Student Seminar on Quantum Integrability - Lecture 4: the Heisenberg XXZ model

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1 Introduction

These notes are written for a student seminar on quantum integrability, held at Utrecht University during the first semester of the academic year 2013/2014. The goal of the seminar was to make the journey from the Coordinate Bethe Ansatz (henceforth abbreviated by CBA) technique applied to Heisenberg models, via the techniques of transfer matrices and the Yang-Baxter equation to the Algebraic Bethe Ansatz technique developed in the 1980s.

The audience was a group of graduate mathematics and theoretical physics students. After two introductory lectures by dr. G. Arutyunov and dr. A. Henriques, the lectures were continued by the students. The first lecture was given by N. Plantz, in which he applied the CBA technique to the Heisenberg XXX model. The second lecture is the subject of these notes.

First a short recapitulation of the previous lecture is given and its important points and conclusion are stressed. Following, the Heisenberg XXZ model is introduced and its physics is discussed. Next, the CBA technique for general M will be applied to the XXZ model. The resulting equations are written in terms of rapidities, in which one encounters them most often. Finally, we conclude with a discussion of the existence and uniqueness of solutions to Heisenberg models in general.

2 Recapitulation of the XXX model and the Coordinate Bethe Ansatz

The Heisenberg XXX model is defined by introducing its Hamiltonian:

$$\hat{H} = -J\sum_{n=1}^{L} \vec{S}_n \cdot \vec{S}_{n+1} = -J\sum_{n=1}^{L}\left(\frac{1}{2}(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) + S_n^z S_{n+1}^z\right), \tag{1}$$

where $S^{\pm}$ are the usual spin flip operators and we take periodic boundary conditions: $S_n^{\alpha} = S_{n+L}^{\alpha}$. It was shown that the XXX Hamiltonian commutes with the total spin operator in all directions, i.e. $[\hat{H}, \sum_i^L S_i^{\alpha}] = 0$, for $\alpha = x, y, z$. As the Hamiltonian is defined with periodic boundary conditions we have translational symmetry. Thus, the symmetry group is given by:

$$G = \mathbb{Z}/L\mathbb{Z} \times SU(2). \tag{2}$$

Using only $U_z(1)$ symmetry, the total spin in the z-direction can be written as $L/2$ minus the number of spin flips M (= # magnons) and the associated Hilbert space can be written as a direct sum:

$$S_{tot}^z = \frac{L}{2} - M \quad \text{and} \quad \mathcal{H} = \bigoplus_{M=0}^{L} \mathcal{H}_M \tag{3}$$

Solving the model for $M = 1$ can be done by making a plane wave Ansatz:

$$|\psi_k\rangle = \sum_n f(n) |n\rangle \text{ with } f(n) = e^{ikn}, \tag{4}$$

using the convenient notation $|n\rangle := S_n^- |0\rangle$, with $|0\rangle := |\uparrow\uparrow \ldots \uparrow\rangle$ the ground state of the system. This then yields an energy of

$$E = E_0 + J(1 - \cos k) \quad \text{with} \quad E_0 := \frac{-JL}{4}. \tag{5}$$

Note that the states $|0\rangle$ and $|\psi(k = 0)\rangle$ have the same energy. This degeneracy is of course a consequence of the fact that we haven't used the full $SU(2)$ symmetry group in our description. For the case $M = 2$ an Ansatz of plane waves turned out to be not enough, i.e.

$$|\psi_{k_1,k_2}\rangle = \sum_{n_2>n_1} f(n_1, n_2) |n_1, n_2\rangle, \tag{6}$$

but the form function is now of the form

$$f(n_1, n_2) = A(k_1, k_2)e^{i(k_1 n_1 + k_2 n_2)} + B(k_1, k_2)e^{i(k_1 n_2 + k_2 n_1)}. \tag{7}$$

Note that the second term, with amplitude B, contains permutations of the two momenta. We will later generalize this to the general M case, yielding $M!$ permutations of momenta and the CBA. Demanding that this new Ansatz is an eigenstate yields a constraint on the amplitudes:

$$e^{i\theta(k_1,k_2)} := \frac{A}{B} = -\left(\frac{e^{i(k_1+k_2)} + 1 - 2e^{ik_1}}{e^{i(k_1+k_2)} + 1 - 2e^{ik_2}}\right) \tag{8}$$

Demanding periodicity of our solutions amounts to: $f(n_1, n_2) = f(n_2, n_1 + L)$, giving:

$$\begin{cases} k_1 L = \theta + 2\pi m_1, & m_1 \in \{0, \ldots, L-1\} \\ k_2 L = -\theta + 2\pi m_2, & m_2 \in \{0, \ldots, L-1\} \end{cases} \tag{9}$$

and an energy of

$$E = J \sum_{i=1}^{M} (1 - \cos k_i) + E_0. \tag{10}$$

Solving this XXX model for $M = 2$ now amounts to two things:

1. Find $1/2L(L-1)$ different pairs $m_i \in \mathbb{Z}/L\mathbb{Z}$ such that
2. equations (1) and (2) can be solved uniquely for $\vec{k} \in \mathbb{C}^2$.

If these conditions are obeyed, equation (3) can be used to find the energy of the eigenstate.

