Introduction to Quantum Spin Chains

Lecture Notes, (56 hours)

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Contents

1 Introduction

The notes are prepared for the lecture course "Introduction to the Quantum Spin Chains" within the post-graduate programm in the Regional Training Center in Theoretical Physics(Bonn-Tbilisi-Yerevan) funding by the Volkswagen Foundation under the Contract nr. 86 260. The lecture course is supposed to cover basic and fundamental principles of the very important part of the modern mathematical physics and theory of strongly correlated system, the exactly solvable quantum spin chains. However, in the present lecture notes the main accent has been made on the physical properties of the quantum spin chain, coordinate Bethe ansatz, ground states, low-lying excitations. Another feature of the lecture notes is that in most cases all calculations are presented very detailed to facilitate the learning for the student of any level and background. The only knowing of the basic of quantum mechanic and statistical mechanics is supposed. For the limited number of academic hours allocated for the course, many important issues left out of the material. But the author did his best to convey the a comprehensive way the main properties of the XY, XXX and XXZ-chain. Probably the notes contain large amount of typos which the author could not mention before hands. Please, don't hesitate to contact the author in case if you found some. During the course of the preparation of the notes the author got substantial aid form the following sources, which are also highly recommended for the readers as well:

- J. B. Parkinson, and D. J.J. Farnell, *An Introduction to Quantum Spin Systems*, Lect. Notes Phys. **816**, Springer, Berlin Heidelberg (2010).
- F. Franchini, *Notes on Bethe Ansatz Technique*, https://people.sissa.it/ ffranchi/BAnotes.pdf
- L. Šamaj, *Introduction to Integrable Many-Body Systems II*, acta phys. slovacia **60**, 155, (2010).
- M. Karbach, and G. Müller, *Introduction to Bethe Ansatz I*, Computers in Physics **11**, 36 (1997). arXiv:cond-mat/9809162.
- M. Karbach, K. Hu, and G. Müller, *Introduction to Bethe Ansatz II*, Computers in Physics **12**, 565 (1998) arXiv:cond-mat/9809163.
- M. Karbach, K. Hu, and G. Müller, *Introduction to Bethe Ansatz III*, arXiv:cond-mat/0008018.

2 The XY Chain

2.1 Introduction

Let us consider the chain with a $S = 1/2$ spins on each site. The spin operators satisfy the standard $SU(2)$ commutation relations for the same site and are commutative if they situated at different sites:

$$[S_j^a,\ S_l^b] = i\delta_{j\,l}\epsilon^{a\,b\,c}S_j^c. \tag{2.1}$$

The standard matrix representation of these spin operators is

$$S^x = \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix}, \quad S^y = \begin{pmatrix} 0 & -i/2 \\ i/2 & 0 \end{pmatrix}, \quad S^z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}. \tag{2.2}$$

Thus, the basis of the spin eigenstates consists of two vectors, corresponding to the $S^z = \pm 1/2$ eigenstates of the z-component of the spin:

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2.3}$$

The Hamiltonian of the XY-chain is

$$\mathcal{H}_{XY} = J \sum_{j=1}^{N} \{(1+\gamma) S_j^x S_{j+1}^x + (1-\gamma) S_j^y S_{j+1}^y\} - B \sum_{j=1}^{N} S_j^z. \tag{2.4}$$

Here, the interaction between the neighbor spins contains only x- nd y-components of the spin operators and the external magnetic field B interacts with the z-component of the spins. The feature of the XY-model and its particular cases ($\gamma = 0$ and $\gamma = 1$) is the possibility to obtain an exact solution using the method which is very different to the Bethe Ansatz. The method involves a transformation form spin variables to spinless fermion operators, which is called the **Jordan-Wigner transformations**. For the technical reasons it is convenient to introduce the following operators:

$$\begin{aligned} S_j^{\pm} &= S_j^x \pm i S_j^y, \\ S_j^{+} &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ S_j^{-} &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{aligned} \tag{2.5}$$

Thus, the operators of the new basis of the spin components on each site satisfy the following relations:

$$\begin{aligned} &(S_j^+)^2 = (S_j^-)^2 = 0, \quad S_j^- S_j^+ + S_j^+ S_j^- = 1, \\ &S_j^- S_j^+ - S_j^+ S_j^- = -2S_j^z, \quad S_j^z S_j^{\pm} - S_j^{\pm} S_j^z = \pm S_j^{\pm} \\ &S_j^+ |\downarrow\rangle = |\uparrow\rangle, \quad S_j^+ |\uparrow\rangle = 0, \\ &S_j^- |\downarrow\rangle = 0, \quad S_j^- |\uparrow\rangle = |\uparrow\rangle, \\ &S_j^z |\downarrow\rangle = -\frac{1}{2} |\downarrow\rangle, \quad S_j^z |\uparrow\rangle = \frac{1}{2} |\uparrow\rangle. \end{aligned} \tag{2.6}$$

Exercise *Verify these relations using the matrix form of the spin-operators.*

The first line of these equations is the evidence of the deep similarity between the fermion creation and annihilation operators on one site as the later satisfy the relations:

$$(c_j)^2 = (c_j^+)^2 = 0, \quad \{c_j, c_j^+\} = c_j c_j^+ + c_j^+ c_j = 1. \tag{2.7}$$

However, one can not just replace the spin operators on each site with the corresponding fermionic operators, because the spin operators form different sites commute, while the fermionic operators must satisfy also the following relations:

$$\{c_j, c_l\} = \{c_j^+, c_l^+\} = 0, \quad \{c_j, c_l^+\} = \delta_{jl}. \tag{2.8}$$

Jordan and Winger showed in 1928 that the spin operators for the whole chain can be represented **exactly** in term of the fermions C_j by the following mapping:

$$\begin{aligned} S_j^- &= \exp\left\{ i\pi \sum_{l=1}^{j-1} c_l^+ c_l \right\} c_j, \\ S_j^+ &= c_j^+ \exp\left\{ -i\pi \sum_{l=1}^{j-1} c_l^+ c_l \right\}, \\ S_j^z &= c_j^+ c_j - 1/2. \end{aligned} \tag{2.9}$$

The appearance of the phase factor with a string along the chain guaranties the commutativity of the spin operators from different sites. It is easy to see that the phase factor can be represented in different form, which is particular convenient for the practical reasons:

$$Q_j = \exp\left\{ i\pi \sum_{l=1}^{j-1} c_l^+ c_l \right\} = \prod_{l=1}^{j-1} \left(1 - 2c_l^+ c_l\right). \tag{2.10}$$

Let us prove this relation. To do so, we have to mention, that for any integer n one have $\left(c_j^+ c_j\right)^n = c_j^+ c_j$ and $\left(c_j^+ c_j\right)^0 = 1$. Then, in is straightforward to show that

$$e^{i\pi c_j^+ c_j} = \sum_{n=0}^{\infty} \frac{(i\pi)^n}{n!} \left(c_j^+ c_j\right)^n = 1 + \left(\sum_{n=1}^{\infty} \frac{(i\pi)^n}{n!} \right) c_j^+ c_j = 1 + \left(e^{i\pi} - 1\right) c_j^+ c_j = 1 - 2c_j^+ c_j \tag{2.11}$$

In order to reverse the relations (2.9) one has to take into account some properties of the operators c_j, c_j^+ and Q_j. First of all, let us establish the connection between the Hilbert spaces of the spin operator and operators c_j and c_j^+. It is easy to see from Eqs. (2.9) that the fermion operators act on the standard spin basis as follows

$$\begin{aligned} &c_j | \uparrow\rangle = | \downarrow\rangle, \quad c_j | \downarrow\rangle = 0, \\ &c_j^+ | \uparrow\rangle = 0, \quad c_j^+ | \downarrow\rangle = | \uparrow\rangle. \end{aligned} \tag{2.12}$$

Thus, defining the particle number operators for each site, $n_j = c_j^+ c_j$, one can identify the spin-down state with the empty site and spin-up with the one-fermion state respectively,

$$n_j | \downarrow\rangle = 0, \quad n_j | \uparrow\rangle = | \uparrow\rangle. \tag{2.13}$$

Here the following comment is in order, as the operators c_j and c_j^+ do not bear any other index but the site index and in virtue of the properties (3.199), they are usually called **spinless fermion operators**. The corresponding quasi-particle do not have any internal degrees of freedom like spin, that is why at each site one can find either 0 or 1 quasi-particle, spinless fermion. The quasi-particles are still fermions because of the fermionic commutation relation between operators c_j and c_j^+. For the further consideration the following relations are useful:

$$
\begin{aligned}
& c_j\left(1-2c_j^+c_j\right) = -c_j, \quad c_j^+\left(1-2c_j^+c_j\right) = c_j^+ \\
& \left(1-2c_j^+c_j\right)c_j = c_j, \quad \left(1-2c_j^+c_j\right)c_j^+ = -c_j^+, \\
& \left(1-2c_j^+c_j\right)^2 = 1, \\
& c_j\left(1-2c_l^+c_l\right) = \left(1-2c_l^+c_l\right)c_j, \ \ l \neq j, \\
& c_j^+\left(1-2c_l^+c_l\right) = \left(1-2c_l^+c_l\right)c_j^+, \ \ l \neq j, \\
& c_jQ_l = Q_lc_j, \ \ l \leq j, \\
& c_j^+Q_l = Q_lc_j^+, \ \ l \leq j, \\
& Q_jQ_{j+1} = 1-2c_j^+c_j, \\
& Q_j^2 = 1.
\end{aligned}
\tag{2.14}
$$

Exercise *Verify these relations*

Exercise *Using relations (2.14) check that the spin operators from Eqs. (2.9) satisfy the standard commutation relations if the operators c_j, c_j^+ satisfy relations (2.7) and (2.8).*

After that is also possible to write down the reciprocal relations for the Jordan-Wigner transformation (2.9). Using Eqs. (2.14) one obtains

$$
\begin{aligned}
c_j &= \prod_{l=1}^{j-1}\left(-2S_j^z\right)S_j^-, \\
c_j^+ &= S_j^+\prod_{l=1}^{j-1}\left(-2S_j^z\right), \\
n_j &= S_j^z - 1/2.
\end{aligned}
\tag{2.15}
$$

2.2 Jordan-Wigner diagonalization

Let us now rewrite the Hamiltonian of the general XY-chain in magnetic field in terms of the spinless fermions using the Jordan-Wigner transformation (2.9). First of all, let us replace the $S^{x,y}$ operators with the operators $S^{\pm}$. The Hamiltonian at this stage has the following form:

$$
\mathcal{H}_{XY} = \frac{J}{2}\sum_{j=1}^{N}\left\{\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) + \gamma\left(S_j^+S_{j+1}^+ + S_j^-S_{j+1}^-\right)\right\} - B\sum_{j=1}^{N}S_j^z. \tag{2.16}
$$

Now, using the Jordan-Wigner transformation (2.9) we can replace all terms according to

$$\begin{aligned} S_j^+S_{j+1}^- &= c_j^+Q_jQ_{j+1}c_{j+1} = c_j^+\left(1-2c_j^+c_j\right)c_{j+1} = c_j^+c_{j+1}, \\ S_j^-S_{j+1}^+ &= Q_jc_jc_{j+1}^+Q_{j+1} = c_jQ_jQ_{j+1}c_{j+1}^+ = c_j\left(1-2c_j^+c_j\right)c_{j+1}^+ = -c_jc_{j+1}^+, \\ S_j^+S_{j+1}^+ &= c_j^+Q_jc_{j+1}^+Q_{j+1} = c_j^+Q_jQ_{j+1}c_{j+1}^+ = c_j^+\left(1-2c_j^+c_j\right)c_{j+1}^+ = c_j^+c_{j+1}^+, \\ S_j^-S_{j+1}^- &= Q_jc_jQ_{j+1}c_{j+1} = c_jQ_jQ_{j+1}c_{j+1} = c_j\left(1-2c_j^+c_j\right)c_{j+1} = -c_jc_{j+1}. \end{aligned} \tag{2.17}$$

There is a problem at the end of the chain. Let us assume the periodic boundary condition, which implies $S_{j+N}^a = S_j^a$. However, the phase factor Q_j does not satisfy the periodic boundary conditions. Thus, for the N-th site which is connected to the first site one obtains:

$$\begin{aligned} S_N^+S_1^- &= Q_Nc_N^+c_1, \\ S_N^-S_1^+ &= Q_Nc_Nc_1^+, \\ S_N^+S_1^+ &= Q_Nc_N^+c_1^+, \\ S_N^-S_1^- &= Q_Nc_Nc_1, \end{aligned} \tag{2.18}$$

The Hamiltonian (2.16) eventually takes the following form:

$$\mathcal{H}_{XY} = \frac{J}{2}\sum_{j=1}^{N}\left\{c_j^+c_{j+1}+c_{j+1}^+c_j+\gamma\left(c_j^+c_{j+1}^++c_{j+1}c_j\right)\right\} - B\sum_{j=1}^{N}\left(c_j^+c_j-1/2\right) \tag{2.19}$$

$$- \frac{J}{2}\left\{c_1^+c_N+c_N^+c_1+\gamma\left(c_N^+c_1^++c_1c_N\right)\right\}$$

$$+ \frac{J}{2}Q_N\left\{c_Nc_1^++c_N^+c_1+\gamma\left(c_N^+c_1^++c_Nc_1\right)\right\}. \tag{2.20}$$

The last two terms do not contain the sum over all sites and, therefore, in the thermodynamic limit $N\to\infty$ they can be neglected.

2.3 Fourier Transform

Thus, we have the Hamiltonian of the lattice spinless fermions,

$$\mathcal{H}_{XY} = \frac{J}{2}\sum_{j=1}^{N}\left\{c_j^+c_{j+1}+c_{j+1}^+c_j+\gamma\left(c_j^+c_{j+1}^++c_{j+1}c_j\right)\right\} - B\sum_{j=1}^{N}\left(c_j^+c_j-1/2\right), \tag{2.21}$$

which is a quadratic form of the fermion operators. The first step in diagonalising it is to make use of the translational invariance by introducing Fourier transformed fermion operators:

$$\begin{aligned} d_k &= \frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{-ijk}c_j, \\ d_k^+ &= \frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{ijk}c_j^+. \end{aligned} \tag{2.22}$$

Here, the quasi-moneta k takes N discrete values from the Brillouin zone:

$$k = \frac{2\pi\lambda}{N}, \quad \lambda = -\frac{N}{2}+1, ... \frac{N}{2}, \quad k \in (-\pi, \pi]\,. \tag{2.23}$$

The reverse transform is

$$\begin{aligned} c_j &= \frac{1}{\sqrt{N}} \sum_{k\in B.Z.} e^{ijk} d_k, \\ c_j^+ &= \frac{1}{\sqrt{N}} \sum_{k\in B.Z.} e^{-ijk} d_k^+. \end{aligned} \tag{2.24}$$

Here the sum ingoing over the Brillouin zone. The operators d_k, d_k^+ satisfy standard fermionic anticommutation relations

$$\{d_k\ , d_q\} = \left\{d_k^+\ , d_q^+\right\} = 0, \ \ \left\{d_k\ , d_q^+\right\} = \delta_{kq}. \tag{2.25}$$

Exercise *Using the commutation relations (2.8) and the consistency condition of the Fourier transforms (2.22) and (2.24),* $\sum_{j=1}^{N} e^{i(k-q)j} = N\delta_{kq}$*, verify the relations (2.25).*

Now we can rewrite the Hamiltonian (2.21) in terms of operators d_k, d_k^+.

$$\begin{aligned} \sum_{j=1}^{N} c_j^+ c_{j+1} &= \sum_{j=1}^{N} \frac{1}{N} \sum_{k\in B.Z.} \sum_{q\in B.Z.} e^{-ikj} e^{iq(j+1)} d_k^+ d_q \\ &= \sum_{k\in B.Z.} \sum_{q\in B.Z.} e^{iq} \underbrace{\frac{1}{N} \sum_{j=1}^{N} e^{i(q-k)j}}_{\delta_{kq}} d_k^+ d_q \\ &= \sum_{k\in B.Z.} e^{ik} d_k^+ d_k \end{aligned} \tag{2.26}$$

In the same way for the rest four four terms of the Hamiltonian (2.21) one obtains:

$$\begin{aligned} \sum_{j=1}^{N} c_{j+1}^+ c_j &= \sum_{k\in B.Z.} e^{-ik} d_k^+ d_k, \\ \sum_{j=1}^{N} c_j^+ c_{j+1}^+ &= \sum_{k\in B.Z.} e^{ik} d_k^+ d_{-k}^+, \\ \sum_{j=1}^{N} c_{j+1} c_j &= \sum_{k\in B.Z.} e^{ik} d_k d_{-k}, \\ \sum_{j=1}^{N} c_j^+ c_j &= \sum_{k\in B.Z.} d_k^+ d_k. \end{aligned} \tag{2.27}$$

Exercise *Prove these relations.*

The final form of the Hamiltonian of the general XY-chain written in terms of the spinless fermion creation and annihilation operators in Brillouin zone is

$$\mathcal{H}_{XY} = \sum_{k \in B.Z.} \left\{ (J\cos k - B)\, d_k^+ d_k + J\gamma \frac{e^{ik}}{2} \left(d_k^+ d_{-k}^+ + d_k d_{-k} \right) \right\} + B\frac{N}{2}. \tag{2.28}$$

At this stage one can see that the Fourier transform diagonalize the Hamiltonian partly. Besides the diagonal part the Hamiltonian contains also the term with the interaction between excitation with moneta k and $-k$, proportional to γ. However, for $\gamma = 0$ which corresponds to the simplest case of the XX-chain, only Fourier transform provides the solution of the problem of diagonalization.

2.4 XX-chain

As was mention above the case of $\gamma = 0$ corresponds to the simplest spin model solvable by means of the Jordan-Wigner transformation to free spinless fermions, to the XX-chain. The Hamiltonian is

$$\begin{aligned} \mathcal{H}_{XX} &= J\sum_{j=1}^{N} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right) - B\sum_{j=1}^{N} S_j^z \\ &= \sum_{k \in B.Z.} \varepsilon_{XX}(k) \left(d_k^+ d_k - 1/2 \right), \end{aligned} \tag{2.29}$$

with

$$\varepsilon_{XX}(k) = (J\cos k - B)\,. \tag{2.30}$$

Takin into account the distribution of the quasi-momenta in the Brillouin zone, one can show that

$$-\sum_{k \in B.Z.} \varepsilon_{XX}(k)\frac{1}{2} = B\frac{N}{2}. \tag{2.31}$$

2.5 Zero-temperature properties of the XX-chain

Let us consider the zero-temperature properties of this model. First of all, let us figure out the value of the Fermi momentum and its dependence on the external magnetic field. First of all, we have to distinguish three cases, $|B| \leq J$, $B < -J$ and $B > J$. As usual for the free fermion system, the value of the Fermi momentum is determined from the condition $\varepsilon_{XX}(k) = 0$ (It must be mentioned, that the magnetic filed in this picture plays the role of the chemical potential for the quasi-particles, spinless fermions). The spectrum

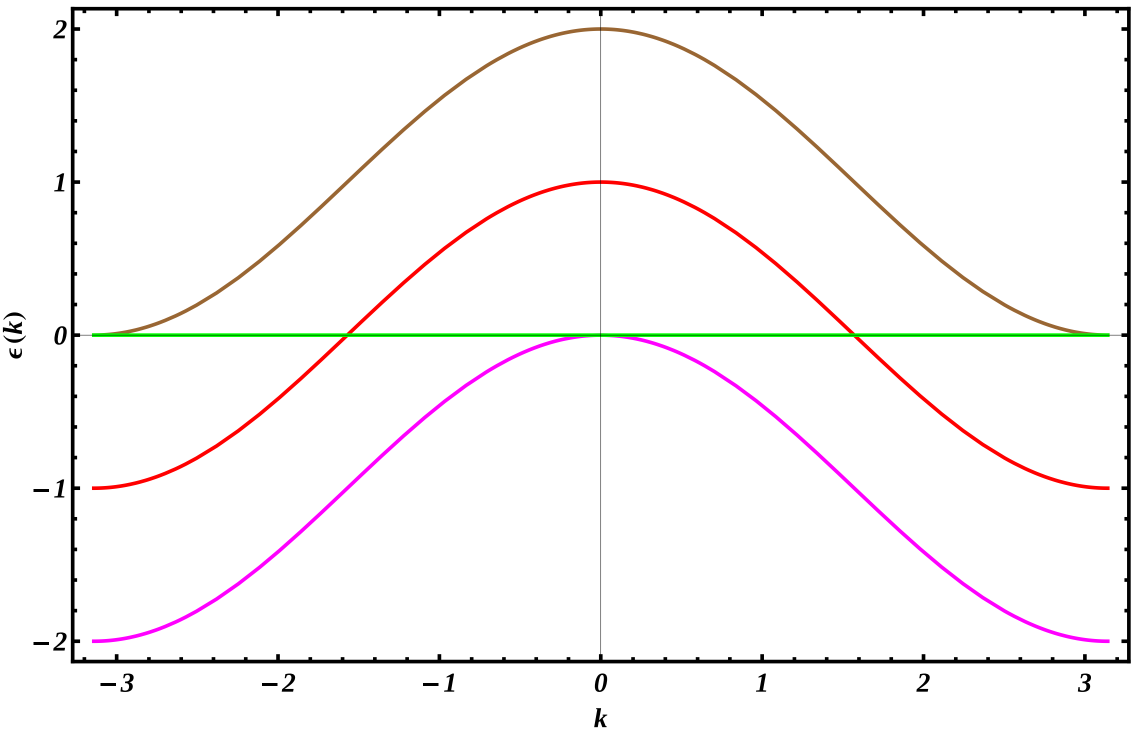

Figure 1: The spectrum of the Xx-chain for different values of the magnetic field B: B=0(red), B=1(brown), B=-1(magenta).

is symmetric with respect to the origin, this means that except the for case $k_F = 0$ in all other situations the Fermi surface consists of two symmetric points, $\pm k_F$. Thus,

$$k_F = \begin{cases} \pi, & B < -J, \\ \arccos \frac{B}{J}, & |B| \leq J, \\ 0, & B > J. \end{cases} \tag{2.32}$$

