained the thermodynamic Bethe-ansatz equations for the XXZ spin chain model [120, 121] predicting correctly the thermodynamic properties of a one-dimensional spin chain system. Following the work of Fowler and Zotos for the massive Thirring model [122] and Hida for the XXZ spin chain [123], where using the normalizability of the wave function they found a rigorous and thorough explanation of the string type solutions that was previously conjectured by TS [121], we obtain restricting conditions for the string type excitations. Consequently, using continued fractions we present the Takakashi-Suzuki theory an elegant formulation for the $\Delta < 1$ spin chain thermodynamics.

Let us start with the Bethe wavefunction:

$$\phi_M(n_1, n_2, ..., n_M) = \Big(\prod_{j=1}^{M} z_j\Big)^{y_1} \sum_{\mathcal{P}\in\mathbb{S}_M}^{M!} A_{\mathcal{P}} \prod_{j=2}^{M} \Big(\prod_{l=j}^{M} z_j\Big)^{y_j}, \tag{5.21}$$

where $y_1 = n_1,\ y_j = n_{j+1} - n_j$ and $z_j = e^{ik_j}$. Moreover, without loss of generality we assume that $\Im k_n \leq \Im k_{n-1} \leq ... \leq \Im k_1$.

The infinite system, ϕ_M, should satisfy the following conditions:

$$\Big|\lim_{n_1,...,n_r\to-\infty} \phi_M(n_1, ..., n_M)\Big| < \infty \tag{5.22}$$

$$\Big|\lim_{n_{M-r+1},...,n_M\to\infty} \phi_M(n_1, ..., n_M)\Big| < \infty. \tag{5.23}$$

From the above conditions we obtain

$$A_{\mathcal{I}} \neq 0,\ A_{\mathcal{P}\neq I} = 0 \quad , \quad |\prod_{j=1}^{n} z_i| = 1,$$

$$|\prod_{l=j+1}^{M} z_l| \leq 1 \quad , \quad j = 1, ..., M-1 \tag{5.24}$$

where we have used the assumption $\Im k_n \leq \Im k_{n-1} \leq ... \leq \Im k_1$.

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \frac{i\zeta}{2}(n+1-2j) + i\frac{p_0}{2}(1-v) \quad , \quad j = 1, ..., n, \tag{5.25}$$

where $v = \pm 1$ and denotes the string parity, while $p_0 = \frac{\pi}{\gamma}$. These are the type of strings that satisfy the normalizability conditions eqs.(5.22,5.23)

Moreover applying the third normalizability condition to eq.(5.25) we get that:

$$
\begin{aligned}
&|\prod_{l=j+1}^{n} z_l| = \frac{\sinh\frac{\gamma}{2}(\lambda_\alpha^n + i(n-2j) + i\frac{\pi}{2}(1-v))}{\sinh\frac{\gamma}{2}(\lambda_\alpha^n + -in + i\frac{\pi}{2}(1-v))}| \Rightarrow \\
&0 < \sqrt{\frac{\cosh\gamma\lambda_\alpha^n - \cos\gamma(n-2j+\frac{p_0}{2}(1-v))}{\cosh\gamma\lambda_\alpha^n - \cos\gamma(n+\frac{p_0}{2}(1-v))}} < 1
\end{aligned} \tag{5.26}
$$

Hence, we obtain two conditions for the two string parities $v = \pm 1$, specifically $\cos\gamma n < \cos\gamma(n-2j)$ for positive string parity and $\cos\gamma n > \cos\gamma(n-2j)$ for negative string parity with $j = 1, ..., n-1$. Additionall,y from the positivity condition we obtain the following condition

$$
\begin{aligned}
&\cos\left(\frac{\pi}{2}(1-v) + (n-2j)\gamma\right) - \cos\left(\frac{\pi}{2}(1-v) + n\gamma\right) = \\
&= 2v\sin(\gamma(n-j))\sin(\gamma j) > 0, j = 1, 2, ..., n-1
\end{aligned} \tag{5.27}
$$

Moreover, the length n of a string should satisfy:

$$
2\sum_{j=1}^{n-1}[\frac{j\gamma}{\pi}] = (n-1)[(n-1)\frac{\gamma}{\pi}], \tag{5.28}
$$

$$
v\sin[(n-1)\gamma] \geq 0 \tag{5.29}
$$

We should mention that Takahashi and Suzuki used a different argumentation in order to arrive the above equations. They argued that if we assume the extreme case, where all magnons are bound in states of string length n, then there is no room to put in more n-particle bound states. For instance, the addition of another bound state is equivalent with the removing of one bound state and reversal of all spins, which in principle has a quite different wave function.

Takahashi and Suzuki showed that in the case where $\gamma/\pi \in (0,1)$ is an arbitrary rational number, we can express it by a continued fraction with length l

$$\frac{\gamma}{\pi} = \cfrac{1}{\nu_1 + \cfrac{1}{\nu_2 + \cfrac{1}{\ddots + \cfrac{1}{\nu_l}}}}, \tag{5.30}$$

where $\nu_1, \nu_2, ..., \nu_{l-1} \geq 1, \nu_l \geq 2$

Furthermore, the following relations are very useful:

$$\begin{aligned} &y_{-1} = 0,\ y_1,,\ y_l = \nu_1,\ y_i = y_{i-2} + \nu_i y_{i-1}, \\ &m_0 = 0 \quad , \quad m_i = \sum_{k=1}^{i} \nu_k,\ N_s = \sum_{k=1}^{l} \nu_k. \end{aligned} \tag{5.31}$$

The parity v_j and string length n are determined by:

$$\begin{aligned} &n_j = y_{i-1} + (j - m_i) y_i,\ v_j = (-1)^{[(n_j-1)/p_0]} \quad , \quad m_i < j < m_{i+1}, \\ &n_{m_l} = y_{l-1},\ v_{m_l} = (-1)^l \end{aligned} \tag{5.32}$$

In the $\Delta < 1$ the logarithmic for of the Bethe-Takahashi equations truncate to a finite set:

$$N\theta_j(\lambda_\alpha^j) = 2\pi I_\alpha^j + \sum_{k=1}^{N_s} \sum_{\beta=1}^{M_k} \Theta_{jk}(\lambda_\alpha^j - \lambda_\beta^k) \quad , \quad \alpha = 1, 2, ..., M_j \tag{5.33}$$

where

$$\begin{aligned} &\theta_j(x) = f(x; n_j, v_j) \quad , \quad \Theta_{jk}(x) = f(x; |n_j - n_k|, v_j v_k) + f(x; n_j + n_k, v_j v_k) + \\ &2 \sum_{i=1}^{\min(n_j,n_k)-1} f(x; |n_j - n_k| + 2i, v_j v_k), \end{aligned} \tag{5.34}$$

$$f(x; n, v) = 2v \tan^{-1}\left[\cot(\frac{n\gamma}{2})^v \tanh(\frac{\gamma x}{2})\right], \tag{5.35}$$

and

$$T_{jk}(x) \equiv \frac{1}{2\pi} \frac{d\Theta_{jk}(x)}{dx} \quad , \quad \alpha_j(x) \equiv \frac{1}{2\pi} \frac{d\theta_j(x)}{dx}. \tag{5.36}$$

where

$$a_j(x) \equiv \frac{1}{2\pi}\frac{d\theta_j(\lambda)}{d\lambda},\ T_{jk} \equiv \frac{1}{2\pi}\frac{d\Theta_{jk}(\lambda)}{d\lambda}, \tag{5.37}$$

Furthermore, note that the functions $a_j(x)$ and also the Fourier transformed functions $a_j(\omega)$ are given by:

$$a_j(\lambda) = \frac{1}{2\pi}\frac{\gamma \sin \gamma q_j}{\cosh \gamma\lambda + \cos \gamma q_j},\ a_j(\omega) = \frac{\sinh q_j\omega}{\sinh p_0\omega}. \tag{5.38}$$

Additionally,

$$\tilde{T}_{jk}(\omega) = \tilde{T}_{kj}(\omega) = 2\sigma_j \frac{\cosh(p_{i+1}\omega)}{\sinh(p_{i+1}\omega)}\frac{\sinh((p_0 - |q_j|)\omega)}{\sinh(p_0\omega)} \tag{5.39}$$

$$q_j \equiv (-1)^i[p_i - (j - m_i)p_{i+1}],\ m_i \leq j < m_{i+1}, \tag{5.40}$$

where

$$p_0 = \frac{\pi}{\gamma},\ p_1 = 1,\ \nu_i = [\frac{p_{i-1}}{p_i}],\ p_i = p_{i-2} - p_{i-1}\nu_{i-1} \tag{5.41}$$

Furthermore, in the thermodynamic limit

$$a_j(x) = \sigma_j(\rho_j(\lambda) + \rho_j^h(\lambda)) + \sum_{k=1}^{m_l} T_{jk} * \rho_k(\lambda),, \tag{5.42}$$

where $\sigma_j \equiv \mathrm{sign}(q_j)$

Minimizing the free energy $\mathcal{F} = E - T\mathcal{S}$ with respect to ρ_j we get:

$$\ln \eta_j(\lambda) = \frac{g_j(\lambda)}{T} + \sum_{k=1}^{m_l} \sigma_k T_{jk} * \ln(1 + \eta_k^{-1}),\ j = 1, ..., m_l \tag{5.43}$$

Equivalently, if $\ln \eta_j \equiv \beta\epsilon_j$

$$\epsilon_j(\lambda) = g_j(\lambda) + T\sum_{k=1}^{m_l} \sigma_k T_{jk} * \ln(1 + e^{-\beta\epsilon_k}),\ j = 1, ..., m_l \tag{5.44}$$

The free energy is given as follows:

$$\mathcal{F} = \Big(\frac{J\Delta}{4} + h\Big) - T\sum_{j=1}^{m_l} \sigma_j \int_{-\infty}^{\infty} a_j(\lambda)\ln(1 + e^{-\beta\epsilon_j})d\lambda. \tag{5.45}$$

In addition, an interesting observation is that the free energy can be expressed using only the ϵ_1 and ϵ_2 excitations

$$\mathcal{F} = -\frac{J\Delta}{4} - \sigma_1 \frac{2\pi \sin\gamma}{\gamma} \int_{-\infty}^{\infty} a_1(\lambda) s_1(x) d\lambda - \\ T \int_{-\infty}^{\infty} \ln(1+e^{\beta\epsilon_1}) d\lambda + \delta_{2m_l} \ln(1+e^{-\beta\epsilon_2}). \tag{5.46}$$

Therefore in the case where $m_l \neq 2$ the free energy can be written only using the ϵ_1 excitation

Finally, one can re-write eq.(5.44) for $h = 0$ in the form of a recurrence relation

$$\begin{aligned}
&\ln(1+e^{\beta\epsilon_0}) = -\frac{2\pi\beta J \sin\theta}{\theta}\delta(\mathrm{x}),\\
&\beta\epsilon_j = (1-\delta_{m_{i-1},j}) s_i \circ \ln(1+e^{\beta\epsilon_{j-1}}) + s_i \circ \ln(1+e^{\beta\epsilon_{j+1}}) \quad , \quad j = 1, ..., m_i - 2,\ j \neq m_l - 2\\
&\beta\epsilon_{m_i-1} = s_i \circ \ln(1+e^{\beta\epsilon_{m_l-2}}) + d_i \circ \ln(1+e^{\beta\epsilon_{m_l-1}}) + s_{i+1} \circ \ln(1+e^{\beta\epsilon_{m_l}}) \quad , \quad i < l\\
&\beta\epsilon_{m_l-2} = (1-2\delta_{m_{l-1},m_l-2}) s_l \circ \ln(1+e^{\beta\epsilon_{m_l-3}}) + s_l \circ \ln(1+2e^{\beta\epsilon_{m_l-1}} + e^{2\beta\epsilon_{m_l-1}}),\\
&\beta\epsilon_{m_l-1} = s_l \circ \ln(1+e^{\beta\epsilon_{m_l-2}}),\\
&\beta\epsilon_{m_l} = -\beta\epsilon_{m_l-1},
\end{aligned} \tag{5.47}$$

where we have used identities given by [121].

5.3 Elements of transport theory for integrable systems

Transport theory is a very intriguing topic with applications in a broad spectrum of scientific fields characterized by its *non-equilibrium* nature. In this section, we are particularly interested in the transport properties of the XXZ model. In general, probing energy/heat transport through a temperature gradient along the material while spin transport through a magnetic field gradient. However novel experimental techniques have revealed.... .

Results within the linear response theory

Considering the XXZ model one can easily calculate the spin and thermal operators using the Heisenberg relation $\partial_t A = i[H, A]$.

The spin current $\mathcal{J}^s = \sum_n j_n^s$ is

$$\partial_t S_n^z = i[H, S_n^z] = (j_n^s - j_{n-1}^s), \tag{5.48}$$

where j_n^s is the local spin current and is found to be given by

$$j_n^s = \frac{iJ}{2}\left(S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+\right). \tag{5.49}$$

in a similar way the thermal current operator is derived

$$\partial_t h_{n,n+1}^z = i[H, h_{n,n+1}^z] = (j_n^{th} - j_{n-1}^{th}) \tag{5.50}$$

It is useful to decompose the hamiltonian as $H = H^0 - h\sum_n S_n^z$ implying that the thermal current will assume the following form:

$$\mathcal{J}^{th} = \mathcal{J}^E - h\mathcal{J}^s. \tag{5.51}$$

The above relation has a very interesting physical consequence, namely that we can generate thermal currents through a combination of temperature and magnetic field gradient manipulations.

