Thermodynamic limit and boundary energy of the spin-1 Heisenberg chain with non-diagonal boundary fields

Zhihan Zheng[1,2], Pei Sun[1,2], Xiaotian Xu[1,2*], Tao Yang[1,2,3,4], Junpeng Cao[4,5,6,7], Wen-Li Yang[1,2,3,4]

1 Institute of Modern Physics, Northwest University, Xi'an 710127, China
2 Shaanxi Key Laboratory for Theoretical Physics Frontiers, Xi'an 710127, China
3 School of Physics, Northwest University, Xi'an 710127, China
4 Peng Huanwu Center for Fundamental Theory, Xi'an 710127, China
5 Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
6 Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China
7 School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China
*xtxu@nwu.edu.cn

Abstract

The thermodynamic limit and boundary energy of the isotropic spin-1 Heisenberg chain with non-diagonal boundary fields are studied. The finite size scaling properties of the inhomogeneous term in the $T-Q$ relation at the ground state are analyzed. Based on the reduced Bethe ansatz equations (BAEs), we obtain the boundary energy of the system. These results can be generalized to the $SU(2)$ symmetric high spin Heisenberg model directly.

Contents

---

1 Introduction

The study of quantum integrable models is an interesting subject in the fields of cold atoms, quantum field theory, condensed matter physics and statistic mechanics [1–5]. The spin-1/2 Heisenberg model can effectively quantify the spin-exchanging interaction and plays an important role in the quantum magnetism and many-body theory. By using the Bethe ansatz method, the one-dimensional (1D) spin-1/2 Heisenberg model can be solved exactly [6]. The typical spin-exchanging couplings in the 1D spin-1 system is characterized by the bilinear biquadratic model, where the Hamiltonian reads

$$H = \sum_{k=1}^{N} \left[J_1 \vec{S}_k \cdot \vec{S}_{k+1} + J_2 (\vec{S}_k \cdot \vec{S}_{k+1})^2 \right]. \tag{1}$$

Here $\vec{S}_k(S_k^x, S_k^y, S_k^z)$ is the spin-1 operator at site k, N is the number of sites and the periodic boundary condition gives $\vec{S}_{N+1} = \vec{S}_1$. If $J_2/J_1 = 1$, the system (1) has the $SU(3)$ symmetry and is integrable. If $J_2/J_1 = -1$, the $SU(2)$ symmetry survives and the system is known as the Zamalodchikov-Fateev (ZF) model [7]. The Bethe ansatz solution and thermodynamic properties of the ZF model are studied by Takhtajan [8] and Babujian [9,10]. If $J_2 = 0$, the system is no longer integrable. Starting from the nonlinear sigma model, Haldane conjectures that the excitation of the system has a gap [11,12]. If $J_2/J_1 = 1/3$, the Hamiltonian (1) degenerates into a projector operator (up to a constant) and the ground state is the famous valence bond solid state [13,14]. If $J_1 = 0$, by using the Temperley-Lieb algebra, the system can be mapped into the XXZ spin chain and is also integrable [15–17].

Besides the periodic boundary condition, the integrable open one is also an interesting subject, which means that the system has magnetic impurity or the boundary magnetic fields [18,19]. In the past few decades, the exact results of high spin models with periodic [7,9,10,20–25] and parallel boundary fields [26–28] have been extensively studied. It is emphasized that the integrable boundary reflection matrix can have non-diagonal elements, which means that the boundary fields are unparallel. Then the $U(1)$ symmetry is broken and it is very hard to study the exact solution of the system. It is known that the integrable systems without $U(1)$ symmetry actually have many applications in the open string theory and the stochastic process of nonequilibrium statistics. Therefore, many interesting works of high spin models with non-diagonal boundary reflections have been done [29–32].