As the dispersion for this case is a convex curve, the filled states are two non-connected sets of states with the gap (forbidden zone) in between, form $-k_F$ to k_F. This means

$$\begin{aligned} n_k &= 1 \quad \text{for} \quad k \in [-\pi, -k_F] \quad \text{and} \quad k \in [k_F, \pi] \\ n_k &= 0 \quad \text{for} \quad k \in [-k_F, k_F]\,. \end{aligned} \tag{2.33}$$

Thus, for the zero-temperature case one can obtain the quasi-particle density and the magnetic moment per one site (magnetization) in the straightforward way:

$$\begin{aligned} \mathcal{N} &= \sum_{k=-\pi}^{-k_F} 1 + \sum_{k=k_F}^{\pi} 1, \\ \mathcal{M} &= \frac{1}{2}\left(\sum_{k=-\pi}^{-k_F} 1 + \sum_{k=k_F}^{\pi} 1\right) - \frac{1}{2}\sum_{k=-k_F}^{k_F} 1. \end{aligned} \tag{2.34}$$

Let us remind the reader that the empty state of the quasi-particle means the $S^z = -1/2$ configuration of the underlying spins form the XX-spin chain, and filled state of the quasi-particle corresponds to the $S^z = 1/2$ state of the spins. Now, we have to make a transition form a discrete sums to the integrals. The integrals can be evaluated much more easily. To to so, one just has to use the standard rules of the integral sums for the integrals on the Brillouin zone:

$$\sum_k f(k) = \sum_k f_k \Delta k \frac{1}{\Delta k} = \frac{N}{2\pi} \sum_k f_k \Delta k \to \frac{N}{2\pi} \int f(k) dk, \tag{2.35}$$

as $\Delta k = \frac{2\pi}{N}(\lambda+1) - \frac{2\pi}{N}(\lambda) = \frac{2\pi}{N}$. Therefore, for the quasi-particle density and magnetization we will have

$$n = \frac{\mathcal{N}}{N} = \frac{1}{2\pi}\left\{\int_{-\pi}^{-k_F} dk + \int_{k_F}^{\pi} dk\right\} = 1 - \frac{k_F}{\pi}, \tag{2.36}$$
$$m = \frac{\mathcal{M}}{N} = \frac{1}{2\pi}\left\{\frac{1}{2}\int_{-\pi}^{-k_F} dk + \frac{1}{2}\int_{k_F}^{\pi} dk - \frac{1}{2}\int_{-k_F}^{k_F} dk\right\} = \frac{1}{2}\left(1 - 2\frac{k_F}{\pi}\right).$$

Using the expressions for the Fermi momentum one obtains

$$n = \begin{cases} 0, & B < J, \\ 1 - \frac{1}{\pi}\arccos(B/J), & |B| \le J, \\ 1, & B > J, \end{cases} \tag{2.37}$$

and

$$m = \begin{cases} -1/2, & B < J, \\ 1/2\left(1 - \frac{2}{\pi}\arccos(B/J)\right), & |B| \le J, \\ 1/2, & B > J, \end{cases} \tag{2.38}$$

It is easy to get the zero-temperature magnetic susceptibility, $\chi = \left(\frac{\partial m}{\partial B}\right)$:

$$\chi = \begin{cases} 0, & B < -J, \\ \frac{1}{J\pi}\left(1 - B^2/J^2\right)^{-1/2}, & |B| \le J, \\ 0, & B > J. \end{cases} \tag{2.39}$$

As the susceptibility has singularities at points $B = -J$ and $B = J$ we deal here with the quantum phase transitions od second order. Thus, the picture of the zero-temperature ground sates of the XX-chain is quite simple: fully polarized spins pointing "down" ($B \le -J$, $k_F = \pi$), fully polarized spins pointing "up" ($B \ge J$, $k_F = 0$) and intermediate state with non-zero magnetization ($|B| < J$, $k_F = \arccos(B/J)$). One can also define the ground state energy of the system per unit site,

$$\varepsilon = E/N = \frac{1}{2\pi}\left\{\int_{-\pi}^{-k_F} (J\cos k - B)\, dk + \int_{k_F}^{\pi} (J\cos k - B)\, dk\right\} + \frac{B}{2} \tag{2.40}$$

or

$$\varepsilon = \begin{cases} B/2, & B < -J, \\ \frac{J}{\pi}\left\{\frac{B}{J}\arccos(B/J) - \sqrt{1 - B^2/J^2}\right\} - \frac{B}{2}, & |B| \le J, \\ -B/2, & B > J, \end{cases} \tag{2.41}$$

2.6 Critical exponents

Let us figure out the behavior of the macroscopic quantities at the vicinities of the quantum phase transition points $B_c = \pm J$, $m_c = \pm 1/2$. First of all, the form of the magnetization curve close to the critical value of the magnetic filed can be easily obtained by expanding the Eq.(2.38) in the vicinity of B_c. So, we have

$$m - m_c \simeq \frac{\sqrt{2}}{\pi}\left(B - B_c\right)^{\frac{1}{2}}, \quad B_c = -J,\ m_c = -1/2, \tag{2.42}$$
$$m - m_c \simeq \frac{\sqrt{2}}{\pi}\left(B_c - B\right)^{\frac{1}{2}}, \quad B_c = J,\ m_c = 1/2.$$

As wee see, the magnetization curve of the XX-chain at zero temperature close to the critical points has square-root form. Thus, the values of the critical index is 2. This critical index, which describes the behavior of the order parameter as a function of a external field at critical point is usually denoted by δ. In the case of magnets we have $m - m_c \simeq (B - B_c)^{\frac{1}{\delta}}$. Another important critical exponent we can obtain from our description of the XX-chain is the critical exponent describing the singularity of the susceptibility at critical points, $\chi \simeq (B - B_c)^{-\gamma}$. Looking at the Eq. (2.39), one can easily see that for the XX-chain $\gamma = 1/2$.

2.7 Bogoliubov transformation

Let us return to the generic case of the XY-chain.

$$\mathcal{H}_{XY} = \sum_{k \in B.Z.} \left\{ \left(J\cos k - B\right) d_k^+ d_k + J\gamma \frac{e^{ik}}{2}\left(d_k^+ d_{-k}^+ + d_k d_{-k}\right) \right\} + B\frac{N}{2}. \tag{2.43}$$

As was mentioned above, the terms proportional to γ are not diagonal. Though, there are no coupling between the states with different $|k|$, the terms describing the coupling between the states with k and $-k$. To diagonalize those terms one has to introduce a new fermion operator which is the linear combination of the d-operators with k and $-k$. A linear combination of this kind is called a **Bogoliubov transformation**. But first, in order to make the symmetry with respect to the origin of the Brillouin zone more explicit let us rewrite the Hamiltonian (2.43) in a bit different form, by combining the k and $-k$ terms and,thus, summing over the one half of the Brillouin zone, $0 \leq k \leq \pi$.

$$\begin{aligned}\mathcal{H}_{XY} &= \sum_{k=0}^{\pi} \left\{ \left(J\cos k - B\right)\left(d_k^+ d_k + d_{-k}^+ d_{-k}\right) + \frac{J\gamma}{2}\left[e^{ik}\left(d_k^+ d_{-k}^+ + d_k d_{-k}\right) + e^{-ik}\left(d_{-k}^+ d_k^+ + d_{-k} d_k\right)\right] \right\} \\ &+ B\frac{N}{2} = \sum_{k=0}^{\pi} \left\{ \left(J\cos k - B\right)\left(d_k^+ d_k + d_{-k}^+ d_{-k}\right) + J\gamma\, i\sin k\left(d_k^+ d_{-k}^+ + d_k d_{-k}\right) \right\} + B\frac{N}{2}. \end{aligned} \tag{2.44}$$

Here we used the following properties od the operators d: $d_{-k}^+ d_k^+ = -d_k^+ d_{-k}^+$ and $d_{-k} d_k = -d_k d_{-k}$. Now, as the summation in the Hamiltonian is going on the positive values of k, the operators with negative k can be considered as the operators corresponding to another kind of the excitation, another quasi-particles. In is also worth mentioning that the Hamiltonian (2.44) can be represented as a Hamiltonian of a two-component fermion field

$$\Psi_k = \begin{pmatrix} d_k \\ d^+_{-k} \end{pmatrix} \tag{2.45}$$

in the following way:

$$\mathcal{H}_{XY} = \sum_{k=0}^{\pi} \left(d_k^+ \; ; d_{-k}\right) \begin{pmatrix} J\cos k - B & J\gamma i \sin k \\ -J\gamma i \sin k & B - J\cos k \end{pmatrix} \begin{pmatrix} d_k \\ d^+_{-k} \end{pmatrix} \tag{2.46}$$

Here the constant term, $\frac{BN}{2}$ is incorporated into the matrix product as a term coming out of the commutation relations of the operators d_k when one brings the Hamiltonian to the form (2.44). Here, we also used the identity $\sum_{k=0}^{\pi} \cos k = 0$. The **Bogoliubov transformation** usually implies the linear transformation mixing the operators d_k and d^+_{-k}:

$$\begin{aligned} \chi_k &= A_k d_k + B_k d^+_{-k}, \\ \chi_{-k} &= C_k d_k^+ + D_k d_{-k}, \end{aligned} \tag{2.47}$$

and

$$\begin{aligned} \chi_k^+ &= A_k^* d_k^+ + B_k^* d_{-k}, \\ \chi^+_{-k} &= C_k^* d_k + D_k^* d^+_{-k}, \end{aligned} \tag{2.48}$$

respectively. Demanding the fermionic anticommutations for the new operators χ one can obtain some relations for the coefficients of the transformations (2.47) and (2.48):

$$\begin{aligned} |A_k|^2 + |B_k|^2 &= 1, \\ |C_k|^2 + |D_k|^2 &= 1, \\ A_k C_k + B_k D_k &= 0. \end{aligned} \tag{2.49}$$

Let us prove the last one.

$$\begin{aligned} &\{\chi_k,\ \chi_{-k}\} = \left(A_k d_k + B_k d^+_{-k}\right)\left(C_k d_k^+ + D_k d_{-k}\right) + \left(C_k d_k^+ + D_k d_{-k}\right)\left(A_k d_k + B_k d^+_{-k}\right) = \\ &A_k C_k \underbrace{\left(d_k d_k^+ + d_k^+ d_k\right)}_{=1} + A_k D_k \underbrace{\left(d_k d_{-k} + d_{-k} d_k\right)}_{=0} + B_k C_k \underbrace{\left(d^+_{-k} d_k^+ + d_k^+ d^+_{-k}\right)}_{=0} = \\ &B_k D_k \underbrace{\left(d^+_{-k} d_{-k} + d_{-k} d^+_{-k}\right)}_{=1} = A_k C_k + B_k D_k = 0. \end{aligned} \tag{2.50}$$

Exercise *Prove two first relations of Eq. (2.49)* (Hint *Demand* $\left\{\chi_k,\ \chi_k^+\right\} = 1$ *and* $\left\{\chi_{-k},\ \chi^+_{-k}\right\} = 1$)

After that one should usually reverse the relations (2.47) and substitute the expressions for d operators into the Hamiltonian and demand the cancelation of non-diagonal terms. But, we would like to present more straightforward and brief method. The matrix form of the Hamiltonian of the XY-chain written is particularly convenient for diagonalization, as one just has to find the eigenvalues of the matrix

$$\mathbf{H}_k = \begin{pmatrix} J\cos k - B & J\gamma i \sin k \\ -J\gamma i \sin k & B - J\cos k \end{pmatrix}. \tag{2.51}$$

The eigenvalues, $\Lambda_k^{\pm}$ are found to be

$$\Lambda_k^{\pm} = \pm\Lambda_k = \pm\sqrt{(J\cos k - B)^2 + J^2\gamma^2 \sin^2 k}. \tag{2.52}$$

This means that there are unitary matrix U_k which satisfies

$$\mathbf{H}_k = \mathbf{U}_k^{+} \begin{pmatrix} \Lambda_k & 0 \\ 0 & -\Lambda_k \end{pmatrix} \mathbf{U}_k \tag{2.53}$$

Then, let us substitute this identity into the Hamiltonian (2.46):

$$\mathcal{H}_{XY} = \sum_{k=0}^{\pi} \Psi_k^{+} \mathbf{H}_k \Psi_k = \sum_{k=0}^{\pi} \Psi_k \mathbf{U}_k^{+} \begin{pmatrix} \Lambda_k & 0 \\ 0 & -\Lambda_k \end{pmatrix} \mathbf{U}_k \Psi_k. \tag{2.54}$$

It is straightforward, now, to define a new two-component fermion field,

$$\Phi_k = \mathbf{U}_k \Psi_k = \begin{pmatrix} \chi_k \\ \chi_{-k}^{+} \end{pmatrix} \tag{2.55}$$

Now, in order to adjust the SU(2)-transformation with matrix $\mathbf{U}_k$ with the Bogoliubov transformation (2.47) and (2.48) we have to consider the later in the following form:

$$\mathbf{U}_k = \begin{pmatrix} A_k & B_k \\ C_k^{*} & D_k^{*} \end{pmatrix}. \tag{2.56}$$

Then, the Hamiltonian (2.54) can be easily rewritten in terms of new fermionic operator:

$$\begin{aligned} \mathcal{H}_{XY} &= \sum_{k=0}^{\pi} \Phi_k^{+} \begin{pmatrix} \Lambda_k & 0 \\ 0 & -\Lambda_k \end{pmatrix} \Phi_k = \sum_{k=0}^{\pi} \Lambda_k \left(\chi_k^{+}\chi_k - \chi_{-k}\chi_{-k}^{+}\right), \\ &= \sum_{k=0}^{\pi} \Lambda_k \left(\chi_k^{+}\chi_k + \chi_{-k}^{+}\chi_{-k} - 1\right) = \sum_{k=-\pi}^{\pi} \Lambda_k \left(\chi_k^{+}\chi_k - 1/2\right). \end{aligned} \tag{2.57}$$

Thus, we diagonalized the Hamiltonian of the XY-chain in terms of composite fermions, Bogoliubov quasi-particles. The energy of the ground state, when there are no quasi-particles in the system can be easily obtained as

$$\begin{aligned} \varepsilon_{XY} &= E_{XY}/N = -\frac{1}{2N}\sum_{k=-\pi}^{\pi} \Lambda_k = -\frac{1}{4\pi}\int_{-\pi}^{\pi} dk \sqrt{(J\cos k - B)^2 + J^2\gamma^2 \sin^2 k} \\ &= -\frac{1}{2\pi}\int_{0}^{\pi} dk \sqrt{(J\cos k - B)^2 + J^2\gamma^2 \sin^2 k}. \end{aligned} \tag{2.58}$$

This is quite general consideration. Setting the values of the parameter γ to specific values one can obtain the important particualr cases of the XY-chain, like $gamma = 0$ for the XX-chain considered above and $\gamma = 1$ for so-called quantum Ising model (Ising chain in a transverse magnetic field), giving by the following Hamiltonian:

$$\mathcal{H}_{qI} = \sum_{j=1}^{N} \left(J S_j^x S_{j+1}^x - B S_j^z \right) = \sum_{k \in B.Z.} \varepsilon_{qI}(k) \left(\chi_k^+ \chi_k - 1/2 \right), \tag{2.59}$$

$$\varepsilon_{qI}(k) = \sqrt{J^2 + B^2 - 2JB \cos k}. \tag{2.60}$$

2.8 Coefficients of the Bogoliubov transformation

Though, we diagonalized the Hamiltonian of the XY-chain and now the spectrum of the Bogoliubov quasi-particles, it is also important to now the coefficients of the transformation, or the entries of the unitary matrix $\mathbf{U}_k$. It is necessary to know the coefficients in order to calculate the correlation functions for the physical operators and in order to express the ground state of the system in terms of the physical quantities related to the operators d and, thus, to the initial spin operators. Let us take a closer look at the Eq. (2.53). Taking into account the form of the unitary matrix $\mathbf{U}_k$ from Eq. (2.56) one can write down the following relation:

$$\begin{pmatrix} a_k & b_k \\ b_k^* & -a_k \end{pmatrix} = \begin{pmatrix} A_k^* & C_k \\ B_k^* & D_k \end{pmatrix} \begin{pmatrix} \Lambda_k & 0 \\ 0 & -\Lambda_k \end{pmatrix} \begin{pmatrix} A_k & B_k \\ C_k^* & D_k^* \end{pmatrix}, \tag{2.61}$$

where

$$a_k = J \cos k - B, \qquad b_k = iJ\gamma \sin k. \tag{2.62}$$

One can derive the following equation for the entries of the unitary matrix $\mathbf{U}_k$:

$$\begin{aligned} |A_k|^2 - |C_k|^2 &= \frac{a_k}{\Lambda_k}, \\ |B_k|^2 - |D_k|^2 &= -\frac{a_k}{\Lambda_k}, \\ A_k^* B_k - C_k D_K^* &= \frac{b_k}{\Lambda_k}. \end{aligned} \tag{2.63}$$

The Bogoliubov transformation constrains given in Eq. (2.49) allow us to look for the entries in the following form:

$$A_k = D_k = \cos \vartheta_k, \quad B_k = C_k^* = i \sin \vartheta_k. \tag{2.64}$$

Then

$$\begin{aligned} \cos 2\vartheta_k &= \frac{a_k}{\Lambda_k} = \frac{J \cos k - B}{\sqrt{(J \cos k - B)^2 + J^2 \gamma^2 \sin^2 k}}, \\ \sin 2\vartheta_k &= \frac{b_k}{i\Lambda_k} = \frac{J\gamma \sin k}{\sqrt{(J \cos k - B)^2 + J^2 \gamma^2 \sin^2 k}}, \end{aligned} \tag{2.65}$$

or

$$\vartheta_k = \frac{1}{2} \arctan\left(\frac{J\gamma \sin k}{J\cos k - B}\right). \tag{2.66}$$

And finally,

$$A_k = \frac{1}{\sqrt{2}} \left(1 + \frac{J\cos k - B}{\sqrt{(J\cos k - B)^2 + J^2\gamma^2 \sin^2 k}}\right)^{1/2}, \tag{2.67}$$

$$B_k = \frac{i}{\sqrt{2}} \left(1 - \frac{J\cos k - B}{\sqrt{(J\cos k - B)^2 + J^2\gamma^2 \sin^2 k}}\right)^{1/2}, \tag{2.68}$$

2.9 Static correlation functions at zero-temperature

As was mentioned above the ground state of the XY-chain in terms of the Bogoliubov quasi-particles can be describe as a vacuum with no occupied stated:

$$\chi_k | 0\rangle = 0, \quad \forall\, k. \tag{2.69}$$

Let us calculate some simple correlation function for the ground state. It is obvious that

$$\begin{aligned} \langle 0\, |\chi_k \chi_q^+ | \,0\rangle &= \delta_{k,q}, \\ \langle 0\, |\chi_k \chi_q | \,0\rangle &= \langle 0\, |\chi_k^+ \chi_q^+ | \,0\rangle = \langle 0\, |\chi_k^+ \chi_q^| \,0\rangle = 0. \end{aligned} \tag{2.70}$$

In order to calculate the correlation functions for the physical free fermion operators one, first of all, has to reverse the relation (2.55).

$$\Psi = \begin{pmatrix} d_k \\ d_{-k}^+ \end{pmatrix} = \mathbf{U}_k^{-1}\Phi = \begin{pmatrix} \cos\vartheta_k & -i\sin\vartheta_k \\ -i\sin\vartheta_k & \cos\vartheta_k \end{pmatrix} \begin{pmatrix} \chi_k \\ \chi_{-k}^+ \end{pmatrix}. \tag{2.71}$$

Therefore, substituting these expressions into the Eqs. (2.70) we get the fundamental correlation functions for the physical spinless fermions:

$$\begin{aligned} \langle 0|\, d_k d_q^+ |\, 0\rangle &= \langle 0| \left(\cos\vartheta_k\ \chi_k - i\sin\vartheta_k \chi_{-k}^+\right)\left(\cos\vartheta_q\ \chi_q^+ + i\sin\vartheta_q \chi_{-q}\right) |\, 0\rangle \\ &= \cos\vartheta_k \cos\vartheta_q \langle 0|\ \chi_k \chi_q^+ |\, 0\rangle = \cos^2\vartheta_k\ \delta_{k,q}, \\ \langle 0|\, d_k^+ d_q |\, 0\rangle &= \sin^2\vartheta_k\ \delta_{k,q}, \\ \langle 0|\, d_k d_q |\, 0\rangle &= -\frac{i}{2}\sin 2\vartheta_k\ \delta_{k,-q} \\ \langle 0|\, d_k^+ d_q^+ |\, 0\rangle &= \frac{i}{2}\sin 2\vartheta_k\ \delta_{k,-q}. \end{aligned} \tag{2.72}$$

Using these expressions one can easily find the following correlation functions of two c operators:

$$\begin{aligned} \langle c_j c_l\rangle = -\langle c_j^+ c_l^+\rangle &= \frac{i}{2\pi}\int_{-\pi}^{\pi} e^{i(l-j)k} \frac{\sin 2\vartheta_k}{2} dk, \\ \langle c_j^+ c_l\rangle &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(l-j)k} \sin^2\vartheta_k dk, \\ \langle c_j c_l^+\rangle &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(l-j)k} \cos^2\vartheta_k dk, . \end{aligned} \tag{2.73}$$

Let us define the static $T = 0$ correlation functions for the spin operators of the XY-chain.

$$\rho^\alpha_{jl} = \langle S^\alpha_j S^\alpha_l \rangle, \tag{2.74}$$

where the angle brackets stand for the expectation value in the ground state of the XY-chain. Now, assuming that $l > j$ we express the correlation functions in terms of the fermionic operators.

$$\begin{aligned}
\rho^x_{jl} &= \frac{1}{4}\langle \left(c^+_j + c_j\right) \prod_{n=j}^{l-1} \left(1 - 2c^+_n c_n\right) \left(c^+_l + c_l\right) \rangle, \\
\rho^y_{jl} &= -\frac{1}{4}\langle \left(c^+_j - c_j\right) \prod_{n=j}^{l-1} \left(1 - 2c^+_n c_n\right) \left(c^+_l - c_l\right) \rangle, \\
\rho^z_{jl} &= \frac{1}{4}\langle \left(1 - 2c^+_j c_j\right) \left(1 - 2c^+_l c_l\right) \rangle.
\end{aligned} \tag{2.75}$$

