Lecture II: BA for the XXZ spin chain

S. Lukyanov

The six vertex model

The story starts with the six vertex model, a statistical mechanics model which describes 2 dimensional ice and other crystals in which hydrogen bonding is responsible for holding the lattice together. The crystal is pictured as a square array of atoms with M rows and N columns. As in ice, between each adjacent pair of atoms there is a hydrogen ion responsible for bonding, located close to one or the other of the two atoms which it binds. They represent the degrees of freedom of the system and can be represented by arrows pointing to one or the other atom along the bond. A configuration of the lattice is defined when an arrow has been placed at each bond, and there are 2^{MN} configurations in total. The partition function is defined as:

$$\mathcal{Z} = \sum_{\text{configurations}} \exp\Big(-\frac{\mathcal{E}}{kT}\Big)\,,$$

where $\mathcal{E}$ is the energy of the configuration.

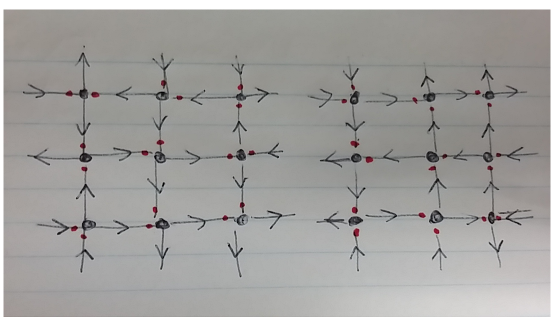


Figure 1: Two possible configurations of a 3×3 lattice. The oxygen atoms are represented by black dots and the hydrogen ions by the red dots

To specify the energy of the lattice, first consider the possible arrow configurations about a specific atom, or vertex. There are $2^4 = 16$ possible ways the arrows can be drawn. In the six vertex model the "ice–rule" is imposed, which states that at each vertex two of the arrows must point towards the vertex and two must point away from the vertex. This is meant to mimic the bonding of H_2O in ice and reduces the 16 possible combinations to just 6 (see figure 2). Each one of these configurations is given a particular energy ϵ_i, so that the total energy of the lattice is just the sum of the energies of each vertex:

$$\mathcal{E} = n_1\,\epsilon_1 + n_2\,\epsilon_2 + \ldots + n_6\,\epsilon_6\,,$$

where n_i is the number of vertices of type i. This is the six vertex model in its most general form. If the crystal is not placed in an external field, so that there is no preferred direction, the energy of a vertex with all arrows reserved should be the same as the

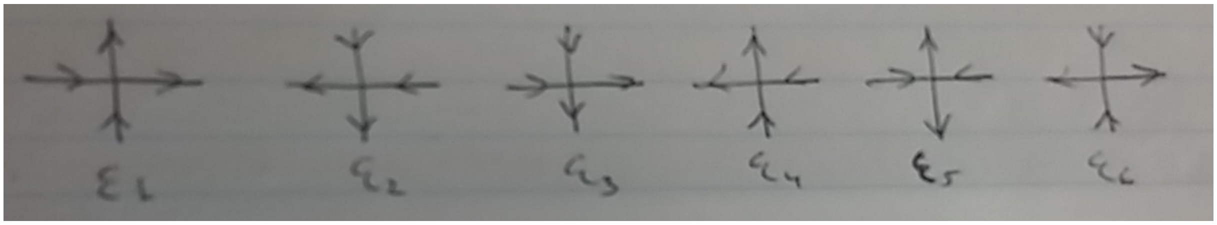


Figure 2: The six possible vertex configurations allowed by the ice–rule

energy of the original vertex. In this case the lattice possesses a $\mathbb{Z}_2$ symmetry, that of the inversion of all arrows, i.e.,

$$\epsilon_1 = \epsilon_2 , \qquad \epsilon_3 = \epsilon_4 , \qquad \epsilon_5 = \epsilon_6 .$$

In this case the model is called the zero–field six vertex model.

Boundary conditions and the Energies

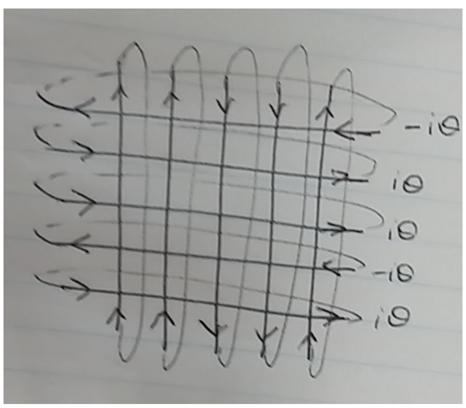


Figure 3: A lattice with twisted boundary conditions displayed

We should also choose boundary conditions for the model. Boundary conditions that will be considered here are called toroidal boundary conditions. For toroidal boundary conditions, the atoms at the opposite boundaries (left, right and top, bottom) are considered to be adjacent (see figure 3). Toroidal boundary conditions imply that $\epsilon_5 = \epsilon_6$ without reference to $\mathbb{Z}_2$ symmetry. Consider a horizontal row. Vertex 5 is a sink for arrows and vertex 6 is a source. The lattice is periodic in the horizontal direction so the number of sources must be equal to the number of sinks. Therefore, ϵ_5 and ϵ_6 only appear in the partition function in the combination $\epsilon_5 + \epsilon_6$ and can be set to be equal to each other.

Toroidal boundary conditions are easily generalized to twisted boundary conditions. In this case, the lattice is periodic in the vertical direction and the horizontal direction, but iθ is added to the energy if the arrow on the horizontal boundary points to the right, and $-$iθ is added if the arrow points to the left (see figure 3). In this report, the six vertex model is assumed to be a zero–field six vertex model with twisted boundary conditions. The partition function is a function of only three Boltzmann weights and the twist parameter:

$$\mathcal{Z} = \mathcal{Z}_\theta(a, b, c) .$$

Given ϵ_i, the problem is to calculate the statistical sum $\mathcal{Z}$ over the possible configurations of arrows which satisfy the ice–rule. The solution to this problem was key in the development of Quantum Integrability.

Solving the model

Relation to particle scattering

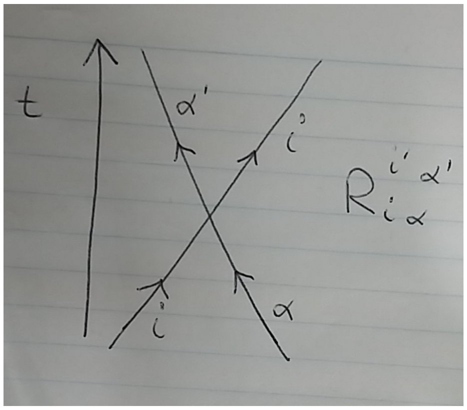


Figure 4: The vertex representing the scattering of two particles. $\boldsymbol{R}^{i'\alpha'}_{i\alpha}$ gives the scattering amplitude for this process.

The vertices of the crystal lattice can be interpreted in terms of the scattering of particles. Consider the vertex turned on its side (see figure 4) and let time point in the vertical direction. There are two types of arrows. An arrow pointing in the direction of positive time is considered to be a particle, and an arrow pointing in the negative direction of time is an anti–particle. The vertex symbolizes scattering and the Boltzmann factors, $\exp\left(\frac{\epsilon_i}{kT}\right)$, are the scattering amplitudes for these processes to occur. The "ice–rule" has the meaning that the "particle charge" is conserved in the interaction, where a particle is assigned a charge of $+1$ and an anti–particle is assigned a charge of -1.

