

## Lecture 3. Solving Bethe ansatz equation

Yunfeng Jiang

### 1 Introduction

In this lecture, we discuss the solution of Bethe ansatz equation (BAE) for the Heisenberg XXX spin chain. Written in terms of rapidities, the BAE of length  $L$  with  $M$  magnons take the following form

$$\left(\frac{u_j + \frac{i}{2}}{u_j - \frac{i}{2}}\right)^L = \prod_{k \neq j}^M \frac{u_j - u_k + i}{u_j - u_k - i}, \quad j = 1, \dots, M. \quad (1.1)$$

Sometimes it is also useful to write the BAE in the polynomial form

$$(u_j + \frac{i}{2})^L \prod_{k=1}^M (u_j - u_k - i) + (u_j - \frac{i}{2})^L \prod_{k=1}^M (u_j - u_k + i) = 0, \quad j = 1, \dots, M. \quad (1.2)$$

Finding solutions of these non-linear algebraic equations is by no means a simple task. Its solution is also related to the fundamental question of completeness of Bethe ansatz. We will discuss these points in detail in this lecture.

### 2 How many solutions do we expect ?

In this section, we count the number of expected solution of BAE with length  $L$  and magnon number  $M$ . We consider a slightly more general situation, which is the  $\text{XXX}_s$  model. Later we will specify to  $s = \frac{1}{2}$ . Let us denote the irreducible spin- $s$  representation by  $\mathcal{D}^{(s)}$ . Taking the  $L$ -fold tensor product, we have the following decomposition

$$[\mathcal{D}^{(s)}]^{\otimes L} = \bigoplus_{J=J_{\min}}^{sL} d_s(L, J) \mathcal{D}^{(J)}. \quad (2.1)$$

where  $J_{\min} = 0$  or  $J_{\min} = 1/2$  depending on whether  $L$  and  $s$  are even or odd. This decomposition can be computed by a repeated application of the Clebsch-Gordan series

$$\mathcal{D}^{(\ell)} \otimes \mathcal{D}^{(\ell')} = \mathcal{D}^{|\ell' - \ell|} \oplus \mathcal{D}^{|\ell' - \ell| + 1} \oplus \dots \oplus \mathcal{D}^{(\ell' + \ell)} \quad (2.2)$$

For example

$$\begin{aligned}
\mathcal{D}^{(1/2)} \otimes \mathcal{D}^{(1/2)} \otimes \mathcal{D}^{(1/2)} &= (\mathcal{D}^{(0)} \oplus \mathcal{D}^{(1)}) \otimes \mathcal{D}^{(1/2)} \\
&= (\mathcal{D}^{(0)} \otimes \mathcal{D}^{(1/2)}) \oplus (\mathcal{D}^{(1)} \otimes \mathcal{D}^{(1/2)}) \\
&= (\mathcal{D}^{(1/2)}) \oplus (\mathcal{D}^{(1/2)} \oplus \mathcal{D}^{(3/2)}) \\
&= (2\mathcal{D}^{(1/2)}) \oplus \mathcal{D}^{(3/2)}.
\end{aligned} \tag{2.3}$$

The spin- $J$  representation is spanned by the states

$$|J, m\rangle, \quad m = -J, -J + 1, \dots, J - 1, J. \tag{2.4}$$

where  $m$  is the magnetization

$$S^z |J, m\rangle = m |J, m\rangle. \tag{2.5}$$

In order to compute the degeneracy  $d_s(L, J)$  in (2.1), let us first compute the number of states  $b_s(L, M)$  for a given magnetization  $m$ . This can be done as follow

$$(z^{-s} + z^{-s+1} + \dots + z^s)^L = \sum_{m=-sL}^{sL} b_s(L, m) z^m \tag{2.6}$$

Now let us compute  $b_s(L, m)$  in another way. Each spin- $J$  representation with  $J \geq |m|$  contains one state with magnetization  $m$ . Since we have  $d_s(L, J)$  spin- $J$  representations, we thus have

$$b_s(L, m) = d_s(L, |m|) + d_s(L, |m| + 1) + \dots + d_s(L, sL). \tag{2.7}$$

From this relation, it is clear that the number of spin- $J$  representations is given by

$$d_s(L, J) = b_s(L, J) - b_s(L, J + 1). \tag{2.8}$$

Now we focus on the Heisenberg XXX spin chain with  $s = \frac{1}{2}$ .

**XXX<sub>1/2</sub> spin chain** For this case, we have

$$(z^{-1/2} + z^{1/2})^L = \sum_{m=-L/2}^{L/2} b_{1/2}(L, m) z^m. \tag{2.9}$$

It is more convenient to write  $m$  in terms of magnon number  $M$ . They are related by

$$m = \frac{L}{2} - M. \tag{2.10}$$

Expanding the left hand side of (2.9), we find

$$b_{1/2}(L, m) = b_{1/2}(L, -m) = \binom{L}{|L/2 - m|} = \binom{L}{M}. \quad (2.11)$$

For a spin- $J$  representation, its highest weight state or primary state is given by  $|J, J\rangle$ , namely it is the state with magnetization  $m = J \geq 0$ . As we have shown in Lecture 2, Bethe states corresponding to *finite solutions*<sup>1</sup> of BAE are primary states (recall that such states are annihilated by  $S^+$ ). For an  $M$ -magnon Bethe state, the magnetization is given by

$$S^z |\mathbf{u}_M\rangle = \left(\frac{L}{2} - M\right) |\mathbf{u}_M\rangle. \quad (2.12)$$

This implies that the  $M$ -magnon Bethe states are the highest weight states of the spin- $(\frac{L}{2} - M)$  representation. Since the spin  $J$  is non-negative, we restrict to the regime  $M \leq \frac{L}{2}$ . We expect that the number of Bethe states  $|\mathbf{u}_M\rangle$  to be the number of spin- $(\frac{L}{2} - M)$  representations, which is given by  $d_{1/2}(L, \frac{L}{2} - M)$ . Therefore the number of expected solutions  $\mathcal{N}(L, M)$  for BAE of length  $L$  and  $M$  magnons is given by

$$\mathcal{N}(L, M) = d_{1/2}(L, L/2 - M) = \binom{L}{M} - \binom{L}{M-1}. \quad (2.13)$$

We will then check whether such an expectation is met.

### 3 Are all solutions acceptable ?

To see whether we can obtain the expected number of solutions, let us consider a concrete example. We take  $L = 4$  and  $M = 2$ . For small quantum numbers, BAE can be solved readily by `Mathematica` or any other standard softwares, which gives 6 solutions :

$$\{u_1, u_2\} = \left\{-\frac{i}{2}, \frac{i}{2}\right\}, \quad \left\{-\frac{1}{2\sqrt{3}}, \frac{1}{2\sqrt{3}}\right\} \quad (3.1)$$

and

$$\{u_1, u_2\} = \left\{\frac{1}{2} \pm \frac{1}{\sqrt{2}}, \frac{1}{2} \pm \frac{1}{\sqrt{2}}\right\}, \quad \left\{-\frac{1}{2} \pm \frac{1}{\sqrt{2}}, -\frac{1}{2} \pm \frac{1}{\sqrt{2}}\right\}, \quad (3.2)$$

Taking  $L = 4$  and  $M = 2$  in (2.13), we expect 2 solutions. So there are too many solutions ! What is going on ? As we shall see shortly, the reason is that some of these solutions are

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<sup>1</sup>As we have shown in Lecture 2, rapidities at infinity corresponds to acting  $S^-$  on the state and thus corresponds to descendant states.

*non-physical*. This means although such solutions indeed satisfy BAE, the corresponding Bethe state is no longer an eigenstate of the Hamiltonian, or transfer matrix. There are two kinds of such solutions, which requires more careful analysis. They have both appeared in our simple example. The first kind are the solutions containing coinciding rapidities, namely solutions of the form  $\underbrace{\{u, \dots, u\}}_K, u_1, \dots, u_M$  and the ones containing multiple sets of coinciding rapidities.

The other kind of solutions are called *singular solutions*, which refer to the solutions containing  $\pm i/2$ , *i.e.* solutions of the form  $\{i/2, -i/2, u_1, \dots, u_M\}$ .

### 3.1 Coinciding rapidities

We first consider solutions with coinciding rapidities. Consider our simple example  $L = 4$ ,  $M = 2$ . If we plug the solutions (3.2) into the state constructed by coordinate Bethe ansatz described in Lecture 1, we find that the Bethe states vanish. This is due to the special choice of the normalization. If, on the other hand, we plug the solutions to the Bethe state constructed by algebraic Bethe ansatz described in Lecture 2, we obtain a finite Bethe states, but we can check easily that these states are *not* eigenstates of the XXX spin chain !