The energy current j_n^E is expressed as

$$j_n^E = J^2 \sum_n \mathbf{S_n} \cdot (\mathbf{S}'_{n-1} \times \mathbf{S}'_{n+1}), \quad \mathbf{S'_n} = (S_n^x, S_n^y, \Delta S_n^z). \tag{5.52}$$

We have already mentioned that spin and thermal currents are generated through a combination of temperature and magnetic field gradient manipulations. Within the *linear response theory*[2] the above statement is mathematically expressed as

$$\begin{pmatrix} \mathcal{J}^s \\ \mathcal{J}^{th} \end{pmatrix} = \begin{pmatrix} C_{th,th} & C_{th,s} \\ C_{s,th} & C_{s,s} \end{pmatrix} \begin{pmatrix} -\nabla T \\ \nabla h \end{pmatrix} \tag{5.53}$$

where the diagonal coefficient $C_{th,th}/C_{s,s}$ corresponds to the thermal/spin thermal conductivity and shall be denoted as k_{th} and σ_s respectively. Additionally, the coefficients

[2] In the context of quantum statistics, the theory states that adding a small perturbation coupled linearly to any observable, e.g. $f(t)\mathcal{O}(t)$ results to a response to the thermal expectation value of any other observable $\mathcal{A}$, in the form of $\langle \delta\mathcal{A}(t)\rangle = -i\int_0^t f(t')\langle[\mathcal{A}(t), \mathcal{O}(t')]\rangle dt'$, known as *Kubo formula*. Note that the non-linear regime to great extent is still unexplored

$C_{i,j}$ are given by

$$C_{i,j} = \lim_{\epsilon \to 0^+} \frac{\beta^r}{L} \int_0^\infty dt e^{-i(\omega - i\epsilon t)} \int_0^\infty d\tau \langle \mathcal{J}^i \mathcal{J}^j (t + i\tau) \rangle \tag{5.54}$$

where $r = 0$ for $j = th$ and $r = 1$ for $j = s$.

Furthermore, the real part of the coefficients C_{ij}, $C'_{i,j}$ can be decomposed into a sharp peak at $\omega = 0$ and regular part:

$$C'_{i,j} = 2\pi D_{i,j} \delta(\omega) + C^{\text{reg}}_{i,j}(\omega), \tag{5.55}$$

where the factors $D_{i,j}$ are called *Drude weights* and C' are evaluated for momentum $q = 0$. In particular, we focus on the diagonal elements, which are denoted as D_s and D_{th}, where the corresponding spin and thermal conductivity relation are

$$\sigma'(\omega) = 2\pi D_s \delta(\omega) + \sigma^{\text{reg}}(\omega). \tag{5.56}$$

$$k'(\omega) = 2\pi D_{th} \delta(\omega) + k^{\text{reg}}(\omega). \tag{5.57}$$

In the thermodynamic limit the spin Drude weight is found to be

$$D_s = \lim_{t \to \infty} \lim_{N \to \infty} \frac{\beta}{2N} \langle \mathcal{J}^s(t) \mathcal{J}^s(0) \rangle, \tag{5.58}$$

while the thermal Drude weight is

$$D_{th} = \lim_{N \to \infty} \frac{\beta^2}{2N} \langle (\mathcal{J}^E)^2 \rangle, \tag{5.59}$$

where we have used that $[\mathcal{J}^E, H] = 0$.

Conservations laws and Mazur's (in)equality

A non-zero Drude spin weight D_s as suggested by Kohn [124] signals diverging dc conductivity. Therefore, regarding the scattering processes into the material we expect that that the spin transport is going to be *ballistic*. In fact, for clean systems, i.e. without impurities ballistic transport is expected at zero temperature since all interactions are frozen. In contrast, a finite Drude weight at non zero temperature is a very interesting and peculiar phenomenon, since scattering processes[3] which are temperature dependent and appear at non-zero temperatures, are expected to broaden

[3]scattering processes can be due to intrinsic spin-spin interactions or due to magnetic impurities, spin-phonon distortions etc.

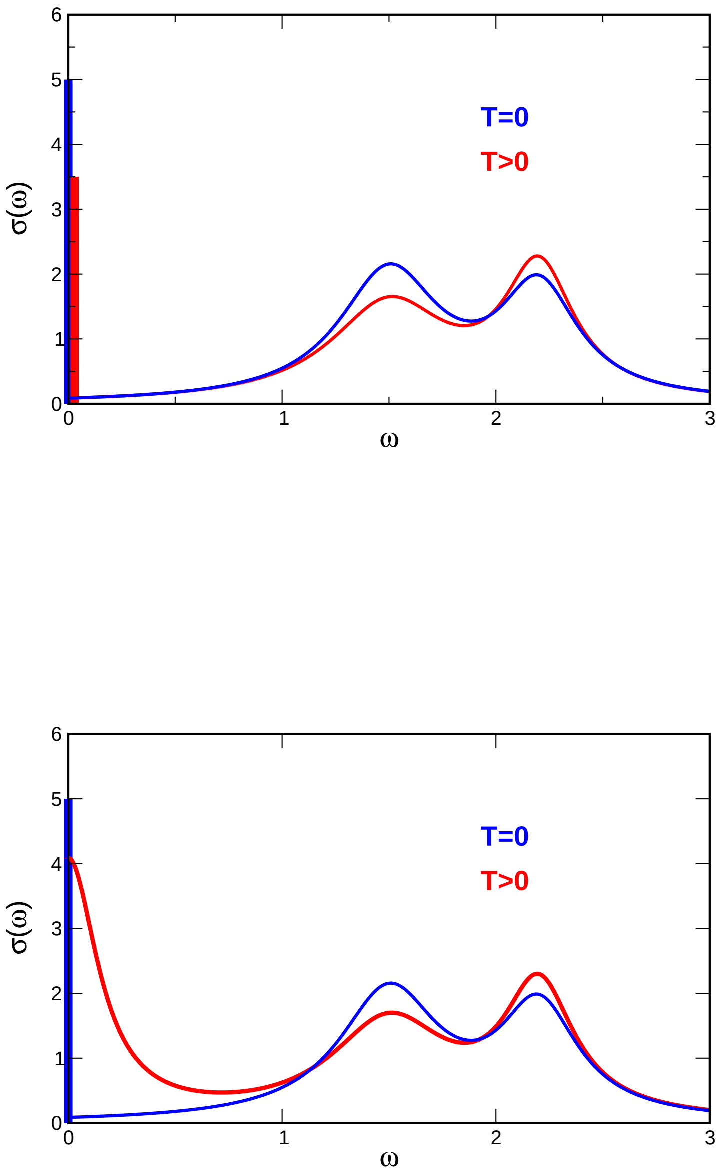

FIGURE 5.1: An illustration of the dc conductivity of an integrable model (top) and a generic non-integrable model (bottom). It is clear that for the non-integrable model the Drude weight vanishes for $T > 0$ resulting in normal transport in contrast to the integrable model where the Drude weight persists even for $T > 0$.

the delta peak, having width analogous to the inverse of the scattering time $\frac{1}{\tau}$, leading to a coexistence between ballistic and diffusive transport. Interestingly, in principle the only way this kind of situation is through a set of constraints that prohibit current relaxation, expressed in the form of conservation laws. The connection of integrable systems with ballistic transport and its contrast with non-integrable, generic systems was made by Zotos, Naef and Prelovsek [95].

Another important result regarding the connection of conservation laws and ballistic transport came from Mazur's work [125]. Specifically, Mazur proposed the following inequality for any hermitian operator $A \in \mathcal{H}$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \langle A(t)A \rangle dt \geq \sum_{n\in\mathbb{N}} \frac{\langle AQ_n \rangle^2}{\langle Q_n^2 \rangle}, \tag{5.60}$$

providing a lower bound for the time averaged correlation function, where $\langle\rangle$ denotes the thermodynamic average and we assume that the all conserved charges are orthogonal to each other, $\langle Q_n Q_m \rangle = \delta_{nm} \langle Q_n^2 \rangle$. This above inequality has an immediate consequence that whenever a charge protecting the operator A exists we get a non-zero value of the above correlation function.

At this point, it is important to mention that if the used set of conserved charges exhaust the Hilbert space, we obtain a strict equality, i.e. a *Mazur equality*. Of course, in general this cannot be done only with the presence of local charges, i.e. operators that act non-trivially to a portion of the physical space, but as shown by Prosen [126] the inclusion of some new charges called *quasilocal charges*[4] are needed.

In particular, for the XXZ model the energy current is analogous to $Q_3 \sim \mathcal{J}^E$, and thus we expect an infinite energy conductivity at any temperature, leading to pure ballistic motion. In contrast, spin current exhibits peculiar characteristics due to the fact that it cannot be expressed as a combination of conservation laws.

Drude weights and Bethe Ansatz calculations

The Bethe Ansatz technique can be useful for calculating the thermal and spin Drude weights. In this section we refer to some well known results which using the thermodynamic Bethe ansatz theory.

Firstly, we provide the thermal Drude weight D_{th} for anisotropies of the form $\Delta =$

[4] quasilocal charges are indeed a new type of conserved quantities, since their density function is not same as in the local case

$\cos(\frac{\pi}{\nu})$. Thermal Drude weight was first calculated by A. Klumper and K. Sakai [25] using the quantum transfer matrix (QTM) formalism, while a pure TBA calculation was carried out by X. Zotos [26]. Let us mention that although the QTM method handles easier all possible values of $0 \leq \Delta < 1$, i.e $\frac{\pi}{\gamma} \notin \mathbb{Q}_+$, the method developed by X. Zotos is a more straightforward approach with more appealing physical interpretation. In short, the trick is to a set of fictitious fields $\{\xi_j\}$ into the total energy of a Bethe Ansatz state (..) and then use the method developed in the aforementioned work.

$$E/N = \sum_j \int_{-\infty}^{\infty} d\lambda(\epsilon_j^{(0)} - hn_j + \xi_j j_j^{(0)})\rho_j, j_j^{(0)} = (\frac{-A}{2\pi})\partial_x \epsilon_j^{(0)}. \tag{5.61}$$

consequently, minimizing the free energy, the extended Bethe ansatz equations for the effective dispersions are obtained,

$$\epsilon_j(\lambda) = g_j(\lambda) - h\nu_j + \xi_j j_j^{(0)} + T\sum_{k=1}^{m_l} \sigma_k T_{jk} * \ln(1 + e^{-\beta\epsilon_k}),\ j = 1, ..., m_l \tag{5.62}$$

Hence, taking the fictitious field to be homogeneous, $\xi_=\xi$, and the magnetic field $h = 0$ we immediately notice that the partition function becomes

$$Z = \mathrm{tr} e^{-\beta H + \xi \mathcal{J}^E}. \tag{5.63}$$

It is immediate that the thermal Drude weight is given by the 2nd derivative with respect to ξ

$$D_{th} = \frac{\beta}{2N}\langle(\mathcal{J}^E)^2\rangle = -\frac{\beta}{2}\frac{\partial^2 f}{\partial \xi^2}|_{\xi=0} \tag{5.64}$$

Performing the calculations we obtain

$$D_{th} = \frac{\beta^2}{2}\sum_j \int_{-\infty}^{\infty} d\lambda(\rho_j + \rho_j^h)O_j(1 - O_j)(j_j^\epsilon)^2, \quad j_j^\epsilon = (\frac{-A}{2\pi})\partial_x \epsilon_j \tag{5.65}$$

Finally, notice that at low temperature the Drude weight scales linearly with temperature, i.e.

$$D_{th} = \frac{\pi v}{6}T, \quad v = J\pi\frac{\sin\gamma}{2\gamma}. \tag{5.66}$$

To evaluate the spin Drude weight D_s we follow the work of X. Zotos [23] and add a fictitious magnetic flux ϕ to the hamiltonian

$$H = J\sum_{i=1}^{N}(\frac{1}{2}e^{i\phi}\sigma_i^+\sigma_{i+1}^- + h.c.) + \frac{\Delta}{4}\sigma_i^z\sigma_{i+1}^z - \frac{h}{2}\sigma_i^z, \tag{5.67}$$

afterwards, we use the Kohn's formula

$$D_s = \frac{1}{2NZ}\sum e^{-\beta E_n}\frac{\partial^2 E_n}{\partial\phi^2}|_{\phi=0}. \tag{5.68}$$

In order to calculate the above equation we must introduce the finite size corrections to the energy eigenvalues due to the magnetic flux.

$$\lambda_N^j = \lambda_\infty^j + \frac{g_{1j}}{N} \tag{5.69}$$

where $\lambda_N^j(\lambda_\infty^j)$ are the rapidities for a system of size $N(N\to\infty)$. To $O(1/N)$,

$$\lambda_j Q_j = \frac{n_j}{2\pi} - \sum_k T_{jk} * (< n_k > Q_k), \quad Q_j = \frac{\partial g_{1j}(\rho_j + \rho_j^h)}{\partial\phi}, \tag{5.70}$$

and we obtain the spin Drude weight,

$$\begin{aligned} D_s &= \frac{\beta}{2}\sum_j\int_{-\infty}^{+\infty} dx(\rho_j+\rho_j^h) < n_j > (1- < n_j >)(j_j^{s2}), \\ j_j^s &= (\frac{1}{\rho_j+\rho_j^h}\frac{\partial\epsilon_j}{\partial x})Q_j, \quad < n_j >= \frac{1}{1+e^{\beta\epsilon_j}}. \end{aligned} \tag{5.71}$$

This expression is in formal analogy to the analogous expression for independent fermions. Solving eq.(6.22) we find that, in the high temperature limit $\beta\to 0$, the bound D_s^{ql} based on quasi-local conservation laws [127]

$$D_s^{ql} = \frac{\sin^2(\frac{\pi l}{m})}{\sin^2(\frac{\pi}{m})}(1 - \frac{l}{2\pi}\sin(\frac{2\pi}{m})), \quad \theta = l/m,\ l = (1+\nu_1\nu_2),\ m = \nu_2 \tag{5.72}$$

Generalized hydrodynamics theory

Generalized hydrodynamics (GHD) has been recently proposed by B. Bertini, M. Collura, J. De Nardis, and M. Fagotti and independently by O. A. Castro-Alvaredo, B.