The scattering amplitudes of a particular interaction can be stored in a matrix, called the $\boldsymbol{R}$–matrix. Each leg represents a two dimensional space spanned by:

$$|+\rangle - \text{a particle} \qquad |-\rangle - \text{an anti–particle} .$$

The bottom legs correspond to incoming particles, and the top legs are the outgoing particles. The $\boldsymbol{R}$–matrix acts from the incoming spaces to the outgoing spaces:

$$\boldsymbol{R} : \mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C}^2 \otimes \mathbb{C}^2$$

Using the basis: $\{|i\rangle \otimes |\alpha\rangle\}$ with $i, \alpha = \pm$ the $\boldsymbol{R}$–matrix is:

$$(\boldsymbol{R})^{i'\alpha'}_{i\alpha} = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & c & 0 \\ 0 & c & b & 0 \\ 0 & 0 & 0 & a \end{pmatrix}$$

where a, b, c are the Boltzmann weights:

$$a = \exp\left(-\frac{\epsilon_1}{kT}\right) \qquad b = \exp\left(-\frac{\epsilon_3}{kT}\right) \qquad c = \exp\left(-\frac{\epsilon_5}{kT}\right) .$$

The transfer matrix

The calculation of the partition function is done by methods that are now standard in Quantum Integrability and can be found in many references. Consider a single row of the

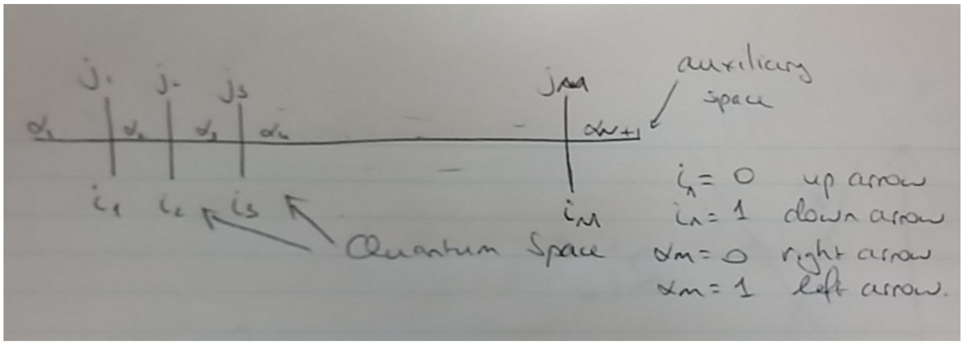


Figure 5: A row of the lattice where the legs are considered as Quantum and Auxiliary Spaces

lattice and use the notation employed in (1). Each vertical leg is considered to be the space $\mathbb{C}^2$ with the basis:

$$|+\rangle \; - \text{up arrow}, \qquad |-\rangle \; - \text{down arrow}\,.$$

This space is denoted as the *quantum space*. The horizontal legs are also considered to be $\mathbb{C}^2$ but is called the *auxiliary space*. It has the basis:

$$|+\rangle \; - \text{arrow pointing right}, \qquad |-\rangle \; - \text{arrow pointing left}\,.$$

The $\boldsymbol{R}$ matrix is an operator that acts on the tensor product of the quantum space and the auxiliary space. Denote the $\boldsymbol{R}$–matrix acting on the i^{th} Quantum Space in the lattice i as $\boldsymbol{R}_i$. Construct the monodromy matrix:

$$\boldsymbol{M} \equiv \begin{pmatrix} \boldsymbol{M}(+,+) & \boldsymbol{M}(+,-) \\ \boldsymbol{M}(-,+) & \boldsymbol{M}(-,-) \end{pmatrix} \qquad \boldsymbol{M} = \boldsymbol{R}_1 \boldsymbol{R}_2 \ldots \boldsymbol{R}_N\,,$$

where the multiplication is carried out in the auxiliary space. Each matrix element $\boldsymbol{M}(\alpha_1, \alpha_N)$ acts on N copies of $\mathbb{C}^2$:

$$\boldsymbol{M}(\alpha_1, \alpha_N) : \underbrace{\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \ldots \otimes \mathbb{C}^2}_{\text{N times}} \to \underbrace{\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \ldots \otimes \mathbb{C}^2}_{\text{N times}}\,.$$

The transfer matrix is defined to be the trace of the monodromy matrix over the auxiliary space:

$$\boldsymbol{T} = \mathrm{Tr}_{\text{auxilary}} \left(\mathrm{e}^{\mathrm{i}\theta\sigma^3} \boldsymbol{M}\right) = \boldsymbol{M}(+,+)\,\mathrm{e}^{\mathrm{i}\theta} + \boldsymbol{M}(-,-)\,\mathrm{e}^{-\mathrm{i}\theta}$$

where $\mathrm{e}^{\mathrm{i}\theta\sigma^3}$ imposes the twisted boundary conditions. The partition function is then expressed in terms of the transfer matrix as:

$$\mathcal{Z}_\theta(a,b,c) = \mathrm{Tr}_{\text{quantum}} \left[\boldsymbol{T}^M\right],$$

and the problem reduces to the calculation of the eigenvalues of $\boldsymbol{T}$. Let $\Lambda_0, \Lambda_1, \Lambda_2 \ldots$ be the eigenvalues of $\boldsymbol{T}$ so that:

$$\Lambda_0 > \Lambda_1 > \Lambda_2 > \ldots$$

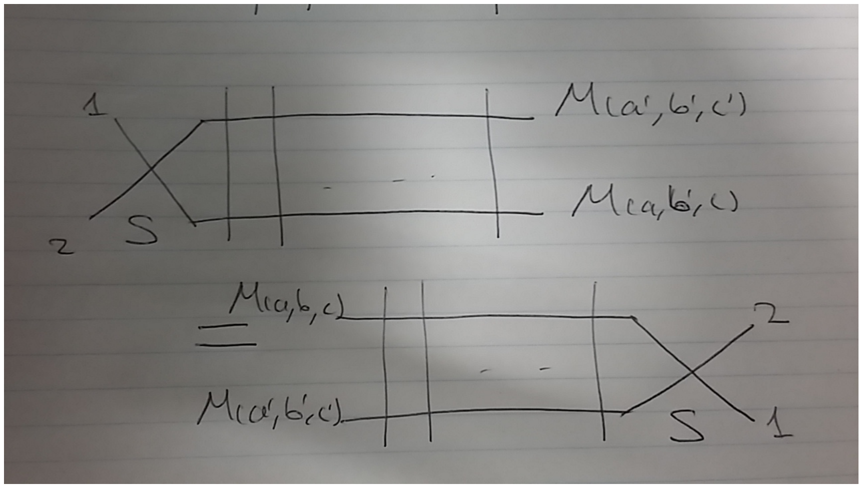


Figure 6: The condition (1) drawn diagrammatically

In the thermodynamic limit, $N, M \to \infty$, the largest eigenvalue gives a dominant contribution:

$$\log \mathcal{Z} \;=\; M \log \Lambda_0 \;+\; \log\left(1 \;+\; \left(\frac{\Lambda_1}{\Lambda_0}\right)^M \;+\; \left(\frac{\Lambda_2}{\Lambda_0}\right)^M \;+\; \ldots\right).$$

