Thermodynamic limit and boundary energy of the $su(3)$ spin chain with non-diagonal boundary fields

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Abstract

We investigate the thermodynamic limit of the $su(n)$-invariant spin chain models with unparallel boundary fields. It is found that the contribution of the inhomogeneous term in the associated $T-Q$ relation to the ground state energy does vanish in the thermodynamic limit. This fact allows us to calculate the boundary energy of the system. Taking the $su(2)$ (or the XXX) spin chain and the $su(3)$ spin chain as concrete examples, we have studied the corresponding boundary energies of the models. The method used in this paper can be generalized to study the thermodynamic properties and boundary energy of other high rank models with non-diagonal boundary fields.

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1 Introduction

Exactly solvable models have played essential roles in many areas of physics, such as ultracold atoms \cite{1}, condensed matter physics \cite{2, 3}, the AdS/CFT correspondence \cite{4, 5}, equilibrium and non-equilibrium statistical physics \cite{6, 7, 8, 9, 10, 11}. The thermodynamic properties of these models, for example, the specific heat, susceptibility and elementary excitations, which can be obtained by using the thermodynamic Bethe ansatz (TBA) \cite{12}, have attracted a great attention due to the analytical results can be compared with experimental data directly \cite{1, 2, 12, 13, 14, 15}.

In the frame of the off-diagonal Bethe ansatz (ODBA) method developed recently \cite{16}, a large class of integrable models without $U(1)$ symmetry, thus lack of obvious reference state, can be solved exactly, which attracts general interest, such as the spin-1/2 chain with arbitrary boundary fields \cite{17, 18, 19, 20, 21}, the $su(n)$ spin chain with non-diagonal boundary fields \cite{22}, the high spin Heisenberg chain \cite{23}, the one-dimensional Hubbard model with arbitrary boundary magnetic fields \cite{24}, the XYZ spin chain with odd site number \cite{25}, the spin-1/2 torus \cite{26} and the Izergin-Korepin Model with generic open boundaries \cite{27}. Naturally, the thermodynamic limit of those models becomes a subject of intense research \cite{28, 29, 30}. However, the corresponding Bethe Ansatz equations (BAEs) obtained by using the ODBA method have much complicated structure due to the inhomogeneous term in the $T$-$Q$ relation, which makes the direct employment of the TBA method to approach the thermodynamic limit of those models very involved \cite{16, 28, 29}.

Nevertheless, some important progresses have been made recently \cite{28, 29, 30}. For the spin-1/2 isotropic quantum spin chain with arbitrary boundary fields, the pioneering work of Jiang et al. \cite{28} showed that the two boundaries are decoupled from each other in the thermodynamic limit. In addition, Nepomechie et al. presented the thermodynamic limit and boundary (or surface) energy of the model with an expansion up to the second order in terms of small non-diagonal boundary terms \cite{29}. For the open XXZ spin chain with generic boundary fields, a method to address this problem was proposed in Refs. \cite{16, 30} based on the fact that the system has some degenerate points, at which the BAEs become the usual production ones and can be studied by the TBA. In the thermodynamic limit, these degenerate points become dense thus we can use the properties at these degenerate points to approach the real thermodynamics of the systems. The thermodynamic limit and surface
energy were calculated for arbitrary imaginary crossing parameter \[30\] and for real crossing parameter with a constraint \[16\], and then applied to the study of the quantum impurities \[31\]. However, the results about the model with arbitrary boundary fields are still missing. Therefore, to obtain the thermodynamic limit and boundary energy of the models solved by the ODBA is still an open question and is worth further study.

In this paper, we study the thermodynamic limit of the \( su(n) \)-invariant spin chain models with unparallel boundary fields by taking the XXX spin-1/2 chain and the \( su(3) \)-invariant chain with unparallel boundary fields \[16\],\[17\] as concrete examples. Because of the difficulties arising from the inhomogeneous term in the \( T-Q \) relation, the first thing should be addressed is the contribution of the inhomogeneous term. Through the analysis of the finite-lattice systems, it is found that the contribution of the inhomogeneous term to the ground state energy does reduce to zero when the size of the system tends to infinity. Namely, the inhomogeneous term in the \( T - Q \) relation can be ignored in the thermodynamic limit. We note that, even though without the inhomogeneous term, the \( T - Q \) relation still contains the non-diagonal boundary fields, whose contribution can be identified by calculating the boundary energy of the model. Comparison of the boundary energy from the analytic expressions with that from the Hamiltonian by the extrapolation method shows that they coincide with each other very well. This further demonstrates that the neglected inhomogeneous term does not affect the physical properties of the studied system in the thermodynamic limit.

The paper is organized as follows. Section 2 serves as an introduction to our notations for the inhomogeneous \( su(n) \)-invariant spin chains with generic boundary fields. In Section 3, we focus on the \( su(2) \)-invariant (or the XXX spin-1/2) open spin chain with the most general non-diagonal boundary terms. With the help of the Bethe ansatz solution for the finite size system, we study the thermodynamic limit and boundary energy of the model. The results for the \( su(3) \)-invariant case are given in Section 4. We summarize our results and give some discussions in Section 5.