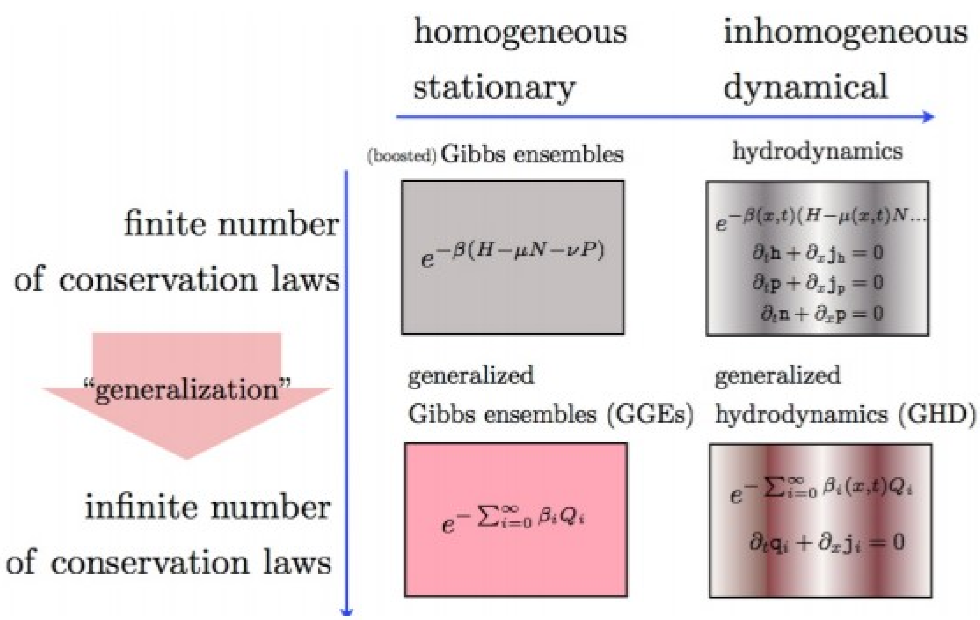

FIGURE 5.2: .
A schematic figure depicting how GHD emerges. Taken from [128]

Doyon, and T. Yoshimura [22, 21] as an alternative way to study non-equilibrium phenomena in various systems such as spin chains, gases or field theories. Specifically, the theory of GHD relies upon the division of the system into "fluid cells" (at mesoscopic scale), where each cell although very small to be observed it is thermodynamically large enough to reach a state of maximum entropy. In general, a gas obeying Galilean transformations can be characterized by three numbers: temperature, chemical potential and a Galilean boost. On the contrary, an integrable system needs an infinite number of quantities for the state to be characterized, and thus the Gibbs ensemble should be replaced with the GGE. In addition, using the assumption of local entropy maximization one can, to good approximation, calculate the expectation value of an operator $\mathcal{O}(x,t)$ [128]

$$\langle \mathcal{O}(x,t)\rangle \simeq \langle \mathcal{O}(0,0)\rangle_{\bar{\beta}(x,t)}, \tag{5.73}$$

where we have used the homogeneity and stationarity of the maximal entropy state $\langle ... \rangle_{\bar{\beta}(x,t)}$ and $\bar{\beta}$ denotes the set of Lagrange multipliers which depend on (x,t). Consequently, as described in [128] one can use the asymptotic scattering states in order to represent these maximal entropy states and then expand the functional form of every physical quantity to become space-time dependent, for instance the quasiparticle and hole densities and will become

$$\rho(\lambda) \to \rho(\lambda, x, t), \quad \rho^h(\lambda) \to \rho^h(\lambda, x, t). \tag{5.74}$$

In addition, assuming that the conserved charges and currents are differentiable we can write down an Euler-Hydrodynamics continuity equation for these quantities

$$\partial_t Q_n + \partial_x J_n = 0, \tag{5.75}$$

where $Q_n \equiv \langle Q_n(0,0)\rangle_{\bar{\beta}(x,t)}$ and $J_n \equiv \langle J_n(0,0)\rangle_{\bar{\beta}(x,t)}$.

The next step is to define the dressing operation $f(\lambda) \to f^{\mathrm{dr}}(\lambda)$. For a single particle species the dressing satisfies the following integral equation

$$f^{\mathrm{dr}}(\lambda) = f(\lambda) + \int_{\mathbb{R}} \frac{d\mu}{2\pi} K(\lambda-\mu) n(\mu) f^{\mathrm{dr}}(\mu), \tag{5.76}$$

while in the case of N_s excitation species a straightforward generalization gives

$$f_j^{\mathrm{dr}}(\lambda) = f_j(\lambda) + \sum_{k=1}^{N_s} \int_{\mathbb{R}} \frac{d\mu}{2\pi} T_{jk}(\lambda-\mu) n_k(\mu) f_k^{\mathrm{dr}}(\mu). \tag{5.77}$$

On this basis, the conserved charge and the current density are defined as

$$Q_n = \int \frac{d\lambda}{2\pi} n(\lambda) h_n^{\mathrm{dr}}(\lambda) \tag{5.78}$$

$$J_n = \int \frac{d\lambda}{2\pi} (E')(\lambda) n(\lambda) h_n^{\mathrm{dr}}(\lambda), \tag{5.79}$$

where, $h_n^{\mathrm{dr}}(\lambda)$ is the dressed quantity of the $h_n(\lambda)$ which is the function which generates the symmetry.

We can rewrite them in the more convenient form

$$Q_n = \int \frac{d\lambda}{2\pi} \rho(\lambda) n(\lambda) h_n(\lambda) \tag{5.80}$$

$$J_n = \int \frac{d\lambda}{2\pi} v^{\mathrm{eff}}(\lambda) n(\lambda) \rho(\lambda) h_n(\lambda) \tag{5.81}$$

where, the effective velocity $v^{\mathrm{eff}}(\lambda) = \frac{(E')^{\mathrm{dr}}(\lambda)}{(p')^{\mathrm{dr}}(\lambda)}$ and has a similar interpretation with the one of a group velocity.

Finally, using eq.(5.75) and making our quantities space-time dependent eq.(5.74) we obtain a set of equations called Bethe-Boltzmann equations

$$\partial_t \rho(x,t,\lambda) + \partial_x \left(u^{\mathrm{eff}}(x,t,\lambda) \rho(x,t,\lambda) \right) = 0. \tag{5.82}$$

The above equations can re-written into a more useful form after going into a diagonal basis

$$\partial_t n(x,t,\lambda) + v^{\mathrm{eff}}(x,t,\lambda) \partial_x n(x,t,\lambda) = 0. \tag{5.83}$$

It is evident, that this non-linear differential equation describes quasiparticles propagating with effective velocity which is functional of the local density, due to the microscopic interactions among the elementary constituents.

Generally, GHD serves as a very interesting extension of TBA to include out-of equilibrium effects. For instance, evaluating currents in non-equilibrium steady states (NeqSS), i.e. states that do not depend on time but are still far from equilibrium. The methodology for the study of such quantities is the partitioning of the physical system into two halves being thermalized into different equilibrium states[5] (for example they are held into different temperatures) which are held separately with no interaction between them. At $t = 0$ the two halves are connected and the system evolves in

[5]This problem is known in the literature as the Riemann problem

accordance with the Hamiltonian of the system. Afterwards, in the absence of diffusion the initial imbalance develops a transport current of physical quantities which can be studied at the long time limit. To this end, many quantities of interest for spin and thermal transport have been calculated such as the Drude weight [24, 27, 129]. Finally, let us mention that GHD equations were successfully applied to many physical systems such as classical mechanical systems [130, 131, 132] and field theories [133, 21], spin chains [22, 129, 134, 135, 136] cold atom systems [137, 138]. Note that this is only a tiny fracture of the vast amount of literature that has appeared over the last few years.

Chapter 6

Dressed Excitations, Thermodynamics and Relaxation

In this chapter, we discuss the low and high temperature contribution of Thermodynamic Bethe Ansatz (TBA) dressed excitations and the energy/magnetization relaxation within the Generalized Hydrodynamics approach in the linear response regime. In particular, we show how the temperature dependent dispersions of the excitations reproduce well known behavior of the specific heat, magnetic susceptibility, spin and energy Drude weights. In this context, we derive a further formulation of the Drude weights from the finite wavevector relaxation. Furthermore, we contrast the TBA description of thermodynamics and dynamics in terms of a multitude of string excitations to that in terms of a single quasi-particle in low energy effective theories.

6.1 Introduction

The framework for studying the thermodynamic properties of the one dimensional spin-1/2 Heisenberg model, in the easy-plane antiferromagnetic regime, was first set in a seminal paper by Takahashi and Suzuki (TS) [121] along the line of the Thermodynamic Bethe ansatz (TBA) proposed by Yang and Yang [44].

The characteristic of the TS formulation was the introduction of an intricate structure of allowed "string excitations" depending on the value of the anisotropy parameter. This structure was originally attributed to the physical requirement of normalizability of the corresponding Bethe ansatz wavefunctions [122, 123] and more recently given a group theoretic interpretation [139]. The specific heat and magnetic susceptibility where mostly obtained by a numerical evaluation of the TBA nonlinear integral equations.

In this work [140], aiming at a physical picture of the (thermo-) dynamics, we look at the low energy dispersions of the underlying string excitations where we find that they are simple expressions in terms of dressed momenta which however are temperature dependent. By reformulating the expressions of the specific heat and magnetic susceptibility we point out that, in contrast to field theoretic approaches, completely different string excitations correspondingly contribute.

On the relaxation functions, a very interesting recent extension of TBA was proposed for space-time dependent densities under the name of Generalized Hydrodynamics approach [22, 21] (GHD). By this novel method the spin and thermal Drude weights [23, 24, 25, 26] were recovered as asymptotic states of a quench from an initial thermal/magnetization step [27]. Here, using the GHD approach in the linear approximation, we analyze the relaxation of wavevector-q dependent thermal/magnetization profiles. As a byproduct we obtain the Drude weights as integrals over frequency of the wavector-q relaxation spectral function, of course closely related to linear response conductivities.

This study provides theoretical background to present and feature experiments in 1D quantum magnets [28], e.g "dynamic heat transport" [29] and "transient grating spectroscopy" experiments [30], that probe the relaxation of magnetization/thermal density profiles.

6.2 TBA formulation and dressed quantities

The XXZ anisotropic Heisenberg Hamiltonian for a chain of N sites with periodic boundary conditions is given by,

$$H = \sum_{i=1}^{N} J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) - hS_i^z, \tag{6.1}$$

where S_i^a are spin-1/2 operators and $S_{N+1}^a = S_1^a$. The region $0 \le \Delta \le 1$ is commonly parametrized by $\Delta = \cos\theta$ and J is taken as the unit of energy. In the following we will closely follow the formulation and notation by TS [121] (see Appendix A).

In the thermodynamic limit, for the simplest case of $\theta = \pi/\nu$, the solutions of the Bethe ansatz equations are grouped into a set of strings of order $l_j = j$ and parity $\zeta_j = +1,\ j = 1, ..., \nu - 1$ and one $l_\nu = +1,\ \zeta_\nu = -1$. More generally the anisotropy parameter θ is expressed as a continued fraction expansion (TS) $\theta = \frac{\pi}{\nu_1 + 1/(\nu_2 + 1/\nu_3 + ...)}$. The densities of excitations $\rho_j(\lambda)$ and holes $\rho_j^h(\lambda)$ (λ is the rapidity of the excitations) are given by,

$$\begin{aligned} a_j &= \sigma_j(\rho_j+\rho_j^h)+\sum_k T_{jk}\circ\rho_k \\ a_j(\lambda) &= \frac{\theta}{2\pi}\frac{v_j\sin(n_j\theta)}{\cosh(\theta\lambda)-v_j\cos(n_j\theta)} \end{aligned} \tag{6.2}$$

with $a\circ b(\lambda)=\int_{-\infty}^{+\infty}a(\lambda-\mu)b(\mu)d\lambda$ and T_{jk} the phase shifts given by TS (Appendix A). The sum over k is constrained over the allowed strings, depending on the value of the anisotropy Δ and $\sigma_j=\zeta_j$. Minimizing the free energy, the standard Bethe ansatz equations for the temperature dependent effective dispersions ϵ_j at temperature T (inverse temperature $\beta=1/k_BT$), are obtained,

$$\begin{aligned} \epsilon_j &= \epsilon_j^{(0)}+hl_j+T\sum_k\sigma_kT_{jk}\circ\ln(1+e^{-\beta\epsilon_k}) \\ \epsilon_j^{(0)} &= -Aa_j,\ A=2\pi\frac{J\sin\theta}{\theta},\ \beta\epsilon_j=\ln\rho_j^h/\rho_j. \end{aligned} \tag{6.3}$$

As the bare momentum of a particle (flipped spin from the ferromagnetic state) is given by,

$$p_1^{(0)}=+i\ln\frac{\sinh\frac{\theta}{2}(\lambda+i)}{\sinh\frac{\theta}{2}(\lambda-i)}, \tag{6.4}$$

and

$$a_1=\frac{1}{2\pi}\frac{\partial p_1^{(0)}}{\partial\lambda}, \tag{6.5}$$

we define "bare" $p_j^{(0)}$ and "dressed" p_j momenta [21],

$$\begin{gathered} \frac{\partial p_j}{\partial\lambda}=2\pi\sigma_j(\rho_j+\rho_j^h)=2\pi\sigma_jr_j,\quad \frac{\partial p_j^{(0)}}{\partial\lambda}=2\pi a_j, \\ r_j=\rho_j+\rho_j^h \end{gathered} \tag{6.6}$$

and rewrite eq.(6.2) as,

$$\frac{\partial p_j}{\partial\lambda}=\frac{dp_j^{(0)}}{d\lambda}-\sum_k\sigma_kT_{jk}\circ n_k\frac{\partial p_k}{\partial\mu}, \tag{6.7}$$

with $n_k=\rho_k/(\rho_k+\rho_k^h)$.