Commuting transfer matrices

Diagonalizing large matrices is a standard problem in Quantum Mechanics which is often tackled by finding operators that mutually commute. A big step towards the solution of the six vertex model was the realization that the transfer matrices for different six vertex models commute. Write the dependence of the transfer matrix on the parameters of the model a, b, c explicitly. The condition that two transfer matrices commute is:

$$\boldsymbol{T}(a,b,c)\,\boldsymbol{T}(a',b',c') \;=\; \boldsymbol{T}(a',b',c')\,\boldsymbol{T}(a,b,c)\ .$$

A sufficient condition is that:

$$\boldsymbol{S}\,\big(\boldsymbol{M}(a,b,c)\otimes\mathbb{I}\big)\,\big(\mathbb{I}\otimes\boldsymbol{M}(a',b',c')\big) \;=\; \big(\mathbb{I}\otimes\boldsymbol{M}(a',b',c')\big)\big(\boldsymbol{M}(a,b,c)\otimes\mathbb{I}\big)\,\boldsymbol{S}\,, \qquad (1)$$

and

$$\left[\boldsymbol{S}, \mathrm{e}^{\mathrm{i}\theta\sigma^3}\otimes\mathrm{e}^{\mathrm{i}\theta\sigma^3}\right] \;=\; 0\,.$$

The condition (1) is shown pictorially in figure 6. This, in turn, is satisfied if the same relation is valid for a single $\boldsymbol{R}$ matrix:

$$\boldsymbol{S}\,\big(\boldsymbol{R}(a,b,c)\otimes\mathbb{I}\big)\,\big(\mathbb{I}\otimes\boldsymbol{R}(a',b',c')\big) \;=\; \big(\mathbb{I}\otimes\boldsymbol{R}(a',b',c')\big)\big(\boldsymbol{R}(a,b,c)\otimes\mathbb{I}\big)\,\boldsymbol{S}\,. \qquad (2)$$

The pictorial representation is given in figure 7. The equation (2) is in fact 64 equations.

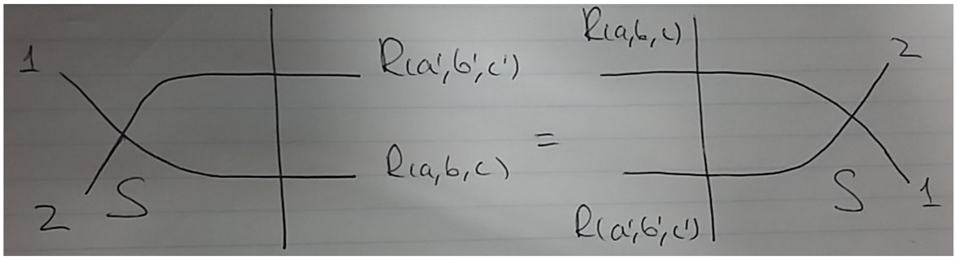


Figure 7: Diagrammatical representation of the RLL relation

It can be shown that the matrix $\boldsymbol{S}$ must have the same form as $\boldsymbol{R}$, i.e.,

$$\boldsymbol{S} = \begin{pmatrix} a'' & 0 & 0 & 0 \\ 0 & b'' & c'' & 0 \\ 0 & c'' & b'' & 0 \\ 0 & 0 & 0 & a'' \end{pmatrix} .$$

Note that this form automatically commutes with $\mathrm{e}^{\mathrm{i}\theta\sigma^3} \otimes \mathrm{e}^{\mathrm{i}\theta\sigma^3}$.

Exercise: Show that the the 64 equations (2) reduce to just 3 non–trivial equations:

$$\begin{aligned} ac'a'' &= bc'b'' + ca'c'' \\ ab'c'' &= ba'c'' + cc'b'' \\ cb'a'' &= ca'b'' + bc'c'' . \end{aligned}$$

A solution for non-zero a'', b'', c'' exists if:

$$\Delta' = \Delta , \qquad \text{where} \quad \Delta = \frac{a^2+b^2-c^2}{2ab} \qquad \Delta' = \frac{a'^2+b'^2-c^2}{2a'b'} .$$

It is convenient to parameterize the weights by:

$$\frac{b}{a} = \frac{\lambda - \lambda^{-1}}{\lambda q^{-1} - \lambda^{-1} q} , \qquad \frac{c}{a} = \frac{q^{-1} - q}{\lambda q^{-1} - \lambda q} , \qquad \Delta = \frac{1}{2}\left(q + q^{-1}\right) . \tag{3}$$

Such a parameterization is convenient because Δ does not depend on λ, which is referred to as the spectral parameter. a'', b'', c'' in $\boldsymbol{S}$ can be solved for and the result is:

$$\boxed{\boldsymbol{R}_{12}(\lambda/\mu)\boldsymbol{R}_{13}(\lambda)\boldsymbol{R}_{23}(\mu) = \boldsymbol{R}_{23}(\mu)\boldsymbol{R}_{13}(\lambda)\,\boldsymbol{R}_{12}(\lambda/\mu)}$$

where the indices denote the spaces on which the $\boldsymbol{R}$ matrices act. This equation is very famous in Quantum Integrability and is known as the Yang–Baxter equation.

Thus we can set

$$\boldsymbol{T}(\lambda) = \big(- \lambda q^{-\frac{1}{2}}\big)^N \mathrm{Tr}\Bigg[\begin{pmatrix} \mathrm{e}^{\mathrm{i}\theta} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\theta} \end{pmatrix} \boldsymbol{R}_1(\lambda)\boldsymbol{R}_2(\lambda)\cdots \boldsymbol{R}_N(\lambda)\Bigg] \tag{4}$$

where

$$\boldsymbol{R}\big(\lambda q^{\frac{1}{2}}\big) = \begin{pmatrix} \lambda q^{-\mathtt{h}/2} - \lambda^{-1} q^{\mathtt{h}/2} & (q^{-1}-q)\,\mathtt{e}_- \\ (q^{-1}-q)\,\mathtt{e}_+ & \lambda q^{\mathtt{h}/2} - \lambda^{-1} q^{-\mathtt{h}/2} \end{pmatrix}$$

and

$$\mathtt{h} = \sigma^z\ , \qquad \mathtt{e}_\pm = \tfrac{1}{2}\,(\sigma^x \pm \mathrm{i}\sigma^y)\ .$$

Notice that the overall factor in (4) is set in such a way that the matrix elements of $\boldsymbol{T}$ are polynomials in λ^2 of order N:

$$(\boldsymbol{T})^{j_1\ldots j_N}_{i_1\ldots i_N} \leftarrow \text{ a polynomial in } \lambda^2 \text{ of order } N\,.$$

The final result is that two transfer matrices of the six vertex model (4) commute, if their anisotropy parameters are the same. This is generally written as:

$$\Big[\boldsymbol{T}(\lambda),\, \boldsymbol{T}(\mu)\Big] \ =\ 0\ .$$

The Heisenberg XXZ spin-chain

A second crucial observation was that the six vertex model was related to the Heisenberg XXZ spin-chain, a model of ferromagnetism solved by Hans Bethe in the 1930's. The XXZ Hamiltonian is defined as a collection of N spins on a lattice which interact via nearest neighbor interactions. The Hamiltonian is:

$$\boldsymbol{H}_{XXZ} \ =\ -J \sum_{i=1}^{N}\ \big(\sigma^x_i\,\sigma^x_{i+1}\ +\ \sigma^y_i\,\sigma^y_{i+1}\ +\ \Delta\,\sigma^z_i\,\sigma^z_{i+1}\big)\,,$$

where σ^a_i are the Pauli spin matrices at site i.