3 Physics of the Heisenberg XXZ model

3.1 Introducing the XXZ model

The Heisenberg XXZ model differs from the XXX model by the introduction of an anisotropy parameter Δ:

$$\begin{aligned}\hat{H}_{XXZ} &= -J\sum_{j=1}^{L}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta(S_j^z S_{j+1}^z - \frac{1}{4})\right) - 2h\sum_{j=1}^{L} S_j^z \\ &= -J\sum_{j=1}^{L}\left(\frac{1}{2}(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) + \Delta(S_j^z S_{j+1}^z - \frac{1}{4})\right) - 2h\sum_{j=1}^{L} S_j^z\end{aligned}$$

Note the differences with the above Hamiltonian and the XXX Hamiltonian 1: besides the introduction of Δ we have shifted the energy by $-E_0$. This will turn out to be convenient later. Furthermore, the last term represents the magnetization of the system due to an external magnetic field. This term comes for 'free' in the model, as it does not make the solving of the model more difficult. Henceforth we will omit it and indicate how the expressions change for $h \neq 0$. One can easily verify that this Hamiltonian only has $U_z(1)$ rotational symmetry:

$$\begin{aligned}[\hat{H}_{XXZ}, \sum_{i=1}^{L} S_j^z] &= -J\sum_{i,j=1}^{L}\left(S_j^x[S_{j+1}^x, S_i^z] + [S_j^x, S_i^z]S_{j+1}^x + S_j^y[S_{j+1}^y, S_i^z] + [S_j^y, S_i^z]S_{j+1}^y + 0\right) \\ &= -Ji\sum_{j=1}^{L}\left(-S_j^x S_{j+1}^y - S_j^y S_{j+1}^x + S_j^y S_{j+1}^x + S_j^x S_{j+1}^y\right) \\ &= 0,\end{aligned}$$

where we used the commutation relations $[S_n^\alpha, S_{n'}^\beta] = i\epsilon_{\alpha\beta\gamma}S^\gamma\delta_{nn'}$. Taking the commutator with the total spin in the x or y direction, one easily sees that precisely because of the anisotropy term Δ, the commutator will not yield zero. Because we still have $U_z(1)$ symmetry we may solve the XXZ Hamiltonian in a similar way as the XXX model, namely by using the $U_z(1)$ symmetry to write the Hilbert space as a direct sum of subspaces. In this case we do not expect degeneracies, as we are using the full available symmetry group. Furthermore, one can show that there exists a similarity transformation U such that:

$$-\hat{H}_{XXZ}(-\Delta) = U\hat{H}_{XXZ}(\Delta)U^{-1}. \tag{11}$$

This unitary similarity transformation is given by (assuming even L):

$$U = \prod_{m=1}^{L/2} S_{2m}^z \qquad \Rightarrow \qquad U^{-1} = U^\dagger = \prod_{m=1}^{L/2} S_{2m}^z. \tag{12}$$

As S^z commutes with itself on every lattice site and $(S_i^z)^2 = \mathrm{id}$, we immediately see that the similarity transformation is trivially satisfied for the third term in the XXZ Hamiltonian. For the first and second term we have to do a little effort:

$$\begin{aligned}
\prod_{m=1}^{L/2} S_{2m}^z \sum_{i=1}^{L} S_i^x S_{i+1}^x \prod_{k=1}^{L/2} S_{2k}^z &= 4\sum_{i=1}^{L/2} S_{2i}^z S_{2i}^x S_{2i+1}^x S_{2i}^z + 4\sum_{i=1}^{L/2} S_{2i}^z S_{2i-1}^x S_{2i}^x S_{2i}^z \\
&= 2i\sum_{i=1}^{L/2} S_{2i}^y S_{2i+1}^x S_{2i}^z - 2i\sum_{i=1}^{L/2} S_{2i}^z S_{2i-1}^x S_{2i}^y \\
&= -\sum_{i=1}^{L/2} \left(S_{2i}^x S_{2i+1}^x + S_{2i-1}^x S_{2i}^x \right) \\
&= -\sum_{i=1}^{L} S_i^x S_{i+1}^x ,
\end{aligned}$$

where we used $(S_i^\alpha)^2 = 4\mathrm{id}$, $S^\alpha := 1/2\sigma^\alpha$, $\sigma^z\sigma^x = i\sigma_y$ and similar relations. For the second part in the Hamiltonian the proof is exactly the same. Thus indeed equation (11) holds. Because we have this similarity transformation, we can conclude that the Hamiltonians $-\hat{H}(-\Delta)$ and $\hat{H}(\Delta)$ can be diagonalized in the same basis. Of course, if they have the same basis, the physics of both is the same. This leads us to the conclusion that the we are only considered with the relative sign of the parameters J and Δ. By letting $-\infty < \Delta < \infty$ we may omit the coupling constant J. Some literature includes it, some does not. In these notes, we choose to include it.

3.2 Some limiting/special cases of the XXZ model

Let us now consider some interesting limiting cases for the anisotropy parameter in the Heisenberg XXZ Hamiltonian.

- $\Delta = 1$: we obtain the XXX Hamiltonian, for which we have already written down the Bethe Ansatz equations.
- $\Delta = 0$ yields the so-called XX model. Via a *Jordan-Wigner transformation*, one can map this model to free fermions on a lattice. To do this, we introduce fermionic

operators:

$$\begin{cases} S_j^- = (-1)^j e^{i\pi\theta_j} c_j^\dagger \\ \\ S_j^+ = (-1)^j e^{-i\pi\theta_j} c_j \\ \\ S_j^z = \frac{1}{2} - c_j^\dagger c_j \\ \\ \theta_j = \sum_{l=1}^{j-1} c_l^\dagger c_l, \end{cases} \tag{13}$$

such that one has $\{c_{j_1}, c_{j_2}^\dagger\} = \delta_{j_1 j_2}$ and we thus indeed have sermonic creation and annihilation operators. Plugging these transformation into the XX Hamiltonian yields

$$\hat{H}_{XX} = \frac{J}{2} \sum_{i=1}^{L} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right). \tag{14}$$

Defining the Fourier transform as

$$c_j = \frac{1}{L} \sum_k e^{ik_n j} \tilde{c}_k$$

(and the hermitian conjugate similar) yields for the Hamiltonian:

$$\hat{H}_{XX} = \frac{J}{L} \sum_k (\cos k) \tilde{c}_k^\dagger \tilde{c}_k, \tag{15}$$

where $J/L \cos k =: \epsilon_k$ is the single particle dispersion relation. We now recognize the standard expression in Fourier space for a Hamiltonian describing non-interacting free fermions on a lattice. The lowest energy excitations are the familiar particle-hole excitations.