To proceed further we introduce the following operators:

$$\begin{aligned}
&A_j = c^+_j + c_j, \quad B_j = c^+_j - c_j, \\
&\{A_j, A_l\} = 2\delta_{jl},\ \{B_j, B_l\} = -2\delta_{jl},\ \{A_j, B_l\} = 0
\end{aligned} \tag{2.76}$$

Thus we have

$$\begin{aligned}
\rho^x_{jl} &= \frac{1}{4}\langle \left(c^+_j + c_j\right) \prod_{n=j}^{l-1} \left(1 - 2c^+_n c_n\right) \left(c^+_l + c_l\right) \rangle \qquad (2.77) \\
&= \frac{1}{4}\langle \left(c^+_j + c_j\right) \left(1 - 2c^+_j c_j\right) \prod_{n=j+1}^{l-1} \left(c^+_n + c_n\right) \left(c^+_n - c_n\right) \left(c^+_l + c_l\right) \rangle \\
&= \frac{1}{4}\langle \left(c^+_j - c_j\right) \prod_{n=j+1}^{l-1} \left(c^+_n + c_n\right) \left(c^+_n - c_n\right) \left(c^+_l + c_l\right) \rangle \\
&= \frac{1}{4}\langle B_j A_{j+1} B_{j+1} A_{j+2} B_{j+2} ... A_{l-1} B_{l-1} A_l \rangle. \qquad (2.78)
\end{aligned}$$

In the same way for the other correlation functions we have

$$\begin{aligned}
&\rho^y_{jl} = (-1)^{l-j} \frac{1}{4}\langle A_j B_{j+1} A_{j+1} B_{j+2} A_{j+2} ... B_{l-1} A_{l-1} B_l \rangle, \\
&\rho^z_{jl} = \frac{1}{4}\langle A_j B_j A_l B_l \rangle.
\end{aligned} \tag{2.79}$$

Since the operators A_j and B_j are anticommuting variables, their expectation values can be evaluated with the Wick's theorem, it terms of the sums of all possible contractions of pairs of operators. With the aid of Eqs. (2.73) we get

$$\begin{aligned}
\langle A_j A_l \rangle &= \delta_{jl} \\
\langle B_j B_l \rangle &= -\delta_{jl}, \\
\langle B_j A_l \rangle &= G_{jl},
\end{aligned} \tag{2.80}$$

where

$$
\begin{aligned}
G_{jl} = G(l-j) &= -\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(l-j)k} e^{i2\vartheta_k} \qquad (2.81)\\
&= -\frac{1}{\pi}\int_{0}^{\pi} \frac{1}{\Lambda_k}\left\{\cos(rk)\left(J\cos k - B\right) - J\gamma\sin(rk)\sin k\right\} dk,\\
& r \equiv l-j.
\end{aligned}
$$

Now we have everything for calculating the correlation functions (2.77) and (2.79) with the aid of Wick's rule. Let us first mention that the contractions of two A and two B operators are different form zero only if both operators belong to the same site. As one can see in the expressions for the correlation function all operators belon to different sites. This means that only the contraction of the form $\langle A_j B_l\rangle$ make a non zero contribution. Then for the application of the Wick's theorem one have only take into account the all possible permutations of the A operators while the B operators are fixed in their positions. Thus, we have

$$
\begin{aligned}
\rho^x_{jl} &= \frac{1}{4}\sum_{P\in S_{l-j}} (-1)^{\mathrm{sgn}(P)} G_{j,P(j+1)} G_{j+1,P(j+2)} \ldots G_{l-1,P(l)} = \frac{1}{4}\det \mathbf{G}^x_{jl}, \qquad (2.82)\\
\rho^y_{jl} &= \frac{1}{4}\sum_{P\in S_{l-j}} (-1)^{\mathrm{sgn}(P)} G_{j+1,P(j)} G_{j+2,P(j+1)} \ldots G_{l,P(l-1)} = \frac{1}{4}\det \mathbf{G}^y_{jl},\\
\rho^z_{jl} &= \frac{1}{4}\left(G_{jj}G_{ll} - G_{jl}G_{lj}\right),
\end{aligned}
$$

where S_{l-j} is a permutation group of $l-j$ indexes, which is case of ρ^x_{jl} corresponds to the following permutations:

$$
P : (j+1, j+2, ..., l-1, l) \mapsto (P(j+1), P(j+2), ..., P(l-1), P(l)) \qquad (2.83)
$$

and in case of ρ^x_{jl} to the following:

$$
P : (j, j+1, ..., l-2, l-1) \mapsto (P(j), P(j+1), ..., P(l-2), P(l-1)) \qquad (2.84)
$$

thus, we see that the correlation functions of the spin operators in the XY chain have the structure of determinants of the certain matrices, in which the entries depend only on the difference of the indexes, $G_{jl} = G(l-j)$.

2.10 Thermodynamics

As the Jordan-Wigner fermionization for the XY-model yields the Hamiltonian of free electrons in is straightforward to describe the thermodynamics of the models exactly. Let us suppose we have a Hamiltonian of a free spinless fermions in the following form:

$$
\mathcal{H} = \sum_{k\in B.Z.} \varepsilon_k \left(c^+_k c_k - 1/2\right). \qquad (2.85)
$$

The specific form the of spectrum does not matter, so far. Let us start with the calculation of the partition function.

$$\begin{aligned}
\mathcal{Z} &= \mathrm{Sp}\, e^{-\beta\mathcal{H}} = \mathrm{Sp}\, e^{-\beta\sum_{k\in B.Z.}\varepsilon_k\left(c_k^+c_k-1/2\right)} = \mathrm{Sp}\left\{\prod_{k\in B.Z.} e^{-\beta\varepsilon_k\left(c_k^+c_k-1/2\right)}\right\} \qquad (2.86)\\
&= \prod_{k\in B.Z.}\sum_{n_k=0,1} e^{-\beta\varepsilon_k(n_k-1/2)} = \prod_{k\in B.Z.}\left(e^{\beta\frac{\varepsilon_k}{2}}+e^{-\beta\frac{\varepsilon_k}{2}}\right) = \prod_{k\in B.Z.} 2\cosh\left(\beta\frac{\varepsilon_k}{2}\right).
\end{aligned}$$

Here, $\beta = 1/T$. Now, we can obtain an expression for the free energy per site in the thermodynamic limit:

$$\begin{aligned}
f &= -\frac{1}{\beta}\lim_{N\to\infty}\frac{\log\mathcal{Z}_N}{N} = -\frac{1}{\beta}\lim_{N\to\infty}\frac{\log\prod_{k\in B.Z.}2\cosh\left(\beta\frac{\varepsilon_k}{2}\right)}{N} \qquad (2.87)\\
&= -\frac{1}{\beta}\lim_{N\to\infty}\frac{1}{N}\sum_{k\in B.Z.}\log\left\{2\cosh\left(\beta\frac{\varepsilon_k}{2}\right)\right\} = -\frac{1}{2\pi\beta}\int_{-\pi}^{\pi}\log\left\{2\cosh\left(\beta\frac{\varepsilon_k}{2}\right)\right\}dk.
\end{aligned}$$

It is also convenient to express the thermodynamic quantities in terms of the standard Fermi distribution function,

$$n_k = \frac{1}{e^{\beta\varepsilon_k}+1}.$$

thus, for the free energy per one site one has

$$f = -\frac{T}{2\pi}\int_{-\pi}^{\pi}\log\left\{2\cosh\left(\beta\frac{\varepsilon_k}{2}\right)\right\}dk = -\frac{T}{2\pi}\int_{-\pi}^{\pi}\log\left\{e^{\beta\frac{\varepsilon_k}{2}}+e^{-\beta\frac{\varepsilon_k}{2}}\right\}dk \qquad (2.88)$$

$$= -\frac{T}{2\pi}\int_{-\pi}^{\pi}\log\left\{e^{-\beta\frac{\varepsilon_k}{2}}\left(e^{\beta\varepsilon_k}+1\right)\right\}dk \qquad (2.89)$$

Thus,

$$f = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{\varepsilon_k}{2}+T\log n_k\right)dk.$$

All thermodynamic functions can be obtained by taking a derivative of the free energy with respect to temperature and to the parameters including into the microscopic model (spin chain). Let us for the time being denote these parameters by J_a. Actually, they include all coupling constants and magnetic field. To get compact and convenient expressions it is suitable to work with the Fermi distribution function and its derivatives:

$$\begin{aligned}
\left(\frac{\partial n_k}{\partial J_a}\right)_{T,\{J_b\}} &= n_k(n_k-1)\,\frac{1}{T}\left(\frac{\partial\varepsilon_k}{\partial J_a}\right)_{J_b}, \qquad (2.90)\\
\left(\frac{\partial n_k}{\partial T}\right)_{\{J_b\}} &= n_k(1-n_k)\,\frac{1}{T^2}\,\varepsilon_k.
\end{aligned}$$

Thus, taking into account these equations one gets

$$\left(\frac{\partial f}{\partial J_a}\right)_{T,\{J_b\}} = \frac{1}{2\pi}\int_{-\pi}^{\pi}(n_k - 1/2)\left(\frac{\partial \varepsilon_k}{\partial J_a}\right)_{\{J_b\}} dk, \tag{2.91}$$

$$\left(\frac{\partial f}{\partial T}\right)_{\{J_b\}} = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\log n_k + \frac{\varepsilon_k}{T}(1-n_k)\right) dk,$$

$$\left(\frac{\partial^2 f}{\partial J_a \partial J_b}\right)_{T,\{J_c\}} = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{1}{T}n_k(n_k-1)\left(\frac{\partial \varepsilon_k}{\partial J_a}\right)_{\{J_c\}}\left(\frac{\partial \varepsilon_k}{\partial J_b}\right)_{\{J_c\}} + (n_k - 1/2)\left(\frac{\partial^2 \varepsilon_k}{\partial J_a \partial J_b}\right)_{\{J_c\}}\right) dk,$$

$$\left(\frac{\partial^2 f}{\partial J_a \partial T}\right)_{\{J_c\}} = \frac{1}{2\pi T^2}\int_{-\pi}^{\pi} n_k(1-n_k)\,\varepsilon_k\left(\frac{\partial \varepsilon_k}{\partial J_a}\right)_{\{J_c\}} dk,$$

$$\left(\frac{\partial^2 f}{\partial T^2}\right)_{\{J_b\}} = -\frac{1}{2\pi T^3}\int_{-\pi}^{\pi}\varepsilon_k^2 n_k(1-n_k)\,dk.$$

Let us now write down these expressions for the general XY-chain, with

$$\varepsilon_k = \sqrt{(J\cos k - B)^2 + J^2\gamma^2\sin^2 k}. \tag{2.92}$$

For the entropy and specific heat one has

$$S = -\left(\frac{\partial f}{\partial T}\right)_B = -\frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\log n_k + \frac{\varepsilon_k}{T}(1-n_k)\right) dk, \tag{2.93}$$

$$C = -T\left(\frac{\partial^2 f}{\partial T^2}\right)_B = \frac{1}{2\pi T^2}\int_{-\pi}^{\pi}\varepsilon_k^2 n_k(1-n_k)\,dk.$$

For the magnetization and susceptibility we get

$$M = -\left(\frac{\partial f}{\partial B}\right)_T = \frac{1}{2\pi}\int_{-\pi}^{\pi}(n_k - 1/2)\,\frac{J\cos k - B}{\sqrt{(J\cos k - B)^2 + J^2\gamma^2\sin^2 k}}\,dk, \tag{2.94}$$

$$\chi = -\left(\frac{\partial^2 f}{\partial B^2}\right)_T =$$

$$-\frac{1}{2\pi}\int_{-\pi}^{\pi}\left\{\frac{1}{T}n_k(n_k-1)\frac{(J\cos k - B)^2}{(J\cos k - B)^2 + J^2\gamma^2\sin^2 k} + \frac{(n_k - 1/2)\,J^2\gamma^2\sin^2 k}{\left((J\cos k - B)^2 + J^2\gamma^2\sin^2 k\right)^{3/2}}\right\} dk.$$

These expressions take especially simple form for the case of XX-chain ($\gamma = 0$):

$$M = \frac{1}{2\pi}\int_{-\pi}^{\pi}(n_k - 1/2)\;dk, \tag{2.95}$$

$$\chi = -\frac{1}{2\pi T}\int_{-\pi}^{\pi} n_k(n_k - 1)\,dk.$$

3 The Heisenberg chain. Coordinate Bethe ansatz

3.1 Introduction

In this section we are going to introduce the coordinate Bethe ansatz method on the example of isotropic Heisenberg and XXZ-spin chain. The Heisenberg spin chain is the prototype model for the application of the coordinate Bethe ansatz technique. Historically, the field development started with the seminal paper of Hans Bethe in 1931, where he uses his intuition for the solution of the quantum-mechanical many-body problem of the isotropic Heisenberg chain. At that time, there was no understating of the nature of quantum integrability. And the method proposed by Bethe for finding the eigenvalues and eigenvectors of the Heisenberg spin chain was considered by him as just a general tool viable also for 2- and 3-dimensional many body problems. Since then, the Heisenberg or XXX-chain have been the bench tools to advance the Bethe idea from one side, and to understand one-dimensional magnetism from the other. We should remark that nowadays we have numerical methods to diagonalize one-dimensional models that are more efficient than the Bethe ansatz approach. However the analytical nature of the latter and the characterization of the states in terms of a set of quantum numbers render this technique very useful for understanding what are the relevant physical processes and to develop even better approximation schemes. Let us start with the very general definition of the model. One can consider the most general form of the S=1/2 spin chain Hamiltonian in the following form:

$$\mathcal{H}_{XYZ} = \sum_{j=1}^{N} \left(J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z \right) - B \sum_{j=1}^{N} S_j^z. \tag{3.96}$$

This model is usually called XYZ-chain. There are four basic possibilities for the coupling constants:

- $J_x = J_y = J_z = J < 0$, the isotropic ferromagnetic XXX Heisenberg chain, solved by Bethe in 1931.
- $Jx = Jy = Jz = J > 0$, the isotropic antiferromagnetic XXX Heisenberg chain, the ground-state energy was obtained by Hulthen in 1938 and the elementary excitations were found by de Cloizeaux and Pearson in 1962.
- $(J_x = J_y = J) \neq J_z$, the XXZ Heisenberg chain, solved by Yang and Yang in 1966.
- $(Jx \neq Jy) \neq J_z$, the fully anisotropic XYZ Heisenberg chain, solved by Baxter in 1971

The simplest case is the isotropic Heisenberg chain The Heisenberg chain is the simples model of the physical quantum S=1/2 spins interacting with each other via the exchange interaction, the specific quantum interaction stemming out form the superposition of the Pauli principle and Coulomb forces. Thus, the physical background behind the Heisenberg model is the simples model of the (anti)ferromagnetism with the localized quantum spins in some spatial lattice interacting with the nearest neighbor only with the exchange interaction, the Hamiltonian of the latter for two neighboring spins are given by

$$V_{ex} = \frac{J}{2} \left(1 + 2\mathbf{S}_1 \, \mathbf{S}_2\right) \tag{3.97}$$

Here, the parameter J is called exchange constant and it depends on the overlap of the spatial part of the electron wave function as well as on the Coulomb interaction matrix elements. The sign of the constant J play crucial role in the macroscopic properties of the model. If it is negative, then the ferromagnetic configuration where all spins are collinear to each other is the ground state for the $B = 0$, otherwise the model is called antiferromagnetic and its properties are much more complicated. So, the Hamiltonian of the Heisenberg model,

$$\mathcal{H}_{Heis} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \, \mathbf{S}_j - \mathbf{B} \sum_j \mathbf{S}_j \tag{3.98}$$

where the sum is going on the pairs of the nearest neighbor sites of some lattice, is the simples relevant model to describe the magnetism of materials. It is one-dimensional variant,

$$\begin{aligned} \mathcal{H}_{XXX} &= J \sum_{j=1}^{N} \left(S_j^x S_j^x + S_j^y S_j^y + S_j^z S_j^z \right) - B \sum_{j=1}^{N} S_j^z, \\ &= J \sum_{j=1}^{N} \left\{ \frac{1}{2} \left(S_j^+ S_j^- + S_j^- S_j^+ \right) + S_j^z S_j^z \right\} - B \sum_{j=1}^{N} S_j^z \end{aligned} \tag{3.99}$$

is integrable and was the first model to be solved by the Bethe ansatz. It is also worth mentioning the link between exchange interaction operator and the permutation operator which change places of two spin states,

$$P_{ij} \mid \psi_i \rangle \otimes \mid \psi_j \rangle = \mid \psi_j \rangle \otimes \mid \psi_i \rangle, \tag{3.100}$$

where ψ stands either for $\uparrow$ or for $\downarrow$. For the SU(2) we have

$$P_{ij} = \frac{1}{2} \left(\mathbb{I} \otimes \mathbb{I} + \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \right). \tag{3.101}$$

Thus, one can write

$$\mathcal{H}_{XXX} = \frac{J}{2} \sum_{j=1}^{N} P_{j,j+1} - B \sum_{j=1}^{N} S_j^z - \frac{NJ}{4}. \tag{3.102}$$

3.2 Isotropic S=1/2 Heisenberg chain

Here we will present the solution of the isotropic Heisenberg chain in term of the coordinate Bethe ansatz. First of all, let us mention some symmetries of the Hamiltonian. It obviously commutes with the operator of the total spin z-projection,

$$\left[\mathcal{H}_{XXX}, \sum_{j=1}^{N} S_j^z \right] = 0, \tag{3.103}$$

so one can classify all eigenstates by the eigenvalue of the total spin z-projection which takes values from $-N/2$ to $N/2$. Therefore, it is very natural and convenient to choose the Ising basis of for the eigenstates. The Ising basis consists of the eigenstates with fixed number of spin "up" and spin "down". It is convenient choose a reference vector in the form of the ferromagnetic state, say, all spins "up". For the ferromagnetic case of negative J it is the ground state. The eigenvalue of the total spin z-projection operator for this eigenstate is the largest, $S^z_{tot} = N/2$. Thus, we will refer to this state as a "vacuum",

$$|\, 0\rangle = |\uparrow\uparrow ... \uparrow\rangle. \tag{3.104}$$

The subspace of the basic vectors with one flipped spin corresponding to $S^z_{tot} = N/2 - 1$ is span by the following N vectors:

$$|\, j\rangle = S^-_j |\, 0\rangle, \quad j = 1, ..., N. \tag{3.105}$$

For the subspace with two flipped spins and $S^z_{tot} = N/2 - 2$ we have C^2_N vectors,

$$|\, j_1, j_2\rangle = S^-_{j_1}\, S^-_{j_2} |\, 0\rangle, \quad j_1, j_2 = 1, ..., N, \;\; j_1 < j_2. \tag{3.106}$$

Therefore, for the subspace with M flipped spins and $S^z_{tot} = N/2 - M$ one has $C^M_N = \frac{N!}{(N-M)!M!}$ vectors of the form

$$|\, j_1, ..., j_M\rangle = S^-_{j_1} ... S^-_{j_M} |\, 0\rangle, \quad j_1, ..., j_M = 1, ..., N, \;\; j_1 < j_2 < ... < j_M. \tag{3.107}$$

These basic vectors spans all the eigenstates, thus, the Hilbert space of the model contains $\sum_{M=0}^{N} C^M_N = 2^N$ states. Obviously, these vectors are not the eigenstates of the Hamiltonian $\mathcal{H}_{XXX}$, but they compose a convenient basis for constructing the eigenstates of the Heisenberg chain. Because of the translational invariance of the Hamiltonian we have to look for the eigenvectors in each S^z_{tot} in the translational invariant form. Let us start from the simples situation with one flipped spin.

3.3 The simplest quasi-particle solution, magnon.

We are looking to the eigenvector in the following form:

$$|\, \Psi_1\rangle = \sum_{j=1}^{N} a(j) |\, j\rangle. \tag{3.108}$$

Then, we can probe the action of the Hamiltonian of the Heisenberg chain to this vector. As the terms corresponding to the interaction with the external magnetic field commute with the rest part of the Hamiltonian describing the interaction of spins with each other it is enough to consider the action only of the latter part of Hamiltonian, as the contribution of the S^z_{tot} operator is just an additive constant to the eigenvalue $E^B_M = -B(N/2 - M)$. The spin-spin interaction part of the Hamiltonian consist of diagonal, $S^z S^z$ and non-diagonal parts $S^+ S^-$. Let us show the action of this part of the Hamiltonian to the pair of the same and different spin states.

$$
\begin{aligned}
S_j^z S_{j+1}^z \,|... \uparrow_j, \uparrow_{j+1}, ...\rangle &= \frac{1}{4}|... \uparrow_j, \uparrow_{j+1}, ...\rangle, \\
S_j^z S_{j+1}^z \,|... \downarrow_j, \downarrow_{j+1}, ...\rangle &= \frac{1}{4}|... \downarrow_j, \downarrow_{j+1}, ...\rangle, \\
S_j^z S_{j+1}^z \,|... \uparrow_j, \downarrow_{j+1}, ...\rangle &= -\frac{1}{4}|... \uparrow_j, \downarrow_{j+1}, ...\rangle, \\
S_j^z S_{j+1}^z \,|... \downarrow_j, \uparrow_{j+1}, ...\rangle &= -\frac{1}{4}|... \downarrow_j, \uparrow_{j+1}, ...\rangle, \\
\frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) \,|... \uparrow_j, \uparrow_{j+1}, ...\rangle &= 0, \\
\frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) \,|... \downarrow_j, \downarrow_{j+1}, ...\rangle &= 0, \\
\frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) \,|... \uparrow_j, \downarrow_{j+1}, ...\rangle &= \frac{1}{2}|... \downarrow_j, \uparrow_{j+1}, ...\rangle, \\
\frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) \,|... \downarrow_j, \uparrow_{j+1}, ...\rangle &= \frac{1}{2}|... \uparrow_j, \downarrow_{j+1}, ...\rangle.
\end{aligned} \tag{3.109}
$$

Now, we can solve the eigenvalues problem for the $\mid \Psi_1\rangle$ eigenstate.

$$
J \sum_{j=1}^{N} \sum_{l=1}^{N} a(l) \left\{ \frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + S_j^z S_{j+1}^z \right\} \mid l\rangle = E_1 \sum_{l=1}^{N} a(l) \mid l\rangle. \tag{3.110}
$$

The eigenvalue corresponding to the reference state $\mid 0\rangle$ is $E_0 = \frac{JN}{4}$. Thus,

$$
\sum_{l=1}^{N} J a(l) \left\{ \frac{1}{2} \mid l-1\rangle + \frac{1}{2} \mid l+1\rangle + \left[\frac{1}{4}(N-2) - \frac{1}{4} 2\right] \mid l\rangle \right\} = E_1 \sum_{l=1}^{N} a(l) \mid l\rangle, \tag{3.111}
$$

this yields

$$
\sum_{l=1}^{N} \left\{ \frac{J}{2} a(l+1) + \frac{J}{2} a(l-1) + (E_0 - E_1 - J)\, a(l) \right\} \mid l\rangle = 0 \tag{3.112}
$$

So, for the coefficients of the wave function we have got the following functional equation:

$$
\frac{J}{2}\, a(l+1) + \frac{J}{2}\, a(l-1) + (E_0 - E_1 - J)\, a(l) = 0 \tag{3.113}
$$

Is it very natural to look for the solution of this equation in the exponential form, $a(l) = Ae^{ikl}$. Substituting this into the Eq. (3.113) we finally get

$$
E_1 - E_0 = -J\,(1 - \cos k)\,. \tag{3.114}
$$

Periodicity condition and translational invariance yield the quantization of the quasi-momenta $k = \frac{2\pi m}{N}$, $m = 0, 1..., N-1$. Note, that the $k = 0$ state is degenerate with the "vacuum" $\mid 0\rangle$. Such an excitation for the ferromagnetic Heisenberg chain where the reference state we adopted here is a real ground state is called **magnon**, the quasi particle with the dispersion given by the Eq. (3.114) and magnetic moment equal to 1.

