Completeness and Bethe root distribution of the spin-$\frac{1}{2}$ Heisenberg chain with arbitrary boundary fields

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Recently, the XXZ spin chain with arbitrary boundary fields was successfully solved via the off-diagonal Bethe ansatz method. The correctness and the completeness of this solution were numerically verified by Nepomechie for one choice of the parameterizations. In this paper, we discuss further the completeness of another parameterization of the Bethe ansatz equations and its reduction to the parallel boundary field case. The numerical results show that when the relative angle between the boundary fields turns to zero, both the $T - Q$ relations and the Bethe ansatz equations are reduced to the ones obtained by the conventional Bethe ansatz methods. This allows us to establish a one-to-one correspondence between the Bethe roots of the unparallel boundary field case and those of the parallel boundary field case. In the thermodynamic limit $N \rightarrow \infty$, those two sets of Bethe roots tend to the same and the contribution of the relative angle to the energy is in the order of $N^{-1}$.

PACS numbers: 75.10.Pq, 03.65.Vf, 71.10.Pm

I. INTRODUCTION

The Heisenberg spin chain model plays a very important role in condensed matter physics since it provides a benchmark for understanding the magnetic properties in one dimension. This model was firstly solved by Bethe with which the so-called Bethe ansatz method was invented. The open boundary problem of this model was initially studied by Gaudin. Thereafter the model with parallel boundary fields was successfully solved in Ref. 6. An important achievement for the integrable models with open boundaries is the reflection equation proposed in Ref. 7 which induces the important result: The spin chain with arbitrary unparallel boundary fields is also integrable! This problem has attracted a lot of attentions not only for its mathematical structure but also for its relevance to the stochastic process and the spin current physics. The density matrix renormalization group (DMRG) analysis showed that the spin-spin correlation in this model may show a spiral behavior and the unparallel boundary fields may induce a “spin voltage”. Though the integrability has been demonstrated for over two decades, the coordinate Bethe ansatz and the algebraic Bethe ansatz encountered a big problem for approaching such a kind of models because those methods strongly rely on the existence of a local vacuum which these model do not possess as the $U(1)$ symmetry is broken by the unparallel boundaries. Until very recently, the model was solved via the off-diagonal Bethe ansatz method. This method overcomes the obstacle of the lack of a reference state and allows to derive the eigenvalues of the transfer matrix only based on some operator product identities. It is shown that the the form of the Bethe ansatz equations (BAEs) is quite different from that of the parallel boundary case and may be parameterized in a variety of different ways. The completeness of the solutions was numerically checked by Nepomechie for a special choice of the parameterizations and the Bethe root distribution in the ground state is also discussed.

In this paper, we examine further the completeness of another parameterization of the BAEs numerically up to lattice number $N = 6$ by comparison of numerically solutions of these equations and the results from the exact diagonalization. In addition, we also consider the reduction of the BAEs to those of the parallel boundary case when the relative angle between the two boundary fields $\alpha \rightarrow 0$. Such a reduction process allows us to establish the one-to-one correspondence between the Bethe roots of the two cases. With this correspondence a perturbation theory can be used to derive the physical effect of the boundary fields.

The paper is organized as follows. In Sec I we give a brief description of the model and the BAEs. The numerical check for the completeness of the BAEs and the distribution of Bethe roots is discussed in Sec II with $N = 3,5$ and $N = 4$ as two examples representing the odd $N$ and even $N$ cases, respectively. The reduction from the case of the unparallel boundary fields to that of the parallel boundary fields is given in Sec III. This allows us to construct the correspondence between the two sets of Bethe roots. Sec IV is attributed to the effect of the relative angle between the boundary fields in the thermodynamic limit $N \rightarrow \infty$. The concluding remarks are given in Sec V.
II. MODEL AND EXACT SOLUTION

The Hamiltonian of the model reads

$$H = \sum_{j=1}^{N-1} \delta_j \delta_{j+1} + \frac{1}{p} \sigma_N^x + \frac{1}{q}(\sigma_N^1 + \xi \sigma_N^2). \quad (1)$$

where \( p, q \) and \( \xi \) are arbitrary real constants and \( \delta_j \) are the Pauli matrices as usual. \( 1/p \) and \( q_0 = q/\sqrt{1 + \xi^2} \) represent the strengths of the two boundary fields, respectively. Notice that we can always choose one boundary field along \( z \)-axis and the other in the \( x-z \) plane without losing generality because of the \( O(3) \)-invariance of the bulk. For convenience, we define the relative angle between the two boundary fields as \( \alpha = \arctan \xi \) and \( \alpha \in (-\pi/2, \pi/2) \).