- $J\Delta \to \infty$ yields the well-known Ising model, of which the ground state is $|\uparrow\uparrow \dots \uparrow\rangle$. The lowest energy excitations have one spin flipped down, which yields a state of the form $|\uparrow\uparrow \dots \uparrow\downarrow\uparrow \dots \uparrow\rangle$. Such a state is referred to as a one-magnon state. All the other ones can be generated by a permutation of the one down spin over the lattice sites. Note that the magnon is a boson as the ground state has total spin $L/2$ in the z-direction, whereas the one-magnon state has total spin $1/2(L-1) - 1/2 = L/2 - 1$. Thus the magnon has spin $S = 1$ and is a boson.

- $J\Delta \to -\infty$ yields an anti-ferromagnetic Ising model, with two ground states: $|\uparrow\downarrow\uparrow\downarrow \dots\rangle$ and $|\downarrow\uparrow\downarrow\uparrow \dots\rangle$, which are called Néel states. The lowest energy excitations of these ground states are called domain walls, which look like $|\uparrow\downarrow\uparrow \dots \uparrow\downarrow\downarrow\uparrow \dots \uparrow\downarrow\rangle$.

- $J\Delta > 0$ and $|\Delta| > 1$ yields a ferromagnet along the z-direction. We can deduce this as the overall sign of the Hamiltonian is negative, yielding a preference for alignment. Furthermore, the fact that $|\Delta| > 1$ represents a dominance of the z-term as opposed to the x and y terms in the Hamiltonian, so that we may neglect the latter two.
- $J\Delta < 0$ and $|\Delta| > 1$ yields an overall plus sign of the Hamiltonian, thus favoring misalignment. Thus we have an anti-ferromagnet along the z-direction.
- $J\Delta \neq 0$ and $|\Delta| < 1$: now the configuarations in the XY-plane energetically dominate those in the z-direction and depending on the overall sign of the Hamiltonian we get (mis)alignment in the XY-plane, also called the planar regime.

4 Coordinate Bethe Ansatz for $\Delta \neq 1$

4.1 Reconsidering the $M = 2$ case

Before we consider the general M case, let us consider the $M = 2$ case briefly and generalize this later on. In the $M = 2$ case it is easiest to consider two separate cases, one being the case of separated down spins and one the case of adjacent down spins. Again we use the expression (6) and demand that $\hat{H}_{XXZ} |\psi\rangle = E_2 |\psi\rangle$. Projecting the resulting equation on the bra $\langle n_1, n_2|$ yields the equation

$$-\frac{J}{2}\left(f(n_1-1,n_2)+f(n_1+1,n_2)+f(n_1,n_2-1)+f(n_1,n_2+1)\right)=(E_2-2J\Delta)f(n_1,n_2). \tag{16}$$

This equation only holds for $2 < n_1 + 1 < n_2 < L$. Following the same procedure, the case of two adjacent down spins yields:

$$-\frac{J}{2}\left(f(n_1-1,n_2)+f(n_1,n_2+1)\right)=(E_2-J\Delta)f(n_1,n_2), \tag{17}$$

which only holds under the condition $2 < n_1 + 1 = n_2 < L$. Note that this second equation is in fact not allowed, as we wrote the eigenstate down for $n_1 < n_2$. For now, we continue and plug into (16) the same Ansatz as the $M = 2$ case for $\Delta = 1$. This immediately yields the energy:

$$E_2 = J(2\Delta - \cos k_1 - \cos k_2). \tag{18}$$

Note the disappearing of the E_0 term because of our shift of the ground state energy and the appearance of the anisotropy parameter Δ. Now the trick is to make a second Ansatz, constituting of extending the first Ansatz to the case $n_1 \leq n_2$. Plugging the obtained energy and the second Ansatz into equation (17) yields a condition of the following form

$$e^{i\phi(k_1,k_2)} := \frac{A}{B} = -\left(\frac{e^{i(k_1+k_2)}+1-2\Delta e^{ik_1}}{e^{i(k_1+k_2)}+1-2\Delta e^{ik_2}}\right), \tag{19}$$

such that our Ansatz is correct if this relation is obeyed. Note again the appearance of the anisotropy parameter in the equation above, as opposed to equation (8). Using this to rewrite our Ansatz we obtain:

$$f(n_1, n_2) = e^{i(k_1 n_1 + k_2 n_2 + \frac{1}{2}\phi(k_1,k_2))} + e^{i(k_1 n_2 + k_2 n_1 - \frac{1}{2}\phi(k_1,k_2))} \tag{20}$$

Demanding periodicity via $f(n_1, n_2) = f(n_2, n_1 + L)$ immediately yields

$$\begin{cases} e^{k_1 L} = -e^{i\phi(k_1,k_2)} \\ e^{ik_2 L} = -e^{-i\phi(k_1,k_2)} \end{cases}, \tag{21}$$

which are called the (exponential) Bethe Ansatz Equations. Taking the logarithm yields the logarithmic Bethe Ansatz Equations:

$$\begin{cases} k_1 L + \phi(k_1, k_2) = 2\pi I_1 & \text{with } I_1 \in \mathbb{N} + \frac{1}{2} \\ k_2 L - \phi(k_1, k_2) = 2\pi I_2 & \text{with } I_2 \in \mathbb{N} + \frac{1}{2} \end{cases}, \tag{22}$$

Now that we understand the $M = 2$ case, we can easily generalize to the general M case.