Recently, a systematic method, i.e., the off-diagonal Bethe ansatz (ODBA) is proposed to solve the models with or without $U(1)$ symmetry [33,34]. The eigenvalues and eigenstates of several typical integrable models are obtained. The next task is to derive the physical quantities in the thermodynamic limit, which is very involved in because the related Bethe ansatz equations (BAEs) are inhomogeneous and the traditional thermodynamic Bethe ansatz can not be employed. In order to overcome this difficulty, an effective method is to study the finite size scaling effects of the inhomogeneous term in the $T-Q$ relation. With the help of this idea, the thermodynamic limit, surface energy and elementary excitations of spin-1/2 XXZ spin chain with arbitrary boundary fields [35,36] or antiperiodic boundary condition [37,38] are studied. The boundary energy of the $SU(3)$ symmetric spin-1 chain with generic integrable open boundaries is also obtained [39]. However, the corresponding thermodynamic properties of the $SU(2)$ symmetric spin-1 Heisenberg model are still missing.

In this paper, we study the thermodynamic limit and boundary energy of the spin-1 isotropic Heisenberg spin chain with non-diagonal boundary reflections. The finite size scaling analysis of the contribution of the inhomogeneous term in the $T-Q$ relation to the ground state energy is studied in detail. In the thermodynamic limit, we find that the most Bethe roots of the reduced BAEs at the ground state form 2-strings, associated with certain boundary strings and the rearrangement of Fermi sea. The different structures of Bethe roots in different regimes of model parameters are given explicitly. Based on them, we obtain the boundary energy induced by the unparallel boundary magnetic fields. We also check the analytic results by the numerical extrapolation, and find that the analytic results and the numerical ones coincide with each other very well. The results given in this paper can be generalized to the $SU(2)$ symmetric spin-s Heisenberg model directly.

This paper is organized as follows. Section 2 serves as an introduction to the notations for the spin-1 Heisenberg model with non-diagonal boundary fields. The ODBA exact solution is also briefly reviewed. In Section 3, we focus on the finite size correction to the ground state energy of the inhomogeneous term in the $T-Q$ relation. In Section 4, by using the patterns of Bethe roots of the reduced BAEs, we study the boundary energy of the model in the thermodynamic limit. We summarize the results and give some discussions in Section 5.

2 Non-diagonal boundary Spin-1 Heisenberg model

The spin-1 Heisenberg model with non-diagonal boundary fields is related with the 19-vertex R-matrix [40]

$$R(u)=\left(\begin{array}{ccc|ccc|ccc}
c(u) & & & & & & & & \\
 & b(u) & & e(u) & & & & & \\
 & & d(u) & & g(u) & & f(u) & & \\
\hline
 & e(u) & & b(u) & & & & & \\
 & & g(u) & & a(u) & & g(u) & & \\
 & & & & & b(u) & & e(u) & \\
\hline
 & & f(u) & & g(u) & & d(u) & & \\
 & & & & & e(u) & & b(u) & \\
 & & & & & & & & c(u)
\end{array}\right), \tag{2}$$

where the non-vanishing elements are

$$\begin{aligned}
&a(u)=u(u+\eta)+2\eta^2,\ b(u)=u(u+\eta),\ c(u)=(u+\eta)(u+2\eta),\\
&d(u)=u(u-\eta),\ e(u)=2\eta(u+\eta),\ f(u)=2\eta^2,\ g(u)=2u\eta,
\end{aligned} \tag{3}$$

u is the spectral parameter and η is the crossing parameter. The R-matrix $R(u)$ satisfies the quantum Yang-Baxter equation (QYBE) [41,42]

$$R_{12}(u-v)R_{13}(u)R_{23}(v)=R_{23}(v)R_{13}(u)R_{12}(u-v). \tag{4}$$

Besides, the R-matrix (2) also enjoys the properties

$$\text{Initial condition}:\ R_{12}(0)=2\eta^2P_{12}, \tag{5}$$

$$\text{Antisymmetry}:\ R_{12}(-\eta)=6\eta^2\,\mathbf{P}^{(0)}_{12}, \tag{6}$$

where P_{12} is the permutation operator and $\mathbf{P}^{(0)}_{12}$ is the projector in the total spin-0 channel. The boundary reflection at one side of the chain is quantified by the reflection matrix