Exercise: Show that $\boldsymbol{H}_{XXZ}(-J,-\Delta)$ can be obtained from $\boldsymbol{H}_{XXZ}(J,\Delta)$ by a unitary transformation, i.e., without loss of generality, the dimensionful coupling constant J can be chosen to be positive.

For the twisted boundary conditions imposed on the six vertex model,

$$\sigma^{\pm}_{N+1} \ =\ \mathrm{e}^{\pm 2\mathrm{i}\theta}\,\sigma^{\pm}_1\,, \qquad\quad (-\pi < 2\theta \leq \pi)\ .$$

the logarithmic derivative of the transfer matrix is equal to the XXZ Hamiltonian up to the addition of an inessential constant.

$$\boldsymbol{H}_{XXZ} = J\ (q-q^{-1})\,\lambda\partial_\lambda \log \boldsymbol{T}(\lambda)\,|_{\lambda=1} - J\ (q-q^{-1})\,N + JN\,\Delta\ .$$

The transfer matrix commutes with the Hamiltonian for any λ and is a continuous family of integrals of motion of the XXZ model. By expanding the transfer matrix in λ, It is possible to construct an infinite number of mutually commuting quantities which also commute with the Hamiltonian. Finding the eigenvalues of $\boldsymbol{T}$ is equivalent to finding the energies of the spin chain as well as the eigenvalues of all the conserved quantities. The transfer matrix is a powerful tool for solving the spin chain.

In 1931, Hans Bethe had derived a method for computing the eigenvalues and eigenvectors of the Heisenberg spin chain. This same method was applied successfully in the 1960s to the six vertex model and goes by the name of the Bethe Ansatz.

The Bethe Ansatz

The method derived by Hans Bethe was to start with a general Ansatz for the eigenvectors, and to use the eigenvalue equation to derive an algebraic system which could be solved for both the eigenvectors and the eigenvalues. However, in the way formulated by Bethe, it is difficult to generalize the Ansatz to other physical problems. The main contribution of Baxter was to interpret the Bethe Ansatz equations as equations for the zeroes of what he called the "auxiliary matrix". This operator is now known as the $\boldsymbol{Q}$–operator, and has become important in the study of Quantum Integrable systems. However, it is not well understood what the $\boldsymbol{Q}$–operator is, and it will only be claimed that such an object exists. The construction of the $\boldsymbol{Q}$ operator is much beyond the scope of these lectures.

The XXZ Hamiltonian as well as the Transfer Matrix commute with the spin operator:

$$\big[\boldsymbol{S}^z, \boldsymbol{T}(\lambda)\big] \;=\; 0\,, \qquad \boldsymbol{S}^z \;=\tfrac{1}{2}\,\sum_j \sigma_j^z\,.$$

Therfore, it is only necessary to consider a particular sector of the transfer matrix with n down spins. Let S^z be the value of the spin operator $\boldsymbol{S}^z$ in this sector.

$$S^z \;=\; \frac{N}{2} - n\;.$$

Since

$$\boldsymbol{V}\boldsymbol{H}_{XXZ}\boldsymbol{V}^{-1} = \boldsymbol{H}_{XXZ}\,, \quad \boldsymbol{V}\boldsymbol{S}^z\boldsymbol{V}^{-1} = -\boldsymbol{S}^z \quad \text{where} \quad \boldsymbol{V} = \exp\Big(\tfrac{\mathrm{i}\pi}{2}\sum_{j=1}^{N}\sigma_j^x\Big)\;,$$

we shall always assume below that $S^z \geq 0$ without loss of generality.

In his work on the 6 vertex model, Baxter found an operator $\boldsymbol{Q}(\lambda)$ which satisfies the following properties:

1. Commutation Relations:

$$\big[\boldsymbol{Q}(\lambda),\, \boldsymbol{T}(\mu)\big] \;=\; \big[\boldsymbol{Q}(\lambda),\, \boldsymbol{Q}(\mu)\big] \;=\; 0\,.$$

2. Its elements are polynomials in λ^2:

$$\boldsymbol{Q}^{j_1\ldots j_N}_{i_1,\ldots i_N} \;=\; \lambda^{\frac{\theta}{\pi g}+S^z} \times \Big(\text{a polynomial in } \lambda^2 \text{ of order } n = \tfrac{N}{2} - S^z\Big)\,. \tag{5}$$

3. It satisfies the TQ–relation:

$$\boldsymbol{Q}(\lambda)\boldsymbol{T}(\lambda q^{\frac{1}{2}}) \;=\; \big(1-\lambda^2 q^{-1}\big)^N \boldsymbol{Q}(\lambda q) \;+\; \big(1-\lambda^2 q\big)^N \boldsymbol{Q}(\lambda q^{-1})\;. \tag{6}$$

The first step is to transform to a basis where $\boldsymbol{Q}$ and $\boldsymbol{T}$ are both diagonal. Note that the eigenvalues of $\boldsymbol{Q}(\lambda)$ will still have the polynomial form (5) since the change of basis matrix can not depend on λ and the TQ–relation remains unchanged. Focus on a particular eigenvalue of $\boldsymbol{Q}$, $Q(\lambda)$, and the corresponding eigenvalue of the transfer matrix, $T(\lambda)$. Let $\{\lambda_k^2\}$ be the zeroes of $Q(\lambda)$. Then it is possible to factorize the polynomial:

$$Q(\lambda) \;=\; \lambda^{\frac{\theta}{\pi g}+S^z} \prod_{j=1}^{\frac{N}{2}-S^z} \Big(1-\frac{\lambda^2}{\lambda_j^2}\Big)$$

Now evaluate the TQ–relation at a zero $\lambda = \lambda_k$. The left hand side is zero since $T(\lambda)$ is an entire function of λ in the complex plane excluding $\lambda = 0$. Equating the right hand side to zero yields:

$$\left(\frac{1-\lambda_k^2\, q}{1-\lambda_k^2\, q^{-1}}\right)^N \;=\; -q^{2S^z}\, \mathrm{e}^{2\mathrm{i}\theta} \prod_{j=1}^{\frac{N}{2}-S^z} \frac{\lambda_j^2 - \lambda_k^2\, q^2}{\lambda_j^2 - \lambda_k^2\, q^{-2}}\;. \tag{7}$$

These are the Bethe Ansatz equations. Solving them, it is possible to find the zeroes λ_k^2 of the $\boldsymbol{Q}$–operator, reconstruct the eigenvalues $Q(\lambda)$ using equation (7) and find the eigenvalues of the transfer matrix $T(\lambda)$ using the TQ–relation (6).

The phase diagram

The exact solution allows one to investigate the physical properties of the model. It turns out that for $\Delta > 1$, the ground state of the Heisenberg magnet is ferromagnetically ordered, $\Delta < -1$ it is anti-ferromagnetically ordered, while $-1 < \Delta < 1$ is the disordered regime of the magnet.