To explain what goes wrong, let us analyze this issue more carefully in the framework of algebraic Bethe ansatz. We consider the case with two magnons. Recall that in algebraic Bethe ansatz, the action of the transfer matrix on the Bethe state is given by

$$T(u)B(u_1) \dots B(u_M)|\Omega\rangle = \tau(u|\mathbf{u}_M)|\Omega\rangle \quad (3.3)$$

$$+ \sum_{k=1}^M g(u, u_k) \left( a(u_k) \prod_{j \neq k}^M f(u_j, u_k) - d(u_k) \prod_{j \neq k}^M f(u_k, u_j) \right) B(u)B(u_1) \dots \widehat{B}(u_k) \dots B(u_M)|\Omega\rangle.$$

where

$$f(u, v) = \frac{u - v + i}{u - v}, \quad g(u, v) = \frac{i}{u - v}. \quad (3.4)$$

For  $M = 2$ , we have

$$T(u)B(u_1)B(u_2)|\Omega\rangle = \tau(u|\mathbf{u}_2)B(u_1)B(u_2)|\Omega\rangle \quad (3.5)$$

$$+ \frac{i}{(u - u_1)(u_2 - u_1)} \left( a(u_1)(u_2 - u_1 + i) - d(u_1)(u_2 - u_1 - i) \right) B(u)B(u_2)|\Omega\rangle$$

$$- \frac{i}{(u - u_2)(u_2 - u_1)} \left( a(u_2)(u_1 - u_2 + i) - d(u_2)(u_1 - u_2 - i) \right) B(u)B(u_1)|\Omega\rangle$$

We can set  $u_2 = u_1 + \epsilon$  and then take the limit  $\epsilon \rightarrow 0$ . This leads to the following result

$$T(u)B^2(u_1)|\Omega\rangle = \tau(u|\{u_1, u_1\})B^2(u_1)|\Omega\rangle - \frac{1}{u - u_1} \left( a(u_1) + d(u_1) \right) B(u)B'(u_1)|\Omega\rangle \quad (3.6)$$

$$+ \frac{i}{u - u_1} \left( 2(a(u_1) - d(u_1)) - i(a'(u_1) - d'(u_1)) - \frac{i}{u - u_1}(a(u_1) + d(u_1)) \right) B(u)B(u_1)|\Omega\rangle$$

As we can see, besides the original vector  $B^2(u_1)|\Omega\rangle$ , we obtain two new vectors on the right hand side, which are  $B(u)B(u_1)|\Omega\rangle$  and  $B(u)B'(u_1)|\Omega\rangle$ . The second vector is special which contains a derivative with respect to  $B(u_1)$  operator. This kinds of term only shows up in the case with coinciding rapidities.

Demanding these additional terms to vanish, we obtain *two* equations

$$a(u_1) + d(u_1) = 0, \quad (3.7)$$

$$2(a(u_1) - d(u_1)) - i(a'(u_1) - d'(u_1)) = 0.$$

Notice that the second equation is independent from the original BAE and is an extra condition. We can check that the four solutions (3.2) satisfy the first equation but not the second. Therefore they do not eliminate the terms  $B(u)B'(u_1)|\Omega\rangle$ . This explains why the resulting Bethe state is not an eigenstate.

What happen for the case of  $M$  magnons is similar. If we have  $u_j = u_k$ , various formula involving  $f(u_j, u_k)$  and  $g(u_j, u_k)$  have singularities. By taking the limit  $u_j \rightarrow u_k$ , we obtain vectors containing derivatives of the  $B$ -operator. We can verify that there are still  $N$  equations ( $N - 1$  BAE and 1 additional condition). Therefore, we always have  $N$  equations, but now we only have  $N - 1$  variables. Therefore, the resulting system is overdetermined. In some cases, one can prove that such overdetermined system do not have solutions.

How to derive the additional constraint when there are coinciding rapidities ? Here we introduce two methods.

**Method 1. RMM relation in the coinciding limit** One straightforward method is using the  $RTT$ -relation in the coinciding limit. We can derive the following commutation relations involving three operators

$$A(u)B^2(v) = f^2(u, v)B^2(v)A(u) + g(u, v)B(u)B'(v)A(v) \quad (3.8)$$

$$+ g(u, v)B(u)B(v) [(1 + f(u, v))A(v) - A'(v)]$$

$$D(u)B^2(v) = f^2(v, u)B^2(v)D(u) + g(u, v)B(u)B'(v)D(v)$$

$$- g(u, v)B(u)B(v) [(1 + f(v, u))D(v) + D'(v)]$$

Together with usual commutation relations, we can compute

$$(A(u) + D(u))B^2(u_1) \prod_{j=2}^N B(u_j)|\Omega\rangle \quad (3.9)$$

by moving  $A$  and  $D$  operators to the right. Demanding the unwanted terms to be zero, we obtain the corresponding constraints.

**Method 2. Polynomiality of transfer matrix** The above derivation is straightforward but tedious. There is a more convenient derivation for the constraints by using polynomiality of the transfer matrix.

Before moving to the cases with coinciding rapidities, let us show that the BAE can actually be derived from polynomiality of the transfer matrix. By construction, we know that the eigenvalue of the transfer matrix should be a polynomial in  $u$ . From algebraic Bethe ansatz, the eigenvalue of the transfer matrix is given by

$$\tau(u|\mathbf{u}_M) = a(u) \prod_{j=1}^M \frac{u - u_j - i}{u - u_j} + d(u) \prod_{j=1}^M \frac{u - u_j + i}{u - u_j} \quad (3.10)$$

where

$$a(u) = \left(u + \frac{i}{2}\right)^L, \quad d(u) = \left(u - \frac{i}{2}\right)^L. \quad (3.11)$$

Looking at (3.10), there seems to be a pole at  $u = u_k$ . To be consistent with the fact that  $\tau(u|\mathbf{u}_M)$  is a polynomial in  $u$ , this pole must be spurious and its residue must be zero. This leads to

$$\text{Res}_{u=u_k} \tau(u|\mathbf{u}_M) = a(u_k) \prod_{j=1}^M (u_k - u_j - i) + d(u_k) \prod_{j=1}^M (u_j - u_k + i) = 0, \quad (3.12)$$

which is exactly the BAE for  $u_k$ .

The cancellation conditions for solutions of coinciding rapidities can be derived by exactly the same logic. Consider the  $K + N$  magnon solution  $\{u_0, u_0, \dots, u_0, u_1, \dots, u_N\}$  where the first  $K$  rapidities are coinciding. The eigenvalue of the transfer matrix is given by

$$\tau(u) = a(u) \left(\frac{u - u_0 - i}{u - u_0}\right)^K \prod_{j=1}^N \frac{u - u_j - i}{u - u_j} + d(u) \left(\frac{u - u_0 + i}{u - u_0}\right)^K \prod_{j=1}^N \frac{u - u_j + i}{u - u_j}. \quad (3.13)$$

By construction,  $\tau(u)$  is a polynomial in  $u$ . Imposing the condition that the residues of the simple pole vanish, we obtain

$$a(u_j)(u_j - u - i)^K \prod_{k=1}^N (u_j - u_k - i) + d(u_j)(u_j - u + i)^K \prod_{k=1}^N (u_j - u_k + i) = 0. \quad (3.14)$$

Imposing that  $u = u_0$  is regular leads to the following  $K$  conditions

$$R_l = \frac{\partial^l}{\partial u^l} \left( \tau(u)(u - u_0)^K \right) \Big|_{u=u_0} = 0, \quad l = 0, \dots, K - 1. \quad (3.15)$$

One can check that these conditions coincide with the ones derived from the first method.

**Different models** To obtain physical solutions with coinciding rapidities, we impose extra conditions apart from BAE. Sometimes such a system do not have solutions, while others do. In the case of Lieb-Liniger model one can *prove* rigorously that the combined system does not have solution [Izergin-Korepin] and therefore in this model repeated roots are not allowed.

For the Heisenberg  $XXX_s$  spin chain where

$$a(u) = (u + is)^L, \quad d(u) = (u - is)^L, \quad (3.16)$$

the situation is more complicated. For our current case, there are good evidence that for  $s = 1/2$  we do not have physical solutions with repeated roots. For  $s \geq 1$ , there are in fact repeated roots which are physical [Hao, Nepomechie]. But it would be nice to prove rigorously that repeated roots are definitely ruled out for  $s = 1/2$ .

### 3.2 Singular solutions

Now we turn to the singular solutions, which take the following form

$$\left\{ \frac{i}{2}, -\frac{i}{2}, u_3, \dots, u_M \right\}. \quad (3.17)$$

In our example of  $L = 4$ ,  $M = 2$ , we have already seen such a solution. We immediately see a problem if we want to compute the eigenvalues corresponding to such solutions. Recall that the energy reads

$$E \sim \sum_{k=1}^M \frac{1}{u_k^2 + 1/4}. \quad (3.18)$$

It is obviously divergent if some of the roots become  $\pm i/2$ . Similarly, we also have singularities in the eigenvector. If we choose the algebraic Bethe ansatz normalization in Lecture 2, we find that  $B(i/2)B(-i/2)|\Omega\rangle$  is a null vector. One can easily prove that this is due to the fact  $B(-i/2)|\Omega\rangle = 0$ . Does this mean we should discard such solutions? This is a bit too quick. As usual, in theoretical physics, when there are singularities, we should first regularize it to obtain finite results and see whether the resulting finite answer makes sense.