Similarly, as the bare particle energies are $\epsilon_j^{(0)} = -Aa_j$ we define dressed energies $E_j = -A\sigma_j(\rho_j + \rho_j^h)$ so that eq.(6.2) becomes,

$$E_j = \epsilon_j^{(0)} - \sum_k \sigma_k T_{jk} \circ \ n_k E_k. \tag{6.8}$$

Notice that the eigenvalues of conserved quantities are obtained by [45]:

$$q_m = \Big(- J\frac{\sin\theta}{\theta}\Big)^m \frac{\partial^m p^{(0)}}{\partial\lambda^m}, \tag{6.9}$$

where $q_0 = p_1^{(0)}$ is the momentum, $q_1 = \epsilon_1^{(0)}$ the energy, $q_2 = j_1^{\epsilon(0)}$ the energy current eigenvalues.

With these definitions the mean value of the total energy is written as,

$$E = \sum_j \int d\lambda \rho_j(\lambda)\epsilon_j^{(0)}(\lambda) = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j \epsilon_j^{(0)} \tag{6.10}$$

or, by using eqs.(6.2,6.8) and a procedure named "dressing" [21],

$$E = \sum_j \int d\lambda \rho_j(\lambda)\epsilon_j^{(0)}(\lambda) = \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi} n_j E_j. \tag{6.11}$$

As the energy current is also a conserved quantity, we can further define the mean value of energy current as,

$$\begin{aligned} J_E &= \sum_j \int d\lambda \rho_j j_j^{\epsilon(0)} = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j j_j^{\epsilon(0)}, \\ j_j^{\epsilon(0)} &= \Big(\frac{-A}{2\pi}\Big)\frac{\partial \epsilon_j^{(0)}}{\partial\lambda} \end{aligned} \tag{6.12}$$

or as in eq.(6.11),

$$J_E = \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi} n_j j_j^{\epsilon}, \quad j_j^{\epsilon} = \Big(\frac{-A}{2\pi}\Big)\frac{\partial \epsilon_j}{\partial\mu}. \tag{6.13}$$

By taking the derivative of eq.(6.3) with respect to the rapidity λ, we obtain an equation for the energy currents with the same structure as eqs.(6.2,6.8).

$$j_j^{\epsilon} = j_j^{\epsilon^{(0)}} - \sum_k \lambda_k T_{jk} \circ n_k j_k^{\epsilon}. \tag{6.14}$$

At this point, it is instructive to introduce an effective velocity of the excitations by [22, 21, 141],

$$v_j = \frac{1}{2\pi\sigma_j(\rho_j + \rho_j^h)} \frac{\partial \epsilon_j}{\partial \mu} = \frac{\partial \epsilon_j}{\partial p_j} \tag{6.15}$$

and rewrite eq.(6.13) in the physical form,

$$J_E = \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi} n_j (v_j E_j). \tag{6.16}$$

6.3 Thermodynamics in the low and high temperature limit

Having presented the basic formalism, we proceed to the low(high) temperature analysis of the dressed excitations and their contribution to thermodynamic quantities of the system in study, in particular the specific heat and magnetic susceptibility. Let us mention, that in this section all calculations are for zero magnetic field ($h = 0$).

Let us begin with the free energy density $f(T)$ [121, 26]

$$\begin{aligned} f &= -T \sum_j \sigma_j \int d\lambda a_j \ln(1 + e^{-\beta\epsilon_j}) \\ &= -T \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi} \ln(1 + e^{-\beta\epsilon_j}). \end{aligned} \tag{6.17}$$

Consequently, we obtain the mean energy density $\epsilon(T)$,

$$\epsilon(T) = \frac{\partial}{\partial \beta}(f/T) = \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi} n_j E_j, \tag{6.18}$$

and by evaluating the equilibrium responses, $\frac{\partial r_j}{\partial \beta}\Big|_{\beta,h}$, $\frac{\partial n_j}{\partial \beta}\Big|_{\beta,h}$ (Appendix D), the specific heat $c(T)$,

$$c = \frac{\partial \epsilon}{\partial T} = \beta^2 \sum_j \int \frac{dp_j}{2\pi} n_j (1 - n_j) E_j^2. \tag{6.19}$$

Similarly, we obtain the mean magnetization density $m(T)$,

$$\begin{aligned} m &= \frac{\partial f}{\partial h} = \sum_j \sigma_j \int d\lambda a_j n_j Q_j \\ &= \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi} n_j Q_j, \quad Q_j = \frac{\partial \epsilon_j}{\partial h}, \end{aligned} \tag{6.20}$$

and the magnetic susceptibility $\chi(T)$,

$$\chi = \frac{\partial m}{\partial h}|_{h \to 0} = \beta \sum_j \int \frac{dp_j}{2\pi} n_j (1 - n_j) Q_j^2. \tag{6.21}$$

The "charges", $Q_j = \partial \epsilon_j / \partial h$ also satisfy,

$$Q_j = Q_j^{(0)} - \sum_k \sigma_k T_{jk} \circ n_k Q_k, \quad Q_j^{(0)} = l_j. \tag{6.22}$$

At low (zero) temperatures (Appendix B) the dispersion relations ϵ_j are relatively simple functions of the dressed momenta p_j, which are of the order of temperature T. At $T = 0$,

$$\begin{aligned} \epsilon_1 &= -v \sin p_1, \quad 0 \le p_1 < \pi \\ \epsilon_j &= 0, \quad j > 1, \end{aligned} \tag{6.23}$$

where $v = J(\pi/2) \sin\theta/\theta$ is the spinon velocity. ϵ_1 is the dispersion of 1-string excitations (holes in the "magnon" Fermi sea) and is the same as the dispersion of spinons, the elementary excitations of the model, [20] but with only one branch.

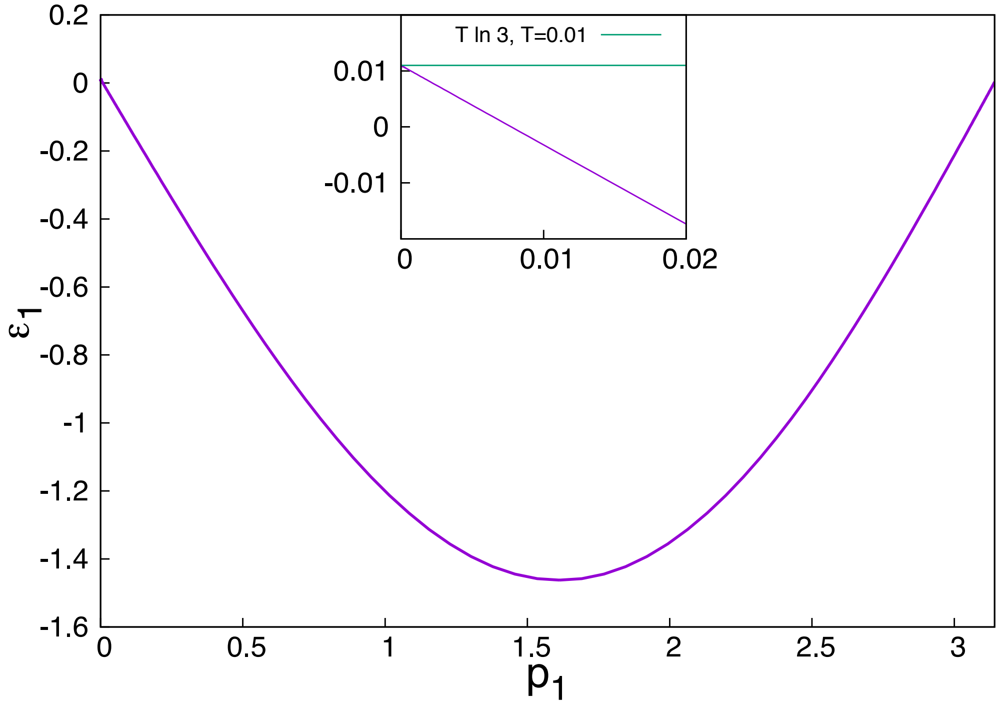

FIGURE 6.1: numerical evaluation of excitation energy ε_1 vs dressed momentum p_1 for $T = 0.01$. The inset show the deviation from the spinon dispersion relation at the region $p_1 \to 0$ where the effective field theory will be generated from

At $T \to 0$ and $\theta/\pi = \nu$, the string excitation thermal energy dispersions ϵ_j form a non-overlapping sequence,

$$\begin{aligned}
\epsilon_1 &\simeq T g(p_1) - v \sin p_1, \quad 0 \leq p_1 \leq \pi \\
\epsilon_j &\simeq T \ln(j^2 - 1) + v|p_j|, \quad j = 2, ..., \nu - 2, \\
|p_j| &\leq p_j^{max}, \quad p_j^{max} = \frac{T}{v} \ln\Big(\frac{(j+1)^2 - 1}{j^2 - 1}\Big), \\
\epsilon_{\nu-1} &\simeq T \ln(\nu - 2) + v|p_{\nu-1}|, \\
|p_{\nu-1}| &< p_{\nu-1}^{max}, \quad p_{\nu-1}^{max} = \frac{T}{v} \ln\Big(\frac{\nu - 1}{\nu - 2}\Big), \\
\epsilon_\nu &= -\epsilon_{\nu-1}, \quad p_\nu^{max} = p_{\nu-1}^{max}.
\end{aligned} \tag{6.24}$$

Note that $\ln 2 \leq g(p_1) \leq \ln 3$, with $g(0) = g(\pi) = \ln 3$ and $g(\pi/2) \simeq \ln 2$ (Appendix B). Additionally the ϵ_j do not overlap as $\epsilon_j(\pm p_j^{max}) = \epsilon_{j+1}(0)$ (the momenta are shifted

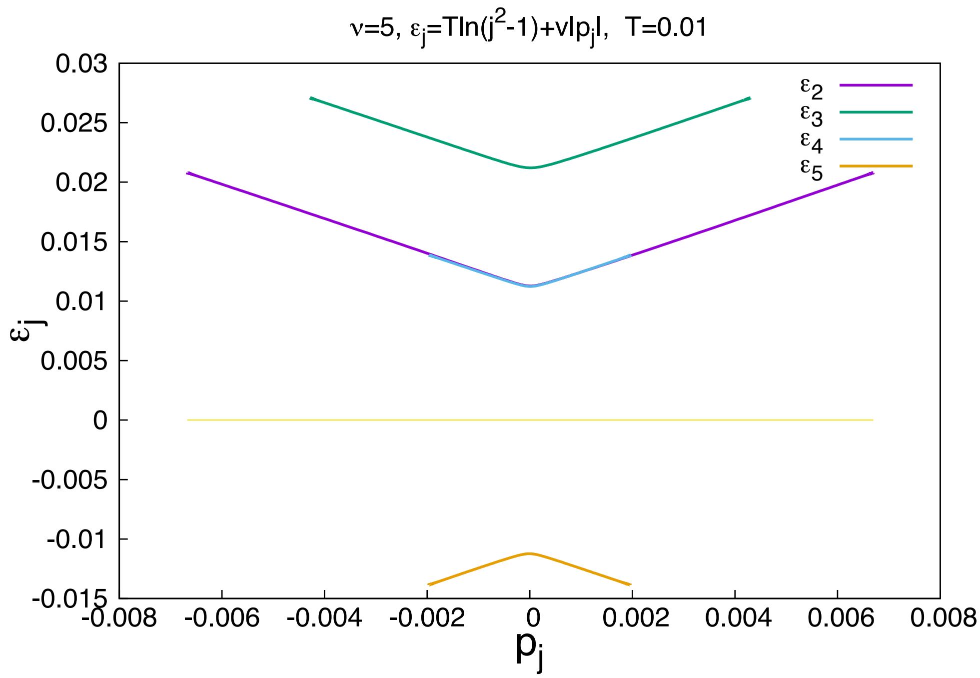

FIGURE 6.2: excitations energies ε_j vs dressed momenta p_j for $T = 0.01$ and $\nu = 5$

by $\pm p_j^{max}$ so that the p_j are symmetric about zero). At $T \to +\infty$ (Appendix C),