## 2 \( su(n) \)-invariant spin chain with generic boundary fields

Let \( V \) denote a \( n \)-dimensional linear space with an orthonormal basis \( \{ |i \rangle |i = 1, \cdots, n \} \), which endows the fundamental representation of \( su(n) \) algebra. The \( su(n) \)-invariant \( R- \)
matrix $R(u) \in \text{End}(V \otimes V)$ is given by \[ R_{12}(u) = u + \eta P_{1,2}, \tag{2.1} \]

where $u$ is the spectral parameter and $\eta$ is the crossing parameter (without losing the generality we set $\eta = 1$ in the following part of this paper). The $R$-matrix satisfies the quantum Yang-Baxter equation (QYBE)

\[ R_{12}(u_1 - u_2)R_{13}(u_1 - u_3)R_{23}(u_2 - u_3) = R_{23}(u_2 - u_3)R_{13}(u_1 - u_3)R_{12}(u_1 - u_2), \tag{2.2} \]

and possesses the following properties:

Initial condition : \[ R_{12}(0) = P_{1,2}, \tag{2.3} \]

Unitarity : \[ R_{12}(u)R_{21}(-u) = \rho_1(u) \text{id}, \quad \rho_1(u) = -(u + 1)(u - 1), \tag{2.4} \]

Crossing-unitarity : \[ R_{12}^{(+)}(u)R_{21}^{(-)}(-u - n) = \rho_2(u) \text{id}, \quad \rho_2(u) = -u(u + n), \tag{2.5} \]

Fusion conditions : \[ R_{12}(-1) = -2P_{1,2}^{(-)}, \quad R_{12}(1) = 2P_{1,2}^{(+)}. \tag{2.6} \]

Here $R_{21}(u) = P_{1,2}R_{12}(u)P_{1,2}$, $P_{1,2}^{(\pm)} = \frac{1}{2}\{1 \mp P_{1,2}\}$ is anti-symmetric (symmetric) project operator in the tensor product space $V \otimes V$, and $t_i$ denotes the transposition in the $i$-th space. Here and below we adopt the standard notation: for any matrix $A \in \text{End}(V)$, $A_j$ is an embedding operator in the tensor space $V \otimes V \otimes \cdots$, which acts as $A$ on the $j$-th space and as an identity on the other factor spaces; $R_{ij}(u)$ is an embedding operator of $R$-matrix in the tensor space, which acts as an identity on the factor spaces except for the $i$-th and $j$-th ones.

Let us introduce the “row-to-row” (or one-row) monodromy matrix $T(u)$, which is an $n \times n$ matrix with operator-valued elements acting on $V^\otimes N$,

\[ T_0(u) = R_{0N}(u)R_{0N-1}(u) \cdots R_{01}(u). \tag{2.7} \]

The QYBE implies that one-row monodromy matrix $T(u)$ satisfies the Yang-Baxter relation

\[ R_{00'}(u - v)T_0(u)T_{0'}(v) = T_{0'}(v)T_0(u)R_{00'}(u - v). \tag{2.8} \]

Integrable open chain can be constructed as follows \[34, 35\]. Let us introduce a pair of $K$-matrices $K^-(u)$ and $K^+(u)$. The former satisfies the reflection equation (RE) \[36, 35\]

\[ R_{12}(u_1 - u_2)K_1^-(u_1)R_{21}(u_1 + u_2)K_2^-(u_2) = K_2^-(u_2)R_{12}(u_1 + u_2)K_1^-(u_1)R_{21}(u_1 - u_2), \tag{2.9} \]
and the latter satisfies the dual RE

\[ R_{12}(u_2 - u_1)K_1^+(u_1)R_{21}(-u_1 - u_2 - n)K_2^+(u_2) = K_2^+(u_2)R_{12}(-u_1 - u_2 - n)K_1^+(u_1)R_{21}(u_2 - u_1). \] (2.10)

For open spin-chains, instead of the standard “row-to-row” monodromy matrix \( T(u) \), one needs to consider the “double-row” monodromy matrix \( \mathcal{J}(u) \)

\[ J_0(u) = T_0(u)K_0^-(u)\hat{T}_0(u), \] (2.11)

\[ \hat{T}_0(u) = R_{01}(u)R_{02}(u)\ldots R_{0N}(u). \]

Then the double-row transfer matrix \( t(u) \) of the open spin chain is given by

\[ t(u) = \text{tr}_0 \{ K_0^+(u)\mathcal{J}_0(u) \}. \] (2.12)

From the QYBE and the (dual) RE, one may check that the transfer matrices with different spectral parameters commute with each other: \([t(u), t(v)] = 0\). Thus \( t(u) \) serves as the generating functional of the conserved quantities, which ensures the integrability of the system described by the Hamiltonian

\[ H = \frac{\partial \ln t(u)}{\partial u} \bigg|_{u=0} = \frac{1}{2} \sum_{j=1}^{N-1} P_{j,j+1} + \frac{\text{tr}_0K_0^+(0)}{\text{tr}_0K_0^-(0)} + \frac{2\text{tr}_0K_0^+(0)P_{0N}}{\text{tr}_0K_0^-(0)} + \{K_1^-(0)\}^{-1}K_1^-(0). \] (2.13)

The commutativity of the transfer matrices with different spectral parameters implies that they have common eigenstates. Let \(|\Psi\rangle\) be a common eigenstate of \( t(u) \), which does not depend upon \( u \), with the eigenvalue \( \Lambda(u) \),

\[ t(u)|\Psi\rangle = \Lambda(u)|\Psi\rangle. \] (2.14)

Using the ODBA method [16, 22], the corresponding eigenvalue \( \Lambda(u) \) is given in terms of an inhomogeneous \( T - Q \) relation [26, 17]. The aim of this paper is to investigate the thermodynamic limit \( (N \to \infty) \) of the model by the exact solutions obtained in [17, 22].
3 Boundary energy of the XXX spin-1/2 chain with arbitrary boundary fields