We shall follow this standard practice. In order to regularized the eigenvector, we choose a different normalization for the Lax matrix. Let us consider

$$\tilde{L}_{an}(u) = \frac{1}{u + i/2} L_{an}(u), \quad L_{an}(u) = (u - \frac{i}{2}) \mathbb{I}_{an} + iP_{an}. \quad (3.19)$$

where  $L_{an}(u)$  is the previous Lax operator defined in Lecture 2. In this new normalization, we have

$$\tilde{M}_a(u) = \frac{1}{(u + i/2)^L} M_a(u). \quad (3.20)$$

In particular,

$$\tilde{B}(u) = \frac{1}{(u + i/2)^L} B(u). \quad (3.21)$$

In this normalization, the Bethe state  $\tilde{B}(i/2)\tilde{B}(-i/2)|\Omega\rangle$  now has a 0/0 ambiguity. Let us first can consider the following *naive* regularization

$$u_1^{\text{naive}} = \frac{i}{2} + \epsilon, \quad u_2^{\text{naive}} = -\frac{i}{2} + \epsilon. \quad (3.22)$$

We plug this solution to the explicit expressions for the eigenvalue and eigenstate. To see whether the regularization makes sense, we perform a direct brute force diagonalization of the Hamiltonian

$$H = \frac{1}{4} \sum_{n=1}^L (\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1) \quad (3.23)$$

and compare with the results we obtain from Bethe ansatz. For the Hamiltonian (3.23), the corresponding eigenvalue is

$$E = -\frac{1}{2} \sum_{k=1}^M \frac{1}{u_k^2 + 1/4}. \quad (3.24)$$

The naive regularization (3.22) yields a finite answer for the eigenvalue in the limit  $\epsilon \rightarrow 0$ , which gives  $E = -1$ . This is indeed one of the eigenvalues from brute force diagonalization.

The naive regularization also leads to a finite vector. However, this finite vector is *not* an eigenvector of the Hamiltonian (3.23) ! After a little bit of thought, we conclude that one should not be surprised by this fact. What we are trying to do is getting a finite answer for

$$\frac{1}{\mathcal{N}(u_1, u_2)} B(u_1)B(u_2)|\Omega\rangle \quad (3.25)$$



in the limit where  $u_1 \rightarrow i/2$  and  $u_2 \rightarrow -i/2$ . However, the finite answer in general depends on *how* the two Bethe roots tend to their limiting values. For example, consider the following limit

$$\lim_{x,y \rightarrow 0} \frac{x-y}{x+y} \quad (3.26)$$

This limit is ambiguous and depends on how  $x$  and  $y$  tend to zero. We can take, for example  $x = 4\epsilon, y = 3\epsilon$ , or  $x = \epsilon^2 + \epsilon, y = -\epsilon^2 + \epsilon$  with  $\epsilon \rightarrow 0$ , which lead to different answers. Therefore, the key point is finding a proper regularization scheme which allows us to obtain the correct eigenvalue and eigenvector. There are two regularizations in the literature.

**Prescription 1** The first one is the following modified regularization

$$u_1 = \frac{i}{2} + \epsilon + c\epsilon^L, \quad u_2 = -\frac{i}{2} + \epsilon, \quad (3.27)$$

where  $c$  is a constant to be determined for different  $L$  and  $M$ . In our  $L = 4, M = 2$  example, it turns out that  $c = 2i$ . Let us analyze this in more detail using ABA. Recall that the action of the transfer matrix on the off-shell Bethe state is given by (we use the new normalization in (3.20))

$$\begin{aligned} \tilde{T}(u)|u_1, \dots, u_M\rangle &= \tau(u|\mathbf{u}_M)|u_1, \dots, u_M\rangle \\ &+ \sum_{k=1}^M F_k(u|\mathbf{u}_M) \tilde{B}(u_1) \cdots \widehat{\tilde{B}(u_k)} \cdots \tilde{B}(u_M) B(u)|\Omega \rangle \end{aligned} \quad (3.28)$$

where  $\tau(u|\mathbf{u}_M)$  is the eigenvalue of the transfer matrix and  $F_k$  are given by

$$F_k(u|\mathbf{u}_M) = \frac{i}{u - u_k} \left[ \prod_{j \neq k}^M \left( \frac{u_k - u_j - i}{u_k - u_j} \right) - \left( \frac{u_k - \frac{i}{2}}{u_k + \frac{i}{2}} \right)^L \prod_{j \neq k}^M \left( \frac{u_k - u_j + i}{u_k - u_j} \right) \right]. \quad (3.29)$$

Let us first focus on the two magnon sector  $M = 2$ . We first consider the naive regularization (3.22) and see what goes wrong. The key observation is that

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \tilde{B}\left(\frac{i}{2} + \epsilon\right) &\sim \text{finite}, \\ \lim_{\epsilon \rightarrow 0} \tilde{B}\left(-\frac{i}{2} + \epsilon\right) &\sim \frac{1}{\epsilon^L} + \text{less singular terms} \end{aligned} \quad (3.30)$$

In order the unwanted terms

$$F_1(u|\mathbf{u}_2) \tilde{B}(u_2)|\Omega\rangle + F_2(u|\mathbf{u}_2) \tilde{B}(u_1)|\Omega\rangle \quad (3.31)$$

to vanish in the  $\epsilon \rightarrow 0$  limit, the coefficients  $F_1(u|\mathbf{u}_2)$  and  $F_2(u|\mathbf{u}_2)$  should go to zero at least at the speed

$$F_1(u|\mathbf{u}_2) \sim \epsilon^{L+1}, \quad F_2(u|\mathbf{u}_2) \sim \epsilon. \quad (3.32)$$

However, explicit calculations show that  $F_1 \sim \epsilon^L$  (instead of  $\epsilon^{L+1}$ ) and  $F_2 \sim 1$  (instead of  $\epsilon$ ). Hence, the unwanted terms are finite in the limit and that's why the corresponding Bethe vector is not an eigenvector.

Now we consider the modified regularization (3.27), explicit calculations lead to

$$\begin{aligned} F_1(u|\mathbf{u}_2) &= \left( \frac{c + 2i^{-L+1}}{u - \frac{i}{2}} \right) \epsilon^L + \mathcal{O}(\epsilon^{L+1}), \\ F_2(u|\mathbf{u}_2) &= \left( \frac{2i - i^{-L}c}{u + \frac{i}{2}} \right) + \mathcal{O}(\epsilon). \end{aligned} \quad (3.33)$$

In order to satisfy (3.32), we require the leading terms in (3.33) to vanish. For even  $L$ , both conditions can be satisfied by taking

$$c = 2i(-1)^{L/2}. \quad (3.34)$$

For odd  $L$ , we cannot satisfy both conditions. Indeed, it is found that in general there are no singular solutions for spin chains with odd length. One can check that the choice (3.34) reproduces the correct eigenvector for  $L = 4$ ,  $M = 2$ .

Encouraged by this example, we consider the general singular solution

$$\left\{ \frac{i}{2}, -\frac{i}{2}, u_3, \dots, u_M \right\}. \quad (3.35)$$

The Bethe equations imply that the last  $M - 2$  Bethe roots obey

$$\left( \frac{u_k + \frac{i}{2}}{u_k - \frac{i}{2}} \right)^{L-1} \left( \frac{u_k - \frac{3i}{2}}{u_k + \frac{3i}{2}} \right) = \prod_{\substack{j \neq k \\ j=3}}^M \frac{u_k - u_j + i}{u_k - u_j - i}, \quad k = 3, \dots, M. \quad (3.36)$$

These equations ensures that  $F_k(u|\mathbf{u}_M) = 0$  for  $k = 3, \dots, M$ . To make sure all the unwanted terms vanish, we require that

$$F_1(u|\mathbf{u}_M) \sim \epsilon^{L+1}, \quad F_2(u|\mathbf{u}_M) \sim \epsilon \quad (3.37)$$

Similarly, these requirement lead to two constraints on the constant  $c$  in the modified regularization. The constraints can be solved readily, yielding

$$c = -\frac{2}{i^{L+1}} \prod_{j=3}^M \frac{u_j - \frac{3i}{2}}{u_j + \frac{i}{2}}, \quad c = 2i^{L+1} \prod_{j=3}^M \frac{u_j + \frac{3i}{2}}{u_j - \frac{i}{2}} \quad (3.38)$$

respectively. For the two equations in (3.38) to be consistent, we must have

$$\prod_{j=3}^M \left( \frac{u_j - \frac{i}{2}}{u_j + \frac{i}{2}} \right) \left( \frac{u_j - \frac{3i}{2}}{u_j + \frac{3i}{2}} \right) = (-1)^L \quad (3.39)$$

Making use of the BAE (3.36), we can rewrite the above consistency condition as

$$\left[ - \prod_{k=3}^M \left( \frac{u_k + \frac{i}{2}}{u_k - \frac{i}{2}} \right) \right]^L = 1. \quad (3.40)$$

The conclusion is that, if the Bethe roots  $\{u_3, \dots, u_M\}$  satisfy both (3.36) and (3.40), we can make sure that all the unwanted terms vanish and obtain correct eigenstates. These solutions are called *singular physical* solutions. If the Bethe roots only satisfy (3.36) but not (3.40), they are called singular non-physical solutions.