3.4 The two-body (two magnon) problem

Let us now consider an eigenstate corresponding to the case of two flipped spins, or two-magnon state. The prominent point here is that the two-magnon subspace, and in general with higher number of quasi-particles, is not a simply superposition of magnons. It can be seen, for example, by counting the number of all possible two-magnon states which can be constructed form the superposition of the one-magnon states, N^2 with the dimension of the subspace with $M = 2$, $\frac{N(N-1)}{2}$. The general form of the eigenvector with $M = 2$ is

$$|\Psi_2\rangle = \sum_{1\leq\, l_1\, <l_2\, \leq N} a(l_1,\ l_2)|\, l_1, l_2\rangle. \tag{3.115}$$

Bethe in 1931 suggested the following ansatz for the coefficients $a(\, l_1, l_2)$:

$$a(\, l_1, l_2) = A_{12}\; e^{\,i(\, k_1 l_1 + k_2 + l_2)} + A_{21}\; e^{\,i(\, k_1 l_2 + k_2 + l_1)} \tag{3.116}$$

Setting $A_{12} = A_{21}$ would lead to a direct superposition of magnons, however, as was mentioned above, it would be an overcompleted set of non-orthogonal and non-stationary states. The picture of the superimposed magnons is in an obvious conflict with the requirement that two flipped spins must be at different sites. The eigenvalue equation for the the wave-function (3.115) lead to the $\frac{N(N-1)}{2}$ equations for the coefficients $a(\, l_1, l_2)$. Here one have to distinguish two cases with two different equations: $l_2 > l_1 + 1$ and $l_2 = l_1 + 1$. Therefore, we have

$$\begin{aligned}
&\frac{J}{2}\left\{a(\, l_1+1, l_2) + a(\, l_1, l_2-1) + a(\, l_1-1, l_2) + a(\, l_1, l_2+1)\right\} + \\
&(E_0 - E_2 - 2J)\, a(\, l_1, l_2) = 0, \quad l_2 > l_1 + 1, \\
&\frac{J}{2}\left\{a(\, l_1-1, l_2) + a(\, l_1, l_2+1)\right\} + (E_0 - E_2 - J)\, a(\, l_1, l_2) = 0, \quad l_2 = l_1 + 1
\end{aligned} \tag{3.117}$$

Substituting Eq. (a(ll)) into the first relation of these equations (for $l_2 > l_1 + 1$) we find that it automatically satisfied by the plane waves (3.116) for arbitrary A_{12}, A_{21}, k_1 and k_2 providing the energy, E_2 depends on the quasi-momenta as follows

$$E_2 - E_0 = -J \sum_{j=1,2} (1 - \cos k_i)\,. \tag{3.118}$$

One can see, that in this case we deal with a superposition of two independent magnons. However, the second relation of the Eq. (3.117), which corresponds to the adjacent flipped spins are not automatically satisfied by the (3.116). But, if we substitute the second relation of Eq. (3.117) into the first one and then set $l_2 = l_1 + 1$ wefind N conditions equivalent to the second relation of the Eq. (3.116):

$$2a(\, l_1, l_1 + 1) = a(\, l_1, l_1) + a(\, l_1 + 1, l_1 + 1). \tag{3.119}$$

Then, we have to claim the solution in the form of the plane waves which is the solution of the eigenvalue equation for $l_2 > l_1 + 1$ satisfy also this relation. This yields the following equation for the amplitudes:

$$2\left(A_{12}e^{ik_2} + A_{21}e^{ik_1}\right) = (A_{12} + A_{21})\left(1 + e^{i(k_1+k_2)}\right). \tag{3.120}$$

Form which we get the ratio

$$\frac{A_{12}}{A_{21}} = -\frac{e^{i(k_1+k_1)} + 1 - 2e^{ik_1}}{e^{i(k_1+k_1)} + 1 - 2e^{ik_2}}. \tag{3.121}$$

It is easy to verify that this ratio is a pure phase:

$$\frac{A_{12}}{A_{21}} = e^{i\theta_{12}} = e^{-i\theta_{21}}. \tag{3.122}$$

Exercise *Prove that this is really the case.* Thus, this phase can be contributed in a symmetric way into the Bethe ansatz solution.

$$a(\ l_1, l_2) = e^{\,i\left(\ k_1 l_1 + k_2 + l_2 + \frac{1}{2}\theta_{12}\right)} + e^{\,i\left(\ k_1 l_2 + k_2 + l_1 + \frac{1}{2}\theta_{21}\right)} \tag{3.123}$$

Thus, the phase factor θ depends of the quasi-momenta k_1 and k_2 and has an obvious meaning of the scattering phase for two magnons. For the phase one can find more convenient expressions just modifying Eq. (3.121):

$$\cot\frac{\theta}{2} = i\frac{e^{i\theta}+1}{e^{i\theta}-1} = i\frac{e^{ik_2} - e^{ik_1}}{1 - e^{ik_1} - e^{ik_2} + e^{i(k_1+k_2)}} = \frac{\sin\left(\frac{k_1-k_2}{2}\right)}{\cos\left(\frac{k_1+k_2}{2}\right) - \cos\left(\frac{k_1-k_2}{2}\right)}. \tag{3.124}$$

Thus,

$$2\cot\frac{\theta_{12}}{2} = \cot\frac{k_1}{2} - \cot\frac{k_2}{2}. \tag{3.125}$$

The quasi-momenta of the Bethe ansatz wave function are not determined yet. It can be done by the imposing the periodic boundary conditions. Demanding the translational invariance of the wave function we have: $a(\ l_1, l_2 + N) = a(\ l_2, l_1)$. Therefore, we get

$$e^{iNk_1} = e^{i\theta_{12}}, \quad e^{iNk_1} = e^{-i\theta_{12}} = e^{i\theta_{21}}, \tag{3.126}$$

or

$$\begin{aligned} Nk_1 &= 2\pi I_1 + \theta(\ k_1, k_2) \\ Nk_2 &= 2\pi I_2 - \theta(\ k_1, k_2) \\ I_1, I_2 &\in \{0, 1, ..., N-1\}\,, \end{aligned} \tag{3.127}$$

here we introduce new notation, $\theta(\ k_1, k_2) \equiv \theta_{12}$ in order to emphasize explicit dependence of the phase on quasi-momenta. It is worth mentioning that the total momentum of this state is

$$k = k_1 + k_2 = \frac{2\pi}{N}\left(I_1 + I_2\right). \tag{3.128}$$

The magnons interaction is reflected in the phase shift θ and in the deviation of the momenta k_1, k_2 from the single (free) magnon wave numbers. This is because the magnons either scatter off each other or form bound states. Note that the momenta $k)1, k_2$ specify the

Bethe ansatz wave function (3.116), while the wave number k is the quantum number associated with the translational symmetry of the Hamiltonian and exists independently of the Bethe ansatz. The allowed (I_1, I_2) pairs are restricted to $0 \le I_1 \le I_2 \le N-1$. Switching I_1 with I_2 simply interchanges k_1 and k_2 and produces no new solution. There are $N(N+1)/2$ pairs that meet the ordering restriction, but only $N(N-1)/2$ of them yield a solution of Eqs. (3.125) and (3.127). The solutions can be determined analytically or computationally. Some of them have real k_1, k_2, and others yield complex conjugate momenta, $k_2 = k_1^*$. The complete spectrum of the $M = 2$ case can be figured out.

- C_1-class of states: one of the Bethe quantum numbers is zero, $I_1 = 0$, $I_2 = 0, 1, ...N-1$. One can show that the solution of the Bethe ansatz equation in this case are: $k_1 = 0$, $k_2 = \frac{2\pi n}{N}$, $n = 0, 1, ..., N-1$, $\theta = 0$. Thus, there are N states of this class.

- C_2-class of states: both I_1, I_2 are non-zero and differ by two or more, $I_2 - I_1 \ge 2$. There are $N(N-5)/1+3$ such pair of quantum numbers. All of them correspond to the real quasi-momenta, k_1 and k_2. To determinate this solution, one has to combine Eqs. (3.125), (3.127) and (3.128) into a single non-linear equation for k_1:

$$2\cot\frac{Nk_1}{2} = \cot\frac{k_1}{2} - \cot\frac{k-k_1}{2}. \tag{3.129}$$

  One has to fix the values of the N and $k = \frac{2\pi n}{N}$ and then find the solutions of this equation numerically. Though, there are several simple cases where the analytic solution is possible.

- C_3-class o f state: non-zero Bethe quantum numbers I_1, I_2 which either equal or differ by unity. There exist $2N-3$ such pairs but only $N-3$ of them are the solutions of (3.125) and (3.127). Most of these solutions are complex. In order to determine them, we suppose

$$k_1 = \frac{k}{2} + iv, \quad k_2 = \frac{k}{2} - iv, \quad \theta = \phi + i\chi. \tag{3.130}$$

  And then substituting this into the Eq. (3.125) we get

$$\cos\frac{k}{2}\sinh(Nv) = \sinh\left[(N-1)\,v\right] + \cos\phi\sinh v, \tag{3.131}$$

  where $\phi = \pi(I_2 - I_1)$, and $\chi = Nv$. It is sufficient to consider only positive v. The energy of any complex solution is

$$E_2 - E_0 = -2J\left(1 - \cosh v\ \cos\frac{k}{2}\right). \tag{3.132}$$

  The detailed analysis of the Eq. (3.131) shows that a complex solution exists for $I_1 = I_2$ if

$$I_1 + I_2 = 2, 4, ..., \frac{N}{2} - 2, \frac{3N}{2} + 2, ...2N-2. \tag{3.133}$$

For $I_2 - I_1 = 1$ a complex solution exists if

$$I_1 + I_2 = \mathcal{I}, \mathcal{I} + 2, ..., \frac{N}{2} - 1, \frac{3N}{2} + 3, ..., 2N - \mathcal{I} + 2, \qquad (3.134)$$

where $\mathcal{I} \approx \sqrt{N}/\pi$. In the case $I_2 - I_1 = 1$ there exists additional real solution

$$I_1 + I_2 = 3, 5, ...\mathcal{I} - 2, 2N - \mathcal{I} + 2, ..., 2N - 3. \qquad (3.135)$$

Thus, we have more $N - 4$ solutions in class C_3.

3.5 The Bethe ansatz

Generalizing the formalism which we have been constructed for the two-body problem to the case of general M we can formulate the solution of the eigenvalues problem for the Heisenberg chain Hamiltonian in terms of the Bethe ansatz. Let us look for the eigenvector in the form

$$|\Psi_M\rangle = \sum_{1 \le j_1 < ... < j_M \le N} a(j_1, ..., j_M) | j_1, ..., j_m\rangle \qquad (3.136)$$

The ansatz proposed by Bethe for the wave-functions is given by the following expression:

$$a(j_1, ..., j_M) = \sum_{P \in S_M} A(P) \exp \left\{ i \sum_{l=1}^{M} k_{P(l)} j_l \right\}, \qquad (3.137)$$

here the sum is going over the $M!$ elements of the M-dimensional symmetric group, S_M. Each element P_r corresponds to certain permutation of the indexes $\{j_l\}$:

$$P_r : \quad (1, ..., M) \mapsto (P(1), ..., P(M)). \qquad (3.138)$$

The periodicity condition for the coefficients $a(j_1, ..., j_M)$ reads

$$a(j_2, ..., j_M, j_1 + N) = a(j_1, j_2, ..., j_M). \qquad (3.139)$$

The eigenvalue problem for this state yields the following equation:

$$\sum_{\{j_k\}} a(j_1, ..., j_M) \left\{ \left(E_0 - \frac{JN_a}{2} \right) |j_1, ..., j_M\rangle + \frac{J}{2} \sum_{\{j'_k\}} |j'_1, ..., j'_M\rangle \right\} \qquad (3.140)$$
$$= E_M \sum_{\{j_k\}} a(j_1, ..., j_M) |j_1, ..., j_M\rangle,$$

where N_a is the number of the pairs of the antiparallel orientated spins in the configuration $|j_1, ..., j_M\rangle$, the summation in the second sum is going over all sets of site $\{j'_k\} = \{j'_1, ..., j'_M\}$ with can be obtained from the configuration $\{j_k\} = j_1, ..., j_M$ by changing of the numbers

j_k by one. The condition that the state (3.136) is an eigenstate of the Hamiltonian (3.99) is

$$\left(E_0 - E_M - \frac{JN_a}{2}\right) a(\,j_1, ..., j_M) + \frac{J}{2}\sum_{\{j'_k\}} a(\,j'_1, ..., j'_M) = 0. \tag{3.141}$$

Generalizing the results for the one and two flipped spins the eigenstate condition can be written in the following way. The coefficient of the eigenvector should satisfy the following functional equation, which can be obtained from (3.141) for the case when none of the numbers $\{j_k\}$ are adjacent $j_k \neq j_{k-1}+1$:

$$\begin{aligned}&(E_0 - E_M - JM)\, a(\,j_1, ..., j_M) \\ &+\frac{J}{2}\sum_{k=1}^{M}\{a(\,j_1, ..., j_k - 1, j_{k+1}, ..., j_M) + a(\,j_1, ..., j_k + 1, j_{k+1}, ..., j_M)\} = 0.\end{aligned} \tag{3.142}$$

Substituting the ansatz for the coefficient $a(\,j_1, ..., j_M)$ into this equations one can immediately make sure that it satisfies for arbitrary $A(P)$ and leads to the following spectrum:

$$E_M - E_0 = -J\sum_{j=1}^{M}(1-\cos k_j) \tag{3.143}$$

Then, considering various combinations of possible adjacent flipped spins, we can obtain the additional M equation to be satisfied by the function $a(\,j_1, ..., j_M)$,

$$\begin{aligned}&2a(\,j_1, ..., j_k, j_{k+1}, ..., j_M) = a(\,j_1, ..., j_k, j_k, ..., j_M) + a(\,j_1, ..., j_{k+1}, j_{k+1}, ..., j_M), \\ &k = 1, ..., M.\end{aligned} \tag{3.144}$$

Substituting in these equations the Bethe ansatz for the wave function we obtain the equation for the coefficients A in the following form:

$$\begin{aligned}&A(P)\left\{e^{i\left(k_{P(j)}+k_{P(j+1)}\right)} - 2e^{ik_{P(j+1)}} + 1\right\} \\ &+A(P\;P_{j,j+1})\left\{e^{i\left(k_{P(j)}+k_{P(j+1)}\right)} - 2e^{ik_{P(j)}} + 1\right\} = 0,\end{aligned} \tag{3.145}$$

where $P_{j,j+1}$ is just a transposition of j and $j+1$. Thus,

$$A(P)/A(PP_{j,j+1}) = e^{i\theta_{jl}} = -\frac{e^{i(k_j+k_l)} + 1 - 2e^{ik_j}}{e^{i(k_j+k_l)} + 1 - 2e^{ik_l}}. \tag{3.146}$$

and we, finally, get the expressions for the coefficients $A(P)$ in therm of the magnon scattering phases:

$$A(P) = \exp\left\{\frac{i}{2}\sum_{l<j}\theta_{P(l)P(j)}\right\}, \tag{3.147}$$

Exercise *Derive these equation in general form*
Where the scattering phases can be represented in a real form as follows:

$$\cot\frac{\theta_{jl}}{2} = \cot\frac{k_j}{2} - \cot\frac{k_l}{2}, \quad j,l = 1,...,M. \tag{3.148}$$

Eventually, one can write down the Bethe's wave function for the Heisenberg chain in the following form:

$$a(\, j_1,...,j_M) = \sum_{P\in\, S_M} \exp\left\{ i\sum_{l=1}^{M} k_{P(l)} j_l + \frac{i}{2}\sum_{l<l'} \theta_{P(l)P(l')} \right\}. \tag{3.149}$$

Exercise *Consider the case of 3 flipped spins $M = 3$ and perform all the evaluations explicitly*
Applying the boundary conditions we get the relation

$$\sum_{l=1}^{M} k_{P(l)} j_l + \frac{1}{2}\sum_{l<l'} \theta_{P(l)P(l')} = -2\pi I_{P'(M)} + \sum_{l=2}^{M} k_{P'(l-1)} j_l + k_{P'(M)}(j_1 + N), \tag{3.150}$$

where the permutations P and P' are connected to each other by $P'(i-1) = P(l)$, $l = 2,...,M$, $P'(M) = P(1)$. As can be seen, all term not involving the index $P'(M) = P(1)$ cancel and we get

$$\frac{1}{2}\sum_{l'} \theta_{P(1)P(l')} = \frac{1}{2}\sum_{l} \theta_{P'(l)P'(M)} - 2\pi I_{P'(M)} + N k_{P'(M)}, \tag{3.151}$$

or, finally, taking into account translational invariance, we can write down the same relation for arbitrary k_j:

$$\begin{aligned} N k_j &= 2\pi I_j + \sum_{l\neq j} \theta_{jl}, \quad j = 1,...,M, \\ I_j &\in \{0, 1, ..., N-1\}. \end{aligned} \tag{3.152}$$

3.6 Rapidities and String solutions

It is easy to see that the scattering phase does not depend on the difference of the quasi-momenta of the excitations. To have the results in a "translational invariant" way is it convenient to introduce the rapidities λ_j to parametrize the quasi-momenta:

$$\lambda_j = \cot\frac{k_j}{2}, \quad \theta_{jl} = 2\mathrm{arccot}\left(\frac{\lambda_j - \lambda_l}{2}\right), \tag{3.153}$$

or

$$\begin{aligned} k_j &= \frac{1}{i}\log\frac{\lambda_j + i}{\lambda_j - i}, \\ e^{i\theta_{jl}} &= \frac{\lambda_j - \lambda_l + 2i}{\lambda_j - \lambda_l - 2i}. \end{aligned} \tag{3.154}$$

Therefore, in terms of rapidities the Bethe ansatz equations (3.152) take the form

$$\left(\frac{\lambda_j + i}{\lambda_j - i}\right)^N = \prod_{l\neq j} \frac{\lambda_j - \lambda_l + 2i}{\lambda_j - \lambda_l - 2i}, \qquad j = 1, ...M. \tag{3.155}$$

And spectrum

$$E_M - E_0 = -2J \sum_{j=1}^{M} \frac{1}{\lambda_j^2 + 1}. \tag{3.156}$$

It turns out that some (actually, the majority of) states are characterized by complex rapidities. The Bethe ansatz equations do not allow the analytic treatment in general case, thus, one has to rely only on numerics. However, standard numerical algorithms to solve the these equations have problems in finding some of their complex solutions or have very low efficiency. Therefore, it is highly important to figure out the general structure of these complex rapidities to develop more appropriate ways to find them. Unfortunately, a complete understanding of this structure is still missing. But we have a fairly good account of what happens in the thermodynamic limit. This structure goes under the name of *string hypothesis*. Let us consider the simplest case with complex solutions, the $M = 2$ situation(two flipped spins). The Bethe equation in term of rapidities read

$$\begin{aligned} \left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^N &= \frac{\lambda_1 - \lambda_2 + 2i}{\lambda_1 - \lambda_2 - 2i}, \\ \left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^N &= \frac{\lambda_2 - \lambda_1 + 2i}{\lambda_2 - \lambda_1 - 2i}, \end{aligned} \tag{3.157}$$

As the total momentum of the state $k = k_1 + k_2 = \frac{1}{i} \log \left(\frac{\lambda_1 + i}{\lambda_1 - i} \frac{\lambda_2 + i}{\lambda_2 - i} \right)$ must be real we have an addition condition

$$\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^N \left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^N = 1. \tag{3.158}$$

Even in this simplest case where we deal only with two equations the complex solution is very difficult to find. However, the situation gets essentially simpler if we take the thermodynamic limit $N \to \infty$. In this limit the roots are organized in a simple structures, known as string hypothesis, as it is still not proven that the string solution we are about to describe exhaust the whole Hilbert space of the model. However, this is commonly believed to the true, at least to the point that the states missed do not contribute significantly to the thermodynamic of the model. As the LHS in Eqs. (3.157) will grow (or decrease) exponentially in N, therefore, in the thermodynamic limit the LHS is strictly zero or infinity and the RHS will have to do the same. Thus, we must have

$$\lambda_1 - \lambda_2 = \pm 2i, \tag{3.159}$$

or

$$\begin{aligned} \lambda_1 &= \lambda \pm i, \\ \lambda_2 &= \lambda \mp i. \end{aligned} \tag{3.160}$$