In Ref. 1, a general expression of the eigenvalue \( \Lambda(u) \) of the transfer matrix was derived based on the operator product identities of the transfer matrix. In this paper, we choose the following extended \( T-Q \) ansatz of \( \Lambda(u) \)

$$\Lambda(u) = \tilde{a}(u) \frac{Q_1(u-1)}{Q_2(u)} + \tilde{d}(u) \frac{Q_2(u+1)}{Q_1(u)} + \tilde{c}(u) \tilde{a}(u) \tilde{d}(u), \quad (2)$$

with

$$\tilde{a}(u) = \sqrt{1 + \xi^2} \frac{u + 1}{u + \frac{1}{2}} (u + p)(u + q_0)(u + 1)^2 N,$$

$$\tilde{d}(u) = \sqrt{1 + \xi^2} \frac{u + 1}{u + \frac{1}{2}} (u + 1 - p)(u + 1 - q_0) u^2 N,$$

$$\tilde{c}(u) = -\frac{\xi_0}{2} \frac{(2u + 1) \beta}{2\sqrt{1 + \xi^2}} \frac{u + 1}{u + p} \frac{1}{u + q_0} \frac{1}{u + p + u + q_0},$$

$$Q_1(u) = \prod_{j=1}^{M} \left( u - i \mu_j + \frac{1}{2} \right), \quad Q_2(u) = \prod_{j=1}^{M} \left( u + i \mu_j + \frac{1}{2} \right),$$

where \( \xi_0 = 4 \sin^2(\alpha/2), \) \( M \geq N \) is an integer and \( \mu_j \)'s are the Bethe roots. \( \Lambda(u) \) possesses the following properties: (1) It is a polynomial of degree \( 2N + 2 \); (2) It satisfies the crossing symmetry relation \( \Lambda(u) = \Lambda(-u - 1) \). Notice that \( \tilde{a}(-u - 1) = \tilde{b}(u), \tilde{c}(-u - 1) = \tilde{c}(u) \) and \( Q_1(-u - 1) = (-1)^M Q_2(u) \) protect the crossing symmetry automatically. Since \( \Lambda(u) \) is a polynomial, the regularity induces the following BAES

$$\xi_0 \left[ \left( \mu_j + \frac{1}{2} \right) \left( \mu_j - \frac{1}{2} \right) \right]^\beta \mu_j \left( \mu_j - \frac{1}{2} \right)^{2N + 1} = (\mu_j + ip') \times \left( \mu_j + iq' \right) \prod_{l=1}^{M} (\mu_j + \mu_l)(\mu_j + \mu_l - i), j = 1, 2, \cdots, M, \quad (3)$$

where \( p' = p - 1/2, q' = q_0 - 1/2 \) and \( \beta = M - N \). Notice that the simplicity of the "poles" is required to keep the self-consistency in deriving the BAES. This requirement gives the following selection rules for the Bethe roots: \( \mu_l \neq \mu_j \) for \( l \neq j \) and \( \mu_j + \mu_l \neq 0,1 \). The integer \( \beta \) here should be nonnegative even number for even \( N \) and positive odd number for odd \( N \). In the numerical verifications, we choose \( M = N \) and \( \beta = 0 \) for even \( N \) and \( M = N + 1 \) and \( \beta = 1 \) for odd \( N \). The eigenvalue of Hamiltonian \( (1) \) is given by

$$E = N - 1 + \frac{1}{p} \frac{1}{q_0} - 2 \sum_{j=1}^{M} \frac{1}{\mu_j + 1/2}. \quad (4)$$

III. COMPLETENESS OF THE BETHE ANSATZ SOLUTIONS

The numerical solutions for Eqs. \( (3) \) are undertaken for some given parameters \( p, q \) and \( \xi \) with small \( N \). The results for \( p = -0.6, q = -0.3, \xi = 1.2 \) and \( N = 3, 4, 5 \) are listed in Table I. The values of the eigenvalue in the tables are calculated from both the Bethe roots and the exact diagonalization.