The Hamiltonian given by (2.13) of the XXX spin-1/2 chain with unparallel boundary fields reads [16, 17]

\[ H = \sum_{j=1}^{N-1} (\vec{\sigma}_j \cdot \vec{\sigma}_{j+1}) + \frac{1}{p} \sigma^z_j + \frac{1}{q} (\sigma^x_N + \xi \sigma^z_N) + N, \]  

(3.1)

where \( \vec{\sigma}_j \) is the Pauli matrix at site \( j \), and \( p, q \) and \( \xi \) are all arbitrary real boundary parameters to ensure a hermitian Hamiltonian. The corresponding \( K \)-matrices \( K^\pm(u) \) are given by

\[ K^-(u) = \begin{pmatrix} p + u & 0 \\ 0 & p - u \end{pmatrix}, \]  

(3.2)

and

\[ K^+(u) = \begin{pmatrix} q + u + 1 & \xi(u+1) \\ \xi(u+1) & q - u - 1 \end{pmatrix}. \]  

(3.3)

The eigenvalue \( \Lambda(u) \) of the corresponding transfer matrix is given in terms of the inhomogeneous \( T - Q \) relation [17]

\[ \Lambda(u) = \frac{2(u+1)^{2N+1}}{2u+1} (u+p) \left[ (1+\xi^2)^{\frac{1}{2}} u + q \right] Q(u-1) Q(u) \]

\[ + \frac{2u^{2N+1}}{2u+1} (u-p+1) \left[ (1+\xi^2)^{\frac{1}{2}} (u+1) - q \right] Q(u+1) Q(u) \]

\[ + 2 \left[ 1 - (1+\xi^2)^{\frac{1}{2}} \right] \frac{[u(u+1)]^{2N+1}}{Q(u)}, \]  

(3.4)

where the function \( Q(u) \) can be parameterized as

\[ Q(u) = \prod_{j=1}^{N} (u - \lambda_j)(u + \lambda_j + 1), \]  

(3.5)

and the \( N \) Bethe roots \( \{\lambda_j | j = 1, \cdots, N\} \) should satisfy a set of BAEs,

\[ \left( \frac{\lambda_j + 1}{\lambda_j} \right)^{2N+1} \frac{(\lambda_j + p) \left[ (1+\xi^2)^{\frac{1}{2}} \lambda_j + q \right]}{(\lambda_j - p + 1) \left[ (1+\xi^2)^{\frac{1}{2}} (\lambda_j + 1) - q \right]} = \]

\[ - \frac{\left[ 1 - (1+\xi^2)^{\frac{1}{2}} \right] (2\lambda_j + 1)(\lambda_j + 1)^{2N+1}}{(\lambda_j - p + 1) \left[ (1+\xi^2)^{\frac{1}{2}} (\lambda_j + 1) - q \right] \prod_{l=1}^{N} (\lambda_j - \lambda_l - 1)(\lambda_j + \lambda_l)} \]

\[ - \prod_{l=1}^{N} \frac{(\lambda_j - \lambda_l + 1)(\lambda_j + \lambda_l + 2)}{(\lambda_j - \lambda_l - 1)(\lambda_j + \lambda_l)}, \quad j = 1, \cdots, N. \]  

(3.6)
The eigenvalue of the Hamiltonian is given in terms of the Bethe roots by
\[ E = \sum_{j=1}^{N} \frac{2}{\lambda_j(\lambda_j + 1)} + 2N - 1 + \frac{1}{p} + \frac{(1 + \xi^2)^{\frac{1}{2}}}{q}. \]  

\[ (3.7) \]

### 3.1 Contribution of the inhomogeneous term to the ground state energy

In order to study the contribution of the inhomogeneous term (the last term in Eq. (3.4)) to the ground state energy, we first consider the \( T - Q \) relation without the inhomogeneous term\(^3\), i.e.,
\[ \Lambda_{\text{hom}}(u) = \frac{2(u + 1)^{2N+1}}{2u + 1}(u + p) \left[ (1 + \xi^2)^{\frac{1}{2}}u + q \right] \frac{Q(u - 1)}{Q(u)} \]
\[ + \frac{2u^{2N+1}}{2u + 1}(u - p + 1) \left[ (1 + \xi^2)^{\frac{1}{2}}(u + 1) - q \right] \frac{Q(u + 1)}{Q(u)}. \]  

\[ (3.8) \]

The singular property of the \( T - Q \) relation (3.8) gives the following BAEs
\[ \left( \frac{\mu_j - \frac{i}{2}}{\mu_j + \frac{i}{2}} \right)^{2N} \left( \frac{\mu_j - i\bar{p}}{\mu_j + i\bar{q}} \right) \left( \frac{\mu_j - i\bar{p}}{\mu_j + i\bar{q}} \right) = \prod_{i\neq j} \left( \frac{\mu_j - \mu_i - i}{\mu_j - \mu_i + i} \frac{\mu_j + \mu_i - i}{\mu_j + \mu_i + i} \right). \]  

\[ (3.9) \]

where we have put \( \lambda = i\mu - \frac{1}{2}, \bar{p} = p - \frac{1}{2} \) and \( \bar{q} = q(1 + \xi^2)^{-\frac{1}{2}} - \frac{1}{2} \).

We define the contribution of the inhomogeneous term to the ground state energy as
\[ E_{\text{inh}} = E_{\text{hom}} - E_{\text{true}}. \]  

\[ (3.10) \]

Here \( E_{\text{hom}} \) is the ground state energy of the XXX spin-1/2 chain calculated by the homogeneous \( T - Q \) relation (3.8). In this case (i.e., without the inhomogeneous term), the number of Bethe roots reduces to \( M = N/2 \), when an even \( N \) is assumed. Then energy \( E_{\text{hom}} \) is given by equation (3.7) with the constraint (3.9). \( E_{\text{true}} \) is the ground state energy of the Hamiltonian (3.1), which can be obtained by either using the density matrix renormalization group (DMRG)\(^7\) or solving the BAEs (3.6) directly. We have checked that the ground state energy \( E_{\text{true}} \) obtained by these two methods are the same.