Bethe Ansatz v.s. exact Bohr-Sommerfeld

The solution of the six vertex model has been reduced to the mathematical problem of analyzing the algebraic system (7). In what follows we will focus on the disordered phase where $-1 < \Delta < 1$, i.e., the parameter q is a pure phase.

$$q = \mathrm{e}^{\mathrm{i}\pi g} \qquad (0 < g < 1)\;.$$

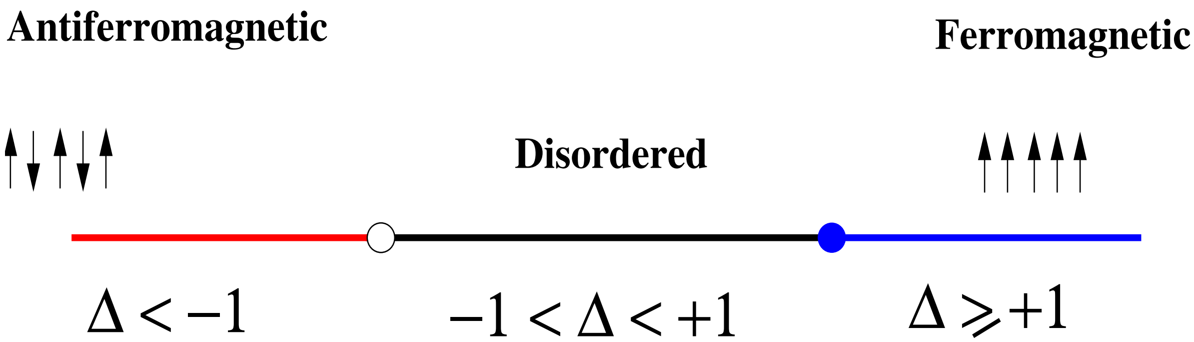


Figure 8: The phase diagram for the XXZ spin chain at zero temperature.

First of all let us make the following formal observation. on the BA equations (7). Assuming that $\lambda_j^2 \sim C_N\ E_{j-1},\ \ C_N = o(N^{-1})$ as $N \to \infty$:

$$\mathrm{e}^{4\pi \mathrm{i} g k}\ \prod_{j=0}^{\infty} \frac{\big(1 - E_n\, q^2/E_j\big)}{\big(1 - E_n\, q^{-2}/E_j\big)} = -1\ , \qquad 2k \equiv \frac{\theta}{g\pi} + S^z\ ,$$

which coincides with the exact Bohr-Sommerfeld quantization condition provided

$$g = \frac{1}{\alpha + 1}, \quad 2k = \ell + \tfrac{1}{2}\ .$$

This gives a hint that the 6-vertex model has a deep relation to the problem discussed in the first lecture.

The Bethe Ansatz equations and scaling

It is convenient to substitute the spectral parameter λ by x:

$$\lambda^2\ =\ -\mathrm{e}^{2x}\ .$$

In these new variables, the Bethe Ansatz equations become:

$$\left[\frac{\cosh\big(x_k\ +\ \frac{\mathrm{i}\pi g}{2}\big)}{\cosh\big(x_k\ -\ \frac{\mathrm{i}\pi g}{2}\big)}\right]^N = -\mathrm{e}^{2\mathrm{i}\theta} \prod_{j=1}^{n} \frac{\sinh\big(x_j - x_k - \mathrm{i}\pi g\big)}{\sinh\big(x_j - x_k + \mathrm{i}\pi g\big)}$$

Taking the logarithm of both sides yields:

$$\frac{1}{2\pi\mathrm{i}}\ N\ \log\left[\frac{\cosh\big(x_k\ +\ \frac{\mathrm{i}\pi g}{2}\big)}{\cosh\big(x_k\ -\ \frac{\mathrm{i}\pi g}{2}\big)}\right]\ =\ I_j\ +\ \frac{\theta}{\pi}\ +\ \frac{1}{2\pi\mathrm{i}} \sum_{j=1}^{n} \log\left[\frac{\sinh\big(x_k - x_j + \mathrm{i}\pi g\big)}{\sinh\big(x_j - x_k + \mathrm{i}\pi g\big)}\right]\ , \qquad (8)$$

where I_j are a set of $n \equiv \frac{N}{2} - S^z$ integers (for n odd) or half–integers (for n even) that arise from the ambiguity of the logarithm function.

Different choices of the half–integers I_j correspond to different sets of solutions of equation (8) for the Bethe roots x_j. Each solution is used to reconstruct a particular eigenvalue of $\boldsymbol{T}$. To solve the Bethe Ansatz equations numerically for a particular eigenvalue, it is important to have some intuition as to where the roots, x_j, corresponding to that eigenvalue lie in the complex plane. Not only will this allow the half–integers I_j to be chosen correctly, but it is needed to construct the numerical algorithm to solve for the roots. For $0 < g < \frac{1}{2}$, Yang and Yang rigorously proved that for the ground state, the roots x_j are real and correspond to the following choice of the I_j's:

$$I_j = -\frac{n+1}{2} + j \qquad (j = 1, \ldots, n)$$

Notice that for zero twist, the roots x_j lie on the real line, symmetrically about the origin, and as closely packed as possible (see figure 9).

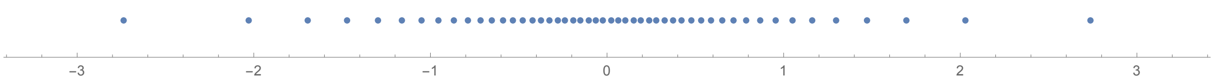


Figure 9: The distribution of the Bethe roots for the ground state in the sector $S^z = 0$, for $N = 100$, $g = \frac{1}{3}$ and $\theta = 0$.

Scaling

Label the Bethe roots in ascending order, so that:

$$x_1 < x_2 < x_3 < \ldots < x_n \ .$$

The following limit is called the scaling limit of the roots:

$$\begin{aligned} \rho_j &= \lim_{N\to\infty} \big(N^{2-2g}\, \mathrm{e}^{+2x_j}\big) \qquad && (j = 1, 2, \ldots - \ \text{fixed}) \\ \bar{\rho}_{\bar{j}} &= \lim_{N\to\infty} \big(N^{2-2g}\, \mathrm{e}^{-2x_{n-\bar{j}}}\big) \qquad && (\bar{j} = 1, 2, \ldots - \ \text{fixed}) \end{aligned} \tag{9}$$

Figure 10 shows how the first four roots approach the limit: as N increases, the left most roots tend to negative infinity according to (9). It is possible to show that

$$\rho_j^{\frac{1}{2(1-g)}} = \pi\, j + O(1)\ , \quad \bar{\rho}_{\bar{j}}^{\frac{1}{2(1-g)}} = \pi\, \bar{j} + O(1) \qquad \text{as} \quad j,\ \bar{j} \to \infty\ . \tag{10}$$

The corresponding scaling limit of the vacuum eigenvalues of the $\boldsymbol{Q}$ operator is:

$$\lim_{N\to\infty} \big(\lambda^{-1} N^{1-g}\big)^{S^z + \frac{\theta}{\pi g}}\, Q\big(N^{g-1}\,\lambda\big) \ = \prod_{j=1}^{\infty} \left(1 - \frac{\lambda^2}{\rho_j}\right) .$$