| \( \mu_{1,2} \) | \( \mu_{3,4} \) | \( E \) | elv |
|----------------|----------------|------|-----|
| \pm 0.40945 \pm 0.01585i | \pm 0.25771 \pm 0.50018i | -9.66040 | 1 |
| \pm 0.36230 - 0.00003i | \pm 3.087841 \pm 0.48274i | -9.66040 | 1 |
| \pm 0.16920 + 0.50006i | \pm 1.577811 \pm 0.71570i | -5.22656 | 2 |
| \pm 1.57984 - 0.84026i | \pm 1.51070 \pm 1.08886i | -5.22656 | 2 |
| \pm 1.61505 + 0.04771i | \pm 0.13230 \pm 0.92111i | -4.27213 | 3 |
| \pm 1.27132 + 0.04315i | \pm 1.27426i \pm 0.04143i | -4.27213 | 3 |
| \pm 0.33201 + 0.50005i | \pm 1.45102i \pm 0.33565i | -2.94645 | 4 |
| \pm 4.11978i - 0.79915i | \pm 1.11160i \pm 0.00355i | -2.94645 | 4 |
| \pm 0.88730 + 0.02945i | \pm 0.69758i \pm 0.00590i | 2.03247 | 5 |
| \pm 0.28427 + 0.00744i | \pm 0.29118i \pm 0.98321i | 2.03247 | 5 |
| \pm 0.41166 + 0.50097i | \pm 0.86138i \pm 0.16936i | 4.25829 | 6 |
| \pm 3.58744i - 0.63526i | \pm 0.69229i \pm 0.00290i | 4.25829 | 6 |
| \pm 0.83111 - 0.04406i | \pm 0.20999i \pm 0.90204i | 6.60218 | 7 |
| \pm 1.13291i - 0.12386i | \pm 0.67782i \pm 0.01441i | 6.60218 | 7 |
| \pm 1.09568i - 0.55876i | \pm 0.19858i \pm 0.89064i | 8.73767 | 8 |
| \pm 5.57838i - 1.52046i | \pm 0.20398i \pm 0.89604i | 8.73767 | 8 |

Even
TABLE II: Bethe roots and the eigen energies for $p = -0.6, q = -0.3, \xi = 1.2, N = 4$.

| $\mu_{1,2}$ | $\mu_{3,4}$ | $E$ elv |
|-------------|-------------|--------|
| $\pm 1.3676 + 0.21035i$ | $\pm 0.26039 + 0.00024i$ | $-10.76127$ |
| $\pm 0.20995 + 0.00021i$ | $\pm 1.69283 - 0.28144i$ | $-9.28939$ |
| $\pm 0.79468 - 0.43736i$ | $\pm 0.70776 + 0.46346i$ | $-6.64726$ |
| $\pm 0.48700 - 0.00183i$ | $\pm 1.35733 - 0.19102i$ | $-5.95319$ |
| $\pm 1.34713 + 0.49238i$ | $\pm 2.62865 - 0.77106i$ | $-4.04791$ |
| $\pm 0.16855 - 0.10453i$ | $\pm 0.12746 + 1.06030i$ | $-3.22515$ |
| $\pm 1.77115 + 0.22696i$ | $\pm 1.15047 - 0.04554i$ | $-2.08666$ |
| $\pm 3.46475 - 0.75587i$ | $\pm 1.14892 - 0.04841i$ | $-1.23956$ |
| $\pm 0.34771 - 0.00294i$ | $\pm 0.78950i + 0.09748i$ | $-0.28153$ |
| $\pm 0.19568 - 0.00928i$ | $\pm 0.26033i + 0.95237i$ | $2.50287$ |
| $\pm 1.56553 + 0.22572i$ | $\pm 0.70522i - 0.01317i$ | $4.46454$ |
| $\pm 0.45669 + 0.01413i$ | $\pm 0.23133i + 0.90518i$ | $5.39498$ |
| $\pm 2.62317 - 0.52576i$ | $\pm 0.71018i - 0.01812i$ | $5.61585$ |
| $\pm 1.37968 - 0.28919i$ | $\pm 0.64194i - 0.05012i$ | $7.22925$ |
| $\pm 1.12382 - 0.10390i$ | $\pm 0.20476i + 0.89676i$ | $8.55124$ |
| $\pm 7.91636 - 2.01412i$ | $\pm 0.20397i + 0.89603i$ | $9.77318$ |

though we cannot demonstrate the completeness of the solutions from the BAEs, the numerical results strongly suggest that the solution is complete. In fact, from the BAEs we learn that there are infinite number of choices of $\beta$. Different choice only gives different parameterization but not different solution. In such a sense, we may believe the solution from the BAESs is complete.