From the fitted curves in Figure 1 we find the power law relation between \( E_{\text{inh}} \) and \( N \), i.e., \( E_{\text{inh}} = \gamma_1 N^{\beta_1} \). Due to the fact that \( \beta_1 < 0 \), the value of \( E_{\text{inh}} \) tends to zero when the size of the system tends to infinity, which means that the inhomogeneous term in Eq. (3.4) can be neglected in the thermodynamic limit.

\(^3\)It should be emphasized that, for a finite \( N \), \( \Lambda_{\text{hom}}(u) \) is different from the exact eigenvalue \( \Lambda(u) \) given by (3.4).
Figure 1: The contribution of the inhomogeneous term to the ground state energy $E_{inh}$ versus the system size $N$. The data can be fitted as $E_{inh} = \gamma_1 N^{\beta_1}$. Due to the fact $\beta_1 < 0$, when the $N$ tends to infinity, the contribution of the inhomogeneous term tends to zero. Here $p = 8$, $q = 4$, (a) $\xi = \frac{1}{8}$, $\gamma_1 = 0.000253$ and $\beta_1 = -0.6334$; (b) $\xi = \frac{5}{8}$, $\gamma_1 = 0.006096$ and $\beta_1 = -0.6521$; (c) $\xi = \frac{25}{8}$, $\gamma_1 = 0.080180$ and $\beta_1 = -0.7297$.

3.2 Boundary energy

Now, the boundary energy is ready to be calculated. We consider the case of $\bar{p}, \bar{q} \geq 0$, in which all the Bethe roots are real at the ground state. Taking the logarithm of equation (3.9), we obtain

$$2 \arctan \left( \frac{2\mu_j}{2\bar{p}} \right) + 2 \arctan \left( \frac{2\mu_j}{2\bar{q}} \right) + 4N \arctan (2\mu_j) = 2\pi I_j + \sum_{l=1}^{M} \left[ 2 \arctan \left( \frac{2(\mu_j - \mu_l)}{2} \right) + 2 \arctan \left( \frac{2(\mu_j + \mu_l)}{2} \right) \right] - 2 \arctan (2\mu_j), \quad (3.11)$$

where $I_j$ is a set of quantum numbers. If we define

$$Z(\mu_j) = \frac{I_j}{2N}. \quad (3.12)$$

It turns to be a continuous function in the thermodynamic limit as the distribution of Bethe roots is continuous, i.e., $Z(\mu_j) \rightarrow Z(u)$. Taking the derivative of $Z(u)$ with respect to $u$, we obtain the density of states as

$$\rho(u) = a_1(u) + \frac{1}{2N} \left[ a_{2p}(u) + a_{2q}(u) + a_1(u) - \delta(u) \right] - \int_{-\infty}^{\infty} a_2(u-v)\rho(v)dv, \quad (3.13)$$

where

$$a_n(u) = \frac{1}{2\pi} \frac{n}{u^2 + \frac{n^2}{4}}. \quad (3.14)$$
The energy density of the ground state is

\[ e_g = -2\pi \int_{-\infty}^{\infty} a_1(\mu)\rho(\mu)d\mu + 1 - \frac{1}{2N} + \frac{1}{2Np} + \frac{(1 + \xi^2)^{\frac{3}{2}}}{2Nq} \]

\[ = 1 - 2\ln(2) + O(N^{-1}). \quad (3.15) \]

The boundary energy is given by [38, 39, 40]

\[ E_b(p, q, \xi) = \lim_{N \to \infty} \left[ E_0(N; p, q, \xi) - 2E_0^{periodic}(N) \right] \]

\[ = -4\pi N \int_{-\infty}^{\infty} \tilde{a}_1(\omega)\tilde{\rho}(\omega)d\omega - 1 + \frac{1}{p} + \frac{(1 + \xi^2)^{\frac{3}{2}}}{q}. \quad (3.16) \]

The density deviation from that of the periodic case satisfies

\[ \delta\rho(u) = \frac{1}{2N} [a_{2p}(u) + a_{2q}(u) + a_1(u) - \delta(u)] - \int_{-\infty}^{\infty} a_2(u - v)\delta\rho(v)dv. \quad (3.17) \]

With the help of the Fourier transformation, we have

\[ \delta\tilde{\rho}(\omega) = \frac{1}{2N} \left( e^{-p|\omega|} + e^{-q|\omega|} + e^{-|\omega|} \right) - 1. \quad (3.18) \]

Therefore, the boundary energy can be calculated as

\[ E_b(p, q, \xi) = -2 \int_0^\infty \frac{e^{-p\omega}}{1 + e^{-\omega}}d\omega - 2 \int_0^\infty \frac{e^{-\sqrt{1+\xi^2}\omega}}{1 + e^{-\omega}}d\omega + \pi - 2\ln 2 - 1 + \frac{1}{p} + \frac{(1 + \xi^2)^{\frac{3}{2}}}{q}. \quad (3.19) \]

As shown in Figure 2, the blue solid lines are the boundary energy calculated by using Eq. (3.19), while the red points are data obtained by employing the BST algorithms [41] to solve the boundary energy of the Hamiltonian (3.1) in the thermodynamic limit. We can see that the analytical and numerical results agree with each other very well for all tunable parameters.