**Prescription 2** The above prescription, although works fine, might be well criticized as somewhat ad hoc. Therefore, here we discuss another way of regularizing the solution which has more clear physical meaning. Let us consider the following equation

$$\left( \frac{u_j + \frac{i}{2}}{u_j - \frac{i}{2}} \right)^L = e^{-i\beta} \prod_{k \neq j}^M \frac{u_j - u_k + i}{u_j - u_k - i}, \quad j = 1, \dots, M. \quad (3.41)$$

This is in fact the Bethe ansatz equation of the XXX spin chain with the following twisted boundary condition

$$\begin{aligned} \sigma_{L+1}^x &= \cos \beta \sigma_1^x - \sin \beta \sigma_1^y, \\ \sigma_{L+1}^y &= \sin \beta \sigma_1^x + \cos \beta \sigma_1^y, \\ \sigma_{L+1}^z &= \sigma_1^z. \end{aligned} \quad (3.42)$$

We assume that for small  $\beta$ , the roots  $\pm i/2$  of physical singular solution acquire some small correction of order  $\beta$ ,

$$u_1 = \frac{i}{2} + c_1 \beta + \mathcal{O}(\beta^2), \quad u_2 = -\frac{i}{2} + c_2 \beta + \mathcal{O}(\beta^2). \quad (3.43)$$

Consider the Bethe equations for  $u_1$  and  $u_2$  in the polynomial form

$$\begin{aligned} (u_1 + \frac{i}{2})^L (u_1 - u_2 - i) \prod_{k=3}^M (u_1 - u_k - i) &= e^{-i\beta} (u_1 - \frac{i}{2})^L (u_1 - u_2 + i) \prod_{k=3}^M (u_1 - u_k + i), \\ (u_2 + \frac{i}{2})^L (u_2 - u_1 - i) \prod_{k=3}^M (u_2 - u_k - i) &= e^{-i\beta} (u_2 - \frac{i}{2})^L (u_2 - u_1 + i) \prod_{k=3}^M (u_2 - u_k + i). \end{aligned}$$

Plugging (3.43) into the above equation, expand both sides in  $\beta$ , and require that these equations are satisfied up to first order in  $\beta$ , we obtain

$$c_1 = c_2. \quad (3.44)$$

Taking the product of all Bethe ansatz equations in (3.41), we obtain

$$\left( \frac{u_1 + \frac{i}{2} u_2 + \frac{i}{2} \prod_{j=3}^M u_j + \frac{i}{2}}{u_1 - \frac{i}{2} u_2 - \frac{i}{2} \prod_{j=3}^M u_j - \frac{i}{2}} \right)^L = e^{-iM\beta} \quad (3.45)$$

Now plugging the expansion (3.43) into the above equation using  $c_1 = c_2$ , we obtain

$$\left( \frac{c_1 \beta + i \prod_{j=3}^M u_j + \frac{i}{2}}{c_1 \beta - i \prod_{j=3}^M u_j - \frac{i}{2}} \right)^L = e^{-iM\beta} \quad (3.46)$$

The limit  $\beta \rightarrow 0$  can be taken readily and leads to

$$\left[ - \prod_{j=3}^M \left( \frac{u_j + \frac{i}{2}}{u_j - \frac{i}{2}} \right) \right]^L = 1. \quad (3.47)$$

This is the same condition as we derived before. The rest rapidities satisfy the usual Bethe equations.

### 3.3 Roots at infinity

Finally, let us discuss roots at infinity. Let us consider the BAE with  $M + 1$  magnons. Suppose we take  $u_{M+1} \rightarrow \infty$ , the BAE corresponding to  $u_{M+1}$  becomes trivial and we are left with  $M$  non-trivial BAE. The dependence on  $u_{M+1}$  in these equations also decouple since

$$\lim_{u_{M+1} \rightarrow \infty} \frac{u_k - u_{M+1} - i}{u_k - u_{M+1} + i} = 1. \quad (3.48)$$

We thus recover a BAE of  $M$  magnons. The magnon with infinite rapidity has zero energy. We see that adding roots at infinity to a Bethe state  $|\mathbf{u}_M\rangle$  does not change the energy or BAE of the original state. But the magnon number is changed.

As we discussed in Lecture 2, adding a root at infinity corresponds to acting a  $S^-$  on the primary state. The existence of such states is related to the fact that Heisenberg XXX spin chain is  $SU(2)$  invariant. If we introduce the twisted boundary condition, which breaks the  $SU(2)$  invariance, we see immediately that roots at infinity are not allowed.

When considering solutions of BAE, we usually only consider the cases where the rapidities are finite. The solutions at infinity can be taken into account straightforwardly by symmetry considerations.

### 3.4 Summary

Let us summarize what we have learned so far

1. When there are coinciding rapidities, extra conditions need to be imposed to ensure all the unwanted terms vanish. These conditions lead to an overdetermined system of equations. In the Heisenberg XXX spin chain, numerical evidence shows that this overdetermined system is not solvable. As a result, coinciding rapidities are not allowed. However, a rigorous proof like the one for the Lieb-Liniger model [1] is still lacking.
2. Singular roots need to be regularized carefully. After proper regularizations, we see that some of the singular solutions are physical while others are not. The physical singular solutions need to satisfy an additional condition (3.40).
3. Roots at infinity are allowed due to  $SU(2)$  invariance. Adding roots at infinity corresponds to acting  $S^-$  on the corresponding Bethe state.

**Completeness conjecture** Let us end this part of the story by a conjecture of completeness formulated by Hao, Nepomechie and Sommesse [2]. For the Bethe equation of length  $L$  and  $M$  magnons, let us denote the solution of non-singular and physical singular without repeated roots by  $\mathcal{N}_1(L, M)$  and  $\mathcal{N}_2(L, M)$ . HNS conjectured is that

$$\mathcal{N}_1(L, M) + \mathcal{N}_2(L, M) = \binom{L}{M} - \binom{L}{M-1}. \quad (3.49)$$

We see the right hand side is precisely the number of solutions that we expect in (2.13). This conjecture, if valid, tells us the following things

- If we solve BAE directly, there are in general too many solutions;
- We need to discard solutions with coinciding rapidities and non-physical singular solutions;
- Bethe ansatz for Heisenberg XXX spin chain is complete.

This conjecture is tested quite non-trivially up to  $L = 14$  in [2].

## 4 Baxter's $TQ$ -relation

In this section, we consider an alternative formulation of the Bethe ansatz equation, which is Baxter's  $TQ$ -relation. Recall that the eigenvalue of the transfer matrix is

$$\tau(u|\mathbf{u}_M) = a(u) \prod_{j=1}^M \frac{u - u_j - i}{u - u_j} + d(u) \prod_{j=1}^M \frac{u - u_j + i}{u - u_j}. \quad (4.1)$$

Let us define the following  $Q$ -polynomial

$$Q(u) = \prod_{j=1}^M (u - u_j), \quad (4.2)$$

whose zeros are the Bethe roots. We can write (from now on, to simplify the notation, we will simply write  $\tau(u|\mathbf{u}_M)$  as  $\tau(u)$ .)

$$\tau(u)Q(u) = a(u)Q(u - i) + d(u)Q(u + i). \quad (4.3)$$

This is called the  $TQ$ -relation. It is equivalent to the Bethe ansatz equation. This can be seen as follows. Evaluate both sides at  $u = u_j$  where  $u_j$  is one of the Bethe roots, we obtain

$$a(u_j)Q(u_j - i) + d(u_j)Q(u_j + i) = 0, \quad (4.4)$$

which is the polynomial form of BAE. Now because both  $\tau(u)$  and  $Q(u)$  are polynomials of degree  $L$  and  $M$  respectively, we can make the following ansatz

$$\tau(u) = \sum_{k=0}^L t_k u^k, \quad Q(u) = u^M + \sum_{k=0}^{M-1} c_k u^k. \quad (4.5)$$

Plugging the ansatz (4.5) into (4.3) and compare the coefficients of  $u^k$ , ( $k = 0, \dots, L$ ) on both sides of the equation, we obtain a set of algebraic equations for  $\{t_j, c_j\}$ . Solving these equations, we obtain  $\{t_j, c_j\}$  simultaneously, which in turn determine  $\tau(u)$  and  $Q(u)$ .

**Example 1** Let us again consider the  $L = 4$ ,  $M = 2$  example. The  $TQ$ -relation reads

$$\begin{aligned} & (t_4 u^4 + t_3 u^3 + t_2 u^2 + t_1 u + t_0) (u^2 + c_1 u + c_0) \\ &= (u + \frac{i}{2})^4 [(u - i)^2 + c_1(u - i) + c_0] + (u - \frac{i}{2})^4 [(u + i)^2 + c_1(u + i) + c_0]. \end{aligned} \quad (4.6)$$

Expanding both sides in  $u$  and compare the coefficients, we obtain the following 7 equations

$$\begin{aligned}
t_4 - 2 &= 0, \\
t_4 c_1 + t_3 - 2c_1 &= 0, \\
t_4 c_0 + t_3 c_1 + t_2 - 2c_0 - 3 &= 0, \\
t_3 c_0 + t_2 c_1 + t_1 - c_1 &= 0, \\
t_2 c_0 + t_1 c_1 + t_0 + 3c_0 - \frac{9}{8} &= 0, \\
t_1 c_0 + t_0 c_1 + \frac{7}{8}c_1 &= 0, \\
t_0 c_0 - \frac{1}{8}c_0 + \frac{1}{8} &= 0.
\end{aligned} \tag{4.7}$$

This set of algebraic equations can be solved straightforwardly, yielding two solutions

$$\begin{aligned}
t_4 = 2, \quad t_3 = 0, \quad t_2 = 3, \quad t_1 = 0, \quad t_0 = \frac{13}{8}, \quad c_1 = 0, \quad c_0 = -\frac{1}{12}, \\
t_4 = 2, \quad t_3 = 0, \quad t_2 = 3, \quad t_1 = 0, \quad t_0 = -\frac{3}{8}, \quad c_1 = 0, \quad c_0 = \frac{1}{4}.
\end{aligned} \tag{4.8}$$

This means we have two possible  $\{\tau(u), Q(u)\}$ , given by

$$t(u) = 2u^4 + 3u^2 + \frac{13}{8}, \quad Q(u) = u^2 - \frac{1}{12}. \tag{4.9}$$

and

$$t(u) = 2u^4 + 3u^2 - \frac{3}{8}, \quad Q(u) = u^2 + \frac{1}{4}. \tag{4.10}$$

To find Bethe roots, we find the zeros of the  $Q(u)$  in (4.9) and (4.10), which are

$$\left\{ \frac{1}{2\sqrt{3}}, -\frac{1}{2\sqrt{3}} \right\}, \quad \left\{ \frac{i}{2}, -\frac{i}{2} \right\}. \tag{4.11}$$

Interestingly, the solutions with coinciding rapidities are automatically eliminated. Why this is so? Recall that both BAE and the extra conditions for the coinciding rapidities (3.15) can be obtained from polynomiality of  $\tau(u)$ . By making the ansatz (4.5), we are explicitly requiring that  $\tau(u)$  to be a polynomial. Since the repeated roots are not allowed (although we do not have a rigorous proof so far), such solutions are automatically eliminated. This is one of the advantages of the  $TQ$ -relation.