$$\begin{aligned} \epsilon_j &\simeq T\ln((j+1)^2-1), \quad j = 1, ..., \nu-2 \\ |p_j| &\leq p_j^{max}, \quad p_j^{max} = \pi\frac{j+1}{(j+1)^2-1} \\ \epsilon_{\nu-1} &\simeq T\ln(\nu-1), \quad p_{\nu-1}^{max} = \frac{\pi}{2}\frac{1}{\nu-1} \end{aligned} \tag{6.25}$$

and thus the top of the dispersions, $\epsilon_j(p_j^{max})/T$, are temperature independent as they coincide with the $T \to 0$ ones. The momentum space is increasing with T at low temperatures, reaching a constant value at high temperatures. It is also interesting to observe that a quasi-particle dispersion of the form, $f(p) = T\ln g - \epsilon_p$ can be interpreted as a dispersion of holes, with degeneracy g,

$$n_h = 1 - n = \frac{g}{g + e^{\beta\epsilon_p}}. \tag{6.26}$$

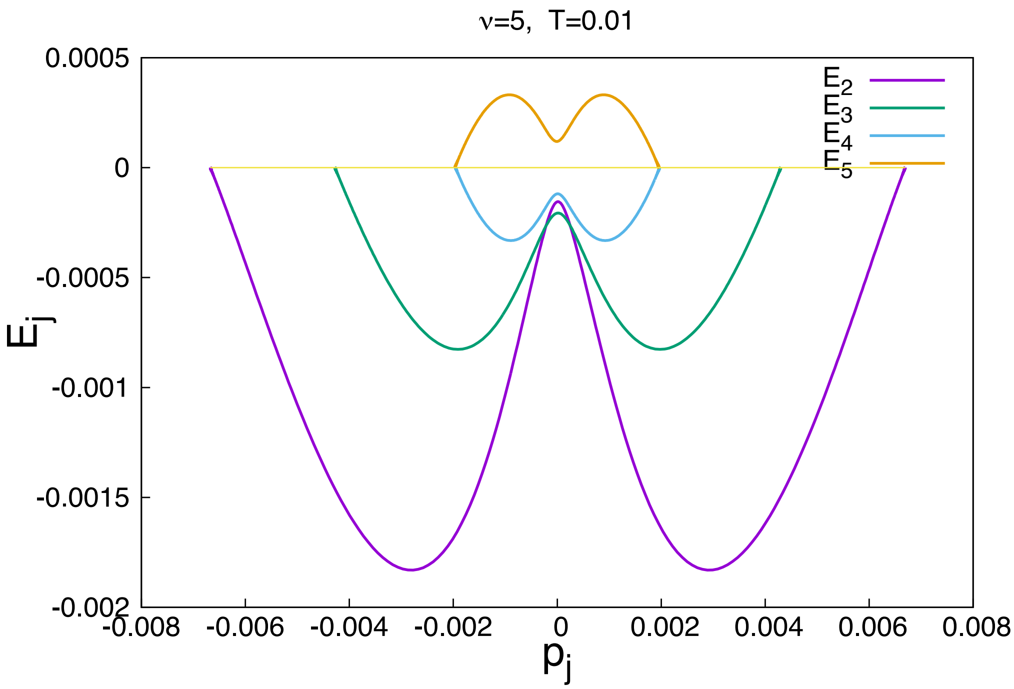

FIGURE 6.3: Dressed excitations energies E_j vs dressed momenta p_j for $T = 0.01$ and $\nu = 5$

Concerning the excitation energies E_j, at $T = 0$, $E_1 = \epsilon_1$ and $E_j = 0,\ j > 1$. At low T, we find numerically that they do not have an accurate simple form, $E_1 \sim -v|\sin p_1|$ and $E_j,\ j > 1$ are of $O(T)$,

$$E_j \sim -T|\sin(\frac{\pi p_j}{p_j^{max}})|, \quad j = \nu - 1, \nu, \quad |p_j| \leq p_j^{max}, \tag{6.27}$$

where p_j^{max} are the same as for the ϵ_j.

At this point it is interesting to compare the commonly used "spinon" description of the specific heat as obtained from a Luttinger liquid or bosonization theory to the TBA description. In the spinon description, the elementary excitations with dispersion $\epsilon = v|\sin p|, -\pi < p \leq \pi$ contribute at low energies to the specific heat by a 4-fold linear dispersion $\epsilon \sim vp$, $c_{spinon} \simeq \frac{\pi}{3}\frac{1}{\beta v}$. On the other hand the TBA 1-string excitations with dispersion $\epsilon_1(p_1) \simeq T\ln 3 - v\sin p_1$ eq.(6.24) and 2-fold linear spectrum at low energies, give

$$c_{TBA}^{(1)} \simeq \beta^2 2 \int_0^{+\infty} \frac{dp_1}{2\pi} \frac{(vp_1)^2}{4\cosh^2 \frac{\beta(T\ln 3 - vp_1)}{2}} \simeq 1.234 \frac{1}{\beta v} \tag{6.28}$$

instead of $\pi/3 \simeq 1.047$. In this calculation we used the $T = 0$ dispersion E_1 which overestimates $c_{TBA}^{(1)}$ as at low temperatures $|E_1| < v \sin p_1$. A complete accurate numerical evaluation of eq.(6.19) reproduces the factor $\pi/3$ and indicates that the contribution of higher order strings is minimal. As $E_j, j > 1$ is $O(T)$ we find from eqs.(6.19,6.24) that $c_{TBA}^{(j)} \sim \frac{1}{\beta v}\frac{1}{j^3}$. Note that this attribution of the low-T specific heat to a single branch of 1-string excitations is not in agreement with the discussion in [142].

To evaluate the magnetic susceptibility, we first note that in the case of zero magnetic field ($h = 0$) the charges Q_j are temperature independent [27, 103, 103] and the evaluation of (6.22) is particularly simple giving $Q_j = 0, j = 1, ..., \nu - 2$ and $Q_{\nu-1} = -Q_\nu = +\nu/2$ (Appendix E). Using the relation (6.21) for the magnetic susceptibility and eq.(6.24) we obtain for $T \to 0$,

$$\chi = \frac{1}{\pi v} K, \quad K = \frac{1}{2} \frac{1}{1 - 1/\nu}, \tag{6.29}$$

where K is the Luttinger liquid parameter. In the high temperature limit, $\beta \to 0$, from eq.(6.25), $\chi = \frac{\beta}{4}$. The fact that the $l_\nu = +1$ excitations with parity $\zeta_\nu = -1$ account for the magnetic susceptibility is not surprising, as they physically correspond to a uniform change of the S^z component of the magnetization by $+1$ [143] and detected e.g. in ESR experiments [144]. Overall, it is important to mention that calculation of these two thermodynamic quantities pose an interesting question: "*What is the relation between the TBA string excitations and the single linear dispersion quasi-particle emerging from the low energy effective theories*?". Indeed, we notice that these apparently different descriptions describe accurately the thermodynamics of the system, thus expecting a relation between the two descriptions. Nevertheless, although as expected the numerical calculations give the correct results, the interpretation of E_j and their relation to the aforementioned quasiparticle is not well understood. The above difficulty could be ascribed to the complex behavior of E_j.

Closing this section, we note that for $\theta/\pi = \nu_1 + 1/\nu_2$ (see Appendix B, C), relations similar to eqs.(6.24,6.25) give the same low/high temperature asymptotic specific heat and magnetic susceptibility.

6.4 Energy - magnetization relaxation

In the GHD approach, the occupations n_j depend on space and time following the continuity equation [21, 22],

$$\frac{\partial n_j(x,t)}{\partial t} + v_j(x,t)\frac{\partial n_j(x,t)}{\partial x} = 0, \tag{6.30}$$

This is conjectured to be valid in the long wavelength - time limit (hereafter, the dependence of quantities in space-time will be explicitly denoted by (x,t), otherwise they will refer to an equilibrium state at a temperature $k_B T = 1/\beta$ and magnetic field h). Notice that this relation follows by making local the conservation of energy for every excitation mode [21],

$$\begin{aligned} \frac{\partial E(x,t)}{\partial t} &+ \frac{\partial J_E}{\partial x} = 0 \\ \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi}\frac{\partial}{\partial t} n_j E_j &+ \sum_j \sigma_j \int \frac{dp_j^{(0)}}{2\pi}\frac{\partial}{\partial x} n_j (v_j E_j) = 0 \\ \frac{\partial}{\partial t}\rho_j &+ \frac{\partial}{\partial x}(v_j \rho_j) = 0, \end{aligned} \tag{6.31}$$

the original form of the GHD equation.

Most of the studies have considered a quench scenario, namely two regions at different temperatures/magnetic fields initially separated by a wall. Here, with view to future experiments on quantum magnets [30], we want to study the energy/ magnetization relaxation, starting from an initial condition where a small sinusoidal field of wavevector-q, $\delta\beta(x) = \delta\beta_q e^{iqx}$ or $\delta h(x) = \delta h_q e^{iqx}$ is applied to the system, resulting in a response with the same wavevector-q (the discussion here is closely related to one in the context of the Lieb-Liniger Bose gas [145]). In the following, we will explicitly denote quantities depending on space-time, otherwise equilibrium ones are implied. We will first consider a temperature perturbation $\delta\beta_q e^{iqx}$ around the equilibrium state at inverse temperature β and magnetic field h, $n_j(x,t) = n_j + \delta n_j(x,t) = n_j + \delta n_j(t)\delta\beta_q e^{iqx}$. Substituting in eq.(6.30) we obtain,

$$\delta n_j(x,t) = \frac{\partial n_j}{\partial \beta}\Big|_{\beta,h} \delta\beta_q e^{iq(x - v_j t)} \tag{6.32}$$

The space-time dependence of the energy eq.(6.10) becomes,

$$\begin{aligned} E(x,t) &= \sum_j \int d\lambda r_j(x,t) n_j(x,t) \epsilon_j^{(0)} \\ &= \sum_j \int d\lambda (r_j + \delta r_j(x,t))(n_j + \delta n_j(x,t)) \epsilon_j^{(0)} \\ E(x,t) &= E + \delta E(x,t) \end{aligned} \tag{6.33}$$

and after linearization (see Appendix D),

$$\begin{aligned} \delta E(x,t) &\simeq \sum_j \int d\lambda (\delta r_j(x,t) n_j + r_j \delta n_j(x,t)) \epsilon_j^{(0)}, \\ \frac{\delta E(x,t)}{\delta \beta_q} &\simeq \sum_j \int d\lambda (\frac{\partial r_j}{\partial \beta}\Big|_{\beta,h} n_j + r_j \frac{\partial n_j}{\partial \beta}\Big|_{\beta,h}) \epsilon_j^{(0)} e^{iq(x - v_j t)}, \\ \frac{\delta E(x,t)}{\delta \beta_q} &\simeq -\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j) E_j^2 e^{iq(x-v_j t)}. \end{aligned} \tag{6.34}$$

Taking a Fourier transform, we obtain,

$$\begin{aligned} \frac{1}{2\pi}\int dt e^{i\omega t} \frac{\delta E(x,t)}{\delta \beta_q} &\simeq \\ -\sum_j \sigma_j \int \frac{dp_j}{2\pi} \quad n_j(1-n_j) \quad & E_j^2 \delta(\omega - q v_j) e^{iqx} \\ &= -S_{EE}(q,\omega) e^{iqx}. \end{aligned} \tag{6.35}$$

$$S_{EE}(q,\omega) = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j) E_j^2 \delta(\omega - q v_j) \tag{6.36}$$

is the energy structure factor in the $q \to 0$ limit within GHD. In this limit, $S_{EE}(q,\omega)$ is related to the specific heat $c(T)$, $c = \beta^2 \int d\omega S_{EE}(q,\omega)$.

In a similar analysis for the energy current J_E we find that,

$$\frac{\delta J_E(x,t)}{\delta \beta_q} \simeq -\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j) E_j j_j^{\epsilon} e^{iq(x-v_j t)}. \tag{6.37}$$

At this point it is interesting to observe that the derivative with respect to time of $\delta J_E(x,t)/\delta \beta_q$ satisfies a continuity equation in q-space,

$$\begin{aligned}
\frac{\partial}{\partial t}\frac{\delta J_E(x,t)}{\delta\beta_q} &\simeq iq\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)E_j j_j^{\epsilon} v_j e^{iq(x-v_j t)} \\
&\simeq iq\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(j_j^{\epsilon})^2 e^{iq(x-v_j t)} \\
\frac{\partial}{\partial t}\frac{\delta J_E(x,t)}{\delta\beta_q} &- iq\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(j_j^{\epsilon})^2 e^{iq(x-v_j t)} = 0
\end{aligned} \tag{6.38}$$

with "current" related to the thermal Drude weight D_{th} [26],

$$\begin{aligned}
D_{th} &= \frac{\beta^2}{2}\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(j_j^{\epsilon})^2 \\
&= \frac{\beta^2}{2}\sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(v_j E_j)^2.
\end{aligned} \tag{6.39}$$

As in the case of the energy, we obtain the energy current structure factor,

$$S_{J_E J_E}(q,\omega) = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(j_j^{\epsilon})^2 \delta(\omega - q v_j), \tag{6.40}$$

which reduces to a δ-function as $q \to 0$ with weight D_{th}. In the low temperature limit $v_j \to v$ and the thermal Drude weight $D_{th} = \frac{v^2}{2}c$. Additionally, taking the time derivative to eq.(6.38) we obtain:

$$\frac{\partial^2}{\partial t^2}\frac{\delta E(x,t)}{\delta\beta_q}\Big|_{x,t=0} \simeq -q^2 D_{th}. \tag{6.41}$$

The above relation is interpreted as ballistic energy transport, where the thermal Drude weight D_{th} can be seen as the inverse of the effective mass, $m_{th} \sim \frac{1}{D_{th}}$.