When \( \xi = 0 \), the non-diagonal boundary condition degenerates into the diagonal one. The boundary energy (3.19) reduce to that of the system with diagonal boundary conditions.
Furthermore, if $\xi$ is small, we can expand the boundary energy (3.19) with respect to $\xi$ as

$$E_b(p, q, \xi) \simeq \frac{1}{p} + \psi^{(0)} \left( \frac{p}{2} \right) - \psi^{(0)} \left( \frac{p+1}{2} \right) + \frac{1}{q} + \psi^{(0)} \left( \frac{q}{2} \right) - \psi^{(0)} \left( \frac{q+1}{2} \right)$$

$$+ \pi - 1 - 2 \ln(2) + \xi^2 \left[ \frac{1}{2q} - \frac{1}{4} q \psi^{(1)} \left( \frac{q}{2} \right) + \frac{1}{4} q \psi^{(1)} \left( \frac{q+1}{2} \right) \right]$$

$$+ \xi^4 \left[ q^3 \psi^{(2)} \left( \frac{q}{2} \right) - q^3 \psi^{(2)} \left( \frac{q+1}{2} \right) + 6q^2 \psi^{(1)} \left( \frac{q}{2} \right) - 6q^2 \psi^{(1)} \left( \frac{q+1}{2} \right) - 4 \right]$$

$$+ O \left( \xi^6 \right),$$

(3.20)

where $\psi^{(m)}(x)$ is the $m$-order derivative of digamma function [42]. The Eq.(3.20) contains only even powers of $\xi$ because the energy is invariant under $\xi \to -\xi$ [29]. It should be remarked that Eq.(3.20) only being effective for small values of $\xi$, while Eq.(3.19) being vailable for general values of $\xi$.

4 Results for the $su(3)$-invariant spin chain with non-diagonal boundary fields

Without losing the generality, we consider a $su(3)$-invariant spin chain (with the fundamental representation of $su(3)$) with non-diagonal boundary fields described by the Hamiltonian
\[ H = 2 \sum_{j=1}^{N-1} P_{j,j+1} + \frac{2\hbar}{2 + \hbar} E_{N}^{13} + \frac{2\hbar}{2 + \hbar} E_{N}^{22} + \frac{2\hbar}{2 + \hbar} E_{N}^{31} 
+ 2\hbar E_{11}^{11} + \frac{2}{3} \bar{h} - h, \]  

(4.1)

where the permutation operator is defined in the tensor space of 3-dimensional linear spaces

\[ P_{j,j+1} = \sum_{\mu,\nu=1}^{3} E_{j}^{\mu,\nu} E_{j+1}^{\nu,\mu}, \quad E_{j}^{\mu,\nu} \text{ is the the Weyl matrix (or the Hubbard operator)} \]

\[ \bar{h} \text{ and } h \text{ are arbitrary real boundary parameters which are related to the boundary fields. The corresponding } K\text{-matrices } K^{\pm}(u) \text{ are given by} \]

\[ K^{-}(u) = 1/h + u \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \]

(4.2)

and

\[ K^{+}(u) = 1/\bar{h} - \left( u + \frac{3}{2} \right) \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}. \]

(4.3)

The eigenvalue \( \Lambda(u) \) of the corresponding transfer matrix is given in terms of the inhomogeneous \( T - Q \) relation \[22\]

\[ \Lambda(u) = z_{1}(u) + z_{2}(u) + z_{3}(u) + x(u), \]

(4.4)

where the functions \( z_{m}(u) \) and \( x(u) \) are defined as

\[ z_{m}(u) = \frac{u \left( u + \frac{3}{2} \right) K^{(m)}(u) Q^{(0)}(u) Q^{(m-1)}(u+1) Q^{(m)}(u-1)}{(u + \frac{m}{2}) \left( u + \frac{m-1}{2} \right)} \frac{Q^{(m-1)}(u) Q^{(m)}(u)}{Q^{(m-1)}(u+1) Q^{(m)}(u+1)}, \quad m = 1, 2, 3, \]  

(4.5)

\[ x(u) = u \left( u + \frac{3}{2} \right) Q^{(0)}(u+1) Q^{(0)}(u) \]

\[ \times \frac{2u \left( u + \frac{1}{2} \right)^{2} (u - \frac{1}{2}) \left( u + \frac{3}{2} \right) (u + 1) Q^{(2)}(-u-1)}{Q^{(1)}(u)}, \]  

(4.6)

\[ ^{4} \text{Without losing the generalization, the } K^{\pm}(u) \text{ given by } [16, 22, 35] \text{ satisfy } [K^{-}(u), K^{\mp}(v)] \neq 0. \text{ This fact gives rise to that they cannot be diagonalized simultaneously (which corresponds to the non-diagonal (or unparallel) boundary fields), and that there is no an obvious reference state on which the conventional Bethe ansatz } [16] \text{ can be performed.} \]
respectively and

\[
K^{(1)}(u) = \left( \frac{1}{\hbar} + \frac{1}{2} - u \right) \left( \frac{1}{\hbar} + u \right),
\]

\[
K^{(2)}(u) = \left( \frac{1}{\hbar} + \frac{3}{2} + u \right) \left( \frac{1}{\hbar} - u - 1 \right),
\]

\[
K^{(3)}(u) = \left( \frac{1}{\hbar} + \frac{3}{2} + u \right) \left( \frac{1}{\hbar} - u - 1 \right).
\]

(4.7)