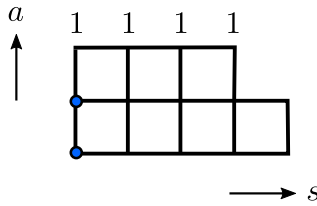
However,  $TQ$ -relation does not eliminate all the non-physical solutions. It does not eliminate the non-physical singular solutions. For example, consider the BAE with  $L = 5$  and  $M = 2$ . From our analysis above, we know that in this case  $\{\frac{i}{2}, -\frac{i}{2}\}$  is not a physical solution because  $L$  is odd. Nevertheless, it shows up in the solution of  $TQ$ -relation. There exists another formalism which eliminates all non-physical solutions, including the singular non-singular solutions. This is the rational  $Q$ -system.

## 5 Rational $Q$ -system

In this section, we discuss the rational  $Q$ -system method for finding Bethe roots. This method was proposed by Marboe and Volin in [3] in 2016.

### 5.1 The formalism

**Young tableaux** For a length  $L$  spin chain with  $M$  magnons, we take a Young tableaux with two rows  $(L - M, M)$  as is shown in figure 5.1. At each node, we associate a polynomial



**Figure 5.1:** Young tableaux corresponding to the BAE of length  $L$  and magnon number  $M$ .

$Q_{a,s}(u)$  whose degree is given by the number of boxes to the upper right of the node.

**Boundary condition** We fix the  $Q$ -functions at the upper and left boundary. The  $Q$ -functions at the upper boundary are fixed to be 1, namely  $Q_{2,s}(u) = 1$ . On the left boundary, we fix

$$Q_{0,0}(u) = u^L, \quad Q_{1,0}(u) = \prod_{j=1}^M (u - u_j). \quad (5.1)$$

where  $Q_{1,0}(u)$  is precisely the  $Q$ -function defined in (4.2). To solve the rational  $Q$ -system in what follows, we will parameterize  $Q_{1,0}(u)$  as

$$Q_{1,0}(u) = u^M + \sum_{k=0}^{M-1} c_k u^k. \quad (5.2)$$

Later we will derive a set of algebraic equations for  $\{c_k\}$ .

**The  $QQ$ -relation** The  $Q$ -functions on the Young tableaux are not independent, they obey the  $QQ$ -relation

$$Q_{a+1,s}(u)Q_{a,s+1}(u) = Q_{a+1,s+1}^+(u)Q_{a,s}^-(u) - Q_{a+1,s+1}^-(u)Q_{a,s}^+(u). \quad (5.3)$$



**Polynomiality of  $Q$ -functions** Now the task is to find the rest  $Q$ -functions using the  $QQ$ -relation and the boundary condition. We make the crucial requirement that *all the  $Q$ -functions should be polynomials*. We will see that this turns out to be a non-trivial requirement and lead to a set of algebraic equations.

## 5.2 From $QQ$ to BAE

Let us show how Bethe ansatz can be derived from the  $QQ$ -relation. To this end, we focus on the first column of the  $QQ$ -relation. We have two such relations

$$\begin{aligned} Q_{1,1}(u) &= Q_{1,0}^+(u) - Q_{1,0}^-(u), \\ Q_{1,0}(u)Q_{0,1}(u) &= Q_{1,1}^-(u)Q_{0,0}^+(u) - Q_{1,1}^+(u)Q_{0,0}^-(u). \end{aligned} \quad (5.4)$$

Here we need to use the important condition that  $Q_{1,0}(u_k) = 0$ . Evaluating the second equation in (5.4) at  $u = u_k$ , we obtain

$$Q_{1,1}^-(u_k)Q_{0,0}^+(u_k) - Q_{1,1}^+(u_k)Q_{0,0}^-(u_k) = 0 \quad (5.5)$$

Next, we want to rewrite  $Q_{1,1}^\pm(u_k)$  in terms of  $Q_{1,0}(u_k)$  and  $Q_{0,0}(u_k)$ . This can be achieved by evaluating the first equation at  $u = u_k \pm i/2$ , which lead to

$$Q_{1,1}^+(u_k) = Q_{1,0}^{++}(u_k), \quad Q_{1,1}^-(u_k) = -Q_{1,0}^{--}(u_k). \quad (5.6)$$

Plugging into (5.5), we obtain

$$Q_{0,0}^+(u_k)Q_{1,0}^{--}(u_k) + Q_{0,0}^-(u_k)Q_{1,0}^{++}(u_k) = 0. \quad (5.7)$$

This is equivalent to

$$\frac{Q_{0,0}^+(u_k)Q_{1,0}^{--}(u_k)}{Q_{0,0}^-(u_k)Q_{1,0}^{++}(u_k)} = -1 \quad (5.8)$$

which is precisely the BAE upon plugging in (5.1).

## 5.3 Solving $QQ$ -relations

Let us solve the rational  $Q$ -system row by row. For  $a = 1$ , the  $QQ$ -relation reads

$$Q_{1,s+1} = Q_{1,s}^- - Q_{1,s}^+. \quad (5.9)$$

This can be solved by

$$Q_{1,s}(u) = D^s Q_{1,0}(u), \quad Df(u) \equiv f(u - \frac{i}{2}) - f(u + \frac{i}{2}). \quad (5.10)$$

We then consider the row  $a = 0$ . The  $QQ$ -relation reads

$$Q_{0,s+1}Q_{1,s} = Q_{1,s+1}^+ Q_{0,s}^- - Q_{1,s+1}^- Q_{0,s}^+ \quad (5.11)$$

The  $Q_{1,s}$  has been computed in the previous step. We have

$$Q_{0,s+1} = \frac{Q_{1,s+1}^+ Q_{0,s}^- - Q_{1,s+1}^- Q_{0,s}^+}{Q_{1,s}} \quad (5.12)$$

In general, the right hand side is a rational function instead of a polynomial. To ensure that all the  $Q$ -functions are polynomials, we need to impose the condition that the remainder of the right hand side of (5.12) is vanishing. This leads to a set of algebraic equations for  $\{c_k\}$  defined in (5.2), which is called *zero remainder condition*. We then solve these equations and determine  $Q_{1,0}(u)$ . Let us see how rational  $Q$ -system works by an example.

**Example 1** Consider again our example  $L = 4, M = 2$ . We first draw the Young tableaux  $(2, 2)$ . We have the following boundary conditions

$$Q_{0,0}(u) = u^4, \quad Q_{1,0}(u) = u^2 + c_1 u + c_0 \quad (5.13)$$

and  $Q_{2,s}(u) = 1$ . We first calculate  $Q_{1,s}(u)$  by (5.10) for  $s = 1, 2$ . They are given by

$$\begin{aligned} Q_{1,1} &= Q_{1,0}^+ - Q_{1,0}^- = i(2u + c_1), \\ Q_{1,2} &= Q_{1,1}^+ - Q_{1,1}^- = -2. \end{aligned} \quad (5.14)$$

Then we move to compute  $Q_{0,s}(u)$  with  $s = 1, 2$ . First consider  $Q_{0,1}$ . From  $QQ$ -relation, we have

$$\begin{aligned} Q_{0,1} &= \frac{Q_{1,1}^+ Q_{0,0}^- - Q_{1,1}^- Q_{0,0}^+}{Q_{1,0}} \\ &= i \frac{[2(u + \frac{i}{2}) + c_1](u - \frac{i}{2})^4 - [2(u - \frac{i}{2}) + c_1](u + \frac{i}{2})^4}{u^2 + c_1 u + c_0} \end{aligned} \quad (5.15)$$

Performing this polynomial division explicitly, we obtain a quotient and a remainder. We take the quotient to be  $Q_{0,1}$

$$Q_{0,1}(u) \equiv 6u^2 - 2c_1 u + (2c_1^2 - 6c_0 + 1). \quad (5.16)$$

The corresponding remainder is given by

$$R_{0,1}(u) = (-2c_1^3 + 8c_1 c_0 - 2c_1) u - \left( 2c_0 c_1^2 - 6c_0^2 + c_0 + \frac{1}{8} \right) \quad (5.17)$$

We then compute  $Q_{0,2}$  by the  $QQ$ -relation

$$Q_{0,2} = \frac{Q_{1,2}^+ Q_{0,1}^- - Q_{1,2}^- Q_{0,1}^+}{Q_{1,1}}. \quad (5.18)$$

Plugging (5.14) and (5.16) into (5.18), we again find a quotient and remainder, given by

$$Q_{0,2}(u) = 12, \quad R_{0,2}(u) = -16i c_1. \quad (5.19)$$

Requiring the remainders  $R_{0,1}(u)$  and  $R_{0,2}(u)$  to vanish for any  $u$ , we obtain the following zero remainder conditions

$$\begin{aligned} -2c_1^3 + 8c_1 c_0 - 2c_1 &= 0, \\ 2c_0 c_1 - 6c_0^2 + c_0 + \frac{1}{8} &= 0, \\ -16i c_1 &= 0. \end{aligned} \quad (5.20)$$

These equations can be solved easily. We obtain two solutions

$$c_1 = 0, \quad c_0 = \frac{1}{4}, \quad \text{and} \quad c_1 = 0, \quad c_0 = -\frac{1}{12}, \quad (5.21)$$

which corresponds to

$$Q_{1,0}(u) = u^2 + \frac{1}{4}, \quad Q_{1,0}(u) = u^2 - \frac{1}{12}. \quad (5.22)$$

Finding the zeros of  $Q_{1,0}(u)$ , we find the correct Bethe roots.