$$K^-(u)=(2u+\eta)\begin{pmatrix} x_1(u) & y_4(u) & y_6(u)\\ y_4(u) & x_2(u) & y_5(u)\\ y_6(u) & y_5(u) & x_3(u)\end{pmatrix}, \tag{7}$$

where the matrix elements are

$$\begin{aligned}
x_1(u) &= (p_- + u + \frac{\eta}{2})\,(p_- + u - \frac{\eta}{2}) + \frac{\alpha_-^2}{2}\,\eta\,(u - \frac{\eta}{2}),\\
x_2(u) &= (p_- + u - \frac{\eta}{2})\,(p_- - u + \frac{\eta}{2}) + \alpha_-^2\,(u + \frac{\eta}{2})\,(u - \frac{\eta}{2}),\\
x_3(u) &= (p_- - u - \frac{\eta}{2})\,(p_- - u + \frac{\eta}{2}) + \frac{\alpha_-^2}{2}\,\eta\,(u - \frac{\eta}{2}),\\
y_4(u) &= \sqrt{2}\,\alpha_-\,u\,(p_- + u - \frac{\eta}{2}),\\
y_5(u) &= \sqrt{2}\,\alpha_-\,u\,(p_- - u + \frac{\eta}{2}), \quad y_6(u) = \alpha_-^2\,u\,(u - \frac{\eta}{2}),
\end{aligned} \tag{8}$$

p_- and α_- are the boundary parameters which measure the strength and direction of the boundary field. The reflection matrix $K^-(u)$ satisfies the reflection equation (RE)

$$R_{12}(u-v)K_1^-(u)R_{21}(u+v)K_2^-(v) = K_2^-(v)R_{21}(u+v)K_1^-(u)R_{12}(u-v). \tag{9}$$

The boundary reflection at the other side is quantified by the dual reflection matrix

$$K^+(u) = K^-(-u-\eta)\Big|_{(p_-,\alpha_-)\to(p_+,-\alpha_+)}, \tag{10}$$

where p_+ and α_+ are the boundary parameters characterizing the strength and direction of the corresponding boundary field. The dual reflection matrix $K^+(u)$ satisfies the dual RE

$$\begin{aligned}
&R_{12}(v-u)K_1^+(u)R_{21}(-u-v-2\eta)K_2^+(v)\\
&\quad = K_2^+(v)R_{21}(-u-v-2\eta)K_1^+(u)R_{12}(v-u).
\end{aligned} \tag{11}$$

From the R-matrix (2), we construct the single row monodromy matrices $T_0(u)$ and $\hat{T}_0(u)$ as

$$\begin{aligned}
T_0(u) &= R_{0N}(u-\theta_N)R_{0N-1}(u-\theta_{N-1})\cdots R_{01}(u-\theta_1),\\
\hat{T}_0(u) &= R_{10}(u+\theta_1)R_{20}(u+\theta_2)\cdots R_{N0}(u+\theta_N),
\end{aligned} \tag{12}$$

where $\{\theta_k, k=1,\cdots,N\}$ are the inhomogeneous parameters, the subscript 0 means the auxiliary space and $1,\cdots,N$ denote the quantum spaces. The single row monodromy matrices $T_0(u)$ and $\hat{T}_0(u)$ are the 3×3 matrices in the auxillary space $\mathbf{V}_0$ and their elements act on the quantum space $\mathbf{V}^{\otimes N}$. The transfer matrix of the system reads

$$t(u) = tr_0\{K_0^+(u)T_0(u)K_0^-(u)\hat{T}_0(u)\}. \tag{13}$$

From the QYBE (4), RE (9) and dual RE (11), one can prove that the transfer matrices with different spectral parameters commute with each other, i.e.,

$$[t(u), t(v)] = 0. \tag{14}$$

Therefore, $t(u)$ serves as the generating functional of all the conserved quantities, which ensures the integrability of the system. The model Hamiltonian is generalized from the transfer matrix $t(u)$ as