4.2 The general M case

Using the analogue of the $M = 2$ case we can immediately write down the generalized equation for no adjacent down spins:

$$-\frac{J}{2}\sum_{a=1}^{M} \left(f(n_1, \ldots, n_a - 1, \ldots n_M) + f(n_1, \ldots, n_a + 1, \ldots, n_M)\right) = (E_M - J\Delta M) f(n_1, \ldots, n_M), \tag{23}$$

which holds for $n_a + 1 < n_a$ and for all $a \in \{1, \ldots M\}$. In the general M case we can have many possible other states, e.g. a block of more than two down spins adjacent and the rest well-seperated or several blocks of down spins. However we again consider the case where only two spins are adjacent, i.e. : there is precisely one $a \in \{1, \ldots M\}$ such that $n_a + 1 = n_{a+1}$. This generalization of the $M = 2$ case is a little less straight forward and yields

$$\begin{aligned} &(E_M - J\Delta) f(n_1, \ldots, n_M) = \\ &-\frac{J}{2}\left(\sum_{a \neq k, k+1}^{M} f(n_1, \ldots, n_a - 1, \ldots, n_M) + f(n_1, \ldots, n_a + 1, \ldots, n_M) - 2\Delta f(n_1, \ldots, n_M)\right) \\ &-\frac{J}{2}\left(f(n_1, \ldots, n_k - 1, n_k + 1, \ldots, n_M) + f(n_1, \ldots, n_k, n_k + 2, \ldots, n_M)\right) \end{aligned} \tag{24}$$

Now let us introduce the Bethe Ansatz for the M-particle sector:

$$f(n_1, \ldots, n_M) = \sum_{\mathcal{P} \in S_M} A_{\mathcal{P}} \exp\left(i \sum_{j=1}^{M} k_{\mathcal{P}(j)} n_j \right), \tag{25}$$

where $\mathcal{P}$ is a permutation of S_M. There are $M!$ of such elements. Plugging this Ansatz into equation (23) yields the energy:

$$E_M = J \sum_{a=1}^{M} (\Delta - \cos k_a). \tag{26}$$

which as an obvious generalizaton of the $M = 2$ case. We can proceed by extending the Ansatz in the same way as we did for $M = 2$. We plug the Ansatz and the formula for the energy into equation (24). Again we find a condition on the amplitudes $A_{\mathcal{P}}$. Consider two permutations $\mathcal{Q}$ and $\mathcal{P}$, which differ by switching the momenta associated to two neighbors [1]

$$\mathcal{Q} = \mathcal{P}_{\mathcal{P}(j), \mathcal{P}(j+1)} \mathcal{P}, \tag{27}$$

such that our Ansatz yields an eigenstate if and only if:

$$A_{\mathcal{P}} = A_{\mathcal{Q}} e^{i\Phi(k_{\mathcal{P}_j}, k_{\mathcal{P}_{j+1}})}, \tag{28}$$

where Φ is the by now familiar *exchange phase*:

$$e^{i\Phi(k,k')} := \frac{A_{\mathcal{P}}}{A_{\mathcal{Q}}} = -\left(\frac{e^{i(k+k')} + 1 - 2\Delta e^{ik}}{e^{i(k+k')} + 1 - 2\Delta e^{ik'}} \right). \tag{29}$$

The momentum vectors k and k' in the equation above differ by one permutation. Again we have found factorized scattering: the sacttering of M particles (magnons) has reduced to the pairwise scattering of two magnons! Using equations (28) and (29) one can find a closed formula for the coefficients $A_{\mathcal{P}}$ as a phase. Just as in the $M = 2$ case we can use this write the Bethe Ansatz more explicitly as:

$$f(n_1, \ldots, n_M) = \sum_{\mathcal{P} \in S_M} (-1)^{|\mathcal{P}|} \exp\left(i \sum_{j=1}^{M} k_{\mathcal{P}(j)} n_j - \frac{i}{2} \sum_{1 \le b < a \le M} \Phi(k_{\mathcal{P}_a}, k_{\mathcal{P}_b}) \right), \tag{30}$$

where $|\mathcal{P}|$ represents the parity of the permutation. By invoking periodicity ($f(n_1, \ldots, n_M) = f(n_2, \ldots, n_M, n_1 + L)$) we can find the exponential Bethe Ansatz equations for the general

[1] Notation and argument taken from section 2.2.2. of *Dynamics of Heisenberg spin chains*, PhD thesis R. Hagemans, supervisor prof. J-S Caux

M case:

$$\begin{aligned}
\sum_{\mathcal{P}} A_{\mathcal{P}} e^{i\sum_{j=1}^{M} k_{\mathcal{P}_j} n_j} &= \sum_{\mathcal{P}} A_{\mathcal{P}} e^{ik_{\mathcal{P}_M} L} e^{i\sum_{j=1}^{M} k_{\mathcal{P}_j} n_j} \Leftrightarrow \\
\sum_{\mathcal{P}} (-1)^{M-1} A_{\mathcal{P}_1\mathcal{P}_M\ldots\mathcal{P}_1\mathcal{P}_2} e^{i\sum_{j=1}^{M} k_{\mathcal{P}_j} n_j} &= \sum_{\mathcal{P}} A_{\mathcal{P}} e^{ik_{\mathcal{P}_M} L} e^{i\sum_{j=1}^{M} k_{\mathcal{P}_j} n_j} \Rightarrow \\
(-1)^{M-1} A_{\mathcal{P}_1\mathcal{P}_M\ldots\mathcal{P}_1\mathcal{P}_2} &= A_{\mathcal{P}} e^{ik_{\mathcal{P}_M} L} \Rightarrow \\
(-1)^{M-1} A_{\mathcal{P}} e^{-i\sum_\alpha \Phi(k_\alpha, k_\beta)} &= A_{\mathcal{P}} e^{ik_{\mathcal{P}_M} L},
\end{aligned}$$

such that we find $\forall \mathcal{A}_{\mathcal{P}}$ the exponential Bethe Ansatz equations:

$$e^{ik_\beta L} = (-1)^{M-1} e^{-i\sum_\alpha \Phi(k_\alpha, k_\beta)}. \tag{31}$$

Again, we can write down the logarithmic Bethe Ansatz equations by carefully taking the complex logarithm:

$$Lk_\alpha + \sum_\alpha \Phi(k_\alpha, k_\beta) = 2\pi I_\alpha \qquad \text{where} \qquad I_\alpha = \begin{cases} \in \mathbb{Z} & \text{when } L-M \text{ odd} \\ \in \mathbb{Z} + \frac{1}{2} & \text{when } L-M \text{ even} \end{cases}, \tag{32}$$

where the values for I_a are chosen such that the minus sign is correctly obtained after taking the complex logarithm. (It effectively follows from the $(-1)^{M-1}$ term in the exponential Bethe Ansatz equations.)