Compared with solving BAE directly or the  $TQ$ -relation, we find that in the rational  $Q$ -system approach, it takes some effort to find what are precisely the equations to solve. This might seem to be a disadvantage of the approach. However, it is definitely worth the pain because it turns out the zero remainder conditions are much efficient to solve. In addition, the other crucial advantage of the approach is that it eliminates all non-physical solutions. By solving rational  $Q$ -system, we obtain all physical solutions at once. This fact is quite remarkable and in the rest of the lecture we will explain why rational  $Q$ -system is able to achieve this.

## 6 Polynomiality of the other solution of $TQ$ -relation

We start to decode the rational  $Q$ -system from this section. Let us recall the  $TQ$ -relation

$$\tau(u)Q(u) = a(u)Q(u-i) + d(u)Q(u+i). \quad (6.1)$$

This can be seen as a second order difference equation for the unknown function  $Q(u)$ . It has two solutions. Let us denote the other one by  $P(u)$ . Here we have made the assumption that both  $\tau(u)$  and  $Q(u)$  are polynomials. However, the other solution  $P(u)$  does not have to be a polynomial in general. We will see that, by requiring  $P(u)$  to be polynomial, we can eliminate the non-physical singular solution from the solution of  $TQ$ -relation. This fact can be stated more precisely as a theorem, which we will prove in this section. Before going to the theorem, let us first prove a lemma following [4].

**Lemma** Given a solution of BAE  $\{u_j\}$ . If there are two Bethe roots, which without loss of generality can be denoted by  $u_1$  and  $u_2$ , satisfy  $u_1 - u_2 = i$ , then we must have  $u_1 = i/2$ ,  $u_2 = -i/2$ .

In another words, this lemma says that for a set of Bethe roots, either it does not contain any two rapidities whose difference is  $i$ , or in the case such pair exists, these two rapidities must be  $\pm i/2$ .

*Proof:* Since  $u_2 - u_1 = i$ , we can write  $u_1 = s + \frac{i}{2}$  and  $u_2 = s - \frac{i}{2}$ . We need to prove that  $s = 0$ .

Let us first consider the case of  $N = 2$  to have an idea how the proof goes. The BAE reads

$$\begin{aligned} \left(\frac{u_1 + \frac{i}{2}}{u_1 - \frac{i}{2}}\right)^L &= \frac{u_1 - u_2 + i}{u_1 - u_2 - i}, \\ \left(\frac{u_2 + \frac{i}{2}}{u_2 - \frac{i}{2}}\right)^L &= \frac{u_2 - u_1 + i}{u_2 - u_1 - i}. \end{aligned} \quad (6.2)$$

Let us analyze the first equation. Due to the condition  $u_1 - u_2 = i$ , the right hand side is divergent. For the equation to hold, the left hand side cannot be finite and we must have  $u_1 = \frac{i}{2}$ . Similarly, we consider the second equation. Due to  $u_1 - u_2 = i$ , the right hand side of the second equation is vanishing. To ensure the left hand side is also vanishing, we must have  $u_2 = -i/2$ . Therefore we have proved the lemma for  $N = 2$ .

Now we consider the case for  $N > 2$ .

Let us consider the BAE for  $u_1$ , which reads

$$\left(\frac{u_1 + \frac{i}{2}}{u_1 - \frac{i}{2}}\right)^L = \frac{u_1 - u_2 + i}{u_1 - u_2 - i} \prod_{k=3}^N \frac{u_1 - u_k + i}{u_1 - u_k - i}. \quad (6.3)$$

The first term on the rhs is divergent. Therefore, either we have  $u_1 = i/2$  as in the  $N = 2$  case, or there exist another Bethe root called  $u_3$  such that  $u_1 - u_3 = -i$ , which produces a 0 that cancels the pole and make the result finite. If the latter case were true, we have  $u_2 = s - \frac{i}{2}$ ,  $u_1 = s + \frac{i}{2}$  and  $u_3 = s + \frac{3i}{2}$ . We can then analyze the BAE for  $u_3$ , which reads

$$\left(\frac{u_3 + \frac{i}{2}}{u_3 - \frac{i}{2}}\right)^L = \frac{u_3 - u_1 + i}{u_3 - u_1 - i} \prod_{k \neq 1,3}^N \frac{u_3 - u_k + i}{u_3 - u_k - i}. \quad (6.4)$$

Since the first term on the rhs is divergent. We either have  $s = -i$  (for the left hand to be zero), or there exist a  $u_4$  such that  $u_3 - u_4 = -i$  (to produce a zero to cancel the pole). In the later case, we can move on to analyze the BAE for  $u_4$ . It is easy to convince oneself by this analysis, for the BAE to be consistent, the possible values of  $s$  are  $s = 0, -i, -2i, \dots, -ni$ , namely it is a non-positive integer times imaginary unit  $i$ .

Let us analyze the BAE in a different way. We start by considering BAE for  $u_2$

$$\left(\frac{u_2 + \frac{i}{2}}{u_2 - \frac{i}{2}}\right)^L = \frac{u_2 - u_1 + i}{u_2 - u_1 - i} \prod_{k=3}^N \frac{u_2 - u_k + i}{u_2 - u_k - i}. \quad (6.5)$$

Now the right hand side is vanishing, so we must have either  $u_2 = -\frac{i}{2}$ , meaning  $s = 0$  or there exists a  $u_3$  such that  $u_2 - u_3 = i$ , which means  $u_3 = s - \frac{3i}{2}$ . Similar to the previous case, we then analyze the BAE for  $u_3$  and conclude that either  $s = i$  or there is a  $u_4$  such that  $u_3 - u_4 = i$ . Repeating this reasoning, we find that the possible values of  $s$  are  $s = 0, i, 2i, 3i, \dots, ni$ . The two ways of analyzing are not compatible with each other unless  $s = 0$ . Therefore, we conclude that  $s = 0$ .

Now we move to prove the main theorem following [4, 5].

**Theorem 1** Consider the  $TQ$ -relation

$$\tau(u)Q(u) = (u + \frac{i}{2})^L Q(u - i) + (u - \frac{i}{2})^L Q(u + i). \quad (6.6)$$

where  $\tau(u)$  is a polynomial. For each polynomial solution  $Q(u)$  with degree  $n \leq L/2$ ,

- If the zeros of  $Q(u)$  does not contain  $\pm i/2$ , there exist a polynomial  $P(u)$  such that

$$P(u + i/2)Q(u - i/2) - P(u - i/2)Q(u + i/2) = u^L \quad (6.7)$$

Notice that such a polynomial is not unique. If  $P_0(u)$  satisfies (6.7), the following polynomials

$$P(u) = P_0(u) + \alpha Q(u) \quad (6.8)$$

where  $\alpha$  is an arbitrary constant, all satisfy (6.7).

- If the zeros of  $Q(u)$  contain  $\pm i/2$ , then there exist a function  $P(u)$  satisfying (6.7). However,  $P(u)$  is in general not a polynomial but take the following form

$$P(u) = P_0(u) + \alpha Q(u)\psi(-iu + 1/2) \quad (6.9)$$

where  $P_0(u)$  is a polynomial,  $\psi(u)$  is the digamma function and  $\alpha$  a constant. The function  $P(u)$  will become a polynomial, namely  $\alpha = 0$  if and only if the following additional condition is satisfied

$$(-1)^L = \prod_{k=3}^N \frac{u_k + \frac{i}{2} u_k + \frac{3i}{2}}{u_k - \frac{i}{2} u_k - \frac{3i}{2}}. \quad (6.10)$$

where  $u_k$  are the rest of the roots (apart from  $\pm i/2$ ) of  $Q(u)$ .

*Proof:* We first divide the two sides of the  $TQ$ -relation (6.6) by  $Q(u - i)Q(u)Q(u + i)$  and obtain

$$\frac{\tau(u)}{Q(u + i)Q(u - i)} = R(u - i/2) + R(u + i/2) \quad (6.11)$$

where

$$R(u) = \frac{u^L}{Q(u - i/2)Q(u + i/2)}. \quad (6.12)$$

Performing a partial fraction decomposition, we can write  $R(u)$  as

$$R(u) = \pi(u) + \frac{q_-(u)}{Q(u - i/2)} + \frac{q_+(u)}{Q(u + i/2)} \quad (6.13)$$

Assuming  $Q(u)$  is of degree  $n$ . We have

$$\deg \pi(u) = L - 2n, \quad \deg q_-(u) < n, \quad \deg q_+(u) < n. \quad (6.14)$$

Plugging (6.13) into (6.11), we obtain

$$\begin{aligned} \frac{\tau(u)}{Q(u + i)Q(u - i)} &= \pi(u - i/2) + \pi(u + i/2) + \frac{q_-(u - i/2)}{Q(u - i)} + \frac{q_+(u + i/2)}{Q(u + i)} \\ &\quad + \frac{q_+(u - i/2) + q_-(u + i/2)}{Q(u)}. \end{aligned} \quad (6.15)$$

Now we need to distinguish two cases.