Evidence for the existence of the limit is illustrated in figure 11. Similarly one has for the right edge of the distribution of the Bethe roots

$$\lim_{N\to\infty} \big(\lambda N^{1-g}\big)^{S^z - \frac{\theta}{\pi g}}\, \big[Q\big(N^{g-1}\,\lambda\big)/(N^{g-1}\lambda)^N\big] \ = \prod_{j=1}^{\infty} \left(1 - \frac{\lambda^{-2}}{\bar{\rho}_{\bar{j}}}\right) .$$

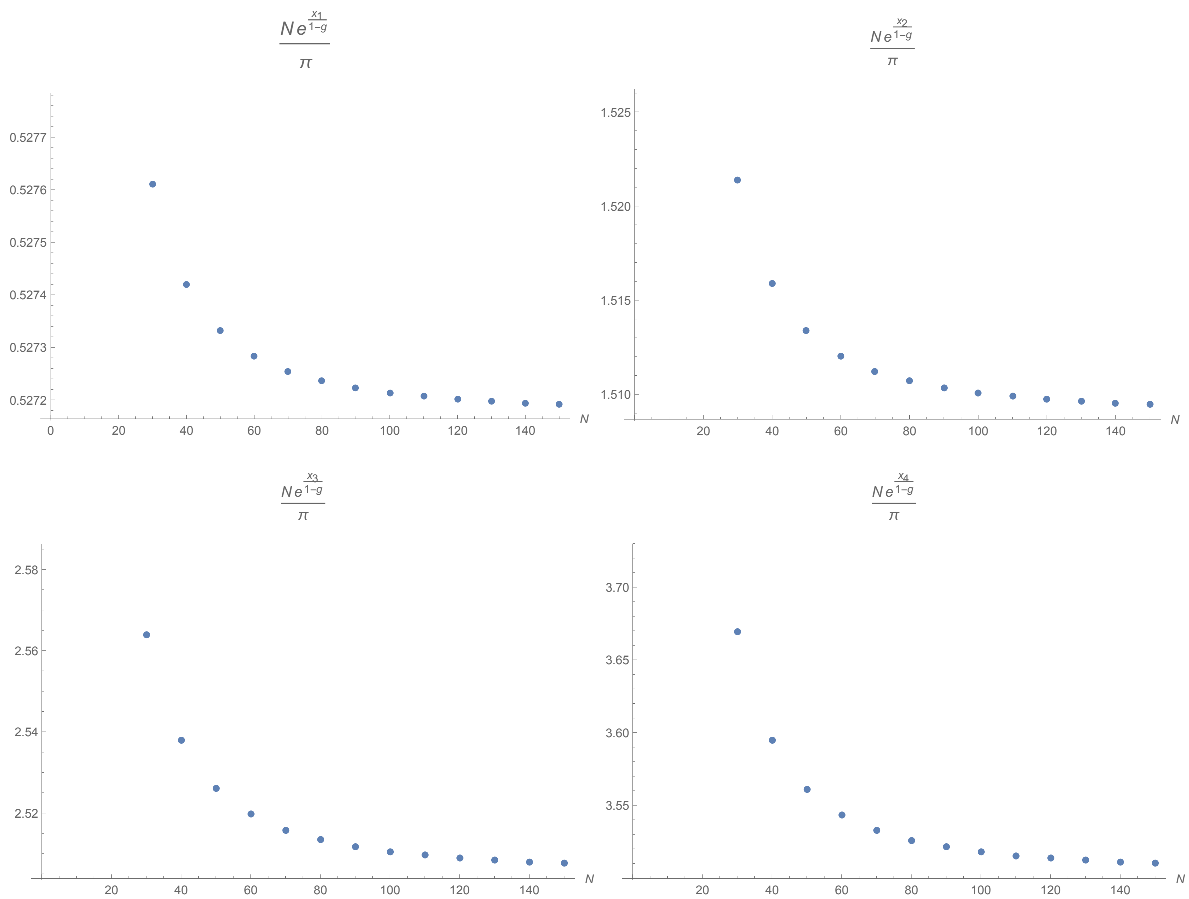


Figure 10: A plot of $\frac{N}{\pi} e^{\frac{2x_j}{1-g}}$ for $j = 1, 2, 3, 4$ as a function of N showing that as $N \to \infty$ a limiting value is approached. The parameters have been set to $g = \frac{1}{3}$, $n = \frac{N}{2}$ and $\theta = 0$.

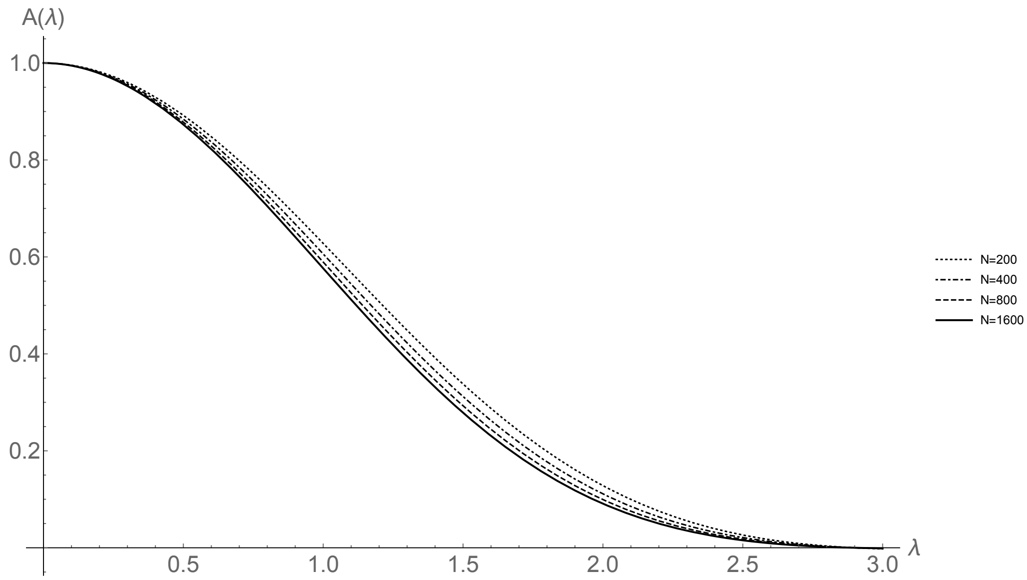


Figure 11: A plot of $A(\lambda) = \left(N^{1-g}\right)^{S^z+\frac{\theta}{\pi g}}\ Q\left(N^{g-1}\lambda\right)$ for $N = 200, 400, 800$ and $N = 1600$. The values of the parameters are: $S^z = 2$, $g = 1/3$, $\theta = -0.1$.