Note that in this procedure we have only considered the two different cases of all spins separated and one pair of spins adjacent. Using only these two cases, we have been able to generalize the exponential and logarithmic Bethe Ansatz equations. In fact we should consider all different possible cases and infer that the equations we found are still consistent. We shall omit this for now.

5 Coordinate Bethe Ansatz equations in terms of rapidities

In this section we will introduce a convenient parametrization of the Bethe Ansatz equations in terms of *rapidities* (denoted by λ). The Bethe Ansatz equations are most often found in this form in the literature. However, there are a lot of different parametrizations floating around, so the reader must take care. The convenience of the parametrization in terms of the rapidities comes from the fact that the two-particle scattering phase becomes a function of the difference: $\Phi(k, k') \Rightarrow \Phi(\lambda, \lambda') = \Phi(|\lambda - \lambda'|)$. In principle, one has to do the parametrization for all values of Δ to have the most general XXZ model. We shall only consider the values of Δ which are most interesting to us: $-1 < \Delta \leq 1$.

5.1 The case $|\Delta| < 1$

In this case we parametrize the anisotropy parameter as

$$\Delta = \cos\zeta \qquad \text{for} \qquad \zeta \in (0, 2\pi). \tag{33}$$

Now one can introduce a rapidity λ_a (belonging to the associated momentum k_a) implicitly as follows:

$$e^{ik_a} = \frac{\sinh(\lambda_a + i\zeta/2)}{\sinh(\lambda_a - i\zeta/2)}, \tag{34}$$

such that we only have to take this to the power L to obtain the right-hand side of the exponential Bethe Ansatz equations (31). For the left-hand side we must do some more work and plug in the above equation for the rapidity into the formula for the exchange phase (29). By writing out the complex exponentials, plugging in the parametrization for the anisotropy parameter Δ in terms of complex exponentials and some tedious book-keeping, one finds that the exchange phase becomes a function of the difference of the rapidities only. This is just as we claimed above:

$$e^{i\Phi(k_a,k_b)} = \frac{\sinh(\lambda_a - \lambda_b + i\zeta)}{\sinh(\lambda_a - \lambda_b - i\zeta)}. \tag{35}$$

Such that we find for the exponential Bethe Ansatz equations in terms of the rapidities:

$$\left(\frac{\sinh(\lambda_a + i\zeta/2)}{\sinh(\lambda_a - i\zeta/2)}\right)^L = \prod_{b\neq a}^{M} \frac{\sinh(\lambda_a - \lambda_b + i\zeta)}{\sinh(\lambda_a - \lambda_b - i\zeta)}. \tag{36}$$

We can also write the logarithmic Bethe Ansatz equations in terms of rapidities. For this we take the logarithm of equation (34):

$$\begin{aligned}
\Phi(\lambda_a, \lambda_b) &= -i\ln\left(-\frac{\sinh(\lambda_a - \lambda_b - i\zeta)}{\sinh(\lambda_a - \lambda_b + i\zeta)}\right) \\
&= -i\ln\left(-\frac{\sin(i(\lambda_a - \lambda_b) + \zeta)}{\sin(i(\lambda_a - \lambda_b) - \zeta)}\right) \\
&= -i\ln\left(\frac{\tan\zeta + i\tanh(\lambda_a - \lambda_b)}{\tan\zeta - i\tanh(\lambda_a - \lambda_b)}\right) \\
&= 2\arctan\left(\frac{\tanh(\lambda_a - \lambda_b)}{\tan\zeta}\right),
\end{aligned}$$

where we used several triogonometic identities for functions of complex numbers, which can be found in appendix A. Similarly, one finds for the momenta:

$$k_a = 2\arctan\left(\frac{\tanh\lambda_a}{\tan(\zeta/2)}\right), \tag{37}$$

such that we obtain for the logarithmic Bethe Ansatz equations in terms of rapidities:

$$L\phi_1(\lambda_a) - \sum_{b=1}^{M} \phi_2(\lambda_a - \lambda_b) = 2\pi I_a, \tag{38}$$

where we defined:

$$\phi_n(\lambda) := 2\arctan\left(\frac{\tanh(\lambda)}{\tan(\frac{n\zeta}{2})}\right). \tag{39}$$

5.2 The case $|\Delta| = 1$

Taking the limit $\Delta \to 1 \Leftrightarrow \zeta \to 0$ in equation (36) yields a pointless expression of the form "1=1". Thus we have to do better than that. We can extend our previous results be defining the $\Delta = 1$ case via a limiting procedure as follows:

$$f(\lambda_{|\Delta|=1}) = \lim_{\zeta\to 0} \frac{f(\lambda_{|\Delta|<1})}{\zeta}, \tag{40}$$

by which we mean that every function, which is a function of the anisotropy, in the case $|\Delta| < 1$, can be extended to a function depending on $\Delta = 1$ by the limiting procedure above. By plugging this into the exponential Bethe Ansatz equations written in terms of rapidities, we get for the right-hand side:

$$\lim_{\zeta\to 0} \frac{\sinh(\zeta(\lambda_a - \lambda_b + i))}{\sinh(\zeta(\lambda_a - \lambda_b - i))} = \lim_{\zeta\to 0} \frac{\cosh(\zeta(\lambda_a - \lambda_b + i))}{\cosh(\zeta(\lambda_a - \lambda_b - i))} \frac{\lambda_a - \lambda_b + i}{\lambda_a - \lambda_b - i} = \frac{\lambda_a - \lambda_b + i}{\lambda_a - \lambda_b - i}, \tag{41}$$

where the reader should note that we plugged in $\lambda_{|\Delta|<1} = \zeta\lambda_{|\Delta|=1}$ (this is legit provided we take the limit, which we do) into the RHS of the Bethe Ansatz equations, omitted the subscript '$|\Delta = 1|$' and calculated the limit by using the rule of l'Hôpital. This leads to the exponential Bethe Ansatz equations in terms of rapidities for the $|\Delta| = 1$ case:

$$\left(\frac{\lambda_a + i/2}{\lambda_a - i/2}\right)^L = \prod_{b\neq a}^{M} \frac{\lambda_a - \lambda_b + i}{\lambda_a - \lambda_b - i} \tag{42}$$