Here the \(Q\)-functions can be parameterized as

\[
Q^{(0)}(u) = u^{2N}, \quad Q^{(3)} = 1,
\]

\[
Q^{(r)}(u) = \prod_{l=1}^{L_r} \left( u - \lambda^{(r)}_l \right) \left( u + \lambda^{(r)}_l + r \right), \quad r = 1, 2,
\]

where \(L_1 = N + L_2 + 3\) and \(0 \leq L_2 \leq N\). Then the energy spectrum of the Hamiltonian (4.1) can be given in terms of the associated Bethe roots by

\[
E = \sum_{l=1}^{L_1} \frac{2}{\lambda^{(1)}_l (\lambda^{(1)}_l + 1)} + 2(N - 1) + \frac{\hbar \hbar + 2\hbar - 2\bar{\hbar}}{2 + \hbar} + \frac{2}{3},
\]

(4.8)

where the Bethe roots \(\{\lambda^{(r)}_j\}\) should satisfy the nested BAEs

\[
1 + \frac{\lambda^{(1)}_l}{\lambda^{(1)}_l + \eta} \frac{(2\bar{\hbar} \lambda^{(1)}_l + 3\bar{\hbar} + 2)(\hbar \lambda^{(1)}_l + h - 1) Q^{(0)}(\lambda^{(1)}_l + \eta)}{(2\hbar \lambda^{(1)}_l - \hbar - 2)(h \lambda^{(1)}_l + 1) Q^{(0)}(\lambda^{(1)}_l)}
\]

\[
\times \frac{Q^{(1)}(\lambda^{(1)}_l + \eta) Q^{(2)}(\lambda^{(1)}_l - \eta)}{Q^{(1)}(\lambda^{(1)}_l - \eta) Q^{(1)}(\lambda^{(1)}_l)} = \bar{c} (\lambda^{(1)}_l)^2 \left( \frac{\lambda^{(1)}_l + \eta}{2} \right)^{\frac{3}{2}} (\lambda^{(1)}_l + \eta)
\]

\[
\times (\lambda^{(1)}_l + \frac{3}{2} \eta) (\lambda^{(1)}_l - \frac{\eta}{2}) \frac{Q^{(0)}(\lambda^{(1)}_l) Q^{(2)}(\lambda^{(1)}_l - \eta)}{Q^{(1)}(\lambda^{(1)}_l - \eta)}, \quad l = 1, \cdots, L_1,
\]

(4.9)

\[
\frac{(\lambda^{(2)}_k + \frac{3}{2} \eta) Q^{(1)}(\lambda^{(2)}_k + \eta) Q^{(2)}(\lambda^{(2)}_k - \eta)}{(\lambda^{(2)}_k + 1 \eta) Q^{(1)}(\lambda^{(2)}_k) Q^{(2)}(\lambda^{(2)}_k + \eta)} = -1, \quad k = 1, \cdots, L_2,
\]

(4.10)

with \(\bar{c} = 4\hbar \hbar / [(2\bar{\hbar} \lambda^{(1)}_l - \hbar - 2)(h \lambda^{(1)}_l + 1)]\).

\[\textbf{4.1 Contribution of the inhomogeneous term}\]

As for the open \(\text{su}(3)\) quantum spin chain case, the contribution of the inhomogeneous term to the ground state energy \(E_{inh}\) is still the same as that defined in the XXX spin-1/2 chain
case, i.e.,

$$E_{\text{inh}} = E_{\text{hom}} - E_{\text{true}},$$  \hspace{1cm} (4.11)

where $E_{\text{true}}$ is the true values of the ground state energy of the Hamiltonian (4.1) and $E_{\text{hom}}$ is the ground state energy calculated from the energy spectrum

$$E = -\sum_{l=1}^{L_1} \frac{2}{(\mu_{l}^{(1)})^2 + \frac{1}{2}} + 2(N-1) + \frac{\hbar \tilde{h} + 2h - 2\tilde{h}}{2 + \tilde{h}} + \frac{2}{3},$$  \hspace{1cm} (4.12)

where the Bethe roots satisfy the associated BAEs

\begin{equation}
\left(\frac{\mu_{l}^{(1)} + i\tilde{f}}{\mu_{l}^{(1)} - i\tilde{f}}\right)\left(\frac{\mu_{j}^{(1)} + i\tilde{f}}{\mu_{j}^{(1)} - i\tilde{f}}\right)\prod_{j=1}^{L_1} \left(\frac{\mu_{l}^{(1)} - \mu_{j}^{(1)} - i}{\mu_{l}^{(1)} - \mu_{j}^{(1)} + i}\right)\left(\frac{\mu_{l}^{(1)} + \mu_{j}^{(1)} - i}{\mu_{l}^{(1)} + \mu_{j}^{(1)} + i}\right) = -1, \quad l = 1, \ldots, L_1,
\end{equation}

\begin{equation}
\left(\frac{\mu_{k}^{(2)} - \mu_{j}^{(1)}}{\mu_{k}^{(2)} + \mu_{j}^{(1)} + i}\right)\prod_{j=1}^{L_1} \left(\frac{\mu_{k}^{(2)} - \mu_{j}^{(1)} + i}{\mu_{k}^{(2)} + \mu_{j}^{(1)} - i}\right) = -1, \quad k = 1, \ldots, L_2.
\end{equation}

Here we have used the relations $\lambda_{l}^{(1)} = i\mu_{l}^{(1)} - \frac{1}{2}, \lambda_{k}^{(2)} = i\mu_{k}^{(2)} - 1, \tilde{f} = -1 - 1/\tilde{h}$ and $f = -\frac{1}{2} + 1/h$. To simplify the computations we constrain ourselves to the regions $h \in (0, 2)$, $\tilde{h} \in (-1, 0)$. The restrictions imposed on $h$ and $\tilde{h}$ are chosen such that $f$ and $\tilde{f}$ are positive with range $(0, \infty)$, for which case all the Bethe roots of the ground state are real.