- For the case of non-singular solutions, namely  $Q(u)$  does not contain  $\pm i/2$  its zeros, we multiply both sides by  $(u - u_k)$  and then take  $u \rightarrow u_k$ . The left hand side is zero. The first four terms on the right hand side are also zero. For the last term to be zero, we require

$$q_+(u_k - i/2) + q_-(u_k + i/2) = 0, \quad k = 1, \dots, n. \quad (6.16)$$

Since the two polynomials satisfy  $\deg(q_{\pm}(u)) < n$ , each of them can be parameterized by  $n$  parameters. The relation (6.16) imposes  $n$  constraints and we are left with  $n$  independent parameters. We can use these  $n$  parameters to define another polynomial of degree  $n - 1$ . Or, put it differently, the constraints (6.16) can be solved by introducing a polynomial  $q(u)$  of degree  $n - 1$  such that

$$q_+(u) = q(u + i/2), \quad q_-(u) = -q(u - i/2). \quad (6.17)$$

Plugging into (6.13), we find

$$R(u) = \pi(u) + \frac{q(u + i/2)}{Q(u + i/2)} - \frac{q(u - i/2)}{Q(u - i/2)} \quad (6.18)$$

The polynomial  $\pi(u)$  can always be written as

$$\pi(u) = \rho(u + i/2) - \rho(u - i/2) \quad (6.19)$$

where  $\rho(u)$  is a polynomial of degree  $L - 2n + 1$ . Notice that  $\rho(u)$  is not unique, but the only important thing is that such a polynomial exists. We can then write

$$R(u) = \frac{u^L}{Q(u + i/2)Q(u - i/2)} = \frac{P(u + i/2)}{Q(u + i/2)} - \frac{P(u - i/2)}{Q(u - i/2)}. \quad (6.20)$$

where

$$P(u) = \rho(u)Q(u) + q(u). \quad (6.21)$$

By construction,  $P(u)$  is a polynomial of degree  $n^* = L + 1 - n$ . From (6.20), we obtain

$$P(u + i/2)Q(u - i/2) - P(u - i/2)Q(u + i/2) = u^L \quad (6.22)$$

Let us denote the zeros of  $P(u)$  as  $\{\tilde{u}_k\}$ . From (6.22), we have

$$P(\tilde{u}_k + i)Q(\tilde{u}_k) = (\tilde{u}_k + i/2)^L, \quad -P(\tilde{u}_k - i)Q(\tilde{u}_k) = (\tilde{u}_k - i/2)^L. \quad (6.23)$$

Taking the ratio of the above two equations, we find that

$$\left(\frac{\tilde{u}_k + i/2}{\tilde{u}_k - i/2}\right)^L = -\prod_{j=1}^{n^*} \frac{\tilde{u}_k - \tilde{u}_j + i}{\tilde{u}_k - \tilde{u}_j - i} \quad (6.24)$$

which implies that the zeros of  $P(u)$  also satisfy Bethe equations of length  $L$  and magnon number  $n^*$ . The solutions  $\{\tilde{u}_k\}$  are called *dual solutions* of  $\{u_k\}$ .

- For the case with singular solutions, let us denote

$$Q(u) = (u - \frac{i}{2})(u + \frac{i}{2})\bar{Q}(u) \quad (6.25)$$

where  $\bar{Q}(u)$  is a polynomial of degree of  $n - 2$ . The equation (6.15) now becomes

$$\begin{aligned} & \frac{1}{(u - \frac{3i}{2})(u + \frac{3i}{2})(u - \frac{i}{2})(u + \frac{i}{2})} \frac{\tau(u)}{\bar{Q}(u+i)\bar{Q}(u-i)} \\ & = \pi(u - i/2) + \pi(u + i/2) + \frac{q_-(u - i/2)}{Q(u - i)} + \frac{q_+(u + i/2)}{Q(u + i)} \\ & \quad + \frac{q_+(u - i/2) + q_-(u + i/2)}{(u + \frac{i}{2})(u - \frac{i}{2})\bar{Q}(u)} \end{aligned} \quad (6.26)$$

Let us denote the zeros of  $\bar{Q}(u)$  by  $\{u_3, \dots, u_n\}$ . We can multiply both sides of (6.26) by  $(u - u_k)$  and then take  $u \rightarrow u_k$ , this leads to the condition

$$q_+(u_k - i/2) + q_-(u_k + i/2) = 0, \quad k = 3, \dots, n. \quad (6.27)$$

Here comes the crucial difference. Now in general  $q_{\pm}(u)$  have  $2n$  parameters. Our condition (6.27) only fixes  $n - 2$  of them. So in total we still have  $n + 2$  parameters. Therefore in this case, the constraint can be solved by

$$\begin{aligned} q_+(u) &= +q(u + i/2) + \frac{1}{2}\bar{Q}(u + i/2)\sigma(u + i/2), \\ q_-(u) &= -q(u - i/2) + \frac{1}{2}\bar{Q}(u - i/2)\sigma(u - i/2). \end{aligned} \quad (6.28)$$

where  $q(u)$  is a polynomial of degree  $\deg q(u) \leq n - 1$  and  $\sigma(u)$  is another polynomial whose degree  $\deg \sigma(u) \leq 1$ . In general we need  $n + 2$  parameters to fix the two polynomials  $q(u)$  and  $\sigma(u)$ . Plugging (6.28) into (6.13), we obtain

$$R(u) = \pi(u) + \frac{q(u + i/2)}{Q(u + i/2)} - \frac{q(u - i/2)}{Q(u - i/2)} + \frac{1}{2} \left( \frac{\sigma(u - i/2)}{u(u - i)} + \frac{\sigma(u + i/2)}{u(u + i)} \right) \quad (6.29)$$

Again, we write  $\pi(u) = \rho(u + i/2) - \rho(u - i/2)$  where  $\rho(u)$  is a polynomial, unique up to an additive constant. Let us denote

$$U(u) = \frac{1}{2} \left( \frac{\sigma(u - i/2)}{u(u - i)} + \frac{\sigma(u + i/2)}{u(u + i)} \right) \quad (6.30)$$



It can be decomposed as

$$U(u) = \frac{a_0}{u} + \frac{b_0^+}{u-i} + \frac{b_0^-}{u+i}. \quad (6.31)$$

We want to write  $U(u)$  in a difference form

$$U(u) = V(u+i/2) - V(u-i/2). \quad (6.32)$$

One choice is

$$V(u) = -i(a_0 + b_0^+ + b_0^-)\psi(-iu + 1/2) + \frac{b_0^-}{u+i/2} - \frac{b_0^+}{u-i/2} \quad (6.33)$$

where  $\psi(x)$  is the digamma function defined by

$$\psi(x) = \frac{d}{dx} \log \Gamma(x). \quad (6.34)$$

Using the property of the digamma function

$$\psi(x+1) - \psi(x) = \frac{1}{x} \quad (6.35)$$

we can verify that (6.32) is indeed valid. We can then write

$$R(u) = \frac{P(u+i/2)}{Q(u+i/2)} - \frac{P(u-i/2)}{Q(u-i/2)} \quad (6.36)$$

where now

$$P(u) = \rho(u)Q(u) + q(u) + Q(u)V(u). \quad (6.37)$$

It satisfies

$$P(u+i/2)Q(u-i/2) - P(u-i/2)Q(u+i/2) = u^L. \quad (6.38)$$

This proves the first part of the theorem. Now we move to the second part of the theorem. In the  $TQ$ -relation, we replace the factors  $(u \pm i/2)^L$  by

$$\begin{aligned} (u-i/2)^L &= P(u)Q(u-i) - P(u-i)Q(u), \\ (u+i/2)^L &= P(u+i)Q(u) - P(u)Q(u+i) \end{aligned} \quad (6.39)$$

and divide both sides by  $Q(u)$ . This gives

$$\tau(u) = P(u+i)Q(u-i) - P(u-i)Q(u+i). \quad (6.40)$$

Evaluate the above equation at  $u = -i/2$ , we obtain

$$\tau(-i/2) = P(i/2)Q(-3i/2) - P(-3i/2)Q(i/2) \quad (6.41)$$

We need to focus on the second term. Since  $Q(u)$  has zeros at  $\pm i/2$ ,  $Q(i/2)$  is vanishing. However, in  $P(-3i/2)$ , there is a term  $\psi(-1)$  which is divergent with residue  $-1$ . This divergence is cancelled by the zero and leads to

$$\tau(-i/2) = P(i/2)Q(-3i/2) + (a_0 + b_0^+ + b_0^-)\bar{Q}(i/2)Q(-3i/2) \quad (6.42)$$

Now evaluating the  $TQ$ -relation at  $u = -i/2$ , we find

$$\tau(-i/2) = -(-i)^L \frac{\bar{Q}(i/2)}{Q(-i/2)} \quad (6.43)$$

Evaluating (6.38) at  $u = i$ , we find that (noticing that  $P(3i/2)$  is finite)

$$P(i/2) = -\frac{i^L}{Q(3i/2)}. \quad (6.44)$$

Plugging into (6.42), we obtain

$$\tau(-i/2) = -i^L \frac{Q(-3i/2)}{Q(3i/2)} + (a_0 + b_0^+ + b_0^-)Q^*(i/2)Q(-3i/2) \quad (6.45)$$

Comparing the rhs of (6.43) and (6.45), we find that  $a_0 + b_0^+ + b_0^- = 0$  if and only if

$$-(-i)^L \frac{\bar{Q}(i/2)}{Q(-i/2)} = -i^L \frac{Q(-3i/2)}{Q(3i/2)} = -i^L \frac{\bar{Q}(-3i/2)}{Q(3i/2)} \quad (6.46)$$

This is precisely

$$\prod_{k=3}^N \frac{u_k + \frac{i}{2}}{u_k - \frac{i}{2}} \frac{u_k + \frac{3i}{2}}{u_k - \frac{3i}{2}} = (-1)^L. \quad (6.47)$$

The same as the condition (3.39) derived from regularization of Bethe roots.