We may similarly show how the argument of the characteristic function $\phi_n(\lambda)$ changes:

$$\lim_{\zeta\to 0} \frac{\tanh(\lambda\zeta}{\tan(n\zeta/2)} = \lim_{\zeta\to 0}(1 - \tanh^2(\lambda\zeta))\cos^2\left(\frac{n\zeta}{2}\right)\frac{n}{2} = \frac{n\lambda}{2}, \tag{43}$$

such that we can define a new characteristic function:

$$\psi_n(\lambda) := 2\arctan\left(\frac{2\lambda}{n}\right), \tag{44}$$

with which the logarithmic Bethe Ansatz equations for the case $|\Delta| = 1$ become:

$$L\psi_1(\lambda_a) - \sum_{b=1}^{M} \psi_2(\lambda_a - \lambda_b) = 2\pi I_a. \tag{45}$$

6 The existence of solutions to the XXZ and the XXX model

6.1 The meaning and nature of existence of solutions

It is very hard to prove the existence and uniqueness of complete solutions to either one of the Heisenberg models. Let us recall what we mean by solutions to these models. For the M-magnon sector we want to find exactly L choose M different $I \in (\mathbb{Z}/L\mathbb{Z})^M$, such that for every I we can find a unique $\vec{\lambda} \in \mathbb{C}^M$ that solves the Bethe Ansatz equations.

Contrary to a physicist's intuition, precisely the high symmetry of the XXX and XXZ model makes it hard to prove that there are solutions. An analogue in atomic physics might make this insightful. For the hydrogen atom, a lot of states are degenerate: they carry the same energy. However, if we put on a magnetic field, the degeneracies are lifted as the electrons with spins in certain orbits (mis)align with the magnetic field. This is the Zeeman effect. Breaking symmetries (in the case of a magnetic field time-reversal symmetry) thus lifts degeneracy. In our Heisenberg models one has a lot of symmetry and thus a lot of degeneracy. Because of this high degeneracy it is hard to find a complete set of eigenstates which can form a basis for the Hilbert space. If enough symmetry is broken, one can prove uniqueness and existence. In fact, in the case of anisotropy, a magnetic field and impurities along the chain length (i.e. no translation invariance) it has been proven that the resulting model has a unique solution [2] In this light we expect that the proof of existence and uniqueness of the XXZ model is easier than for the XXX case. This is indeed the case: the proof for the XXX has not been given yet, whereas there are proofs for the XXZ model.

Finally we should note that physicists are able to find complete, unique solutions to both the XXX and XXZ model for a given chain length L and given other parameters. However, a mathematician (or maybe a very ambitious theoretical physicist) would like to see a proof of existence and uniqueness for general parameters.

Let us now introduce some basic definitions and theorems on convexity, as we shall need this later for a flawed proof of the existence of a real, unique solution to the logarithmic Bethe Ansatz equations.

6.2 Some basic defintions and theorems concerning convexity

If we have a function $f : \mathbb{R} \to \mathbb{R}$ and we know $f(\bar{x}) = 0$, then knowing that $d^2f/dx^2 > 0$ globally makes us conclude that $\bar{x}$ is a global minimum of the function f. Can we generalize to the case at hand? For this we need some mathematical theorems and definitions. Proofs and more elaborate material of the following can be found e.g. in *"Nonlinear Programming:*

[2] See the article by Tarasov and Varchenko: *Completeness of Bethe Vectors and Difference Equations with Regular Singular Points*, Int. Math. Res., Nov 13 (1996), pp 637-669.

Theory and Algorithms" (3rd edition) by Bazaraa, Sherali and Shetty.

Definition 1. *A set $S \subset \mathbb{R}^n$ is called* convex *if $\forall x, y \in S$ and $\forall \lambda \in [0,1]$ we have that $\lambda x + (1-\lambda)y \in S$.*

Examples of convex sets are intervals $[a,b] \in \mathbb{R}$ and disks in $\mathbb{R}^2$. The unit circle $S^1 \subset \mathbb{R}^2$ is not convex.

Definition 2. *Let S be a convex set. A function $f : S \to \mathbb{R}$ is called a* convex function *if we have $\forall x, y \in S$ and $\forall \lambda \in [0,1]$ that $f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y)$.*

Definition 3. *Let S be a convex set. A function $f : S \to \mathbb{R}$ is called a* strictly convex function *if we have $\forall x \neq y \in S$ and $\forall \lambda \in (0,1)$ that $f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y)$.*

Convex functions can be interpreted as functions for which one can draw a line from one point on the graph of the function to another, such that the resulting line is lying above the graph in between the two points. Of course, it is important that one can do this for any two points. A simple convex function is $f(x) = x^2$, whereas a simple non-convex function is $f(x) = x^4 - x^2$.

Theorem 1. *Let S be a convex set, let $f : S \to \mathbb{R}$ be convex and let $\bar{x}$ be a local minimzer of f. Then $\bar{x}$ is a global minimzer of f over S.*

Proof. Suppose $\exists \bar{y} \in S$ such that $f(\bar{y}) < f(\bar{x})$. Define $y(\lambda) = \lambda\bar{x} + (1-\lambda)y$ and note that $y(\lambda) \in S$ for $\lambda \in [0,1]$. We have that $y(\lambda) \to \bar{x}$ as $\lambda \to 1$. Thus we have:

$$\begin{aligned} f(y(\lambda)) &= f(\lambda\bar{x} + (1-\lambda)y) \\ &\leq \lambda f(\bar{x}) + (1-\lambda)f(y) \\ &< \lambda f(\bar{x}) + (1-\lambda)f(\bar{x}) = f(\bar{x}) \qquad \forall \lambda \in (0,1) \end{aligned}$$

But then $\bar{x}$ is not a local minimizer. Proof by contradiction.