\[\text{相似 as the } su(2)\text{-case discussed in the previous section, it is believed that the contribution of the inhomogeneous term to the ground state energy should vanish in the thermodynamic limit for other choices of values of } h \text{ and } \tilde{h}.\]
Taking the logarithm of BAEs (4.13)-(4.14), we obtain

\[
2 \arctan \left( \frac{\mu_1^{(1)}}{f} \right) + 2 \arctan \left( \frac{\mu_1^{(1)}}{f} \right) + 2(2N + 1) \arctan \left( 2\mu_1^{(1)} \right) - 2 \sum_{j=1}^{L_1} \arctan \left( \mu_1^{(1)} - \mu_j^{(1)} \right) + \arctan \left( \mu_1^{(1)} + \mu_j^{(1)} \right) \\
+ 2 \sum_{j=1}^{L_2} \arctan \left( \mu_j^{(1)} + \mu_j^{(2)} \right) + \arctan \left( \mu_j^{(2)} - \mu_j^{(2)} \right) = 2\pi I_l, \tag{4.15}
\]

\[
2 \arctan \left( 2\mu_k^{(2)} \right) + 2 \sum_{j=1}^{L_1} \arctan \left( \mu_k^{(2)} - \mu_j^{(1)} \right) + \arctan \left( \mu_k^{(2)} + \mu_j^{(1)} \right) \\
- 2 \sum_{j=1}^{L_2} \arctan \left( \mu_k^{(2)} - \mu_j^{(2)} \right) + \arctan \left( \mu_k^{(2)} + \mu_j^{(2)} \right) = 2\pi J_k, \tag{4.16}
\]

where \(I_l\) and \(J_k\) are both quantum numbers which determine the eigenenergy and the corresponding eigenstates. It is well-known that the size of the system \(N\), with either even or odd value, gives the same thermodynamic properties. For simplicity, we set \(N\) as an even number and parameterize it as \(N = 6(n - 1) + \alpha\), where \(\alpha = 2, 4, 6\). Then we find that the values of \(L_1\) and \(L_2\) in BAEs (4.15)-(4.16) at the ground state are given by

\[
L_1 = L_1^{(\alpha)} + 4(n - 1), \quad L_2 = L_2^{(\alpha)} + 2(n - 1), \tag{4.17}
\]

respectively, where \(L_1^{(2)} = 2, L_2^{(2)} = 1, L_1^{(4)} = 3, L_2^{(4)} = 1, L_1^{(6)} = 4\) and \(L_2^{(6)} = 2\).

To show the finite size effects, we plot the values of \(E_{\text{inh}}\) versus the system size \(N\) with the choice of \(\bar{h} = -\frac{1}{63}, \bar{h} = -\frac{1}{15}\) and \(\bar{h} = -\frac{1}{3}\), while keeping \(h = 0.5\) and \(h = 1.2\) in Figure 3 respectively. As shown in Figure 3, the contribution of the inhomogeneous term to the ground state energy \(E_{\text{inh}}\) is a function of the size of the system size \(N\) in the form of \(E_{\text{inh}} = \gamma_2 N^{\beta_2}\), where \(\beta_2 < 0\) is negative, which is the same form as the XXX spin-1/2 chain case but with different values of the parameters. In the limiting case where \(N\) tends to infinity, the contribution of \(E_{\text{inh}}\) to the ground state energy of the system can be ignored.

We have checked our results numerically to show that when \(\bar{h} = 0\) the system degenerates to the situation of the diagonal boundary fields, i.e., \(E_{\text{inh}} = 0\).
4.2 Boundary energy of the open $su(3)$ quantum spin chain

We have shown in previous section that the contribution of the inhomogeneous term in the $T - Q$ relation Eq. (4.4) to the ground state energy of the system can be ignored at least in the thermodynamic limit. This fact allows one to use the homogeneous $T - Q$ relation $\Lambda_{\text{hom}}(u) = \sum_{m=1}^{3} z_m(u)$, instead of inhomogeneous one (4.4), to calculate the ground state energy of the system in the thermodynamic limit by standard method [2]. Here, let us consider the case of $f, \bar{f} \geq 0$. Following the standard method [2], let us introduce the so-called the counting functions associated with the two sets of Bethe roots as follows:

\[
Y(u^{(1)}) = \frac{1}{2\pi} \left\{ \Xi_1 (u^{(1)}) + \frac{1}{2N} \left[ \Xi_1 (u^{(1)}) + \Xi_2 (u^{(1)}) + \Xi_2 (u^{(1)}) \right] \right\}
- \frac{1}{2\pi} \sum_{l=1}^{L_1} \left[ \Xi_2 (u^{(1)} - u_l^{(1)}) + \Xi_2 (u^{(1)} + u_l^{(1)}) \right]
+ \frac{1}{2\pi} \sum_{k=1}^{L_2} \left[ \Xi_1 (u^{(1)} + u_k^{(2)}) + \Xi_1 (u^{(1)} - u_k^{(2)}) \right],
\]

(4.18)

\[
Z(u^{(2)}) = \frac{1}{4N\pi} \left\{ \Xi_1 (u^{(2)}) \right\} + \frac{1}{2\pi} \sum_{l=1}^{L_1} \left[ \Xi_1 (u^{(2)} - u_l^{(1)}) + \Xi_1 (u^{(2)} + u_l^{(1)}) \right]
- \frac{1}{2\pi} \sum_{k=1}^{L_2} \left[ \Xi_2 (u^{(2)} - u_k^{(2)}) + \Xi_2 (u^{(2)} + u_k^{(2)}) \right],
\]