## 7 Demystifying rational $Q$ -system

In the previous section, we have mentioned that rational  $Q$ -system gives precisely all the physical Bethe roots that we want. In addition, we also proved that the requirement that both solutions to the  $TQ$ -relation are polynomials gives the additional condition under which singular physical solutions are physical. In this section, we will see that this polynomiality is encoded in the rational  $Q$ -system, which explains why it only gives physical solutions. Let us first prove the following theorem.

**Theorem 2** The zeros of Baxter polynomial  $Q(u)$  is a physical solution to the Bethe ansatz equation if and only if the functions  $T_0(u)$  and  $T_1(u)$  in the following two  $TQ$ -relations are polynomials

$$\begin{aligned} T_0(u)Q(u) &= W_0(u - i/2)Q(u + i) + W_0(u + i/2)Q(u - i), \\ T_1(u)DQ(u) &= W_1(u - i/2)DQ(u + i) + W_1(u + i/2)DQ(u - i), \end{aligned} \quad (7.1)$$

where

$$\begin{aligned} DQ(u) &= Q(u - i/2) - Q(u + i/2), \\ W_0(u) &= u^L, \\ W_1(u) &= (u + \frac{i}{2})^L + (u - \frac{i}{2})^L - T_0(u). \end{aligned} \quad (7.2)$$

Proof: From Theorem 1 we have

$$\begin{aligned} (u + \frac{i}{2})^L &= P(u + i)Q(u) - P(u)Q(u + i), \\ (u - \frac{i}{2})^L &= P(u)Q(u - i) - P(u - i)Q(u). \end{aligned} \quad (7.3)$$

From (6.40), we have

$$T_0(u) = P(u + i)Q(u - i) - P(u - i)Q(u + i) \quad (7.4)$$

Plugging (7.3) and (7.4) into the definition of  $W_1(u)$  (7.2), we obtain

$$W_1(u) = DQ(u - i/2)DP(u + i/2) - DQ(u + i/2)DP(u - i/2) \quad (7.5)$$

We can then plug  $W_1(u)$  into (7.1) and find that

$$T_1(u) = DP(u + i)DQ(u - i) - DP(u - i)DQ(u + i) \quad (7.6)$$

Using the general form of  $P(u)$ , we have

$$\begin{aligned} DP(u) &= P(u - i/2) - P(u + i/2) \\ &= DP_0(u) + \alpha_0 Q(u - i/2)\psi(-iu) - \alpha_0 Q(u + i/2)\psi(-iu + 1) \end{aligned} \quad (7.7)$$

Here we focus on the case of singular solution because this is the tricky case. Using the property of the digamma function (6.35), we can write the above quantity as

$$DP(u) = DP_0(u) - i\alpha_0 \frac{Q(u + i/2)}{u} + \alpha_0 DQ(u) \psi(-iu) \quad (7.8)$$

Now consider

$$T_1(0) = DP(i) DQ(-i) - DP(-i)DQ(i) \quad (7.9)$$

we see that  $DP(-i)$  has a pole because  $\psi(-iu)$  has a pole at  $u = -i$ . The corresponding residue is  $-i\alpha_0 DQ(i) DQ(-i)$ . Now

$$\begin{aligned} DQ(i) &= Q(i/2) - Q(3i/2) = -Q(3i/2), \\ DQ(-i) &= Q(-3i/2) - Q(-i/2) = Q(-3i/2). \end{aligned} \quad (7.10)$$

For singular solutions,  $Q(\pm 3i/2)$  cannot be zero. Otherwise this will contradict our lemma, which says the only possible roots whose difference is  $i$  are  $\pm i/2$ . On the other hand, if  $T_1(u)$  is a polynomial, there should be no pole at  $u = 0$ . Therefore, to ensure  $T_1(u)$  to be a polynomial, we must have  $\alpha_0 = 0$ , which in term means  $P(u)$  is a polynomial. According to Theorem 1, the zeros of  $Q(u)$  is a physical solution if and only if  $P(u)$  is a polynomial.

**Why rational  $Q$ -system works** Now let us see that the equations (7.2) appears naturally in the rational  $Q$ -system.

Let us first consider the box whose lower left corner is at  $(a, s) = (0, 0)$ . The corresponding  $QQ$ -relation is given by

$$Q_{1,0}Q_{0,1} = Q_{1,1}^+Q_{0,0}^- - Q_{1,1}^-Q_{0,0}^+ \quad (7.11)$$

Plugging in the boundary conditions

$$Q_{1,0}(u) = Q(u), \quad Q_{0,0}(u) = u^L, \quad (7.12)$$

we obtain

$$\begin{aligned} Q_{0,1}(u)Q(u) &= (u - \frac{i}{2})^L Q_{1,1}^+(u) - (u + \frac{i}{2})^L Q_{1,1}^-(u) \\ &= (u - \frac{i}{2})^L [Q(u) - Q^{++}(u)] - (u + \frac{i}{2})^L [Q^{--}(u) - Q(u)] \end{aligned} \quad (7.13)$$

where we have used the  $QQ$ -relation in the second equality

$$[(u - \frac{i}{2})^L + (u + \frac{i}{2})^L - Q_{0,1}(u)] Q(u) = (u - \frac{i}{2})^L Q^{++}(u) + (u + \frac{i}{2})^L Q^{--}(u). \quad (7.14)$$

Defining

$$T_0(u) = (u + \frac{i}{2})^L + (u - \frac{i}{2})^L - Q_{0,1}(u), \quad Q_{0,1}(u) = W_1(u), \quad (7.15)$$

we have

$$T_0(u)Q(u) = (u - \frac{i}{2})^L Q^{++}(u) + (u + \frac{i}{2})^L Q^{--}(u). \quad (7.16)$$

This is the first  $TQ$ -relation in (7.2).

Now we consider the block at  $(a, s) = (0, 1)$  with the corresponding  $QQ$ -relation

$$\begin{aligned} Q_{1,1}Q_{0,2} &= Q_{1,2}^+Q_{0,1}^- - Q_{1,2}^-Q_{0,1}^+ \\ &= W_1^- Q_{1,2}^+ - W_1^+ Q_{1,2}^- \\ &= W_1^- (Q_{1,1} - Q_{1,1}^{++}) - W_1^+ (Q_{1,1}^{--} - Q_{1,1}) . \end{aligned} \tag{7.17}$$

This can be rewritten as

$$(W_1^+ + W_1^- - Q_{0,2}) Q_{1,1} = W_1^- Q_{1,1}^{++} + W_1^+ Q_{1,1}^{--} \tag{7.18}$$

Noticing that  $Q_{1,1}(u) = DQ(u)$  and defining

$$T_1(u) = W_1^+(u) + W_1^-(u) - Q_{0,2}(u) , \tag{7.19}$$

we can rewrite (7.18) as

$$T_1(u) DQ(u) = W_1^-(u) DQ^{++}(u) + W_1^+(u) DQ^{--}(u) . \tag{7.20}$$

This is the second  $TQ$ -like equation in (7.2). Therefore, according to Theorem 2, the zeros of  $Q(u) = Q_{1,0}(u)$  are physical solutions of Bethe ansatz equations. This explains why the rational  $Q$ -system works so well.

Notice that we only used the  $QQ$ -relations in the first two columns of the Young tableaux to derive the two  $TQ$ -like relations in Theorem 2. This means that the  $QQ$ -relations for the rest of the boxes in the Young tableaux is redundant.

## 8 On completeness of Bethe ansatz

After a long discussion on Bethe ansatz equations of the XXX spin chain, let us summarize the situation about the completeness problem of Bethe ansatz. The conclusion is that Bethe ansatz is complete for XXX spin chain. However, this is not a simple result proven in a single work, but rather a conclusion we can draw from several works in the past decade.

- The original BAE has too many solutions. There are two kinds of non-physical solutions: coinciding rapidities and non-physical singular solutions. This is discussed in detail in [2].
- These two kinds of solutions can be eliminated by considering  $TQ$ -relations and require that both solutions of  $TQ$ -relations are polynomials. This is explained in [4].

- There is a final important result, which we did not discuss in this lecture. It is proven by Mukhin, Tarasov and Varchenko [6] that the number of solutions for a the  $TQ$ -relation with two polynomial solutions is given by

$$\mathcal{N}_{L,M} = \binom{L}{M} - \binom{L}{M-1} \quad (8.1)$$

where  $L$  is the degree of  $T(u)$  and  $M$  is the degree of  $Q(u)$ . Notice that (8.1) is precisely the number of primary states (2.13) that we need for the Bethe ansatz to be complete, derived at the beginning of the lecture.

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