The ODE/IM correspondence

Let $\left\{ E_{j-1} \right\}_{j=1}^{\infty}$ and $\left\{ \bar{E}_{\bar{j}-1} \right\}_{\bar{j}=1}^{\infty}$ be ordered spectral sets of eigenvalues of the operators,

$$\boldsymbol{H} = -\frac{\mathrm{d}^2}{\mathrm{d}z^2} + U_{\text{eff}}(z) \qquad \bar{\boldsymbol{H}} = -\frac{\mathrm{d}^2}{\mathrm{d}\bar{z}^2} + \bar{U}_{\text{eff}}(\bar{z})$$

where

$$U_{\text{eff}}(z) = \frac{\ell(\ell+1)}{z^2} + z^{2\alpha}\ , \qquad \bar{U}_{\text{eff}}(\bar{z}) = \frac{\bar{\ell}(\bar{\ell}+1)}{\bar{z}^2} + \bar{z}^{2\alpha}\ ,$$

then

$$\boxed{\lim_{N\to\infty} \left(N^{2-2g}\ \lambda_j^2 \right) = -C\, E_{j-1} \qquad \lim_{N\to\infty} \left(N^{2-2g}\ \lambda_{n-\bar{j}}^{-2} \right) = -C\ \bar{E}_{\bar{j}-1}}$$

provided

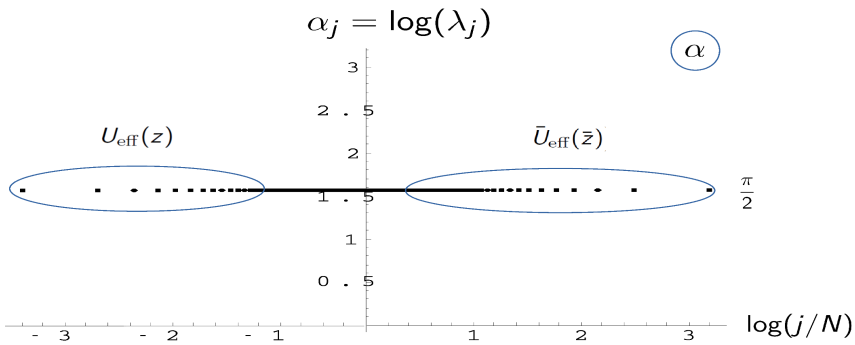
$$\alpha = \frac{1}{g} - 1\,, \qquad \ell = S^z + \frac{\theta}{\pi g} - \frac{1}{2}\ , \qquad \bar{\ell} = S^z - \frac{\theta}{\pi g} - \frac{1}{2}\ , \tag{11}$$

and

$$C = \pi^{\frac{2\alpha}{1+\alpha}}/C_0 = \left[\frac{2\Gamma\left(\frac{3}{2} + \frac{1}{2\alpha}\right)}{\sqrt{\pi}\Gamma\left(1 + \frac{1}{2\alpha}\right)} \right]^{-\frac{2\alpha}{1+\alpha}}\ . \tag{12}$$

Notice that the explicit form of the proportionality coefficient C_0 follows from the WKB asymptotic for E_n (see Exercise I.3) and eq.(10).

The correspondence stated here is only valid for the vacuum states in the given spin sector of the XXZ spin chain. The correspondences for the excited states are the same, except that the potential $U_{\rm eff}(z)$ has extra terms added to it.



Bethe states for the edges of the roots distribution $\leftrightarrow$ **pairs of the "monster" potentials** $\big(U_{\rm eff}(z), \bar{U}_{\rm eff}(\bar{z})\big)$

Exercises

Exercise II.1. Consider the "monodromy matrix"

$$\mathbb{M}(\lambda) = \mathbb{R}_1(\lambda)\mathbb{R}_2(\lambda)\cdots\mathbb{R}_N(\lambda) \ , \tag{13}$$

where

$$\mathbb{R}(\lambda) = \begin{pmatrix} \lambda q^{-\mathtt{h}/2} - \lambda^{-1} q^{\mathtt{h}/2} & (q^{-1} - q)\, \mathtt{e}_- \\ (q^{-1} - q)\, \mathtt{e}_+ & \lambda q^{\mathtt{h}/2} - \lambda^{-1} q^{-\mathtt{h}/2} \end{pmatrix}$$

and $\mathtt{h}$, $\mathtt{e}_\pm$ stand for the formal operators satisfying commutation relations

$$[\mathtt{h}, \mathtt{e}_\pm] = 2\, \mathtt{e}_\pm \ , \qquad [\mathtt{e}_+, \mathtt{e}_-] = \frac{q^{\frac{\mathtt{h}}{2}} - q^{-\frac{\mathtt{h}}{2}}}{q^{\frac{1}{2}} - q^{-\frac{1}{2}}} \ . \tag{14}$$

Show that $\mathbb{M}(\lambda)$ obeys the Yang-Baxter algebra of the form

$$\boldsymbol{R}(\lambda/\mu)\big(\mathbb{M}(\lambda)\otimes\mathbb{I}\big)\big(\mathbb{I}\otimes\mathbb{M}(\mu)\big) = \big(\mathbb{I}\otimes\mathbb{M}(\mu)\big)\big(\mathbb{M}(\lambda)\otimes\mathbb{I}\big)\boldsymbol{R}(\lambda/\mu) \tag{15}$$

where

$$(\boldsymbol{R})^{i'\alpha'}_{i\alpha} = \begin{pmatrix} \lambda q^{-1} - \lambda^{-1} q & 0 & 0 & 0 \\ 0 & \lambda - \lambda^{-1} & q^{-1} - q & 0 \\ 0 & q^{-1} - q & \lambda - \lambda^{-1} & 0 \\ 0 & 0 & 0 & \lambda q^{-1} - \lambda^{-1} q \end{pmatrix}$$

Exercise II.2: Show that $\boldsymbol{H}_{XXZ}(-J,-\Delta)$ can be obtained from $\boldsymbol{H}_{XXZ}(J,\Delta)$ by a unitary transformation, i.e., without loss of generality, the dimensionful coupling constant J can be chosen to be positive.

Solution

$$\boldsymbol{H}_{XXZ}(-J,-\Delta) = \boldsymbol{U}\, \boldsymbol{H}_{XXZ}(J,\Delta)\, \boldsymbol{U}^{-1} \ , \qquad \boldsymbol{U} = \exp\Big(\frac{\mathrm{i}\pi}{2}\sum_{j=1}^{N} j\, \sigma^z_j\Big)$$

Exercise II.3: Show that the energies in the XXZ spin chain can be calculated using the formula

$$E_{XXZ}/J = -N\Delta + 4\sum_{j=1}^{\frac{N}{2}-S^z}\big(\Delta - \cos(p_j)\big) \ , \tag{16}$$

where

$$\mathrm{e}^{\mathrm{i}p_j} = q\, \frac{1 - q^{-1}\lambda_j^2}{1 - q\lambda_j^2} \ . \tag{17}$$

Exercise II.4: (a) Show that the BA equations (8) with $I_j = -\frac{n+1}{2}+j$ can be brought to the form of the extremum condition

$$\frac{\partial Y^{(N)}}{\partial x_j} = 0 \tag{18}$$

for the so-called the Yang-Yang functional

$$Y^{(N)}(x_1,\ldots,x_n) = \sum_j \Big(V(x_j) - \frac{\theta x_j}{\pi}\Big) + \frac{1}{2}\sum_{j\neq l} U(x_j - x_l)\ . \tag{19}$$

Here $V(x)$ and $U(x)$ stand for the functions

$$V(x) = -\frac{N}{2\pi}\,⨍_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega^2}\ \frac{\sinh(\frac{\pi\omega g}{2})}{\sinh(\frac{\pi\omega}{2})}\ \mathrm{e}^{\mathrm{i}\omega x}\ , \tag{20}$$

and

$$U(x) = \frac{1}{\pi}\,⨍_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega^2}\ \frac{\sinh(\frac{\pi\omega g}{2})\cosh(\frac{\pi(1-g)\omega}{2})}{\sinh(\frac{\pi\omega}{2})}\ \mathrm{e}^{\mathrm{i}\omega x}\ , \tag{21}$$

where the symbol $⨍$ denotes the principal value integral.