Let us write down the total momentum and energy, corresponding to these rapidities

$$k = k_1 + k_2 = \frac{1}{i}\log\frac{\lambda + 2i}{\lambda - 2i}, \quad \lambda = 2\cot k \tag{3.161}$$

$$E_2 - E_0 = -\frac{4J}{\lambda^2 + 4}, \tag{3.162}$$

or, substituting the expression for the total momentum of these state into the spectrum one can get the energy of thee excitation, which is obviously the bound state of two flipped spins:

$$E_2 - E_0 = -\frac{J}{2}(1 - \cos k) \tag{3.163}$$

It is turns out, that the energy of this bound state in the ferromagnetic regime ($J < 0$) lays bellow any other state with two flipped spins. Let us consider the upper and lower bonds of the state with two flipped spins and real solution, the scattering state of two magnons with the total momenta $k = k_1 + k_2$. In the thermodynamic limit all these state form a *two-magnon continuum* between these two curves(for negative J):

$$E_2 - E_0 = 2|J|\left(1 - \cos\frac{k}{2}\right), \tag{3.164}$$

$$E_2 - E_0 = 2|J|\left(1 + \cos\frac{k}{2}\right),$$

In the Fig.(2) one can see the corresponding plots. The one-magnon state dispersion is also presented for comparison, as the two-magnon scattering state when one of the quantum number equals to zero is degenerate with the one-magnon state. For $M > 2$ more possible complex solutions can be appear. They can be described in the similar way. They are usually called **Bethe complexes** or **Bethe strings**. The μ-string or the string of the length μ is the set of $2\mu + 1$ rapidities characterized by the same value of the of the real part λ_μ and different but equidistant imaginary parts. Here μ can be integer or half-integer and the stirng solution has the following form:

$$\lambda_{\mu,m} = \lambda_\mu + 2im, \quad -\mu < m < \mu. \tag{3.165}$$

Let us denote the total number of the μ-stings by ν_μ. Then, for a given number of flipped spins we have

$$M = \sum_\mu (2\mu + 1)\,\nu_\mu. \tag{3.166}$$

It is important to notice that the existence and structure of the string solution is strictly valid only in the thermodynamic limit $N \to \infty$ and as long as the number and length of the strings is not comparable to N. The fact that the complexes that we described are sufficient to exhaust the whole Hilbert space is not a proven fact and goes under the name of **string hypothesis**. For finite system sizes significant deviations from the string hypothesis are known to exist and have been observed even for very (very) large systems. When the number

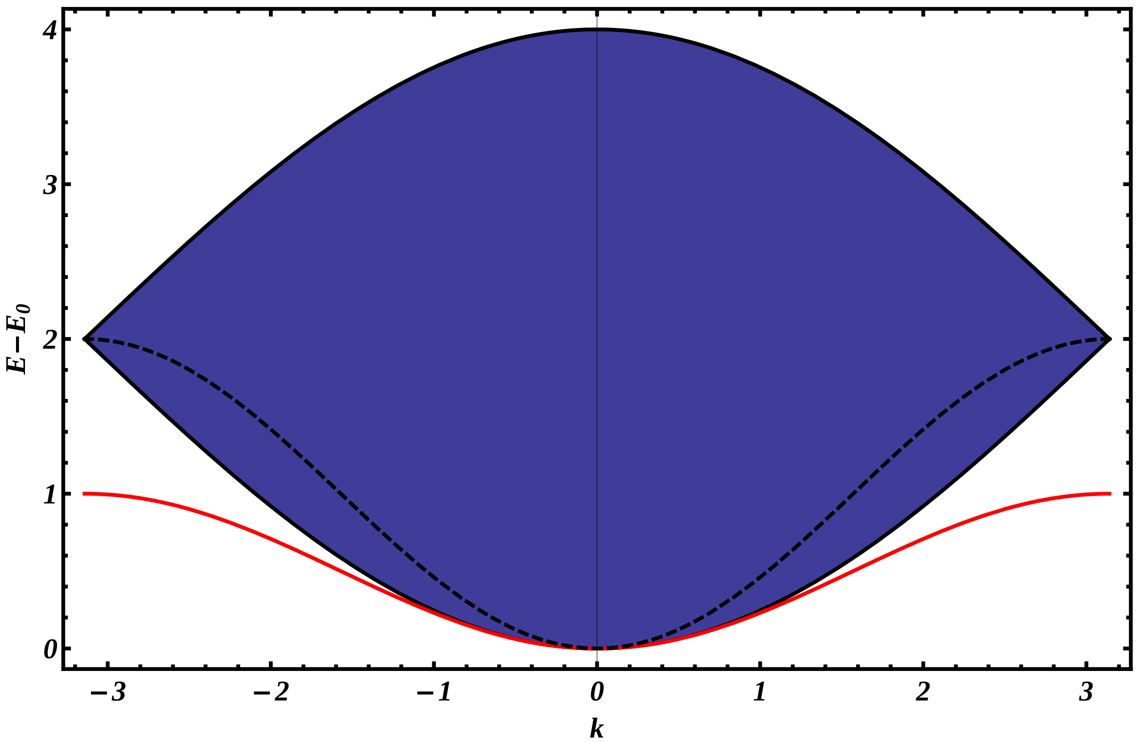

Figure 2: The comparison of the two-magnon continuum(blue region) and the the bound state (red curve) in the thermodynamic limit $N \to \infty$ for the ferromagnetic ($J < 0$) XXX-chain. For the finite chain the allowed two-magnon scattering states form a lattice inside the blue region. The one-magnon disperion curve(black dashed) is presented as well. It lays inside the two-magnon continuum, as the two-magnon scattering states when one of the quantum numbers is zero is degenerate with the one-magnon state.

of strings becomes comparable with N, additional solution that cannot classified within the given structure could arise, but they are believed to be too few to contribute significantly to the thermodynamic of the model. Let us therefore study a bit more carefully these string solutions. The first thing to notice is that the rapidities belonging to a complex can be grouped together and treated as a single entity. In fact, all the interactions of individual rapidities can be factorized and summed over separately in the interactions between the complexes. The energy and momentum of a μ-complex can be obtained by summing over all rapidities in the complex:

$$k_\mu(\lambda_\mu) = \frac{1}{i} \log \frac{\lambda_\mu + i(2\mu+1)}{\lambda_\mu - i(2\mu+1)}, \tag{3.167}$$

$$E_\mu - E_0 = \frac{-2J(2\mu+1)}{\lambda_\mu^2 + (2\mu+1)^2} = \frac{-J}{2\mu+1}\left(1 - \cos k_\mu\right). \tag{3.168}$$

Exercise *Derive these relations.*

3.7 Antiferromagnetic ground state. The Hulthén Integral Equation

Let us now figure out some physical properties of the ground state of the Heisenberg chain for antiferromagnetic regime ($J > 0$). The progress in this issue was achieved by Hulthén in 1938. First of all, as was mentioned above, for the ferromagnetic case ($J < 0$) the reference state of the coordinate Bethe ansatz technique is the real ground state. Of cause, it is degenerate with the zero-momentum one-magnon eacitations, but the excited state can be constructed in terms of magnons and strings, the bound stated of magnon, over the magnon vacuum, $|\,0\rangle = |\uparrow\uparrow ... \uparrow\rangle$. However, for the antiferromagnetic case the situation is crucially different. Let us mention the classical antiferromagnetic state which is just the alternation of parallel and antiparallel spins to the z-axis. The corresponding quantum analog is called the **Néel state**, $|\uparrow\downarrow\uparrow\downarrow ... \downarrow\rangle$, is obviously not an eigenstate of the Heisenberg chain Hamiltonian, but it is a basis state. The true ground state of the antiferromagnetic Heisenberg chain will not be orthogonal to the Néel state since it is the state with $S^z_{tot} = 0$, this means that in the ground state we will have the half of all spins flipped, $M = N/2$. Thus, the corresponding equations we need to solve for the determination of the antiferromagnetic ground state are

$$\begin{aligned} &k_j = \frac{2\pi}{N} I_j + \frac{1}{N}\sum_{l\neq j}\theta_{j\,l}, \\ &2\cot\frac{\theta_{j\,l}}{2} = \cot\frac{k_j}{2} - \cot\frac{k_l}{2}, \\ &j = 1, ...N/2. \end{aligned} \tag{3.169}$$

As we know, the complex values of the rapidities correspond to the spin complexes in which, roughly speaking, the probability for the neighboring spins to point in the same direction in very high. However, in the antiferromagnetic case these configuration will have higher energies. Therefore, the Bethe string of the length more than 1 is very unfavorable. Thus, for the quantum numbers one will have situation with all I_j are different, real and $|I_j - I_l| \geq 2$ for all j, l. There are two possibilities

$$\begin{aligned} &\{I_j\} = \{0, 2, 4, ..., N-2\}, \\ &\{I_j\} = \{1, 3, 5, ..., N-1\}, \end{aligned} \tag{3.170}$$

obviously, $I_j + N$ is equivalent to I_j. The first of these has$I_1 = 0$ and it can be shown that this gives a state in which $S_{tot} = 1$ with $S^z_{tot} = 0$, while the second choice gives a state with $S_{tot} = 0$ and $S^z_{tot} = 0$. The second of these is the correct one since the first is degenerate with other states with $S_{tot} = 1$ and $S^z_{tot} = \pm 1$ which lie higher in energy. We see that the distribution of the quantum number in the interval $[0, N]$ is uniform. So, let us introduce a new variable

$$x_j = \frac{2j-1}{N} = \frac{I_j}{N} \tag{3.171}$$

This variable become continuous in the limit $N \to \infty$ and take values in the interval $(0, 1)$. Likewise we can regard the momenta as a continuous functions. Thus,

$$x_j \to x, \quad k_j \to k(x), \quad k_l \to k(y), \quad x, y \in (0, 1). \tag{3.172}$$

Thus, the equation for the scattering phases becomes

$$2\cot\frac{\theta(x,y)}{2} = \cot\frac{k(x)}{2} - \cot\frac{k(y)}{2}. \tag{3.173}$$

The function θ is restricted to lie in the interval $(-\pi, \pi)$. The equation for the momenta becomes an integral equation

$$k(x) = 2\pi x + \frac{1}{2}\int_0^1 \theta(x,y)\, dy, \tag{3.174}$$

The factor 1/2 appears here because

$$\Delta y = \frac{2(i+2)-1}{N} - \frac{2i-1}{N} = \frac{2}{N}. \tag{3.175}$$

When $x = y$, $\cot\frac{\theta(x,y)}{2} = 0$, so $\theta = \pm\pi$ and at this points the value of the θ jumps from $-\pi$ to π. Therefore, it is convenient to divide the integral in two sections:

$$k(x) = 2\pi x + \frac{1}{2}\int_0^x \theta(x,y)\, dy + \frac{1}{2}\int_x^1 \theta(x,y)\, dy. \tag{3.176}$$

Now differentiate this equation with respect to x

$$\begin{aligned} \frac{dk}{dx} &= 2\pi + \frac{1}{2}\left\{\theta(x,y)|_{y\to x^-} - \theta(x,y)|_{y\to x^+}\right\} + \frac{1}{2}\int_0^x \frac{\partial\theta}{\partial x}dy + \frac{1}{2}\int_x^1 \frac{\partial\theta}{\partial x}dy \\ &= \pi + \frac{1}{2}\int_0^1 \frac{\partial\theta}{\partial x}dy, \end{aligned} \tag{3.177}$$

as

$$\begin{aligned} \theta(x,y)|_{y\to x^-} &= -\pi, \\ \theta(x,y)|_{y\to x^+} &= \pi. \end{aligned} \tag{3.178}$$

Then, we introduce the functions

$$\begin{aligned} \xi(x) &= \cot\frac{k(x)}{2}, \quad \eta(y) = \cot\frac{k(y)}{2}, \\ f(\xi) &= -\frac{dx}{d\xi}, \quad f(\eta) = -\frac{dy}{d\eta}. \end{aligned} \tag{3.179}$$

and remember also that

$$\theta = 2\cot^{-1}\left\{\frac{\xi-\eta}{2}\right\}, \tag{3.180}$$

we can calculate

$$\begin{aligned} \frac{dk}{dx} &= \frac{dk}{d\xi}\frac{d\xi}{dx} = -\frac{1}{f(\xi)}\frac{dk}{d\xi} = \frac{1}{f(\xi)}\frac{2}{1+\xi^2}, \\ \frac{\partial\theta}{\partial x} &= \frac{\partial\theta}{\partial\xi}\frac{d\xi}{dx} = -\frac{1}{f(\xi)}\frac{\partial\theta}{d\xi} = \frac{1}{f(\xi)}\frac{1}{1+\frac{1}{4}(\xi-\eta)^2}, \\ dy &= \frac{dy}{d\eta}d\eta = -f(\eta)d\eta. \end{aligned} \tag{3.181}$$

Substituting these results into the integral equation we get

$$\frac{1}{f(\xi)}\frac{2}{1+\xi^2} = \pi - \frac{1}{2f(\xi)}\int \frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2} \tag{3.182}$$

This is now an integral over η instead of y. As y goes from 0 to 1, $k(y)$ goes from 0 to 2π (not proved here but can be shown from Eq. (3.174)) so $\cot\frac{k(y)}{2}$ goes from $+\infty$ to $-\infty$ Therefore

$$\frac{1}{f(\xi)}\frac{2}{1+\xi^2} = \pi + \frac{1}{2f(\xi)}\int_{-\infty}^{\infty} \frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2} \tag{3.183}$$

And finally we can obtain the fundamental integral equation for the function $f(\xi)$,

$$f(\xi) = \frac{2}{\pi(1+\xi^2)} - \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2} \tag{3.184}$$

Now, we have to solve this integral equation. As we deal here with a linear integral equation it can be solved by Fourier transform. Defining

$$F(q) = \int_{-\infty}^{\infty} e^{iq\xi} f(\xi)d\xi, \quad f(\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\xi}F(q)dq,$$

Then, the fundamental integral equation becomes

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\xi}F(q)dq = \frac{2}{\pi(1+\xi^2)} - \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\eta}F(q)dq\right)\frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2}. \tag{3.185}$$

Now, we can implement the integration over η in the r.h.s. To do so, we have to make a substitution $z = \frac{1}{2}(\xi-\eta)$. Then

$$\begin{aligned} \text{r.h.s} &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} F(q)dq \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-iq\eta}d\eta}{1+\frac{1}{4}(\xi-\eta)^2} && (3.186)\\ &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} F(q)dq\frac{1}{2\pi}2e^{-iq\xi}\int_{-\infty}^{\infty}\frac{e^{2iqz}dz}{1+z^2} \\ &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} F(q)dq\frac{1}{2\pi}2e^{-iq\xi}\pi e^{-2q}. && (3.187)\end{aligned}$$

Thus,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\xi}F(q)dq = \frac{2}{\pi(1+\xi^2)} - \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\xi}e^{-2q}F(q)dq. \tag{3.188}$$

Integrating both site by ξ from $-\infty$ to ∞ with the function $e^{ip\xi}$ we get

$$F(p) = \frac{2}{\pi}\int_{-\infty}^{\infty}\frac{e^{ip\xi}d\xi}{1+\xi^2} - e^{-2p}F(p), \tag{3.189}$$

or

$$(1+e^{-2p})F(p) = \frac{2}{\pi}\pi e^{-p}$$

thus

$$F(q) = \frac{1}{\cosh q}.$$

And finally we get

$$f(\xi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-iq\xi}}{\cosh q} = \frac{1}{2\cosh\left(\frac{\pi\xi}{2}\right)}.$$

Now we are in a position to calculate the ground state energy for the infinite antiferromagnetic Heisenberg chain. As, the spectrum for the finite chain with N site is given by

$$E_{GS} - E_0 = -J \sum_j (1 - \cos k_j)$$

in the limit $N \to \infty$ we have to transform the sum into the integral according to

$$k_j \to k(x), \quad \sum_{j=1}^{N/2} \to \frac{N}{2} \int_0^1 dx$$

Let us represent the spectrum as an integral over the function $f(\xi)$.

$$1 - \cos k(x) = 2\sin^2 \frac{k(x)}{2} = \frac{2}{1 + \cot^2 \frac{k(x)}{2}} = \frac{2}{1 + \xi^2} \tag{3.190}$$

$$dx = \frac{dx}{d\xi} d\xi = -f(\xi) d\xi \tag{3.191}$$

Then,

$$\begin{aligned} E_{GS} - E_0 &= -\frac{JN}{2} \int_{-\infty}^{\infty} \frac{2f(\xi)d\xi}{1+\xi^2} = -JN \int_{-\infty}^{\infty} \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iq\xi} F(q) dq \right\} \frac{d\xi}{1+\xi^2} \\ &= -\frac{JN}{2} \int_{-\infty}^{\infty} F(q) e^{-|q|} dq = -2JN \int_0^{\infty} \frac{e^{-q}}{e^q + e^{-q}} dq = -JN \log 2 \end{aligned} \tag{3.192}$$

Here and above we used the following integrals:

$$\int_{-\infty}^{\infty} \frac{e^{\pm iq\xi} d\xi}{1 + \xi^2} = \pi e^{-|q|}.$$

Thus,

$$E_{GS} = -JN \log 2 + \frac{JN}{4}$$

This is the famous result of Hulthén and the first example of the real physical application of the Bethe ansatz. The numerical estimation gives

$$\frac{E_{GS}}{JN} = -0.443147$$

3.8 Antiferromagnetic Excitations. Spinons

As was shown above, the ground state of the antiferromagnetic Heisenberg chain is made up of a linear combination of the of basis states with exactly half the spin reversed, $M = N/2$. Let us now investigate the issue of the elementary excitations over the antiferromagnetic ground state. In contrast to the ferromagnetic case, where the deviations from the ground state (all spins are aligned) can be just in the way of lowering the S^z_{tot}, here both directions are possible. Thus, the low-lying excitation has $N/2 \pm 1$ spins reversed. That is why the picture of the low-lying excitation in the antiferromagnetic case is more complicated. And even for the simplest case the derivation demands much more effort. The lowest-lying excited states (the elementary excitations) have $S_{tot} = 1$ and $S^z_{tot} = 0, \pm 1$. Let us recall that within the subspace $S^z_{tot} = 1$ the lowest-lying states belongs to class C_2: all quantum number are real and differ by 2 or more. The partly all completely bounded states lie higher in energy. As for a state with $S^z_{tot} = 1$ one should have $N/2 - 1$ deviations from the fully polarized state, we have to deal with the $N/2 - 1$ values of momenta k_j and hence the quantum numbers I_j. Let us recall the quantum numbers of the antiferromagnetic ground state

$$\{I_j\} = \{1, 3, 5, ..., N-3, N-1\}.$$

Now we have to specify all variants of extracting one number from this sequence.

- The one number can be extracted from the middle giving rise to a gap of size 4:

  $$\{I_j\} = \{1, 3, 5..., L, L+4, L+6, ..., N-3, N-1\} \tag{3.193}$$

  where L is an odd number. Here, the quantum number $L+2$ are extracted.

- It is also possible to have two gaps of size 3:

  $$\{I_j\} = \{1, 3, 5..., L_1, L_1+3, L_1+5, ..., L_2, L_2+3, L_2+5, ..., N-3, N-1\}, \tag{3.194}$$

  here L_1 is an odd number and $L_2 \geq L1 + 3$ is an even number.

- There are two possibilities to have gap at the beginning:

  $$\begin{aligned} \{I_j\} &= \{3, 5, 7, ..., N-3, N-1\} \\ \{I_j\} &= \{2, 4, 6, ..., L, L+3, L+5, ..., N-3, N-1\} \end{aligned} \tag{3.195}$$

  L is an even number.