Similarly to the energy, the mean value of the magnetization Q is given by,

$$Q = \sum_j \int d\lambda \rho_j(\lambda) Q_j^{(0)} = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j Q_j^{(0)} \tag{6.42}$$

and applying a space-time dependent magnetic field $\delta h(x) = \delta h_q e^{iqx}$ we obtain a relaxation,

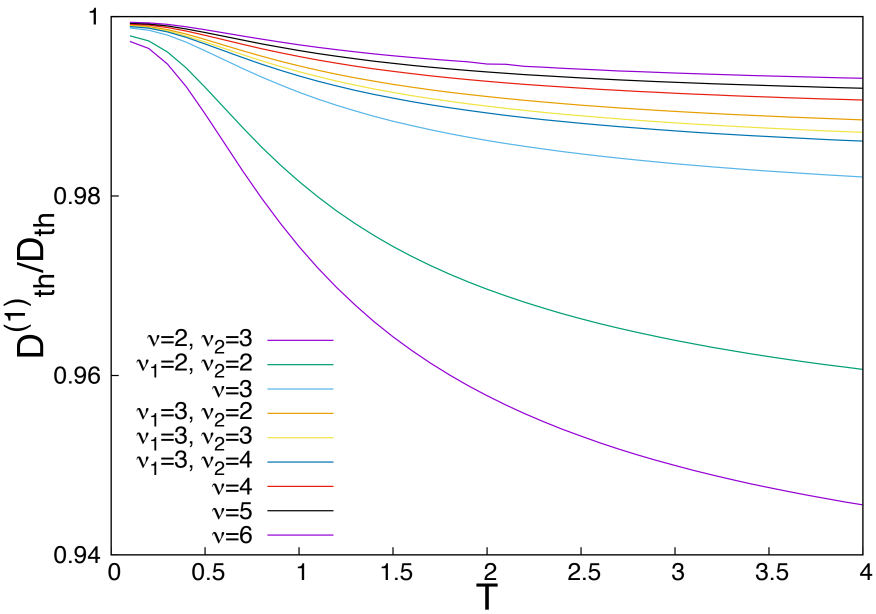

FIGURE 6.4: The fraction of one string thermal Drude weight $D_{th}^{(1)}$ over the total D_{th} versus temperature T for various (ν_1, ν_2) combinations

$$\begin{aligned} \frac{\delta Q(x,t)}{\delta h_q} &\simeq -\beta \sum_j \int d\lambda r_j n_j (1-n_j) Q_j^2 e^{iq(x-v_j t)} \\ &\simeq -\beta \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j (1-n_j) Q_j^2 e^{iq(x-v_j t)}. \end{aligned} \tag{6.43}$$

Finally, taking a Fourier transform, we obtain,

$$\begin{aligned} \frac{1}{2\pi} \int dt e^{i\omega t} \frac{\delta Q(x,t)}{\delta h_q} &\simeq \\ -\beta \sum_j \sigma_j \int \frac{dp_j}{2\pi} \quad n_j(1-n_j) \quad & Q_j^2 \delta(\omega - q v_j) e^{iqx} \\ &= \quad -\beta S(q,\omega) e^{iqx}, \end{aligned} \tag{6.44}$$

with $\beta S(q,\omega)e^{iqx}$ the magnetization relaxation function [146] obtaining $S(q,\omega)$ the $q \to 0$ spin structure factor within GHD.

$$S(q,\omega) = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j) Q_j^2 \delta(\omega - qv_j). \tag{6.45}$$

Again, in this limit, $S(q,\omega)$ is related to the magnetic susceptibility χ, $\chi(T) = \beta \int d\omega S(q,\omega)$.

The spin current however is not a conserved quantity in the XXZ Heisenberg model, it has been conjectured though within GHD and recently rigorously proven [24] that its mean value is given by,

$$J_S = \sum_j \int d\lambda \rho_j (v_j Q_j^{(0)}) = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j (v_j Q_j^{(0)}). \tag{6.46}$$

A similar analysis as for the energy current leads to,

$$\frac{\partial}{\partial t}\frac{\delta J_S(x,t)}{\delta h_q} - iq \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(v_j Q_j)^2 e^{iq(x-v_j t)} = 0, \tag{6.47}$$

with "current" related to the spin Drude weight D_s [23],

$$D_s = \frac{\beta}{2} \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(v_j Q_j)^2. \tag{6.48}$$

Moreover, the corresponding spin current structure factor is

$$S_{J_S J_S}(q,\omega) = \sum_j \sigma_j \int \frac{dp_j}{2\pi} n_j(1-n_j)(v_j Q_j)^2 \delta(\omega - qv_j). \tag{6.49}$$

In the zero temperature limit, using eq.(6.24), D_s is easily evaluated giving the known $T=0$ result [147],

$$D_s = \chi \frac{v^2}{2} = \frac{1}{2\pi} vK. \tag{6.50}$$

The high temperature limit is particularly interesting, since eq.(6.48) implies a "fractal" behavior [126, 127, 148, 27, 24] as a function of the anisotropy Δ. In this limit

(Appendix C), for $\Delta = \cos\pi/(\nu_1 + 1/\nu_2) = \cos(\pi m/l), l = 1 + \nu_1\nu_2, m = \nu_2$,

$$\begin{aligned}
\epsilon_{\nu_1+\nu_2-1} &= -\epsilon_{\nu_1+\nu_2} = T \ln \frac{l-\nu_1}{\nu_1} \\
Q_{\nu_1+\nu_2-1} &= -Q_{\nu_1+\nu_2} = \frac{l}{2} \\
p^{max}_{\nu_1+\nu_2-1} &= p^{max}_{\nu_1+\nu_2} = \frac{\pi}{2}\frac{1}{(l-\nu_1)\nu_1} \\
v_{\nu_1+\nu_2-1} &= -v_{\nu_1+\nu_2} = \alpha \sin(\lambda p_{\nu_1+\nu_2-1}) \\
\alpha &= \frac{\sin\pi m/l}{\sin\pi/l},\ \lambda = \frac{2\nu_1(l-\nu_1)}{l},
\end{aligned} \tag{6.51}$$

$$\begin{aligned}
&D_s = \frac{\beta}{2}(\frac{l}{2})^2 \cdot (1-\frac{\nu_1}{l})(\frac{\nu_1}{l}) \cdot \Big(\sum_{j=\nu_1+\nu_2-1}^{\nu_1+\nu_2} \sigma_j \int_{-p_j^{max}}^{+p_j^{max}} \frac{dp_j}{2\pi} {v_j}^2\Big) \\
&D_s = \chi\frac{\bar{v}^2}{2} = \frac{\beta}{2}\frac{\sin^2(\frac{\pi m}{l})}{\sin^2(\frac{\pi}{l})}(1-\frac{\sin\frac{2\pi}{l}}{\frac{2\pi}{l}}), \\
&\chi = \beta/4, \quad \bar{v}^2 = \int_{-1}^{+1} dt\alpha^2 \sin^2(\frac{\pi t}{l}),
\end{aligned} \tag{6.52}$$

which traces the singular "fractal" behavior of D_s to the velocities of the $\nu_1 + \nu_2 - 1, \nu_1 + \nu_2$ excitations in contrast to the regular behavior of χ.

Analogously with eq.(6.41), a similar relation to can be derived

$$\frac{\partial^2}{\partial t^2}\frac{\delta Q(x,t)}{\delta h_q}\Big|_{x,t=0} \simeq -q^2 D_s \tag{6.53}$$

In conclusion, in low energy effective theories one quasi-particle with linear dispersion and effective velocity [73, 149] accounts for both the specific heat, magnetic susceptibility and dynamic structure factors. In contrast, in the ν TBA string excitations, the 1-strings mostly contribute to the specific heat, while the $\nu - 1, \nu$ to the magnetic susceptibility and corresponding dynamic structure factors. As all string excitations have the same characteristic velocity at low energies, effective field theories seem as a re-summation of the string contributions, but further work is necessary to reconcile the two pictures.

6.5 Appendix

6.5.1 Appendix A: Dynamics in the $T \to 0$ limit

First consider the $T = 0$ case. We can easily see that

$$E_1 = \epsilon_1, \quad E_{j>1} = 0 \tag{6.54}$$

$$n_1 = \frac{1}{1 + e^{\beta\epsilon_1}} = 1, \tag{6.55}$$

where we have used that $\epsilon_1 < 0$.

Therefore, using eqs.(6.6,6.7) and the Fourier transform we obtain :

$$\frac{\partial p_1}{\partial \lambda} = \frac{\partial p_1^{(0)}}{\partial \lambda} - T_{11} \circ \frac{\partial p_1}{\partial \lambda}(\omega) \Rightarrow \frac{\partial p_1}{\partial \lambda}(\omega) = \frac{\partial p_1^{(0)}}{\partial \lambda}(\omega) - T_{11}(\omega) \cdot \frac{\partial p_1}{\partial \lambda}(\omega). \tag{6.56}$$

Additionally we have that:

$$\frac{\partial p_1^{(0)}}{\partial \lambda}(\omega) = 2\pi a_1(\omega), \quad 1 + T_{11}(\omega) = 2\cosh(\omega) \cdot a_1(\omega) \tag{6.57}$$

$$\frac{\partial p_1}{\partial \lambda}(\omega) = \frac{\pi}{\cosh(\omega)} \Rightarrow \frac{\partial p_1}{\partial \lambda} = \frac{\pi/2}{\cosh(\pi\lambda/2)} \tag{6.58}$$

$$p_1(\lambda) = \tan^{-1}(\sinh\frac{\pi\lambda}{2}), \quad -\pi/2 \leq p_1(\lambda) \leq +\pi/2 \tag{6.59}$$

Hence,

$$E_1 \;=\; (-J\frac{\sin\theta}{\theta})\frac{\partial p_1}{\partial \lambda} = -v \cdot \sin p_1, \quad v = J\frac{\pi}{2} \cdot \frac{\sin\theta}{\theta} \quad , \quad 0 \leq p_1 \leq \pi \tag{6.60}$$

$$v_1 = \frac{\partial\epsilon_1/\partial\lambda}{\partial p_1/\partial\lambda} = -v \cdot \cos p_1, \quad 0 \leq p_1 \leq \pi. \tag{6.61}$$

Therefore, we obtain that at zero temperature, $\epsilon_1 = E_1$ is a spinon excitation as presented in eq.(6.23).

Let us continue with the $T \to 0$ limit. In this case in order to have a consistent set of equations we need to include terms of $\mathcal{O}(T)$ order. In fact the spinon excitation acquires a part which comes from the scattering with higher string species. Therefore the ϵ_1 excitation can be written as

$$\epsilon_1(\lambda) = -\frac{v}{\cosh(\frac{\pi\lambda}{2})} + g(\lambda)T. \tag{6.62}$$

The exact calculation of $g(\lambda)$ is difficult, but we can instead calculate the asymptotic and $\lambda = 0$ values of $g(\lambda)$

If we assume that all physical quantities of interest reach a fixed value at the limit, $\lambda \to \pm\infty$ then the convolution $A \circ B(\lambda)|_{\lambda\to\pm\infty}$, where $A(\lambda)$ vanishes rapidly at infinity can be written as:

$$A \circ B(\lambda)|_{\lambda\to\pm\infty} = B_{\pm\infty} \int_{-\infty}^{\infty} A(\mu)d\mu, \tag{6.63}$$

where $B_{\pm\infty} \equiv \lim_{\lambda\to\pm\infty} B(\mu)$.

Therefore, we can transform a set of non-linear integral equations such as eqs.(6.3,5.47) into a set of algebraic equations.

As a simple example let us consider the simplest non-trivial case, $\nu = 3$

Using eqs.(6.3,5.47) and the fact that $\int_{-\infty}^{\infty} T_{ij}(\mu)d\mu = \frac{1}{\pi}\Theta_{ij}(\infty)$ we obtain:

$$g_\infty = -\tfrac{1}{3}g_\infty + \tfrac{1}{3}\ln(1 + e^{g_\infty}) + \tfrac{2}{3}\ln 2 + \tfrac{2}{3}\ln(1 + \cosh\beta\epsilon_2), \tag{6.64}$$
$$\beta\epsilon_2 = \tfrac{1}{2}\ln(1 + e^{g_\infty}). \tag{6.65}$$

Substituting $g_\infty = \ln\alpha$, $\alpha \neq 1$ we obtain the following equation:

$$w^3 - 6w^2 + 9w - 4 = 0, \tag{6.66}$$

where we have defined that $w \equiv \alpha + 1$.