We can extend this result to an even more powerful result:

Theorem 2. *Let S be a convex set, let $f : S \to \mathbb{R}$ be strictly convex and let $\bar{x}$ be a local minimzer of f. Then $\bar{x}$ is a unique global minimzer of f over S.*

It is the uniqueness and existence of the above theorem we shall use in our proof for the Heisenberg XXZ model. We only need one more definition and one more theorem:

Definition 4. *A symmetric nxn real matrix M is called* positive definite *if $z^T M z > 0$ for any non-zero real column vector z.*

Theorem 3. *Let X be a non-empty, convex open set and let $f \in C^2(X, \mathbb{R})$. Then: f is strictly convex $\Leftrightarrow$ the Hessian of f is positive definite $\forall x \in X$.*

Proving that a function is convex has now become easy: one just needs to prove that it is positive definite. We shall use this in the following and combine it with the theorem on global, unique minimizers.

6.3 A flawed proof for the existence of solutions to the XXZ model

In this we follow the book by Korepin, Bogoliubov, Izergin. The reader is encouraged the find the mistake himself, before it is revealed at the end of these notes. Let us start by considering a god given so-called Yang-Yang action[3] $S : \mathbb{R}^M \to \mathbb{R}$ defined by

$$S(\lambda) = \sum_{a=1}^{M} \left(L\hat{\phi}_1(\lambda_a) - 2\pi I_a \lambda_a \right) + \frac{1}{2} \sum_{a,b=1}^{M} \hat{\phi}_2(\lambda_a - \lambda_b), \tag{46}$$

where we also defined

$$\hat{\phi}_n(\lambda) = \int_0^\lambda \phi_n(\mu) d\mu = 2 \int_0^\lambda \arctan\left(\frac{\tanh(\mu)}{\tan(\frac{n\zeta}{2})} \right) d\mu. \tag{47}$$

If we calculate the extreme points of the Yang-Yang action we find:

$$\frac{\partial S}{\partial \lambda_g} = \sum_{a=1}^{M} (L\phi_1(\lambda_a)\delta_{ag} - 2\pi I_a \delta_{ag}) + \frac{1}{2} \sum_{a,b=1}^{M} (\phi_2(\lambda_a - \lambda_b)\delta_{ag} - \phi_2(\lambda_a - \lambda_g)\delta_{bg}) \tag{48}$$

$$= L\phi_1(\lambda_g) - \sum_{a=1}^{M} \phi_2(\lambda_g - \lambda_a) - 2\pi I_g. \tag{49}$$

Lo and behold: the extreme points of the Yang-Yang action are precisely given by the logarithmic Bethe Ansatz equations. Might this have been the motivation to introduce the Yang-Yang action in the first place? Surely! Note that the derivative of $\hat{\phi}_n(\lambda)$ yields precisely $\phi_n(\lambda)$ because $\phi_n(0) = 0$. Furthermore note that we used $\phi_n(-\lambda) = -\phi_n(\lambda)$ in the above.

Because it is in general pretty hard to prove a function is convex, we use the last theorem stated in the previous section to show that the Yang-Yang action is strictly convex. Restricting ourselves to $\lambda \in \mathbb{R}^M$, this means that if we have a local minimum of the Yang-Yang action, it is a global minimum and also unique. For the following, we let $v \in \mathbb{R}^M$ be a random column vector and we denote v_α for one element of that column vector. First

[3] In fact, it is a function, but physicists love the call things an 'action'. In this case it is just a mapping from $\mathbb{R}^M$ to $\mathbb{R}$. If it were a mapping from some Banach space to the real numbers, then calling it an action would have been appropriate, because we would be dealing with a linear functional.

we look for the derivative of the characteristic function $\phi_n(\lambda)$:

$$\begin{aligned}
\frac{d\phi_n(\lambda_a)}{d\lambda_a} &= \frac{d}{d\lambda_a}\left(2\arctan\left(\frac{\tanh(\lambda_a)}{\tan(\frac{n\zeta}{2})}\right)\right) \\
&= 2\left(1+\frac{\tanh^2\lambda_a}{\tan^2(n\zeta/2}\right)^{-1}\left(\frac{1}{\cosh^2\lambda\tan(n\zeta/2)}\right) \\
&= \frac{2\tan(n\zeta/2)}{\cosh^2\lambda_a(\tan^2(n\zeta/2)+\tanh^2\lambda_a)}.
\end{aligned}$$

We note that the derivative of $\phi_n(\lambda_a)$ is well-defined $\forall\lambda_a\in\mathbb{R}$ and $\forall n\in\mathbb{N}_+$. We can now investigate whether the Hessian matrix of the Yang-Yang action is postive definite:

$$\begin{aligned}
\sum_{\delta,\gamma} v_\delta v_\gamma \frac{\partial^2 S}{\partial\lambda_\gamma\partial\lambda_\delta} &= L\sum_\gamma \frac{2\tan(\zeta/2)v_\gamma^2}{\cosh^2\lambda_\gamma(\tan^2(n\zeta/2)+\tanh^2(\lambda_\gamma))} \\
&+\sum_{\delta,\gamma}\frac{2\tan(\zeta)v_\delta v_\gamma}{\cosh^2(\lambda_\gamma-\lambda_\delta)(\tan^2(\zeta/2)+\tanh^2(\lambda_\gamma-\lambda_\delta)} \\
&= L\sum_\gamma \frac{2\tan(\zeta/2)v_\gamma^2}{\cosh^2\lambda_\gamma(\tan^2(n\zeta/2)+\tanh^2(\lambda_\gamma))} \\
&+\sum_{\delta>\gamma=1}\frac{2\tan(\zeta)(v_\delta+v_\gamma)^2}{\cosh^2(\lambda_\gamma-\lambda_\delta)(\tan^2\zeta+\tanh^2(\lambda_\gamma-\lambda_\delta)}.
\end{aligned}$$