- The similar gaps can be at the end:

  $$\begin{aligned} \{I_j\} &= \{1, 3, 5, ..., N-5, N-3\} \\ \{I_j\} &= \{1, 3, 5, ..., L, L+3, L+5, ..., N-4, N-2\} \end{aligned} \tag{3.196}$$

As one can see all these possibilities lead to a huge number of excited states. They form a continuum in the limit $N \to \infty$. Now the problem is to define the lowest state for a given total momentum k. Des Cloiseaux and Pearson in 1962 investigating the finite chain numerically, found out that for $-\pi < k < 0$ the second line of Eq. (**??**) corresponds to the lowest energy, while for $0 < k < \pi$ the correct choice is second line of Eq. (3.196). Let us construct the lowest energy excitation for the case $-\pi < k < 0$. It is convenient to work in the $S^z_{tot} = 0$ subspace. The state with $S_{tot} = 1$ and $S^z_{tot} = 0$ has additional $I = 0$, corresponding to additional extra $k_j = 0$. So, let us write down the corresponding set of the quantum numbers

$$\{I_j\} = \{0, 2, 4, 6, ..., 2n, 2n+3, ..., N-3, N-1\} \tag{3.197}$$

Here we denoted L by $2n$ for convenience. As usual, the total momentum is

$$k = \frac{2\pi}{N}\sum_{j=1}^{N/2} I_j = \frac{2\pi}{N}\left(\frac{N^2}{4} - n\right) = -\frac{2\pi n}{N} \mod 2\pi \tag{3.198}$$

Here, we suppose that N is a multiple of 4, but as we are going to take the limit $N\infty$, it is not a significant restriction. We also used the formula of the arithmetic sum, $1 + 3 + 5 + ... + (N-3) + (N-1) = \frac{N^2}{4}$ and the fact that in the sum of all quantum numbers form Eq. (3.197) the first n terms are reduced by 1 with respect this series. The further derivation is very similar to that we have done in the previous section. First of all we can express n as

$$n = \frac{|k|N}{2\pi} \tag{3.199}$$

Now we are going to pass to the continuum limit regarding $x_j = \frac{2j-1}{N}$ as a continuous variable in the limit $N \to \infty$. The only one difference in that now $x_j \neq I_j/N$ as the quantum numbers are not evenly spaced anymore. Instead, we have

$$\begin{aligned} I_j &= \frac{2j-2}{N} = \frac{x_j}{N} - \frac{1}{N}, \quad j \leq n \\ I_j &= \frac{2j-1}{N} = \frac{x_j}{N}, \quad j > n. \end{aligned} \tag{3.200}$$

Thus, one can define the function of x instead of x in the following way

$$I(x) = x - \frac{1}{N}\Theta\left(\frac{|k|}{\pi} - x\right), \tag{3.201}$$

where $\Theta(x)$ is the step function. Now the calculations are very similar to those for the antiferromagnetic ground state with the only one difference in the definition of the function $I(x)$. Thus, the continuous variant of the equation for the spectrum lead to the following relation:

$$k(x) = 2\pi\left(x - \frac{1}{N}\Theta\left(\frac{|k|}{\pi} - x\right)\right) + \frac{1}{2}\int_0^x \theta(x,y)\, dy + \frac{1}{2}\int_x^1 \theta(x,y)\, dy. \tag{3.202}$$

Then, taking the derivative with respect to x we have

$$\frac{dk}{dx} = \pi + \frac{2\pi}{N}\delta(x_0 - x) + \frac{1}{2}\int_0^1 \frac{\partial\theta}{\partial x} dy, \tag{3.203}$$

here we used $\frac{d}{dx}\Theta(\frac{|k|}{\pi}-x) = -\delta(\frac{|k|}{\pi}-x)$ and put $x_0 = \frac{|k|}{\pi}$. Now, making the same change of variables like in the previous section and taking into account that $\delta(x_0 - x) = \delta(\xi_0 - \xi)\frac{d\xi}{dx} = -\frac{1}{f(\xi)}\delta(\xi_0 - \xi) = \frac{1}{f(\xi)}\delta(\xi - \xi_0)$ we get

$$\frac{2}{1+\xi^2}\frac{1}{f(\xi)} = \pi + \frac{2\pi}{Nf(\xi)}\delta(\xi-\xi_0) - \frac{1}{2f(\xi)}\int_{-\infty}^{\infty}\frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2}, \tag{3.204}$$

which yields the following modification of the fundamental integral equation from the previous section:

$$f(\xi) = \frac{2}{\pi(1+\xi^2)} + \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2} - \frac{2}{N}\delta(\xi-\xi_0). \tag{3.205}$$

Thus, the only difference form the equation, describing antiferromagnetic ground state is the additional delta-function type driving term in the integral equation. This delta-function comes ut from the choice of the sequence of the quantum numbers I_j. Using the same method as in the previous section we get the equation

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\xi}F(q)dq = \frac{2}{\pi(1+\xi^2)} - \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iq\xi}e^{-2q}F(q)dq - \frac{2}{N}\delta(\xi-\xi_0). \tag{3.206}$$

Multiplying both sides by $e^{ip\xi}$ and integrating by ξ from $-\infty$ to ∞ we obtain

$$F(p) = \frac{2}{\pi}\int_{-\infty}^{\infty}\frac{e^{ip\xi}d\xi}{1+\xi^2} - F(p)e^{-2p} - \frac{2}{N}e^{ip\xi_0} \tag{3.207}$$

or

$$(1+e^{-2p})F(p) = \frac{2}{\pi}\pi e^{-p} - \frac{2}{N}e^{ip\xi_0}. \tag{3.208}$$

And finally,

$$F(p) = \frac{1}{\cosh p} - \frac{2e^{ip\xi_0}}{N(1+e^{-2p})}. \tag{3.209}$$

Now, we ahve to substitute the solution of the integral equation into the continuous limit of the expression for the energy of the excited state.

$$\begin{aligned} E_1 - E_0 &= -\frac{JN}{2}\int_{-\infty}^{\infty}\frac{2f(\xi)d\xi}{1+\xi^2} && (3.210)\\ &= -2JN\int_{-\infty}^{\infty}\frac{e^{-q}}{e^q+e^{-q}}dq + J\int_{-\infty}^{\infty}\frac{e^{-|q|}e^{iq\xi_0}}{1+e^{-2q}}dq \\ &= -JN\log 2 + \frac{J\pi}{2\cosh\left(\frac{\pi\xi_0}{2}\right)}. && (3.211)\end{aligned}$$

The first term here is the antiferromagnetic ground state energy, thus, the second one in the energy of the excitations above the ground state. Now we have to relate the parameter

ξ_0 to the momentum of the excitation k. To do so let us recall the definition of the function $f(\xi)$

$$f(\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(q)e^{-iq\xi}dq = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{\cosh q}e^{-iq\xi}dq - \frac{1}{\pi N}\int_{-\infty}^{\infty}\frac{e^{iq\xi_0}}{1+e^{-2q}}e^{-iq\xi}dq,$$
$$-\frac{dx}{d\xi} = f(\xi) \tag{3.212}$$

This expression differs form that for the ground state just by the term of order $1/N$. We can neglect it and recover the relation from the previous section

$$f(\xi) = \frac{1}{2\cosh\left(\frac{\pi\xi}{2}\right)}. \tag{3.213}$$

Then, as $\xi = \cot\frac{k(x)}{2}$ we have $\xi = \infty$ when $x = 0, k(x) = 0$, thus

$$\int_0^{x_0} dx = -\int_{\infty}^{\xi_0} f(\xi)d\xi = -\int_{\infty}^{\xi_0}\frac{d\xi}{2\cosh\left(\frac{\pi\xi}{2}\right)} = -\frac{2}{\pi}\arctan e^{\frac{\pi\xi}{2}}\,|_{\infty}^{\xi_0}\,. \tag{3.214}$$

Thus,

$$\frac{|k|}{\pi} \equiv x_0 = 1 - \frac{2}{\pi}\arctan e^{\frac{\pi\xi_0}{2}} \tag{3.215}$$

or

$$e^{\frac{\pi\xi_0}{2}} = \cot\frac{|k|}{2} = |\cot\frac{k}{2}| \tag{3.216}$$
$$\frac{1}{2\cosh\left(\frac{\pi\xi}{2}\right)} = \frac{1}{|\tan\frac{k}{2}| + |\cot\frac{k}{2}|} = \frac{1}{2}|\sin k| \tag{3.217}$$

Finally we have

$$E_1 - E_0 = -JN\log 2 + \frac{J\pi}{2}|\sin k| \tag{3.218}$$

This is the exact result obtained by Des Cloizeaux and Pearson for the energy of the antiferromagnetic spin-waves or magnons in the spin-1/2 chain with isotropic Heisenberg exchange. Let us remind the reader that this dispersion corresponds to the specific choice of the set of quantum numbers $\{I_j\}$, corresponding to the law lying excitation above the antiferromagnetic ground state in the thermodynamic limit, and for $-\pi < k < 0$. It can be shown that for the positive values of k within the Brillouin zone the similar calculations give the same result. Thus, for the whole Brillouin zone we have the same dispersion relation (3.218). It is also possible to chose another set of quantum numbers $\{I_j\}$ corresponding to $N/2 - 1$ deviations from the totally aligned state and belonging to the same class of the solution of the Bethe ansatz equations. But Des Cloizeaux and Pearson numerically proved that all other other state are higher in energies and they compose a continuum bounded form above by the function(See Fig. 3)

$$E_1^{max} - E_0 + JN\log 2 = J\pi|\sin\frac{k}{2}|. \tag{3.219}$$

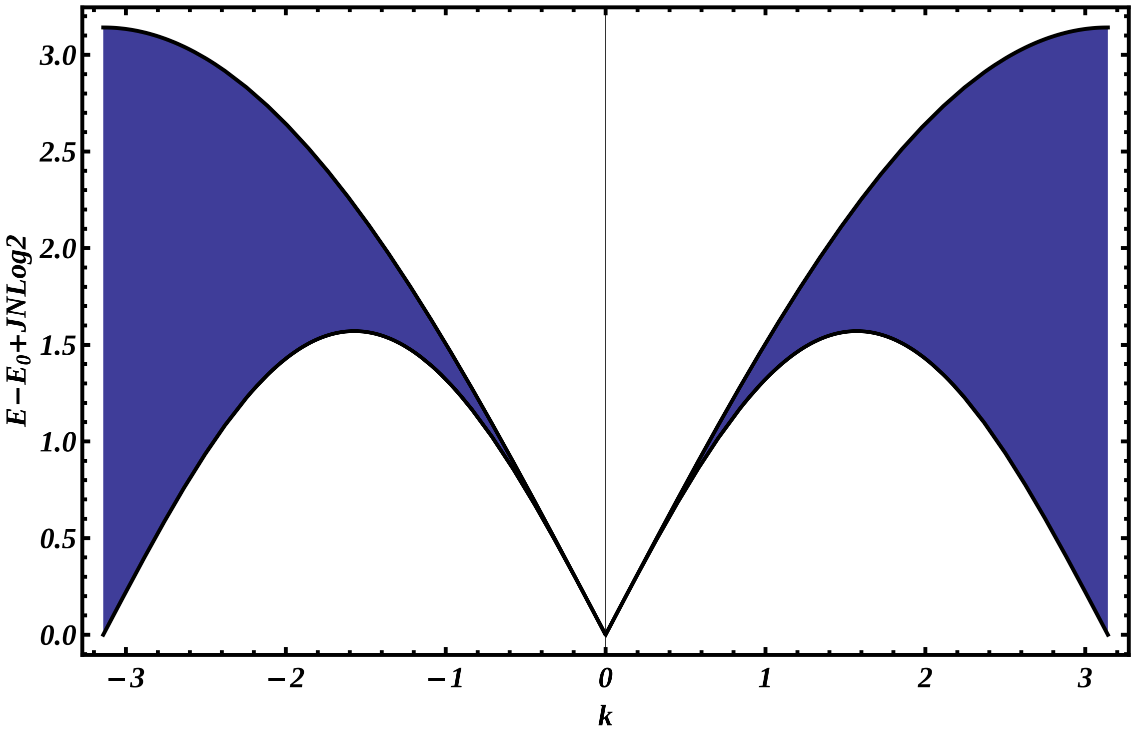

Figure 3: Elementary excitation energies in a spin-1/2 chain with antiferromagnetic isotropic Heisenberg exchange. The blue region corresponds to the continuum of states. The states on the lower boundary are the antiferromagnetic spin waves.

In is worth mentioning that there are numerous states which are not the pure independent antiferromagnetic magnons but have one or more bound multiplets and which lie in general at higher energy. Nevertheless the des Cloizeaux and Pearson result is extremely important and in fact the response to a probe, for example by neutron scattering, is strongest at this lower boundary. There is one important and unusual feature of the antiferromagnetic magnons in Heisenberg chain. In 1981 Faddeev and Takhtajan argued that the spin of the antiferromagnetic spin wave in the Heisenberg chain is rather 1/2 that 1. Their argumentation was based of the calculation of the number of free parameters for the configurations, i.e. the solution of the Bethe ansatz equations corresponding to the low-lying excitations found by des Cloizeaux and Pearson. Thus, it turned out that only the one-particle excitations above the antiferromagnetic ground state is a doublet od spin-1/2 spin waves with the dispersion

$$\frac{J\pi}{2}\sin k, \quad 0 \leq k \leq 0. \tag{3.220}$$

This excitation is a kink rather that an ordinary quasi-particle. All eigenstates of the Hamiltonian contain an even number of kinks and the quasi-momentum of an individual link runs through the half of the Brillouin zone. This particle with spin-1/2 form which the antiferromagnetic spin wave "consist" is called **spinon**.

4 The XXZ-chain

4.1 Introduction

Now we are going to consider the model, describing by the following Hamiltonian:

$$\mathcal{H}_{XXZ} = J\sum_{j=1}^{N}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right) - B\sum_{j=1}^{N} S_j^z. \quad (4.221)$$

As usual, we suppose the periodic boundary conditions, $S_{j+N}^{\alpha} = S_j^{\alpha}$. The model is usually called **XXZ-chain**. The anisotropy parameter, Δ makes the model different form the isotropic Heisenberg chain considered in the previous section. The Hamiltonian of , $\Delta = 1$ corresponds to the isotropic case. The physical origin of the anisotropy lays in the influence of the ligand filed (crystal field) on the exchange interaction which breaks the symmetry of the interaction from SO(3) to SO(2). The parameter J set only the energy scale and only its sign really matters. One can distinguish antiferromagnetic ($J > 0$) and ferromagnetic ($J < 0$) regimes in the $x - y$ plane. The parameter Δ is responsible for the strength and nature of the uniaxial anisotropy. One can distinguish planar($|\Delta| > 1$) and axial ($|\Delta| < 1$) regimes of the anisotropy. For instance, for the $|\Delta| > 1$ and $J\Delta < 1$ the system exhibits a ferromagnetic ordering along the z-axis, while for the case $J\Delta > 1$ we will have a z-axis antiferromagnet. Thus, usually one can speak about **planar** and **axial** regimes of the XXZ-chain. The zero-temperature ground state phase diagram of the $S = 1/2$ XXZ-chain in a magnetic filed, thus, consist of three regions: ferromagnetic, fully polarized ground state; gapless Luttinger liquid ground state and Neèl or antiferromagnetic ground state(See Fig. (4)). The quantum phase transition line between gapless Luttinger liquid phase and polarized phase and between Luttinger liquid phase and Neèl phase are given by the following equations:

$$\begin{aligned} B/J &= 1 + \Delta, \\ B/J &= \sinh\eta \sum_{k=-\infty}^{\infty} \frac{(-1)^k}{\cosh(k\,\eta)}, \\ \eta &= \cosh\Delta. \end{aligned} \quad (4.222)$$

It is easy to see that the ground state phase diagram of the XXZ-chain also has several interesting points: $\Delta = 0$, corresponding to the limit of the XX-chain considered above and which can be represented as a system of non-interacting spinless fermions; $\Delta \to \pm\infty$, corresponding to the classical Ising model limit:

$$\mathcal{H}_{Ising} = J\sum_{j=1}^{N} S_j^z S_{j+1}^z - B\sum_{j=1}^{N} S_j^z. \quad (4.223)$$

This simplest model of the interacting spin chains is indeed a classical one, as the operators S_j^z are diagonal and one can replace them by their eigenvalues and consider them as just classical variables takin values $\pm 1/2$. Any eigenvector of the Ising Hamiltonian is just a direc product of the spin-up and spin-down states on each site, which excludes any possibility of quantum correlations.

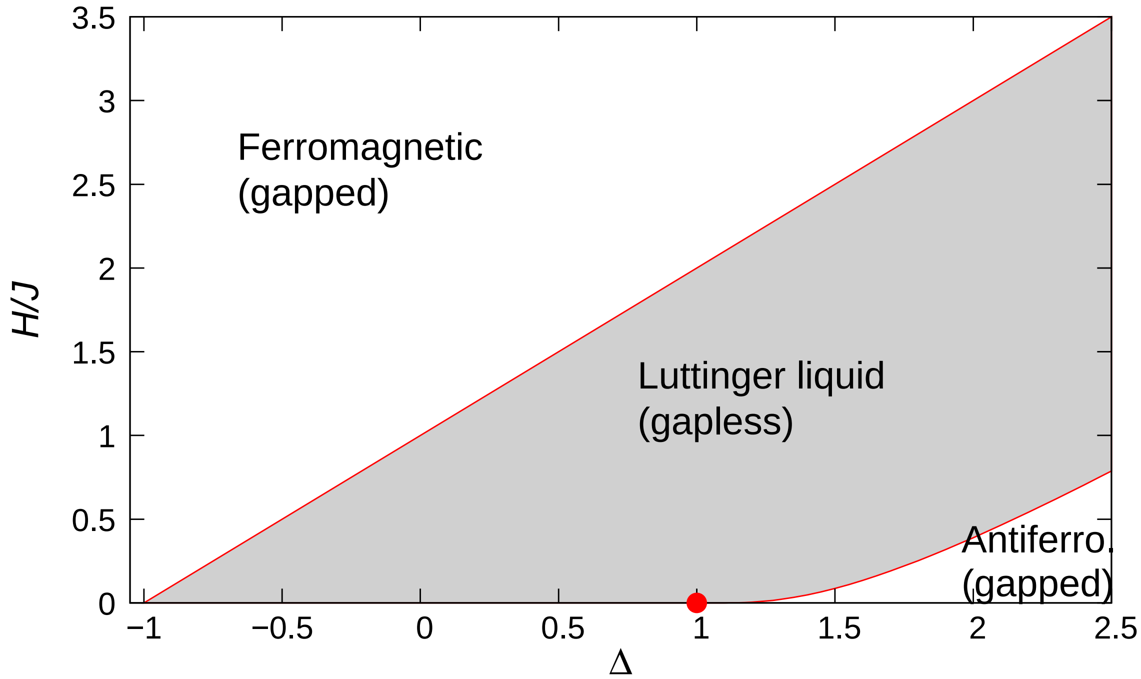

Figure 4: Zero-temperature phase diagram of the spin- 1/2 XXZ chain in a magnetic field.

4.2 Coordinate Bethe ansatz solution

As in the case of isotropic Heisenberg chain, here we the z-projection of the total spin is a conserved quantity:

$$S^z_{tot} = \sum_{j=1}^{N} S^z_j, \qquad [\mathcal{H}_{XXZ}, S^z_{tot}] = 0. \tag{4.224}$$

Thus, here the any eigenstate contains the fixed number of spins pointing up. So, we are going to play the same game as in the case of Bethe ansatz solution of the Heisenberg chain. First of all let us define the reference state, which is the **highest weight state** defined by

$$S^+_j|0\rangle = 0., \quad j = 1, ..., N \tag{4.225}$$

Obviously,

$$|0\rangle = |\uparrow\uparrow\uparrow ... \uparrow\rangle. \tag{4.226}$$

The corresponding eigenvalue, the energy of the reference state is

$$E_0 = \left(\frac{J\Delta}{4} - \frac{B}{2}\right) N. \tag{4.227}$$

This is the unique state with $S^z_{tot} = N/2$. It is the true vacuum or the ground state for the ferromagnetic regime. Then, we have the simplest one-particle states with $S^z_{tot} = N/2 - 1$:

$$|\Psi_1\rangle = \sum_{l=1}^{N} e^{ikl} S^-_l |0\rangle. \tag{4.228}$$

The corresponding eigenvalue, the energy of the one-particle excitation, can be found very easily

$$\begin{aligned}\mathcal{H}_{XXZ}|\Psi_1\rangle &= \sum_{l=1}^{N} e^{ikl}\mathcal{H}_{XXZ}|\,l\rangle \qquad (4.229)\\ &= \sum_{l=1}^{N} e^{ikl}\left\{(E_0 - J\Delta + B)\,|\,l\rangle + \frac{J}{2}\,(|\,l-1\rangle + |\,l+1\rangle)\right\} = E_1\sum_{l=1}^{N} e^{ikl}|\,l\rangle\end{aligned}$$

or

$$\sum_{l=1}^{N}\left\{e^{ikl}\,(E_0 - J\Delta + B - E_1) + \frac{J}{2}\left(e^{ik(l-1)} + e^{ik(l+1)}\right)\right\}|\,l\rangle = 0 \qquad (4.230)$$

And finally we get

$$E_1 - E_0 = -J\,(\Delta - \cos k) + B, \qquad k = \frac{2\pi}{N}I, \quad I = 0, 1, ...N-1. \qquad (4.231)$$

The rest eigenstates are constructed in accordance with the Bethe ansatz method. Thus, the subsector of the Hilbert space corresponding to the M flipped spins is spanned by the following vectors:

$$|\Psi_M\rangle = \sum_{1\le l_1\le ...\le l_M\le N} a(\,l_1, ..., l_M) S^-_{l_1} S^-_{l_2} ... S^-_{l_M}|0\rangle \qquad (4.232)$$

Where the functions $a(\,l_1, ..., l_M)$ are given in the same form as in the case of XXX-model:

$$\begin{aligned}a(\,l_1, ..., l_M) &= \sum_{\mathcal{P}\in S_M} A(\mathcal{P})\exp\left\{i\sum_{j=1}^{M} k_{\mathcal{P}(j)} l_j\right\} \qquad (4.233)\\ &= \sum_{\mathcal{P}\in S_M}\exp\left\{i\sum_{j=1}^{M} k_{\mathcal{P}(j)} l_j + \frac{i}{2}\sum_{j'<j}\Theta(k_{\mathcal{P}(j)}, k_{\mathcal{P}(j')})\right\},\end{aligned}$$

Where $\mathcal{P}$ is the element of the symmetric group, S_M of permutations of M indexes, $\{1, 2, ..., M\}$. The form of the functions $a(\,l_1, ..., l_M)$ is obtained form the eigenvalue equation for the Bethe wave function (4.232):

$$\begin{aligned}&\sum_{\{l\}} a(\,l_1, ..., l_M)\left\{\frac{J}{2}\sum_{\{l'\}}|\,l'_1, ..., l'_M\rangle + \left[\frac{J\Delta}{4}\,(N_p - N_a) - \frac{B}{2}\,(N-2M)\right]|\,l_1, ..., l_M\rangle\right\}\\ &= E_M\sum_{\{l\}} a(\,l_1, ..., l_M)|\,l_1, ..., l_M\rangle, \qquad (4.234)\end{aligned}$$

here by $\{l\}$ we denote the sum over the ordered sequence of indexes, $1 \le l_1 \le ... \le l_M \le N$, the $\{l'\}$ stands for the summation over the all possible groups of indexes which can be obtained form $\{l\}$ just by the shifting of the one of them left or right, N_p is the number of the pair of the parallel spins, ↑↑ or ↓↓, N_a is the number of the pairs of the antiparallel spins, ↑↓ or ↓↑ in the configuration $\mid l_1, ..., l_M\rangle$. Obviously, $N_p + N_a = N$. Taking into account the equation (4.227) the equation for the functions $a(\ l_1, ..., l_M)$ can be written in the following form:

$$\left(E_0 - E_M - \frac{J\Delta}{2} N_a + BM\right) a(\ l_1, ..., l_M) + \frac{J}{2} \sum_{\{l'\}} a(\ l'_1, ..., l'_M) = 0. \tag{4.235}$$

Repeating the same procedure as we did for the isotropic Heisenberg chain, Eqs. (3.141)-(3.143) we arrive at the expression for the coefficient $A(\mathcal{P})$ in the form of scattering phases for the quasi-particles. First of all, we write down the eigenvalue equation (4.234) for the case when where are no neighboring reversed spins, $l_{k+1} \neq l_k + 1$. As in this case $N_a = 2M$ we have

$$\begin{aligned} &(E_0 - E_M - MJ\Delta + BM)\, a(\ l_1, ..., l_M) \qquad (4.236)\\ + \quad &\frac{J}{2} \sum_{j=1}^{M} \{a(\ l_1, ..., l_{j-1}, l_j - 1, l_{j+1}, ..., l_M) + a(\ l_1, ..., l_{j-1}, l_j + 1, l_{j+1}, ..., l_M)\} = 0. \end{aligned}$$