(4.19)
with $\Xi_m(x) = 2 \arctan \left( \frac{2x}{m} \right)$. Then the BAEs (4.15)-(4.16) become

$$Y(\mu^{(1)}_1) = \frac{I_t}{2N}, \quad Z(\mu^{(2)}_k) = \frac{J_k}{2N}$$

(4.20)

In the thermodynamic limit, the Bethe roots (e.g. the solutions to the above equations) for the ground state will become dense on the real line. This allows one to define the densities of the particles ($\rho(u)$ and $\sigma(u)$) and holes ($\rho^h(u)$ and $\sigma^h(u)$),

$$\rho(u) + \rho^h(u) = \frac{d}{du} Y(u), \quad \sigma(u) + \sigma^h(u) = \frac{d}{du} Z(u).$$

(4.21)

Taking the derivative of BAEs (4.20) in the thermodynamic limit, we obtain the functional equations of the densities at the ground state

$$\rho(u) = a_1(u) + \frac{1}{2N} \left[ a_1(u) + a_2f(u) + a_2f(u) - \delta(u) \right]$$

$$- \int_{-\infty}^{\infty} a_2(u - \lambda) \rho(\lambda) d\lambda + \int_{-\infty}^{\infty} a_1(u - v) \sigma(v) dv, \quad \sigma(v) = \frac{1}{2N} \left[ a_1(v) - \delta(v) \right] + \int_{-\infty}^{\infty} a_1(v - \lambda) \rho(\lambda) d\lambda$$

$$- \int_{-\infty}^{\infty} a_2(v - \mu) \sigma(\mu) d\mu.$$  

(4.22)

(4.23)

By using Fourier transformation, we obtain $\rho(u)$ as

$$\rho(u) = \frac{1}{\sqrt{3} (2 \cosh (\frac{2\pi u}{3}) - 1)}.$$  

(4.24)

Thus the ground state energy takes the form

$$E_0(N; h, \bar{h}) = -4\pi N \int_{-\infty}^{\infty} a_1(\mu) \rho(\mu) d\mu + 2(N - 1) + \frac{h\bar{h} + 2h - 2\bar{h}}{2 + \bar{h}} + \frac{2}{3},$$

(4.25)

and the energy density of ground state chooses the value

$$e_g = \lim_{N \to \infty} \left[ \frac{E_0(N; h, \bar{h})}{N} \right] = -4\pi \int_{-\infty}^{\infty} a_1(\mu) \rho(\mu) d\mu + 2 + \mathcal{O}(N^{-1}) \simeq -1.406424.$$  

(4.26)

The boundary energy is given by [38, 39, 40]

$$E_b(h, \bar{h}) = \lim_{N \to \infty} \left[ E_0(N; h, \bar{h}) - 2E_0^{\text{periodic}}(N) \right],$$

(4.27)

For the ground state, the densities of the holes vanish, namely, $\rho^h(u) = \sigma^h(u) = 0$. 

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[65x686]
where $E_{\text{periodic}}(N)$ is the ground state energy of the system with periodic boundary conditions, which can be obtained by the nested algebraic Bethe ansatz. Using the similar method for the $su(2)$-case in the previous section, after some tedious calculation, we obtain the boundary energy for the $su(3)$ spin chain with non-diagonal boundary terms as

$$E_b(h, \bar{h}) = -2 \int_0^\infty \frac{e^{\frac{1}{2} \omega - f \omega} + e^{-\frac{1}{2} \omega - f \omega}}{1 + e^{-\omega} + e^{-2\omega}} d\omega$$

$$-2 \int_0^\infty \frac{e^{\frac{1}{2} \omega - f \omega} + e^{-\frac{1}{2} \omega - f \omega}}{1 + e^{-\omega} + e^{-2\omega}} d\omega + \frac{4\pi}{3\sqrt{3}} + \frac{h\bar{h} + 2h - 2\bar{h}}{2 + h} - \frac{4}{3}. \quad (4.28)$$

Figure 4: Boundary energy as a function of boundary fields. The blue curves are the theoretical results plotted by using equation (4.28), while the red points are the boundary energies obtained by the numerical exact diagonalization and the BST extrapolation. Here (a) $h = 1.2$; (b) $\bar{h} = -\frac{1}{13}$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

As shown in Figure 4, the boundary energies with respect to varying boundary fields $h$ ($\bar{h}$) which are calculated numerically by using exact diagonalization (red dots), where the BST algorithms to obtain the large-N extrapolation of the boundary energy is employed, coincide with the analytical results obtained from Eq. (4.28) very well. This also means that the inhomogeneous term in the $T-Q$ relation (4.4) can be neglected in the thermodynamic limit.

5 Conclusions

In this paper, we have studied the thermodynamic limit and boundary energy of the XXX spin-1/2 chain as well as the $su(3)$-invariant spin chain with unparallel boundary fields. It
is shown that the contribution of the inhomogeneous term in the associated $T - Q$ relation (obtained by the ODBA method) to the ground state energy does vanish in the thermodynamic limit. This fact allows us to study the thermodynamics of the model. As concrete examples, we have calculated the boundary energy (3.19) for the XXX spin-1/2 open chain and (4.28) for the $su(3)$ open chain. The method used in this paper can be generalized to study the thermodynamic properties and boundary energy of other high rank models with non-diagonal boundary fields.

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