We note that the above expression is strictly larger than zero when both $\tan(\zeta/2)$ and $\tan(\zeta/2)$ are larger than zero. If we want to have both larger than zero, we must have $\zeta\in(0,\pi/2)$. Recall that we parametrized $\Delta=\cos\zeta$, we conclude that the Yang-Yang Hessian matrix is positive definite for $0<\Delta<1$. We may thus conclude that for these values of Δ the Yang-Yang action is strictly convex. So if we have a local minimizer, then this is a global, unique minimum. Provided that we restrict $\lambda\in\mathbb{R}^M$ we thus have proven that given a specified $I\in(\mathbb{Z}/L\mathbb{Z})^M$ the logarithmic Bethe Ansatz equations have a global unique minimum $\lambda\in\mathbb{R}^M$.

As indicated beforehand, this proof is flawed. The point is we do not know whether the logarithmic Bethe Ansatz equations are actually local minimizers of the Yang-Yang action. In fact, the proof above is circular: we calculate the logarithmic Bethe Ansatz equations and do not know whether they have solutions (the Yang-Yang action might have no extrema!), but then we continue as if we have the solutions to the Bethe Ansatz equations and that they are minimizers (and not maximizers). A counter example would be $f(\lambda)=e^\lambda$. This function is strictly convex, but never attains a global minimum.

Furthermore, one should note that if the proof above was correct, we would only have done a small part of proving the existence of solutions to the XXZ-model. Firstly, we assumed a given $I \in (\mathbb{Z}/L\mathbb{Z})^M$. Then we restricted ourselves to $\lambda \in \mathbb{R}^M$, whereas the general setting would be $\lambda \in \mathbb{C}^M$. We have not touched upon the problem of completeness. Recall that we should find L choose M different I, such that every single I has a different solution $\lambda \in \mathbb{C}^M$. Still, if the proof would have been correct, one would have been a step closer to the existence of solutions to the XXZ model.

Finally, we note that even though the proof was flawed, the $\Delta = 1$ is explicitly not contained in the values for which the Yang-Yang Hessian matrix is positive definite. This confirms our previous statement that the existence of a solution to the XXX model is more difficult than the XXZ model. One can define a similar Yang-Yang actian and do the same computations using the characteristic $\psi_n(\lambda)$ function (instead of $\phi_n(\lambda)$ in the $\Delta = 1$ case, leading to:

$$\sum_{\delta,\gamma} v_\delta v_\gamma \frac{\partial^2 S}{\partial\lambda_\gamma \partial\lambda_\delta} = L \sum_\gamma \frac{2v_\gamma^2}{1+4\lambda_\gamma^2} - \sum_{\gamma\neq\alpha} \frac{(v_\alpha - v_\gamma)}{1+(\lambda_\alpha-\lambda_\gamma)^2}, \tag{50}$$

which is explicitly not positive definite for arbitrary $v \in \mathbb{R}^M$.

A non-flawed proof requires some more care. It can be found in an article by the inventors of the Yang-Yang action [4].

7 Literature

These notes are based on the following literature:

- Introduction to the Bethe Ansatz I - Michael Karbach, Gerhard Muller - ArXiv: cond-mat/9809162
- Introduction to the Bethe Ansatz II - Michael Karbach, Gerhard Muller - ArXiv: cond-mat/9809163
- Introduction to the Bethe Ansatz III - Michael Karbach, Gerhard Muller - ArXiv: cond-mat/0008018
- Singularities in the Structure Factor of the anisotropic Heisenberg spin-1/2 chain - MSc thesis by P.M. Adamopoulou, supervisor: prof. J-S Caux - `http://www.science.uva.nl/onderwijs/thesis/centraal/files/f395501439.pdf`
- Dynamics of Heisenberg spin chains - PhD thesis Rob Hagemans, supervisor prof. J-S Caux

[4]See: Yang, Yang: *One-Dimensional Chain of Anisotropic Spin-Spin Interactions I, Proof of Bethe's Hypothesis for Ground State in a Finite System*, Phys. Rev. 150 (1966), pp 321-327.

- Lecture Notes on Bethe Ansatz Techniques - F. Franchini - `http://people.sissa.it/~ffranchi/BAnotes.pdf`
- Nonlinear Programming: Theory and Algorithms, Bazaraa, Sherali and Shetty, 3rd edition, John Wiley and Sons (2006)
- Quantum Inverse Scattering Method and Correlation Functions - Korepin, Bogoliubov, Izergin - Cambridge University Press (1993)
- One-Dimensional Chain of Anisotropic Spin-Spin Interactions I, Proof of Bethe's Hypothesis for Ground State in a Finite System, Yang and Yang, Phys. Rev. 150 (1966), pp 321-327
- Completeness of Bethe Vectors and Difference Equations with Regular Singular Points, Tarasov and Varchenko, Int. Math. Res., Nov 13 (1996), pp 637-669.

8 Appendix A: Handy triogonometric formulas

We list several handy trigonometric formulas for complex arguments below [5]. For $x, y \in \mathbb{R}$:

$$\cosh(x+iy) = \cosh x \cos y + i \sinh x \sin y \tag{51}$$

$$\sinh(x+iy) = \sinh x \cos y + i \cosh x \sin y \tag{52}$$

$$\ln\left(\frac{x+iy}{x-iy}\right) = 2i \arctan\left(\frac{y}{x}\right) \tag{53}$$

$$\frac{\sin(x+iy)}{\sin(x-iy)} = \frac{\tan x + i \tanh y}{\tan x - i \tanh y} \tag{54}$$

[5] For derivations and more explanations, see for instance: `http://www.math.ethz.ch/education/bachelor/lectures/fs2012/other/ka_itet/TrigHypFunktionen.pdf`