IV. REDUCTION TO THE PARALLEL BOUNDARY FIELD CASE

When $\alpha$ tends to zero, the Hamiltonian is reduced to the case studied in Refs. 6 and 7. The BAES obtained from the off-diagonal Bethe ansatz should also be reduced to those of the parallel boundary field case. For a very small $\alpha$, $\xi_\alpha = \alpha^2 + O(\alpha^3)$. From Eq. [3], we can see that the left hand side must be also very small. Thus, in the small $\alpha$ limit, we can divide the $\mu$ into two classes

$$
\mu^+ = \pm x_l + i \delta^+_{l}, \quad l = 1, 2, \cdots, M_1;
\mu^- = \pm y_l + i/2 + i \delta^-_{l}, \quad l = 1, 2, \cdots, M_2.
$$

(5)

where $\mu^+ + \mu^- = 2i \delta^+_{l}$, $\mu^+_l + \mu^-_l = 2i \delta^-_{l}$, $\delta^{x,y}$ are small numbers and $M = 2(M_1 + M_2)$. Based on this classification of $\mu_j$, both the $T-Q$ relation and the BAES can be reduced to those of the parallel boundary field case. For $\alpha = 0$, $\delta^{x,y} = 0$. Submitting these results into Eq. [2], the extended $T-Q$ relation is reduced to

$$
A(\mu) = \bar{a}(\mu) \frac{Q(\mu - 1)}{Q(\mu)} + \bar{d}(\mu) \frac{Q(\mu + 1)}{Q(\mu)}.
$$

(6)

where

$$
\bar{Q}(u) = \prod_{j=1}^{M} \left( \mu - i x_j + \frac{1}{2} \right) \left( \mu + i x_j + \frac{1}{2} \right),
$$

(7)

which is just the $T-Q$ relation for the parallel boundary field case.

Now let us check the BAES. Submitting Eq. [4] into Eq. [3], we get four sets of equations of $\mu^+_l$ and $\mu^-_l$ respectively. Keeping the leading order of $\delta^{x,y}$, we get the following four equations:

$$
(x_j - \frac{1}{2})^{2N+1} = \frac{x_j + ip^j x_j + iq^j q_{l}}{x_j - ip^j x_j - iq^j q_{l}} \prod_{l',r} x_j + r x_j - i,
$$

(8)
\[
\begin{align*}
\left(\frac{y_j + 1}{y_j + \frac{1}{2}}\right)^\beta y_j - \frac{1}{2} & = - \frac{y_j + i\beta y_j + ig}{y_j - i\beta y_j - ig} \prod_{i,r} M_j y_j + ry_j - 1 \\
i\delta_j^x = \eta_\alpha \left[\left(\frac{x_j + \frac{1}{2}}{x_j - \frac{1}{2}}\right)^\beta (x_j - \frac{1}{2})^{2N+1}\right] \prod_{i,r} M_j (x_j + rx_j) \\
\times \prod_{i,r} \frac{1}{x_j + rx_j - 1} & = \prod_{i,r} \frac{1}{x_j + ry_j - 1} \\
i\delta_j^y = \eta_\alpha \left[\left(\frac{y_j + \frac{1}{2}}{y_j - \frac{1}{2}}\right)^\beta (y_j - \frac{1}{2})^{2N+1}\right] \prod_{i,r} M_j (y_j + ry_j) \\
\times \prod_{i,r} \frac{1}{y_j + ry_j - 1} & = \prod_{i,r} \frac{1}{y_j + rx_j - 1} \\
\end{align*}
\]

where \( r = \pm \). Notice that in Eqs. (8) and (9) \( x_j \) and \( y_j \) are decoupled from each other. When \( \alpha = 0 \), \( \xi_0 = 0 \), \( \delta^{x,y} = 0 \), from the energy expression (11), we can see that only \( x_j \) contribute and \( y_j \) are irrelevant. The equations about \( x_j \) are just the BAEs of the parallel boundary field case.

For the traditional BAEs, to find the complete solutions we need to choose \( M_j \) from 0 to \( N \). To get a complete reduction, we can set \( \beta \geq N \), for example \( M = 2N \). The correctness of this reduction process is also checked numerically for \( p = 0.6 \), \( q_0 = 0.6 \) and \( N = 10 \). The ground state Bethe root distributions for \( \alpha = 0 \), \( \xi_0 = 0 \), \( \delta^{x,y} = 0 \), from the energy expression (14) we can see that the Bethe roots tend to the values of \( \alpha = 0 \) case.

V. THE THERMODYNAMIC LIMIT

In the thermodynamic limit \( N \to \infty \), the contribution of \( \alpha \) should become smaller and smaller with the increasing \( N \). From Eq. (20) we get

\[
\begin{align*}
\frac{\xi_\alpha' + \beta \mu_j' + \frac{1}{2}}{\mu_j + \frac{1}{2}} & + \frac{\mu_j' + (2N + 1 + \beta) \mu_j'}{2} \mu_j - \frac{1}{2} = \mu_j' = \frac{\mu_j' + i\beta}{2} \\
+ \frac{\mu_j' + 1}{\mu_j + i\beta} & + \sum_l \left( \frac{2}{\mu_j + \mu_l} + \frac{2}{\mu_j + \mu_l - 1} \right) - \frac{2}{\mu_j - \frac{1}{2}}
\end{align*}
\]