(b) Show that $U(x)$ and $V(x)$ for $x\in\mathbb{R}$, are real, continuous, even functions such that

$$\begin{aligned} U(x) &\ \to\ -g\,|x| + O\big(\mathrm{e}^{-2|x|}\big)\ , &\qquad \text{as}\quad x\to\pm\infty \\ V(x) &\ \to\ +\frac{Ng}{2}\,|x| + O\big(\mathrm{e}^{-2|x|}\big)\ , &\qquad \text{as}\quad x\to\pm\infty\ . \end{aligned} \tag{22}$$

Thus the BA eqs.(8) with $I_j = -\frac{n+1}{2}+j$ can be interpreted as an equilibrium condition for the system of N one-dimensional "electrons" in the presence of confining and linear external potentials. For large separations, $x \gg 1$, the 2-body potential $U(x)$ (21) is essentially a 1D repulsive Coulomb potential slightly modified at short distances. At the same time $V(x)$ (20) can be interpreted as the potential produced by the heavy positive charge $+\frac{Ng}{2}$ placed at $x=0$. In order to have an equilibrium configuration, the external linear potential $-\frac{\theta}{\pi}\,x$ should be sufficiently weak:

$$\tfrac{|\theta|}{\pi g} < \tfrac{N}{2} - n + 1 = S^z + 1\ . \tag{23}$$

(c) Show that for $0<g<\frac{1}{2}$ the Hessian of the system (19), $\frac{\partial^2 Y^{(N)}}{\partial x_j \partial x_n}$, is positive definite.

Exercise II.5. (a) Show that for $g=\frac{1}{2}$, the vacuum Bethe roots are given by equation

$$\mathrm{e}^{2x_j} = \tan\Big[\tfrac{\pi}{N}\Big(j - \tfrac{1}{2} + \big(\tfrac{\theta}{2\pi g} + \tfrac{1}{2}\,S^z\big)\Big)\Big]\qquad (j=1,2,\ldots,n)\ . \tag{24}$$

Notice that x_1 goes to $-\infty$ as $\big(-\frac{\theta}{2\pi g}\big) \to \frac{1}{2}\,(S^z+1)$. Using the result of the previous exercise interpret this observation. Also notice that, in the case $g=\frac{1}{2}$

$$
\begin{aligned}
\rho_j &= \lim_{N\to\infty} N\mathrm{e}^{+2x_j} = \pi\,\Big[\,j-\tfrac{1}{2}+\big(+\tfrac{\theta}{2\pi g}+\tfrac{1}{2}\,S^z\big)\Big] \qquad (j=1,2,\ldots\ -\ \text{fixed}) \qquad (25)\\
\bar{\rho}_{\bar{j}} &= \lim_{N\to\infty} N\mathrm{e}^{-2x_{n-\bar{j}}} = \pi\,\Big[\,\bar{j}-\tfrac{1}{2}+\big(-\tfrac{\theta}{2\pi g}+\tfrac{1}{2}\,S^z\big)\Big] \qquad (\bar{j}=1,2,\ldots\ -\ \text{fixed})
\end{aligned}
$$

(b) Show that the vacuum energy for the XXZ spin chain with $\Delta=0$ is given by

$$
E_{XXZ} = -4J\sum_{j=1}^{\frac{N}{2}-S^z}\cos(p_j)\ , \qquad p_j = \tfrac{\pi}{2}-\tfrac{2\pi}{N}\Big(j-\tfrac{1}{2}+\big(\tfrac{\theta}{\pi}+\tfrac{1}{2}\,S^z\big)\Big)\ . \tag{26}
$$

Exercise II.6. Using the results of the previous two exercises, write a code for the iterative solution of the vacuum BA equations for $0<g<\frac{1}{2}$. The initial position of the roots can be approximated by

$$
x_j \approx (1-g)\,\log\bigg(\tan\Big[\tfrac{\pi}{N}\Big(j-\tfrac{1}{2}+\big(\tfrac{\theta}{2\pi g}+\tfrac{1}{2}\,S^z\big)\Big)\Big]\bigg) \qquad (j=1,2,\ldots,n)\ . \tag{27}
$$

Exercise II.7. In the thermodynamic limit, $N\to\infty$, the number of Bethe roots goes to infinity and they form a density. Using the numerical solution of the BA equation demonstrate that for large N and finite S^z, the distribution of the BA roots

$$
D^{(N)}(x_{n+\frac{1}{2}}) = \frac{2}{N(x_{n+1}-x_n)} \qquad \big(\,x_{n+\frac{1}{2}} \equiv \tfrac{1}{2}\,(\,x_{n+1}+x_n\,)\,\big)\ , \tag{28}
$$

is well approximated by the continuous density $D(x)$.

(a) Using the result of Exercise II.5 show that for $g=\frac{1}{2}$

$$
D(x) = \frac{2}{\pi}\,\frac{1}{\cosh(2x)}\ . \tag{29}
$$

(b) Show that for any $0<g<1$.

$$
D(x) = \frac{1}{\pi(1-g)}\,\frac{1}{\cosh(\frac{x}{1-g})}\ . \tag{30}
$$

Exercise II.8. Show that

$$
\rho_j^{\frac{1}{2(1-g)}} = \pi\,j+O(1)\ , \quad \bar{\rho}_{\bar{j}}^{\frac{1}{2(1-g)}} = \pi\,\bar{j}+O(1) \qquad \text{as}\quad j,\ \bar{j}\to\infty\ . \tag{31}
$$

Exercise II.8. One also has the following relations involving the function $\Theta_k(\omega)$ introduced in Exercise I.5:

$$
\begin{aligned}
\sum_{j=1}^{\infty}\rho_j^{-\frac{\mathrm{i}\,\omega}{2(1-g)}} &= \frac{\Gamma(\frac{\mathrm{i}\omega}{2\alpha})\Gamma(-\frac{1}{2}+\frac{\mathrm{i}\omega}{2})}{\sqrt{\pi}\ 2^{1+\mathrm{i}\omega}\ \Gamma(\frac{\mathrm{i}(1+\alpha)\omega}{2\alpha})}\,(C)^{-\frac{\mathrm{i}\omega(1+\alpha)}{2\alpha}}\ \Theta_k(\omega)\\
\sum_{j=1}^{\infty}\bar{\rho}_j^{-\frac{\mathrm{i}\,\omega}{2(1-g)}} &= \frac{\Gamma(\frac{\mathrm{i}\omega}{2\alpha})\Gamma(-\frac{1}{2}+\frac{\mathrm{i}\omega}{2})}{\sqrt{\pi}\ 2^{1+\mathrm{i}\omega}\ \Gamma(\frac{\mathrm{i}(1+\alpha)\omega}{2\alpha})}\,(C)^{-\frac{\mathrm{i}\omega(1+\alpha)}{2\alpha}}\ \Theta_{\bar{k}}(\omega)\ ,
\end{aligned}
$$

where it is assumed that $\Im m(\omega) < -1$ and

$$k = \tfrac{1}{2}\left(S^z + \tfrac{\theta}{g}\right) , \qquad \bar{k} = \tfrac{1}{2}\left(S^z - \tfrac{\theta}{g}\right) . \tag{32}$$

References

[1] R. J. Baxter, "Exactly solved models in statistical mechanics"