Substituting Eq. (4.233) into this equation we immediately get the eigenvalue,

$$E_M - E_0 = \sum_{j=1}^{M} \{B - J\,(\Delta - \cos k_j)\} \tag{4.237}$$

Exercise *Show that the the eigenvalue equation (4.236) is satisfied for arbitrary coefficients $A(\mathcal{P})$ provided the equation (4.237) takes the place.*

In order the Eq. (4.236) to be valid for arbitrary arrangement of the reversed spins we have to impose M additional conditions into the wave functions $a(\ l_1, ..., l_M)$:

$$\begin{aligned} &2\Delta\ a(\ l_1, ..., l_j, l_j + 1, ..., l_M) = a(\ l_1, ..., l_j, l_j, ..., l_M) + a(\ l_1, ..., l_j + 1, l_j + 1, ..., l_M),\\ &j = 1, ..., M. \qquad (4.238) \end{aligned}$$

These equations are just the consistency condition for the case of the two neighboring reversed spins. These additional conditions are enough for complete determination of the wave function. Considering the configurations where three or more flipped spins are on the adjacent sites does not give more information that the cases of two neighboring reversed spins. Substituting the Bethe wave function into the Eqs. (4.238) we get the following equations for the amplitudes:

$$\begin{aligned} &\sum_{\mathcal{P}\in S_M} A(\mathcal{P}) \left\{2\Delta\ e^{ik_{\mathcal{P}(j+1)}} - 1 - e^{i(k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})}\right\} e^{i\left(k_{\mathcal{P}(1)}l_1 + ... + (k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})l_j + ... + k_{\mathcal{P}(M)}l_M\right)} = 0,\\ &j = 1, ..., M. \qquad (4.239) \end{aligned}$$

We have the sum over all permutation of the M indexes and we can peak the terms which leaves the exponential outside the brackets intact. Obviously, for the each element of the permutation group $\mathcal{P}$ the permutation which differs form $\mathcal{P}$ just by permutation of the indexes j and $j+1$, i.e. $\mathcal{P}\mathcal{P}_{j,j+1}$ corresponds to the same exponential outside the brackets in Eqs. (4.239). Thus, we can rearrange the summation and sum over the quotient group $S_M/P_{j,j+1}$ for each j, thus, getting two term for each exponential outside the brackets:

$$\sum_{\mathcal{P}\in S_M/P_{j,j+1}} \left[A(\mathcal{P})\left\{2\Delta\, e^{ik_{\mathcal{P}(j+1)}} - 1 - e^{i(k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})}\right\}\right. \tag{4.240}$$

$$\left.+A(\mathcal{P}\mathcal{P}_{j,j+1})\left\{2\Delta\, e^{ik_{\mathcal{P}(j)}} - 1 - e^{i(k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})}\right\}\right] e^{i\left(k_{\mathcal{P}(1)}l_1+\ldots+(k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})l_j+\ldots+k_{\mathcal{P}(M)}l_M\right)} = 0.$$

Thus, for each j the consistency condition (4.238) leads to $\frac{M!}{2}$ equations for the amplitudes:

$$A(\mathcal{P})/A(\mathcal{P}\mathcal{P}_{j,j+1}) = e^{i\Theta(k_{\mathcal{P}(j)},k_{\mathcal{P}(j+1)})} \tag{4.241}$$

where the scattering phases are given by the expressions

$$e^{i\Theta(k_{\mathcal{P}(j)},k_{\mathcal{P}(j+1)})} = -\frac{e^{i(k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})} - 2\Delta\, e^{ik_{\mathcal{P}(j)}} + 1}{e^{i(k_{\mathcal{P}(j)}+k_{\mathcal{P}(j+1)})} - 2\Delta\, e^{ik_{\mathcal{P}(j+1)}} + 1}. \tag{4.242}$$

Taking into account all possible values of j we can decide that the unique solution (up to a constant multiplier) of the equation is

$$A(\mathcal{P}) = \exp\left\{\frac{i}{2}\sum_{j<j'}\Theta(k_{\mathcal{P}(j)}, k_{\mathcal{P}(j')})\right\}. \tag{4.243}$$

The relation between the scattering phases and the quasi-momenta is

$$\theta(k_j,k_l) = \pi - \Theta(k_j,k_l) = 2\arctan\frac{\Delta\sin\left(\frac{k_j-k_l}{2}\right)}{\cos\left(\frac{k_j+k_l}{2}\right) - \Delta\cos\left(\frac{k_j-k_l}{2}\right)}, \tag{4.244}$$

or

$$e^{i\Theta(k_j,k_l)} = -e^{-i\theta(k_j,k_l)} \tag{4.245}$$

For the determination of the quasi-momenta one have to exploit the cyclic boundary condition we impose on the Bethe wave function, $a(\, l_2,...,l_1+N) = a(\, l_1,...,l_M)$. Let us mention, that in case of the infinite chain where is no restriction of the possible value of k_j (continuous spectrum) and Eq. (4.244) gives us the value of the scattering phases of any two excitations depending of their momenta. However, for the finite chain we have the system of coupled equations for the quasi-momenta and phases (Bethe Equations) originating from the cyclic boundary conditions:

$$\sum_{\mathcal{P}\in S_M} A(\mathcal{P})\exp\left\{i\sum_{j=1}^{M}k_{\mathcal{P}(j)}l_j\right\} = \sum_{\mathcal{P}\in S_M} A(\mathcal{P})\exp\left\{i\sum_{j=1}^{M-1}k_{\mathcal{P}(j)}l_{j+1} + k_{\mathcal{P}(M)}(l_1+N)\right\} \tag{4.246}$$

This lead to the following conditions to the amplitudes:

$$A(\mathcal{P}) = A(\mathcal{P}\mathcal{P}_C)e^{ik_{\mathcal{P}(1)}N}, \tag{4.247}$$

where $\mathcal{P}_C \in S_M$ is the cyclic permutation,

$$\mathcal{P}_C(j) = j + 1. \tag{4.248}$$

Now, for the amplitude (4.243) we have

$$\begin{aligned} A(\mathcal{P}\mathcal{P}_C) &= \exp\left\{\frac{i}{2}\sum_{1\le j'<j<M}\Theta\left(k_{\mathcal{P}(j'+1)},k_{\mathcal{P}(j+1)}\right)+\frac{i}{2}\sum_{1\le j'<M}\Theta\left(k_{\mathcal{P}(j'+1)},k_{\mathcal{P}(1)}\right)\right\} \\ &= \exp\left\{\frac{i}{2}\sum_{1<j'<j<M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(j)}\right)+\frac{i}{2}\sum_{1<j'<M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(1)}\right)\right\} \\ &= \exp\left\{\frac{i}{2}\sum_{1\le j'<j\le M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(j)}\right)+i\sum_{1\le j'\le M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(1)}\right)\right\} \\ &= A(\mathcal{P})\exp\left\{i\sum_{j=1}^{M}\Theta\left(k_{\mathcal{P}(j)},k_{\mathcal{P}(1)}\right)\right\}. \end{aligned} \tag{4.249}$$

Here we used the following intermediate transformations of the sums:

$$\begin{aligned} \frac{i}{2}\sum_{1\le j'<j<M}\Theta\left(k_{\mathcal{P}(j'+1)},k_{\mathcal{P}(j+1)}\right) &= \frac{i}{2}\sum_{2\le j'<j\le M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(j)}\right)+\frac{i}{2}\sum_{j'\le M}\Theta\left(k_{\mathcal{P}(1)},k_{\mathcal{P}(j')}\right) \\ -\frac{i}{2}\sum_{j'\le M}\Theta\left(k_{\mathcal{P}(1)},k_{\mathcal{P}(j')}\right) &= \frac{i}{2}\sum_{1\le j'<j\le M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(j)}\right)+\frac{i}{2}\sum_{j'\le M}\Theta\left(k_{\mathcal{P}(j')},k_{\mathcal{P}(1)}\right) \end{aligned} \tag{4.250}$$

Finally, the periodic boundary condition yields

$$A(\mathcal{P}) = A(\mathcal{P})\exp\left\{i\sum_{j=1}^{M-1}\Theta\left(k_{\mathcal{P}(j)},k_{\mathcal{P}(1)}\right)+ik_{\mathcal{P}(1)}N\right\}. \tag{4.251}$$

As this must be valid for arbitrary permutation $\mathcal{P}$ we come at

$$\exp\left\{iNk_j+i{\sum_{j'=1}^{M}}'\Theta\left(k_{j'},k_j\right)\right\}=1, \quad j=1,...,M, \tag{4.252}$$

where the prime over the sum means that $j' = j$ is excluded. Thus, for determining the spectrum of the excitation with the M reversed spins for the XXZ-chain one has to solve the following system of relations:

$$Nk_j = 2\pi I_j + {\sum_{j'=1}^{M}}'\Theta\left(k_j,k_{j'}\right), \quad j=1,...,M, \tag{4.253}$$

where $I_j = 0, \pm1, \pm2, ...$ As it will be seen later, it is also convenient to use a bit different scattering phases just shifted by π (See Eq. (4.244)). Thus we get:

$$\begin{aligned} \exp\left\{iNk_j+i{\sum_{j'=1}^{M}}'\Theta\left(k_{j'},k_j\right)\right\} &= \exp\left\{iNk_j+i{\sum_{j'=1}^{M}}'\left(\pi-\theta\left(k_{j'},k_j\right)\right)\right\} \\ &= \exp\left\{iNk_j+i\pi(M-1)-i\sum_{j'=1}^{M}\theta\left(k_{j'},k_j\right)\right\}=1, \quad j=1,...,M, \end{aligned} \tag{4.254}$$

here we can omit the prime over the las sum, as $\theta(k_j, k_j) = 0$. The last fact makes the equations for the spectrum written in terms of shifted phase more convenient. From here we get

$$Nk_j = 2\pi\mathcal{I}_j - \sum_{j'=1}^{M} \theta(k_j, k_{j'}), \quad j = 1, ..., M, \tag{4.255}$$

Here, $\mathcal{I}_j = I_j - \frac{M-1}{2}$ are integer or half integer depending on the value of M. It is also convenient to rewrite the conditions for the determination of the spectrum in the following form:

$$e^{iNk_j} = (-1)^{M-1} \prod_{j'=1}^{M} e^{-i\theta\left(k_j, k_{j'}\right)}. \tag{4.256}$$

4.3 Rapidities and different regimes

Looking at the expression for the two-body scattering phase (4.244) one can note a very unwanted property. It is not explicitly translational invariant for shift of the momenta. This fact makes it very difficult to show the factorization of the scattering matrix. In order to fix this problem it is convenient to reparametrize the quasi-momenta by a change of variable $k_j \to \lambda_j$ to introduce proper **rapidities**. Let us introduce the substitution

$$e^{ik_j} = \frac{\sin\left[\frac{\eta}{2}(\lambda_j + i)\right]}{\sin\left[\frac{\eta}{2}(\lambda_j - i)\right]}, \tag{4.257}$$

where η is a yet-undetermined parameter. We will define the connection of this parameter with the parameter of the model under consideration by substituting the Eq. (4.257) into the expression for the scattering phase (4.242) and demanding its translational invariance for the shifts of rapidities λ_j.

$$\frac{e^{i(k_j+k_l)} - 2\Delta\, e^{ik_j} + 1}{e^{(ik_j+k_l)} - 2\Delta\, e^{ik_l} + 1} = \tag{4.258}$$
$$\frac{\cos[\frac{\eta}{2}(\lambda_j - \lambda_l)] - \Delta\cos[\frac{\eta}{2}(\lambda_j - \lambda_l + 2i)] - (\cosh\eta - \Delta)\cos[\frac{\eta}{2}(\lambda_j + \lambda_l)]}{\cos[\frac{\eta}{2}(\lambda_j - \lambda_l)] - \Delta\cos[\frac{\eta}{2}(\lambda_j - \lambda_l - 2i)] - (\cosh\eta - \Delta)\cos[\frac{\eta}{2}(\lambda_j + \lambda_l)]}$$

To eliminate the terms violating the translational invariance one has to set

$$\cosh\eta \equiv \Delta \tag{4.259}$$

Thus,

$$\begin{aligned} \frac{e^{i(k_j+k_l)} - 2\Delta\, e^{ik_j} + 1}{e^{(ik_j+k_l)} - 2\Delta\, e^{ik_l} + 1} &= \frac{\cos[\frac{\eta}{2}(\lambda_j - \lambda_l)] - \Delta\cos[\frac{\eta}{2}(\lambda_j - \lambda_l + 2i)]}{\cos[\frac{\eta}{2}(\lambda_j - \lambda_l)] - \Delta\cos[\frac{\eta}{2}(\lambda_j - \lambda_l - 2i)]} \\ &= -\frac{\sin[\frac{\eta}{2}(\lambda_j - \lambda_l + 2i)]}{\sin[\frac{\eta}{2}(\lambda_j - \lambda_l - 2i)]}. \end{aligned} \tag{4.260}$$

Exercise *Derive the equations (4.258)-(4.260).*

Let us now show some useful relations resulting form the Eq. (4.257). First of all, the limit of the Heisenberg model, $\Delta = 1$ or $\eta = 0$ can be easily taken leading to the result we obtained in the previous chapter:

$$\lim_{\eta \to 0} \frac{\sin\left[\frac{\eta}{2}(\lambda_j + i)\right]}{\sin\left[\frac{\eta}{2}(\lambda_j - i)\right]} = \frac{\lambda_j + i}{\lambda_j - i}. \tag{4.261}$$

Another direct consequence of the Eq. (4.257) is

$$\cot\frac{k_j}{2} = \coth\frac{\eta}{2}\tan\left(\frac{\eta\lambda_j}{2}\right) \tag{4.262}$$

Again one can easily take the Heisenberg chain limit, $\Delta = 1$ or $\eta = 0$, reproducing the result from the previous Section:

$$\lim_{\eta \to 0}\coth\frac{\eta}{2}\tan\left(\frac{\eta\lambda_j}{2}\right) = \lambda_j \tag{4.263}$$

But to describe the properties od the excitations of the XXZ-chain for all values of the anisotropy parameter Δ one has to start form the appropriate choice of rapidities for different regions. One has to distinguish the following cases: axial $\Delta > 1$; axial $\Delta < 1$; planar, $|\Delta| \leq 1$, the last case oslo contains two specific isotropic cases $\Delta = \pm 1$. For this purposes we star with the proper parametrization of the momenta making the scattering phase(here we introduce the notation $\theta_{jl} \equiv \theta(k_j, k_l)$) explicitly translational invariant.

$$\tan\frac{\theta_{jl}}{2} = \frac{\Delta\sin\left(\frac{k_j - k_l}{2}\right)}{\cos\left(\frac{k_j + k_l}{2}\right) - \Delta\cos\left(\frac{k_j - k_l}{2}\right)} = \frac{\Delta\left(\cot\frac{k_l}{2} - \cot\frac{k_j}{2}\right)}{(1-\Delta)\cot\frac{k_j}{2}\cot\frac{k_l}{2} - (1+\Delta)}. \tag{4.264}$$

Two simplest cases are obvious.

1. $\Delta = 1$ **Isotropic antiferromagnet**

$$\begin{aligned} \tan\frac{\theta_{jl}}{2} &= \frac{1}{2}(\lambda_j - \lambda_l) \\ \lambda_j &= \cot\frac{k_j}{2}, \quad k_j = 2\mathrm{arccot}\lambda_j, \\ e^{ik_j} &= \frac{\lambda_j + i}{\lambda_j - i}, \quad e^{-i\theta_{jl}} = -\frac{\lambda_j - \lambda_l + 2i}{\lambda_j - \lambda_l - 2i} \end{aligned} \tag{4.265}$$

Thus, the Bethe equations reads

$$\left(\frac{\lambda_j + i}{\lambda_j - i}\right)^N = \prod_{l \neq j}\frac{\lambda_j - \lambda_l + 2i}{\lambda_j - \lambda_l - 2i}, \quad j = 1, ..., M. \tag{4.266}$$

And the spectrum is

$$E_M - E_0 = BM - J\sum_{j=1}^{M}\frac{dk_j}{d\lambda_j} = BM + 2J\sum_{j=1}^{M}\frac{1}{1+\lambda_j^2}, \tag{4.267}$$
$$E_0 = \left(\frac{J}{4} - \frac{B}{2}\right)N,$$

2. $\Delta = -1$ **Isotropic ferromagnetic**

$$\tan\frac{\theta_{jl}}{2} = \frac{1}{2}(\lambda_l - \lambda_j) \tag{4.268}$$
$$\lambda_j = \tan\frac{k_j}{2}, \quad k_j = 2\arctan\lambda_j, \quad -\pi \le k_j \le \pi, \quad ,-\infty < \lambda_j < \infty,$$
$$e^{ik_j} = -\frac{\lambda_j - i}{\lambda_j + i}, \quad e^{-i\theta_{jl}} = -\frac{\lambda_j - \lambda_l - 2i}{\lambda_j - \lambda_l + 2i}$$

The Bethe equations and the spectrum are

$$\left(\frac{\lambda_j - i}{\lambda_j + i}\right)^N = \prod_{l\neq j}\frac{\lambda_j - \lambda_l - 2i}{\lambda_j - \lambda_l + 2i}, \quad j = 1, ..., M. \tag{4.269}$$

$$E_M - E_0 = BM - J\sum_{j=1}^{M}\frac{dk_j}{d\lambda_j} = BM - 2J\sum_{j=1}^{M}\frac{1}{1+\lambda_j^2}, \tag{4.270}$$
$$E_0 = \left(-\frac{J}{4} - \frac{B}{2}\right)N$$

3. $\Delta > 1$ **Antiferromagnetic (Axial Case)**

$$\tan\frac{\theta_{jl}}{2} = \coth\frac{\eta}{2}\tan\left[\frac{\eta}{2}(\lambda_j - \lambda_l)\right], \quad \Delta \equiv \cosh\eta, \tag{4.271}$$
$$k_j = 2\ \mathrm{arccot}\left[\coth\frac{\eta}{2}\tan\left(\frac{\eta\lambda_j}{2}\right)\right],$$
$$e^{ik_j} = \frac{\sin\left[\frac{\eta}{2}(\lambda_j + i)\right]}{\sin\left[\frac{\eta}{2}(\lambda_j - i)\right]}, \quad e^{-i\theta_{jl}} = -\frac{\sin\left[\frac{\eta}{2}(\lambda_j - \lambda_l + 2i)\right]}{\sin\left[\frac{\eta}{2}(\lambda_j - \lambda_l - 2i)\right]}$$
$$\left(\frac{\sin\left[\frac{\eta}{2}(\lambda_j + i)\right]}{\sin\left[\frac{\eta}{2}(\lambda_j - i)\right]}\right)^N = \prod_{l\neq j}\frac{\sin\left[\frac{\eta}{2}(\lambda_j - \lambda_l + 2i)\right]}{\sin\left[\frac{\eta}{2}(\lambda_j - \lambda_l - 2i)\right]}$$

4. $|\Delta| < 1$ **Paramagnetic (Planar Case)**
The only formal difference from the previous case is the purely imaginary value of the parameter η. Let us introduce $\phi = i\eta$, then

$$\cos\phi \equiv \Delta, \quad |\Delta| < 1, \tag{4.272}$$

and

$$
\begin{aligned}
&\tan\frac{\theta_{jl}}{2} = \cot\frac{\eta}{2}\tanh\left[\frac{\eta}{2}(\lambda_j-\lambda_l)\right], \qquad (4.273)\\
&k_j = 2\,\text{arccot}\left[\cot\frac{\eta}{2}\tanh\left(\frac{\eta\lambda_j}{2}\right)\right],\\
&e^{ik_j} = \frac{\sinh\left[\frac{\eta}{2}(\lambda_j+i)\right]}{\sinh\left[\frac{\eta}{2}(\lambda_j-i)\right]}, \quad e^{-i\theta_{jl}} = -\frac{\sinh\left[\frac{\eta}{2}(\lambda_j-\lambda_l+2i)\right]}{\sinh\left[\frac{\eta}{2}(\lambda_j-\lambda_l-2i)\right]}\\
&\left(\frac{\sinh\left[\frac{\eta}{2}(\lambda_j+i)\right]}{\sinh\left[\frac{\eta}{2}(\lambda_j-i)\right]}\right)^N = \prod_{l\neq j}\frac{\sinh\left[\frac{\eta}{2}(\lambda_j-\lambda_l+2i)\right]}{\sinh\left[\frac{\eta}{2}(\lambda_j-\lambda_l-2i)\right]}
\end{aligned}
$$

5. $\Delta < -1$ **Ferromagnetic (Axial Case)**
   Here, the structure of all equations are the same as in the case of $\Delta > 1$, with the only difference in the shift of the variable η, $\eta \to \eta + i\pi$

To express the spectrum by rapidities one has to use the definition

$$E_M - E_0 = MB + \sum_{j=1}^{M} C(\eta)\frac{dk_j}{d\lambda_j}, \qquad (4.274)$$

where the coefficient $C(\eta)$ can be found form the direct comparison:

$$
\begin{aligned}
&k = 2\text{arccot}\left[\coth\frac{\eta}{2}\tan\left(\frac{\eta\lambda}{2}\right)\right], \qquad (4.275)\\
&\frac{dk}{d\lambda} = -\frac{\eta\sinh\eta}{\cosh\eta-\cos(\eta\lambda)},\\
&\Delta-\cos k = \cosh\eta - \frac{1}{2}(e^{ik}+e^{-ik}) = \cosh\eta - \frac{1}{2}\left(\frac{\sin\left[\frac{\eta}{2}(\lambda+i)\right]}{\sin\left[\frac{\eta}{2}(\lambda-i)\right]} + \frac{\sin\left[\frac{\eta}{2}(\lambda-i)\right]}{\sin\left[\frac{\eta}{2}(\lambda+i)\right]}\right)\\
&= \frac{\sinh^2\eta}{\cosh\eta-\cos(\eta\lambda)}
\end{aligned}
$$