where \( \mu_j' = \partial_{\alpha} \mu_j \) and \( \xi_\alpha' = \partial_{\alpha} \xi_\alpha \). From Eq. (12), we can see that when \( \hat{N} \) is very large, \( \mu_j' \) are very small. Up to the leading order the above equations can be written as

\[
\mu_j' \approx \frac{1}{N^2 \xi_\alpha'} \left[ \frac{1}{N} \sum_l \left( \frac{2}{\mu_j + \mu_l} + \frac{2}{\mu_j + \mu_l - 1} \right) - \frac{2}{\mu_j - \frac{1}{2}} \right]^{-1}
\]

which indicate that \( \mu_j' \) are in the order of \( 1/N \). This means that for two different \( \alpha \) the maximum difference of \( \mu_j \) for the corresponding state is \( \Delta \mu_j \ll 1/N \).

The numerical results in TABLE (IV) for \( N = 10 \) also support this indication. When the lattice number \( N \) is very large, the boundary fields only affect the spins close to the ends. Indeed, the DMRG results showed that the correlations of the spin at the ends and the ones in the bulk are almost independent of the angle \( \alpha \). To show the contribution of \( \alpha \) to the energy, we divide the eigenvalue energy of the Hamiltonian (1) into two parts

\[
E(p, q_0, \alpha) = E(p, q_0, 0) + \Delta E(p, q_0, \alpha),
\]

\( E(p, q_0, 0) \) is the energy for \( \alpha = 0 \) and \( \Delta E \) is the contribution of nonzero \( \alpha \). For a large boundary field angel \( \alpha = \pi/2 \), we plot \( \Delta E \) in FIG. (I) and FIG. (I) (a) gives the \( \Delta E \) and FIG. (I) (b) gives the \( \hat{N} \Delta E \). The numerical fitting shows that \( \Delta E \) is of the order \( 1/N \). For the contribution of the boundary fields to the energy is of order \( O(N^0) \), in the thermodynamic limit we can omit the contribution of \( \alpha \) up to the leading order. In fact, the two boundaries are decoupled from each other completely when \( N \to \infty \).

VI. CONCLUSION

In conclusion, we numerically verified the completeness and the correctness of the off-diagonal Bethe ansatz solutions for the Heisenberg spin chain model with arbitrary boundary fields. The one-to-one correspondence between the Bethe roots of the unparallel boundary field case and those of the parallel boundary field case is established based on the reduction process. This correspondence allows us to study the physical effect of the relative angle \( \alpha \) by a proper perturbation approach, since the Bethe root...
distribution of the parallel boundary field case is already well known. It is shown that the contribution of $\alpha$ to the energy is of order $N^{-1}$, which is negligible small in the thermodynamic limit $N \to \infty$. We remark that such correspondence and perturbation procedure are also suitable for other models solved via the off-diagonal Bethe ansatz.

The financial support from the National Natural Science Foundation of China (Grant Nos.11174335, 11075126, 11031005, 11375141, 11374334), the National Program for Basic Research of MOST (973 project under grant No.2011CB921700) and the State Education Ministry of China (Grant No. 20116101110017 and SRF for ROCS) are gratefully acknowledged.

| $\alpha$ | $\mu_{1,1}^{x}$ | $\mu_{1,2}^{x}$ | $\mu_{1,3}^{x}$ | $\mu_{1,4}^{x}$ | $\mu_{1,5}^{x}$ |
|--------|----------------|----------------|----------------|----------------|----------------|
| 0.0\pi | 0.06215 + 0.00000i | 0.13790 + 0.00000i | 0.23440 + 0.00000i | 0.36296 + 0.00000i | 0.56279 + 0.00000i |
| 0.1\pi | 0.05834 + 0.00942i | 0.14116 + 0.01253i | 0.24263 + 0.01139i | 0.37557 + 0.00980i | 0.58306 + 0.00826i |
| 0.3\pi | 0.05426 + 0.02488i | 0.14343 + 0.03075i | 0.24972 + 0.03269i | 0.39081 + 0.03666i | 0.62243 + 0.04782i |
| 0.4\pi | 0.05337 + 0.02967i | 0.14382 + 0.03605i | 0.25099 + 0.03927i | 0.39382 + 0.04611i | 0.63233 + 0.06678i |
| 0.5\pi | 0.05278 + 0.03332i | 0.14408 + 0.04004i | 0.25180 + 0.04427i | 0.39569 + 0.05347i | 0.63838 + 0.08281i |