Hence, the approved solution is $w = 4$. Additionally, due to symmetry we get the following result :

$$\lim_{\lambda\to\pm\infty} g(\lambda) = \ln 3. \tag{6.67}$$

Also, we find that :

$$\lim_{\lambda\to\pm\infty} \epsilon_2 = T\ln 2. \tag{6.68}$$

The above results can also be derived in closed form, for the more general case $\pi/\theta = \nu_1 + 1/\nu_2$, $\nu_2 > 1$. To this end, we take the asymptotic limit to eq.(5.47), and using eq.(6.63) we reduce the system into a difference equation for $\beta\epsilon_j$. Actually the difference equation, and of course the solution, is the same as the one we obtain to $\mathcal{O}(T)$ order by taking the high temperature limit $T \to \infty$. The physical explanation for this coincidence is that in the high temperature limit, the system excites large values of the rapidity λ, i.e. $\lambda \to \infty$, and thus to dominant order the two limits are equivalent. Therefore, the asymptotic solutions for the ϵ_j excitations are given by [121]

$$\begin{aligned} &\lim_{\lambda\to\pm\infty} \epsilon_j = T\ln\Big((j+1)^2-1\Big) \quad , \quad j=1,...,\nu-2 \\ &\lim_{\lambda\to\pm\infty} \epsilon_{\nu-1} = T\ln(\nu-1) \quad , \quad \epsilon_\nu = -\epsilon_{\nu-1} \end{aligned} \tag{6.69}$$

in the case $\nu_1 = \nu - 1$, $\nu_2 = 1$ and

$$\begin{aligned} &\lim_{\lambda\to\pm\infty} \epsilon_j = T\ln\Big((j+1)^2-1\Big) \quad , \quad j=1,...,\nu_1-1 \\ &\lim_{\lambda\to\pm\infty} \epsilon_j = T\ln\Big((\frac{1+(j-\nu_1)\nu_1+\nu_1}{\nu_1})^2-1\Big) \quad , \quad j=\nu_1,...,\nu_1+\nu_2-2 \\ &\lim_{\lambda\to\pm\infty} \epsilon_{\nu_1+\nu_2-1} = T\ln(\frac{\nu_1\nu_2-\nu_1+1}{\nu_1}) \quad , \quad \epsilon_{\nu_1+\nu_2} = -\epsilon_{\nu_1+\nu_2-1} \end{aligned} \tag{6.70}$$

when $\nu_2 > 1$.

Let us follow the same procedure in order to calculate the $g(0)$ value which is also important for the low temperature dynamics of the excitations. This time however, our result will clearly no longer be exact, but due to the fact that at $T \to 0$ the quantities $\ln(1+e^{\beta\epsilon_j})$ are slowly varying around $\lambda = 0$ and the rapidly vanishing form of the functions s_i, d_i we expect this to be a valid approximation

Similarly, with the previous case let us consider the simplest case, $\nu = 3$.

Since $\epsilon_1(0) = -v + g(0)T$, eq.(5.47) gives that $\beta\epsilon_2 \simeq 0$, when $T \to 0$. Additionally, eq.(6.3) gives

$$\frac{4}{3}g(0) = \frac{2}{3}\ln 2 + \frac{2}{3}\ln(1+\cosh(\beta\varepsilon_2)) \tag{6.71}$$

which yields the solution $g(0) = \ln 2$. Similarly we can find a closed form that holds for all $\pi/\theta = \nu > 3$. Nevertheless, note that with increasing ν the numerical value will slightly differ from our analytical approximation. Using the same procedure that we used in the asymptotic case in order to arrive at a difference equation and the fact that this time $\epsilon_1(0) = -v + g(0)T$ and $e^{\beta\epsilon_1(0)} \simeq 0$, at $T \to 0$, we obtain that the $\lambda = 0$

values of the ϵ_j excitations are the following:

$$\begin{aligned} &\epsilon_1(0) \simeq -v + T\ln 2 \\ &\epsilon_j(0) = T\ln\left(j^2-1\right) \quad , \quad j=2,...,\nu-2 \\ &\epsilon_{\nu-1}(0) = T\ln(\nu-2) \quad , \quad \epsilon_\nu = -\epsilon_{\nu-1}, \end{aligned} \tag{6.72}$$

Note that, a similar but more complicated relation can be constructed for the fractal case ($\nu_2 > 1$).

Next let us consider the ϵ_j excitations as functions of p_j. To this end, we start from the definition of the excitation velocities:

$$\frac{\partial \epsilon_j}{\partial p_j}(\lambda) = v_j(\lambda) \tag{6.73}$$

In order to continue we assume that $v_j,\ j=2,...,\nu$ converge very quickly to their asymptotic values. This is plausible since $s_1(\lambda)$ vanishes rapidly, i.e. for $|\lambda| > \delta$, $s_1(\lambda)$ can be considered negligible, with $\delta > 0$. The above is also justified by numerical calculations. In addition using eqs.(6.7,6.14) we find that $|v_j| = v$, $j=2,...,\nu$, for $|\lambda| > \delta_j$, where the numerical values of δ_j are close to δ. Moreover from equations (6.3,6.7,6.14) we notice that $\frac{\partial \epsilon_j}{\partial \lambda}$ is an antisymmetric function, while $\frac{\partial p_j}{\partial \lambda}$ and ϵ_j are symmetric functions. Therefore for rapidities $|\lambda| > \delta_j$ we obtain that:

$$|\frac{\partial \epsilon_j}{\partial \lambda}| = v\frac{\partial p_j}{\partial \lambda}. \tag{6.74}$$

Since ϵ_j is a symmetric function we obtain that:

$$\epsilon_j = v|p_j - p_j(0)| + \Delta_j \quad , \quad j \geq 2, \tag{6.75}$$

At this point, it is important to mention that eq.(6.75) is not true for a small interval around $p_j(0)$, due to the fact that eq.(6.74) does not hold. This is expected since ϵ_j are everywhere differentiable. Nevertheless, it is supported by the numerics that $p_j(|\lambda| < \delta_j)$ is approximately constant, and thus this interval is indeed a narrow one around $p_j(0)$.

Substituting eqs.(6.69,6.72) into eq.(6.75) it yields:

$$\begin{aligned}
\epsilon_j &\simeq T\ln(j^2-1)+v|p_j|, \quad j=2,...,\nu-2,\\
|p_j| &\le p_j^{max}, \quad p_j^{max}=\frac{T}{v}\ln\Big(\frac{(j+1)^2-1}{j^2-1}\Big),\\
\epsilon_{\nu-1} &= T\ln(\nu-2)+v|p_{\nu-1}|,\\
|p_{\nu-1}| &\le p_{\nu-1}^{max}, \quad p_{\nu-1}^{max}\simeq\frac{T}{v}\ln\Big(\frac{\nu-1}{\nu-2}\Big),\\
\epsilon_\nu &= -\epsilon_{\nu-1}, \qquad (6.76)
\end{aligned}$$

where p_j is shifted such that ϵ_j are symmetric about zero and $p_j^{max} = \frac{1}{2}\lim_{\lambda\to\infty}|p_j(\lambda)| = |p_j(0)|$.

6.5.2 Appendix B: Dynamics in the $\beta \to 0$ limit

First, we consider the non-fractal case, $\nu_2 = 1$. To begin with, in Appendix B we discussed that the dominant term of the high temperature behavior of ϵ_j coincides with the asymptotic limit, $\lambda \to \infty$, given by eq.(6.69). The first correction to this behavior can be found by following the method applied in Appendix C by Takahashi and Suzuki [121]. Hence, using eq.(5.47) the first order correction, $\mathcal{O}(1)$, for zero magnetic field $h = 0$ is given by:

$$\begin{aligned}
\epsilon_j^{(1)}(\lambda) &= -\frac{A}{2(j+1)}(1+e^{-\beta\epsilon_j})[(j+2)\alpha_j(\lambda)-j\alpha_{j+2}(\lambda)] \quad j=1,...,\nu-2\\
\epsilon_{\nu-1}^{(1)}(\lambda) &= -\frac{A}{2}(1+e^{-\beta\epsilon_{\nu-1}})\alpha_{\nu-1}(\lambda), \quad \epsilon_\nu^{(1)} = -\epsilon_{\nu-1}^{(1)}. \qquad (6.77)
\end{aligned}$$

Consequently, the dominant contribution of $\frac{\partial\epsilon_j}{\partial\lambda}$ is given by:

$$\frac{\partial\epsilon_j}{\partial\lambda} = \frac{\partial\epsilon_j^{(1)}}{\partial\lambda}, \qquad (6.78)$$

A careful examination of eq.(6.7) and eq.(6.14) shows that the set of integral equations corresponding to $\frac{\partial\epsilon_j}{\partial\lambda}$ and $\frac{\partial p_j}{\partial\lambda}$ are essentially the same with the substitution of the driving term, $-A\frac{\partial\alpha_j}{\partial\lambda}$ to $2\pi\alpha_j$. Hence, the dominant term of $\frac{\partial p_j}{\partial\lambda}$ will be given by:

$$\frac{\partial p_j}{\partial\lambda} = \frac{\pi}{(j+1)}(1+e^{-\beta\epsilon_j})[(j+2)\alpha_j - j\alpha_{j+2}] \quad j = 1,...,\nu-2$$
$$\frac{\partial p_{\nu-1}}{\partial\lambda} = \pi(1+e^{-\beta\epsilon_{\nu-1}})\alpha_{\nu-1}, \quad \frac{\partial p_\nu}{\partial\lambda} = -\frac{\partial p_{\nu-1}}{\partial\lambda} \tag{6.79}$$

Therefore, the momentum p_j is given by:

$$p_j(\lambda) = \frac{1}{2(j+1)}(1+e^{-\beta\epsilon_j})\Big[(j+2)\Big(f(\lambda;l_j,\zeta_j)+f_j^\infty\Big) - j\Big(f(\lambda;\lambda_{j+2},\zeta_{j+2})+f_{j+2}^\infty)\Big)\Big], \; j=1,...,\nu-2$$
$$p_{\nu-1}(\lambda) = \frac{1}{2}(1+e^{-\beta\epsilon_{\nu-1}})\Big[f(\lambda;l_j,\zeta_j)+f_{\nu-1}^\infty\Big], \quad p_\nu = -p_{\nu-1} \tag{6.80}$$

where $f(\lambda;l_j,\zeta_j)$ is given by eq.(5.35) and $f_j^\infty = \lim_{\lambda\to\infty} f(\lambda;l_j,\zeta_j)$.

$p_j^{max} = |p_j(0)|$ is given by

$$p_j^{max} = \pi\frac{j+1}{(j+1)^2-1}, \; j = 1,...,\nu-2$$
$$p_{\nu-1}^{max} = \frac{\pi}{2}\frac{1}{\nu-1} \quad , \quad p_\nu^{max} = p_{\nu-1}^{max} \tag{6.81}$$

The $\nu-1$ excitation velocity is given by:

$$v_{\nu-1} = -\frac{A}{2\pi}\frac{\partial\alpha_{\nu-1}}{\partial\lambda}\frac{1}{\alpha_{\nu-1}}. \tag{6.82}$$

Let us rewrite $\theta\lambda$ in terms of the momentum $p_{\nu-1}$

$$\theta\lambda = 2\,\mathrm{atanh}\,\Big(\tan(\frac{\nu-1\pi}{2\nu})\cdot\tan(\frac{\nu-1}{\nu}p_{\nu-1})\Big), \tag{6.83}$$

where we have shifted the momenta $p_{\nu-1}$ by $p_{\nu-1}^{max}$.

If $p_{\nu-1}\simeq 0$ we obtain that

$$\theta\lambda \simeq 2\frac{\nu-1}{\nu}\tan(\frac{\nu-1\pi}{2\nu})p_{\nu-1}. \tag{6.84}$$

Therefore in this limit

$$v_{\nu-1} \simeq \frac{\sin\theta}{1+\cos\theta}\theta\lambda = \tan\frac{\pi}{2\nu}\cdot\theta\lambda \tag{6.85}$$

Substituting eq.(6.84) into eq.(6.85) we obtain

$$v_{\nu-1} \simeq 2\frac{\nu-1}{\nu}p_{\nu-1}. \tag{6.86}$$

On the other hand, asymptotically $|v_{\nu-1}| = \sin\theta$. Therefore, a suitable function that satisfies both regions is

$$v_{\nu-1} = \sin(2\frac{\nu-1}{\nu}p_{\nu-1}) \tag{6.87}$$

By directly plotting $v_j(\lambda)$ as a function of $p_{\nu-1}(\lambda)$ we find that $v_{\nu-1}$ is indeed described by the above form.