Thus

$$C(\eta) = J\frac{\sinh\eta}{\eta}. \qquad (4.276)$$

Finally for the spectrum of excitation we have the following representation in terms of rapidities:

- $\Delta > 1$

$$E_M - E - 0 = MB - J\sum_{j=1}^{M}\frac{\sinh^2\eta}{\cosh\eta-\cos(\eta\lambda_j)}, \quad \cosh\eta = \Delta \qquad (4.277)$$

- $|\Delta| < 1$

$$E_M - E - 0 = MB + J\sum_{j=1}^{M} \frac{\sin^2\phi}{\cos\phi - \cosh(\phi\lambda_j)}, \quad \cos\phi = \Delta \tag{4.278}$$

4.4 Another choice of rapidities, Orbach Parametrization

There are another way of the introduction of rapidities du to reparametrization of the momenta, making the phase factors(two quasi-particle S-matrix) translational invariant. It is very similar to the previous one, however some equations become a bit simpler and at the same time the limits of $\Delta = \pm 1$ are not a continues anymore. The Orbach parametrization is

$$e^{ik_j} = \frac{e^{i\lambda_j} - e^{\eta}}{e^{i\lambda_j + \eta} - 1} = \frac{\sin\left[\frac{1}{2}\left(\lambda_j + i\eta\right)\right]}{\sin\left[\frac{1}{2}\left(\lambda_j - i\eta\right)\right]} \tag{4.279}$$

The scattering phase is

$$e^{-i\theta_{jl}} = -\frac{\sin\left[\frac{1}{2}\left(\lambda_j - \lambda_l + 2i\eta\right)\right]}{\sin\left[\frac{1}{2}\left(\lambda_j - \lambda_l - 2i\eta\right)\right]} \tag{4.280}$$

Thus, one can see, that in order to change the parametrization from the presented above to the Orbach parametrization one has to rescale the rapidities

$$\eta\lambda_j \to \lambda_j. \tag{4.281}$$

Though, the Orbach parametrization is not continuous at $\Delta = \pm 1$ it is very suitable for the description and manipulation the string solution of the Bethe ansatz equations. In the next subsection we are going to describe the string solutions we have already mentioned in the section about XXX-chain. That is why we hereafter pass to the Orbach parametrization. Let us just write down the main equations and relations for axial and planar regimes of the XXZ-chain.

$$\begin{aligned}
&\Delta = \arccos\eta > 1, \\
&\cot\frac{k_j}{2} = \coth\frac{\eta}{2}\tan\frac{\lambda_j}{2}, \\
&\left(\frac{\sin\left[\frac{1}{2}\left(\lambda_j + i\eta\right)\right]}{\sin\left[\frac{1}{2}\left(\lambda_j - i\eta\right)\right]}\right)^N = \prod_{l\neq j} \frac{\sin\left[\frac{1}{2}\left(\lambda_j - \lambda_l + i2\eta\right)\right]}{\sin\left[\frac{1}{2}\left(\lambda_j - \lambda_l - i2\eta\right)\right]} \\
&E_M - E - 0 = MB - J\sum_{j=1}^{M} \frac{\sinh^2\eta}{\cosh\eta - \cos\lambda_j},
\end{aligned} \tag{4.282}$$

The Orbach parametrization is very suitable if one investigate the $\Delta \to 0$ or $\Delta \to \infty$ limits of the solutions of the Bethe ansatz equations, because the parameter η is explicitly appears in the expressions for the Bethe strings, while for the parametrization presented in the previous subsection the imaginary part of the strings has the same structure as in the case of XXX-chain. And finally let us write down another form of the Bethe equations for the spectrum (Eq. (4.255)) in which the all regions of the anisotropy parameter Δ can be included. Defining the functions

$$\theta_n(\lambda) = \begin{cases} 2\arctan\left(\cot\frac{\phi n}{2}\tanh\frac{\lambda}{2}\right) & 0 \le \Delta < 1 \\ 2\arctan\frac{\lambda}{n}, & \Delta = 1 \\ 2\arctan\left(\coth\frac{\eta n}{2}\tan\frac{\lambda}{2}\right) & \Delta > 1 \end{cases} \tag{4.283}$$

for the Orbach parametrization. And

$$\theta_n(\lambda) = \begin{cases} 2\arctan\left(\cot\frac{\phi n}{2}\tanh\frac{\phi\lambda}{2}\right) & 0 \le \Delta < 1 \\ 2\arctan\frac{\lambda}{n}, & \Delta = 1 \\ 2\arctan\left(\coth\frac{\eta n}{2}\tan\frac{\eta\lambda}{2}\right) & \Delta > 1 \end{cases} \tag{4.284}$$

for the parametrization which is smooth at $\Delta \to 1$. Then, the Bethe equations read

$$N\theta_1(\lambda_j) = 2\pi I_j + \sum_{l\neq j}^{M} \theta_2(\lambda_j - \lambda_l), \quad j = 1, ..., M. \tag{4.285}$$

where the Bethe quantum numbers I_j are integer or half-integer.

4.5 Simplest string solution. Normalizability of the Bethe wave functions.

In the previous section about XXX-chain we have already presented in a nutshell the concept of the string solutions of the Bethe ansatz equations. Here we are going to give more profound and comprehensive analysis. As was mentioned above, in general case of finite N in it quite complicated to handle the solution of the Bethe ansatz equations. However, one can achieve substantially simplified picture in the thermodynamic limit $N\infty$. Stings are the regular structures in the complex spectral-parameter space which corresponds to bound state on the magnons. They are low-lying excitations form the ground state in the ferromagnetic region. Let us start the $N \to \infty$ analysis of the solution of the Bethe ansatz equations for the simplest isotropic case $\Delta = 1$. Let us start with the two-particle state $M = 2$, as the case of $M = 1$ is trivial and does not differ form the free particle situation, when the possible values of the momenta k just cover continuously the whole interval $(0, 2\pi)$. For the $M = 2$ we have to equations

$$\begin{aligned} \left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^N &= \frac{\lambda_1 - \lambda_2 + 2i}{\lambda_1 - \lambda_2 - 2i}, \\ \left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^N &= \frac{\lambda_2 - \lambda_1 + 2i}{\lambda_2 - \lambda_1 - 2i}. \end{aligned} \tag{4.286}$$

Searching for the real solutions first we mention that the r.h.s. of these equations are a pure phases. Thus,

$$e^{iNk_1} = e^{i\Phi}, \quad e^{iNk_2} = e^{-i\Phi} \tag{4.287}$$

and again in the limit $N \to \infty$ we have two independent magnons with k_1 and k_2 covering continuously the interval $(0, 2\pi)$. Thus, the effects of the interaction disappear for the infinitely long chain. But equations (4.286) also admit a complex solution. Let us assume

$$\lambda_1 = u_1 + iv_1, \quad \lambda_2 = u_2 + iv_2, \tag{4.288}$$

where $u_{1,2}$ and $v_{1,2}$ are real numbers. Comparing the modulus of the both parts of the first equation of (4.286) we have

$$\left(\frac{u_1^2 + (v_1 - 1)^2}{u_1^2 + (v_1 + 1)^2}\right)^N = \frac{(u_1 - u_2)^2 + (v_1 - v_2 - 2)^2}{(u_1 - u_2)^2 + (v_1 - v_2 + 2)^2}. \tag{4.289}$$

Assuming that $v_1 > 0$ and taking the limit $N \to \infty$ we see that the l.h.s of the previous equation goes exponentially to zero, so must do the r.h.s., which implies

$$u_1 = u_2 = u, \quad v_1 - v_2 = 2. \tag{4.290}$$

To determine the possible value of the imaginary part of the solution let us multiply two equations in (4.286) and substitute there Eq. (4.290)

$$\left(\frac{u + i(v_1 + 1)}{u + i(v_1 - 3)}\right)^N = 1. \tag{4.291}$$

In the limit $N \to \infty$ we have $v_1 = 1, u \in \mathbb{R}$. Thus, we get the simplest string solutio, 2-string

$$\lambda_1 = u + i, \quad \lambda_2 = u - i \tag{4.292}$$

which corresponds to the bound state of two magnons with the total moment given by

$$k = k_1 + k + 2 = \frac{1}{i}\log\frac{u + 2i}{u} + \frac{1}{i}\log\frac{u}{u - 2i} = \frac{1}{i}\log\frac{u + 2i}{u - 2i} \tag{4.293}$$

with the energy

$$E_2 - E_0 = -2J\left(\frac{1}{1 + (u + i)^2} + \frac{1}{1 + (u - i)^2}\right) = -\frac{4J}{u^2 + 1} = -\frac{J}{2}(1 - \cos k) \tag{4.294}$$

This the result we have already obtained in the previous section. In can be shown that the string solution (4.292) is the only complex solution for rapidities which ensures the normalizability of the Bethe wave function in the limit of infinite chain. Let us write down the wave function for the $M = 2$ sector in terms of rapidities

$$\begin{aligned} a(l_1, l_2) &\propto \left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^{l_1}\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^{l_2}(\lambda_1 - \lambda_2 + 2i) - \left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^{l_2}\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^{l_1}(\lambda_2 - \lambda_1 + 2i) \\ &= \left\{\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)\right\}^{l_1}\left((\lambda_1 - \lambda_2 + 2i)\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^{l_2 - l_1} - (\lambda_2 - \lambda_1 + 2i)\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^{l_2 - l_1}\right) \end{aligned} \tag{4.295}$$

As in the limit of the infinite chain the site label l_1 can be arbitrary large, the normalizability of the wave function implies that

$$\left|\left(\frac{\lambda_1+i}{\lambda_1-i}\right)\left(\frac{\lambda_2+i}{\lambda_2-i}\right)\right| = 1 \tag{4.296}$$

The next condition the wave function must satisfy is regularity under the asymptotically large distance between reversed spins $l_2 - l_1 \to \infty$. From this requirement we see that one of the terms in the rhs of the Eq. (4.295) must disappear.For the string solution considered here we have

$$\left|\left(\frac{\lambda_1+i}{\lambda_1-i}\right)\left(\frac{\lambda_2+i}{\lambda_2-i}\right)\right| = \left|\frac{u+2i}{u-2i}\right| = 1, \tag{4.297}$$

which is the case for the real u. Then,

$$\left|\frac{\lambda_1+i}{\lambda_1-i}\right| = \left|\frac{u+2i}{u}\right| > 1, \quad \left|\frac{\lambda_2+i}{\lambda_2-i}\right| = \left|\frac{u}{u-2i}\right| < 1 \tag{4.298}$$

For the string considered here the coefficient at the unwanted term vanishes, and thus, we have

$$|a(\ l_1, l_2)|^2 \propto \left(\frac{u}{u^2+4}\right)^{2(l_2-l_1)}, \tag{4.299}$$

which is normalizable and exhibits exponential decay when the distance between reversed spin is growing. This is indeed the picture of a bound state of two magnons.

4.6 General string solutions

In can be shown in general, that in order the Bethe wave function for arbitrary M flipped spins be normalizable in the limit of infinite long chain the complex solutions must be organize in the following structures:

$$\lambda_u^{M,l} = u + i(M+1-2l), \quad l = 1, 2, ..., M, \tag{4.300}$$

Which is called the string of the length M. The real parameter u is called the center of the string. In many regards the strings behave like a single entity and whey obviously corresponds to the bound states of M-magnon. Generalizing the normalizability condition for the Bethe wave function for arbitrary M

$$a(\ l_1, ..., l_M) = \left(\prod_{j=1}^{M}\frac{\lambda_j+i}{\lambda_j-i}\right)^{l_1} \sum_{\mathcal{P}\in S_M}(-1)^{\mathrm{sgn}(\mathcal{P})}A(\mathcal{P})\prod_{j=1}^{M-1}\left(\prod_{l=j+1}^{M}\frac{\lambda_{\mathcal{P}(j)}+i}{\lambda_{\mathcal{P}(j)}-i}\right)^{l_{j+1}-l_j} \tag{4.301}$$

we have

$$\left|\prod_{l=1}^{M}\frac{\lambda_u^{M,l}+i}{\lambda_u^{M,l}-i}\right| = \left|\prod_{l=1}^{M}\frac{u+i(M+2-2l)}{u+i(M-2l)}\right| = \left|\prod_{l=1}^{M}\frac{u+iM}{u-iM}\right| = 1 \tag{4.302}$$

In order to ensure that the wave function is regular for the large distances between the flipped spins there must hold

$$\left| \prod_{l=j+1}^{M} \frac{\lambda_l + i}{\lambda_l - i} \right| < 1 \tag{4.303}$$

Substituting the string solution we get

$$\left| \prod_{l=j+1}^{M} \frac{\lambda_l + i}{\lambda_l - i} \right| = \left| \frac{u + i(M - 2j)}{u - iM} \right| < 1. \tag{4.304}$$

which is satisfied for all $j = 1, 2, ..., M - 1$. Each string of length M is also characterized by a total momentum

$$k = \frac{1}{i} \sum_{j=1}^{M} \log \left(\frac{\lambda_l + i}{\lambda_l - i} \right) = \frac{1}{i} \sum_{l=1}^{M} \log \left(\frac{u + i(M + 2 - 2l)}{u + i(M - 2l)} \right) = \frac{1}{i} \sum_{l=1}^{M} \log \left(\frac{u + iM}{u - iM} \right) \tag{4.305}$$

and energy

$$E_M - E_0 = -2J \sum_{j=1}^{M} \frac{1}{1 + \lambda_j^2} = -2J \sum_{l=1}^{M} \frac{1}{1 + (u + i(M + 1 - 2l))^2} = -\frac{2JM}{u^2 + M^2}. \tag{4.306}$$

Then, using the relation which stems from Eq. (4.305)

$$u = iM \frac{e^{ik} + 1}{e^{ik} - 1} = M \cot \frac{k}{2} \tag{4.307}$$

we finally found

$$E_M - E_0 = -\frac{J}{M} (1 - \cos k). \tag{4.308}$$

4.7 String solutions for $\Delta \neq 1$

The results obtained for the string solutions in case of isotropic Hamiltonian can be directly generalized to the cases of $\Delta \neq 1$. Generally speaking, one can transform all results obtained for the stings in isotropic case to other cases just by making the formal replacement

$$\frac{\lambda + iA}{\lambda - iA} \mapsto \frac{\sin \left[\frac{1}{2} (\lambda + i\eta A) \right]}{\sin \left[\frac{1}{2} (\lambda - i\eta A) \right]} \tag{4.309}$$

in case of Orbach parametrization, and

$$\frac{\lambda + iA}{\lambda - iA} \mapsto \frac{\sin \left[\frac{\eta}{2} (\lambda + iA) \right]}{\sin \left[\frac{\eta}{2} (\lambda - iA) \right]} \tag{4.310}$$

in case of rescalled Orbach parametrization. Let as start from axial case.

- $\Delta > 1$ Imposing the same normalizability conditions on the Bethe wave function

$$a(\, l_1, ..., l_M) = \left(\prod_{j=1}^{M} \frac{\sin\left[\frac{1}{2}(\lambda_j + i\eta)\right]}{\sin\left[\frac{1}{2}(\lambda_j - i\eta)\right]} \right)^{l_1} \sum_{\mathcal{P} \in S_M} (-1)^{\mathrm{sgn}(\mathcal{P})} A(\mathcal{P}) \prod_{j=1}^{M-1} \left(\prod_{l=j+1}^{M} \frac{\sin\left[\frac{1}{2}\left(\lambda_{\mathcal{P}(j)} + i\eta\right)\right]}{\sin\left[\frac{1}{2}\left(\lambda_{\mathcal{P}(j)} - i\eta\right)\right]} \right)^{l_{j+1}-l_j} \tag{4.311}$$

with

$$A(\mathcal{P}) = \prod_{j<l} \sin\left[\frac{1}{2}\left(\lambda_{\mathcal{P}(j)} - \lambda_{\mathcal{P}(l)} + 2i\eta\right)\right] \tag{4.312}$$

The normalizability conditions are satisfied only if the solutions have the following string structure

$$\lambda_j = u + i\eta\,(M + 1 - 2l)\,, \quad l = 1, 2, ..., M. \tag{4.313}$$

Then,

$$\left| \prod_{j=1}^{M} \frac{\sin\left[\frac{1}{2}(\lambda_j + i\eta)\right]}{\sin\left[\frac{1}{2}(\lambda_j - i\eta)\right]} \right| = \left| \prod_{l=1}^{M} \frac{\sin\left[\frac{1}{2}(\lambda_j + i\eta(M+2-2l))\right]}{\sin\left[\frac{1}{2}(\lambda_j + i\eta(M-2l))\right]} \right| = \left| \frac{\sin\left[\frac{1}{2}(\lambda_j + i\eta M)\right]}{\sin\left[\frac{1}{2}(\lambda_j - i\eta M)\right]} \right| = 1. \tag{4.314}$$

and

$$\left| \prod_{l=j+1}^{M} \frac{\sin\left[\frac{1}{2}(\lambda_j + i\eta(M+2-2l))\right]}{\sin\left[\frac{1}{2}(\lambda_j + i\eta(M-2l))\right]} \right| = \left| \frac{\sin\left[\frac{1}{2}(\lambda_j + i\eta(M-2j))\right]}{\sin\left[\frac{1}{2}(\lambda_j - i\eta M)\right]} \right| < 1 \tag{4.315}$$

The total momentum and the energy are given by

$$k = \frac{1}{i} \sum_{l=1}^{M} \log\left[\frac{\sin\left[\frac{1}{2}(u + i\eta(M+2-2l))\right]}{\sin\left[\frac{1}{2}(u + i\eta(M-2l))\right]} \right] = \frac{1}{i} \log\left[\frac{\sin\left[\frac{1}{2}(u + i\eta M)\right]}{\sin\left[\frac{1}{2}(u - i\eta M)\right]} \right], \tag{4.316}$$

$$E_M - E_0 = -J \sum_{l=1}^{M} \frac{\sinh^2 \eta}{\cosh\eta - \cos\left[u + i(M+1-2l)\right]} = -J \frac{\sinh\eta \sinh(\eta M)}{\cosh(\eta M) - \cos u}$$

The useful relation is

$$\cos k = \frac{1 - \cosh(\eta M)\cos u}{\cosh(\eta M) - \cos u}. \tag{4.317}$$

with the aid of which we finally get

$$E_M - E_0 = -J \frac{\sinh\eta}{\sinh(\eta M)} \left\{ \cosh(\eta M) - \cos k \right\} \tag{4.318}$$

- $|\Delta| < 1$ For the paramagnetic region we put $\eta = i\phi$ and then using the same argumentation as in the previous cases and formal replacement all sin functions by $i \sinh$ one can investigate the structure of sting solutions in this case. The analysis of the normalizability conditions shows that in this case we have two type of strings: the strings with their centers on the real axis, or with the positive "parity", $v = 1$

$$\lambda_j = u + i\phi(M + 1 - 2l), \quad l = 1, 2, ..., M \tag{4.319}$$

and string with the center shifted to the $i\pi$ axis or with the negative parity $v = -1$

$$\lambda_j = u + i\pi + i\phi(M + 1 - 2l), \quad l = 1, 2, ..., M \tag{4.320}$$

For a given value of the anisotropy parameter ϕ and the parity v, there exist strong restriction on possible length M of the strings. The Orbach parametrization in this case is

$$e^{ik_j} = \frac{e^{i\phi} - e^{\lambda_j}}{e^{i\phi+\lambda_j} - 1} = \frac{\sinh\left[\frac{1}{2}(i\phi - \lambda_j)\right]}{\sinh\left[\frac{1}{2}(i\phi + \lambda_j)\right]} \tag{4.321}$$

Let us write down the normalizability condition for the string with positive parity

$$\begin{aligned} 1 \;&>\; \left|\prod_{l=j+1}^{M} \frac{\sinh\left[\frac{1}{2}(i\phi(2l - M)) - u\right]}{\sinh\left[\frac{1}{2}(i\phi(M + 2 - 2l)) + u\right]}\right| = \left|\frac{\sinh\left[\frac{1}{2}(i\phi(2j - M)) - u\right]}{\sinh\left[\frac{1}{2}(i\phi M + u)\right]}\right| \\ &=\; \sqrt{\frac{\cosh u - \cos\phi(M - 2j)}{\cosh u - \cos(\phi M)}} \end{aligned} \tag{4.322}$$

This condition is equivalent to the following inequalities

$$\cos(\phi M) < \cos\phi(M - 2j), \quad \text{for } j = 1, 2, ..., M - 1, \;\; v = 1 \tag{4.323}$$

The normalizability conditions for the string with negative parity ($v = -1$) are

$$1 > \left|\frac{\cosh\left[\frac{1}{2}(i\phi(2j - M)) - u\right]}{\cosh\left[\frac{1}{2}(i\phi M + u)\right]}\right| = \sqrt{\frac{\cosh u + \cos\phi(M - 2j)}{\cosh u + \cos(\phi M)}} \tag{4.324}$$

which implies

$$\cos(\phi M) > \cos\phi(M - 2j), \quad \text{for } j = 1, 2, ..., M - 1, \;\; v = -1 \tag{4.325}$$

Both restriction can be cast into one

$$0 < 2v \sin\phi(M - j)\sin(\phi j), \quad j = 1, 2, ..., M - 1 \tag{4.326}$$

The total momentum, energy and dispertion relation are

$$k = \frac{1}{i}\log\frac{\sinh\left[\frac{1}{2}(i\phi M - u - i(1 - v)\frac{\pi}{2})\right]}{\sinh\left[\frac{1}{2}(i\phi M + u + i(1 - v)\frac{\pi}{2})\right]}, \tag{4.327}$$

$$E_M - E_0 = J\frac{\sin\phi\sin(\phi M)}{v\cosh u - \cos(\phi M)},$$

$$E_M - E_0 = J\frac{\sin\phi}{\sin(\phi M)}\left\{\cos(\phi M) + \cos k\right\}. \tag{4.328}$$

- $\Delta \leq -1$ Since the energy spectrum of the Hamiltonians with Δ and $-\Delta$ are related by the reflection around $E = 0$, the string solutions in the cases of negative Δ both isotropic and anisotropic are basically the same as their solution for positive Δ. The fundamental difference is the these are not low-lying excitations form the ground state in the antiferromagnetic region.