Next we move to the $\nu_2 > 1$ case. Initially, let us mention that the dominant term of the excitation energies ϵ_j is given by eq.(6.70). In this case we prove that the excitation velocity $v_{\nu_1+\nu_2-1}$ appears to have a fractal behavior consistent with the findings for the spin Drude weight D_s at high temperatures. A simple generalization of the previous case shows that $\frac{\partial\epsilon_j}{\partial\lambda}$ and momentum $\frac{\partial p_j}{\partial\lambda}$ are given by:

$$\begin{aligned}
\frac{\partial\epsilon_j}{\partial\lambda} &= -\frac{A}{2(n_j+1)}(1+e^{-\beta\epsilon_j})\Big[(n_j+2)\frac{\partial\alpha_j}{\partial\lambda} - n_j\frac{\partial\alpha_{j+2}}{\partial\lambda}\Big], \quad j=1,...,\nu_1-1 \\
\frac{\partial\epsilon_j}{\partial\lambda} &= -\frac{A}{2\nu_1(n_j+\nu_1)}(1+e^{-\beta\epsilon_j})\Big[(n_j+2\nu_1)\frac{\partial\alpha_j}{\partial\lambda} - n_j\frac{\partial\alpha_{j+2}}{\partial\lambda}\Big], \quad j=\nu_1,...,\nu_1+\nu_2-2 \\
\frac{\partial\epsilon_{\nu_1+\nu_2-1}}{\partial\lambda} &= -\frac{A}{2\nu_1}(1+e^{-\beta\epsilon_{\nu_1+\nu_2-1}})\frac{\partial\alpha_j}{\partial\lambda}, \quad \frac{\partial\epsilon_{\nu_1+\nu_2}}{\partial\lambda} = -\frac{\partial\epsilon_{\nu_1+\nu_2-1}}{\partial\lambda}
\end{aligned} \tag{6.88}$$

$$\begin{aligned}
\frac{\partial p_j}{\partial\lambda} &= \frac{\pi}{(n_j+1)}(1+e^{-\beta\epsilon_j})\Big[(n_j+2)\alpha_j - n_j\alpha_{j+2}\Big], \quad j=1,...,\nu_1-1 \\
\frac{\partial p_j}{\partial\lambda} &= \frac{\pi}{\nu_1(n_j+\nu_1)}(1+e^{-\beta\epsilon_j})\Big[(n_j+2\nu_1)\alpha_j - n_j\alpha_{j+2}\Big], \quad j=\nu_1,...,\nu_1+\nu_2-2 \\
\frac{\partial p_{\nu_1+\nu_2-1}}{\partial\lambda} &= \frac{\pi}{\nu_1}(1+e^{-\beta\epsilon_{\nu_1+\nu_2-1}})\alpha_{\nu_1+\nu_2-1}, \quad \frac{\partial p_{\nu_1+\nu_2}}{\partial\lambda} = -\frac{\partial p_{\nu_1+\nu_2-1}}{\partial\lambda},
\end{aligned} \tag{6.89}$$

where n_j are given by eq.(5.32)

Furthermore a careful calculation shows that $p^{max}_{\nu_1+\nu_2-1}$ is

$$p^{max}_{\nu_1+\nu_2-1} = \frac{1}{2\nu_1}(1+e^{-\beta\epsilon_{\nu_1+\nu_2-1}})|f^{\infty}_{\nu_1+\nu_2-1}| = \frac{\pi}{2}\frac{1}{(1+\nu_1\nu_2-\nu_1)\nu_1}. \tag{6.90}$$

Note that we have used the fact that $\zeta_{\nu_1+\nu_2-1} = (-1)^{\nu_2}$.

Performing a linear approximation the velocity and momentum can be written as:

$$v_{\nu_1+\nu_2-1} = \frac{\sin\theta}{1+\cos\frac{\theta}{\nu_2}}\theta\lambda \tag{6.91}$$

$$p_{\nu_1+\nu_2-1} \simeq \frac{1}{\lambda}\zeta_{\nu_1+\nu_2-1}\cot\left(\frac{1+(\nu_2-1)\nu_1}{2}\theta\right)^{\zeta_{\nu_1+\nu_2-1}}\theta\lambda, \tag{6.92}$$

where we have substituted eq.(6.70) into eq.(6.82) and $\lambda = 2\nu_1\frac{(1+\nu_1\nu_2-\nu_1)}{1+\nu_1\nu_2}$.

Therefore using eq.(6.92) and eq.(6.91) we conclude that:

$$v_{\nu_1+\nu_2-1} = \zeta_{\nu_1+\nu_2-1}\frac{\sin\theta}{1+\cos\frac{\theta}{\nu_2}}\tan\left(\frac{1+(\nu_2-1)\nu_1}{2}\theta\right)^{\zeta_{\nu_1+\nu_2-1}}\lambda p_{\nu_1+\nu_2-1} \tag{6.93}$$

One can easily prove that:

$$\zeta_{\nu_1+\nu_2-1}\frac{\sin\theta}{1+\cos\frac{\theta}{m}}\tan\left(\frac{l-\nu_1}{2}\theta\right)^{\zeta_{\nu_1+\nu_2-1}} = -\frac{\sin m\pi/l}{\sin\pi/l}, \tag{6.94}$$

where $m = \nu_2$ and $l = 1+\nu_1\nu_2$.

$$v_{\nu_1+\nu_2-1} \simeq -\frac{\sin m\pi/l}{\sin\pi/l}\lambda p_{\nu_1+\nu_2-1}, \tag{6.95}$$

which proves the fractal behavior of the velocity. Moreover, asymptotically $|v_{\nu_1+\nu_2-1}| = \sin m\pi/l$. Plotting $v_{\nu_1+\nu_2-1}$ as a function of $p_{\nu_1+\nu_2-1}$ reveals that it can be described as

$$v_{\nu_1+\nu+2-1} = -\frac{\sin m\pi/l}{\sin\pi/l}\sin\lambda p_{\nu_1+\nu_2-1} \tag{6.96}$$

6.5.3 Appendix C: Proof of relation (34)

To arrive at eq.(6.34), it is convenient to use a matrix notation for the integral over rapidity λ, sum over string index j and employ standard manipulations [21, 131], using the convention that $[a]$ is a vector column, $tr[A] = \sum_j\int d\lambda A_j(\lambda)$ and $[T][A] = \sum_k(T_{jk}\circ A_k)$

$$\frac{\delta E(x,t)}{\delta\beta_q} = tr\Big\{[\epsilon^{(0)}e^{iq(x-vt)}][\frac{\partial r}{\partial\beta}n] + [\epsilon^{(0)}e^{iq(x-vt)}][\frac{\partial n}{\partial\beta}r]\Big\}, \tag{6.97}$$

solve eq.(6.2) for $[n\frac{\partial r}{\partial \beta}]$,

$$\begin{aligned} &[r] = [\lambda a] - [\lambda T][nr] \\ &[n\frac{\partial r}{\partial \beta}] = -[\lambda n T]([n\frac{\partial r}{\partial \beta}] + [r\frac{\partial n}{\partial \beta}]) \\ &[n\frac{\partial r}{\partial \beta}] = -[I + \lambda n T]^{-1}[\lambda n T][r\frac{\partial n}{\partial \beta}] \end{aligned} \tag{6.98}$$

solve eq.(6.8),

$$[E] = [I + \lambda n T]^{-1}[\epsilon^{(0)}] \tag{6.99}$$

and from eq.(6.3) and eq.(6.8) we find that $\partial(\beta\epsilon_j)/\partial\beta = E_j$.

6.5.4 Appendix D: Charges Q_j

We can readily show this in the simple case $\theta = \pi/\nu$ by using the recursion relations of TS for the phase shifts T_{jk}, and rewriting eq.(6.22) as $(Q_0 = n_0 = 0)$,

$$\begin{aligned} Q_j &= s_1 * Q_{j-1}(1 - n_{j-1}) + s_1 * Q_{j+1}(1 - n_{j+1}) \\ &+ \delta_{\nu-2,j} s_1 * Q_\nu n_\nu, \quad 1 \le j \le \nu - 2 \\ Q_{\nu-1} &= \frac{\nu}{2} + s_1 * Q_{\nu-2}(1 - n_{\nu-2}) \\ Q_{\nu-1} - Q_\nu &= \nu. \end{aligned} \tag{6.100}$$

For $h = 0$, $n_{\nu-1} + n_\nu = 1$ from eq.(6.3), so we can eliminate the $Q_j, n_j, \quad j = \nu - 1, \nu$ from eq.(6.100) obtaining a homogeneous system of equations for $Q_j, n_j, \quad j = 1, \nu - 2$ with solution $Q_j = 0, \ j = 1, ..., \nu - 2$. An algebraic approach of this result was given in [27, 24]. When the magnetic field is nonzero $(h \neq 0)$ the Q_j's are in general functions of the rapidity λ.

For completeness, we also study the case $\pi/\theta = \nu_1 + 1/\nu_2$ $(\nu_2 > 1)$

Using that σ_j is positive in the region $1 \leq j \leq \nu_1 - 1, j = \nu_1 + \nu_2$, the recursion relations eq.(6.22) take the form,

$$\begin{aligned}
Q_j &= s_1 * Q_{j-1}(1-n_{j-1}) + s_1 * Q_{j+1}(1-n_{j+1}), \quad 1 \leq j \leq \nu_1 - 2 \\
Q_{\nu_1-1} &= s_1 * Q_{\nu_1-2}(1-n_{\nu_1-2}) + d_1 * Q_{\nu_1-1}(1-n_{\nu_1-1}) \\
&- s_2 * Q_{\nu_1}(1-n_{\nu_1}) \\
Q_j &= s_2 * Q_{j-1}(1-n_{j-1}) + s_2 * Q_{j+1}(1-n_{j+1}) \\
&+ \delta_{\nu_1+\nu_2-2,j} s_2 * Q_{\nu_1+\nu_2} n_{\nu_1+\nu_2}, \quad \nu_1 \leq j \leq \nu_1+\nu_2-2 \\
Q_{\nu_1+\nu_2-1} &= -\frac{1+\nu_1\nu_2}{2} + s_2 * Q_{\nu_1+\nu_2-2}(1-n_{\nu_1+\nu_2-2}), \quad j = \nu_1+\nu_2-1 \\
& Q_{\nu_1+\nu_2} - Q_{\nu_1+\nu_2-1} = 1 + \nu_1\nu_2.
\end{aligned} \tag{6.101}$$

Similarly as before, in the zero field case ($h = 0$) the solution of eq.(6.101) is $Q_j = 0$ for $1 \leq j \leq \nu_1 + \nu_2 - 2$

Chapter 7

Epilogue

We briefly summarize the most important results of this thesis.

(I) On the spinon scattering by potentials

(a) Scattering matrix elements: We studied the scattering matrix elements from three prototype potentials, a longitudinal, a transverse and a spin-phonon interaction. We found that even for a single-site potential the matrix elements do not behave as those of a regular particle and are non-trivial functions of the system size N as well as the spinon's momentum. We attribute this behavior to the strongly antiferromagnetic nature of the spinon. In addition, we found that there are two dominant matrix elements that play crucial role to the scattering procedure. Both of the them are on-shell matrix elements with the one flipping the spinon velocity and the other being a π-transition.

(b) Transmission coefficient for the scattering by a single-site potential: By summing the Born Series we calculated the transmission coefficient for the scattering of a single spinon by the aforementioned potentials. It is interesting that for an even chain the spinon is fourfold degenerate and therefore we have to introduce two different types of transmission probability the diagonal one $\mathcal{T}(Q,Q)$ and the non-diagonal one $\mathcal{T}(Q+\pi,Q)$, where the total transmission is the sum of the above probabilities. In particular, when the barrier strength the diagonal decreases while the non-diagonal increases. This peculiar effect remind us the Klein paradox where the barrier itself creates particles. However, this is due to the fact that in an even spin chain the lowest branch includes two spinons with the one having zero energy. Moreover, we should mention that although the dominant matrix elements describe accurately the two transmission probabilities including only the lowest branch matrix elements is not sufficient to produce a physically acceptable scattering process since $\mathcal{T}_{tot}(Q) \to 1$ as $N \to \infty$. This is solved by including the whole two spinon spectrum which makes $\mathcal{T}_{tot} \to (Q)$ a function of the spinon energy ε_Q leading us to the conclusion that these $\mathcal{O}(N^2)$ matrix elements serve as a spinon "cloud" regulating scattering to a non-trivial result. Furthermore, interestingly we find that for $\Delta = 0$ and a longitudinal potential low energy spinons behave as a one-dimensional massless Dirac particle, while for $0 < \Delta \leq 1$ the longitudinal potential breaks criticality and spinon behaves as a quadratic particle, implying there is an induced mass. In addition, the gapped case provides new information since criticality is absent and the spinon becomes a localized object. We found that the previous results holds, leading to the conclusion that the dominant effect is the strong antiferromagnetic correlation of our system combined with the many body nature of spinons.

(c) Transmission coefficient for the scattering by an extended potential: We found a "healing" effect, i.e. $\mathcal{T}_{tot} \to 1$ when $\varepsilon_Q \to 0$ when the relation $\sum_n (-1)^n g_n |V_{\pi\pi+Q}|^2 = 0$ holds. In any other case, a "cutting" effect is present at low energies and in fact the transmission coefficient follows a very similar curve to the single site potential case. It is interesting that we can easily manipulate the low energy Transmission probability by simply changing the magnetic field.

(II) On the Dressed excitations, thermodynamics and relaxation

(a) Dressed excitations and spinon thermodynamics: We introduced new energy and momentum dressing relations for the XXZ model along the lines of the GHD formulation. Using these relations we studied the low and high temperature thermodynamics. In particular, we found that in the low temperature limit the most important excitation is the spinon excitation, however even if $T \to 0$ scattering with the rest of the string excitations is also important and it cannot be decoupled from the rest of the excitations making the construction of *a spinon thermodynamics theory* a difficult task. In addition, we calculated the low temperature specific heat and magnetic susceptibility using the analytical results for the string excitations. All the above indicate that further work is needed for a reconciliation of the effective field theory picture and the string excitations (TBA) picture.

(b) Dynamics and relaxation: we studied the energy/magnetization relaxation of XXZ critical spin chain, starting from an initial condition where a small temperature/magnetic field of wavevector-q, is applied to the system, resulting in a same wavevector-q response. With the use of linear-response approximation we were able to derive the Drude weight. Specifically, a temperature perturbation of the form $\delta\beta(x)\delta = \beta_q exp(iqx)$ results in the derivation of the thermal Drude weight and a magnetic field perturbation of the form $\delta h(x)\delta = h_q exp(iqx)$ in the corresponding spin Drude weight. Finally, using the dynamics of the excitation analysis we revealed that the underlying cause for the fractal behavior of the spin Drude weight is the fractality of the string excitation velocities.

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