$$
\begin{aligned}
H &= \partial_u \{\ln u(u+\eta)\, t(u)\}\,\big|_{u=0,\{\theta_k\}\to 0} \\
&= \frac{1}{\eta^2}\sum_{k=1}^{N-1}\left[\vec{S}_k\cdot\vec{S}_{k+1}-(\vec{S}_k\cdot\vec{S}_{k+1})^2\right] \\
&\quad +\frac{1}{p_-^2-\frac{1}{4}(1+\alpha_-^2)\eta^2}\Big[2p_-\alpha_-S_1^x+2p_-S_1^z+\frac{1}{2}(\alpha_-^2\eta-2\eta)(S_1^z)^2 \\
&\qquad -\frac{1}{2}\alpha_-^2\eta[(S_1^x)^2-(S_1^y)^2]-\alpha_-\eta[S_1^zS_1^x+S_1^xS_1^z]\Big] \\
&\quad +\frac{1}{(3p_+^2-\frac{3}{4}(1+\alpha_+^2)\eta^2)\eta^2}\big[6p_+\alpha_+\eta S_N^x-6p_+\eta S_N^z \\
&\qquad +3\alpha_+\eta^2[S_N^xS_N^z+S_N^zS_N^x]-(2p_+^2-\frac{3}{2}(1-\alpha_+^2)\eta^2)(S_N^x)^2 \\
&\qquad -(2p_+^2-\frac{3}{2}(1+\alpha_+^2)\eta^2)(S_N^y)^2-(2p_+^2+\frac{3}{2}(1-\alpha_+^2)\eta^2)(S_N^z)^2\big] \\
&\quad +\frac{\eta(1+\alpha_+^2)}{3p_+^2-\frac{3}{4}(1+\alpha_+^2)\eta^2}+\frac{\eta}{p_-^2-\frac{1}{4}(1+\alpha_-^2)\eta^2}+3N\frac{1}{\eta^2}+\frac{4}{\eta}. \qquad (15)
\end{aligned}
$$

Now, we seek the exact solution of the system (15). Let $|\Psi\rangle$ be an arbitrary eigenstate of $t(u)$ with the eigenvalue $\Lambda(u)$, i.e.,

$$t(u)|\Psi\rangle=\Lambda(u)|\Psi\rangle. \qquad (16)$$

Using the ODBA method and hierarchy fusion, in the homogeneous limit $\{\theta_k=0\}$, the eigenvalue $\Lambda(u)$ can be expressed as the inhomogeneous $T-Q$ relation [34, 40],

$$\Lambda(u) = \Lambda^{(\frac{1}{2},1)}(u+\frac{\eta}{2})\Lambda^{(\frac{1}{2},1)}(u-\frac{\eta}{2})-\delta^{(1)}(u+\frac{\eta}{2}), \qquad (17)$$

$$\Lambda^{(\frac{1}{2},1)}(u) = a^{(1)}(u)\frac{Q(u-\eta)}{Q(u)}+d^{(1)}(u)\frac{Q(u+\eta)}{Q(u)}+cu(u+\eta)\frac{F^{(1)}(u)}{Q(u)}, \qquad (18)$$

where

$$
\begin{aligned}
a^{(1)}(u) &= d^{(1)}(-u-\eta) \\
&= \frac{2u+2\eta}{2u+\eta}(\sqrt{1+\alpha_+^2}u+p_+)(\sqrt{1+\alpha_-^2}u-p_-)\left(u+\frac{3\eta}{2}\right)^{2N}, \qquad (19)\\
F^{(1)}(u) &= (u-\frac{\eta}{2})^{2N}(u+\frac{\eta}{2})^{2N}(u+\frac{3\eta}{2})^{2N}, \qquad (20)\\
\delta^{(1)}(u) &= a^{(1)}(u)\, d^{(1)}(u-\eta), \qquad (21)\\
c &= 2(\alpha_-\alpha_+-1-\sqrt{(1+\alpha_-^2)(1+\alpha_+^2)}), \qquad (22)\\
Q(u) &= \prod_{k=1}^{2N}(u-u_k)(u+u_k+\eta)=Q(-u-\eta), \qquad (23)
\end{aligned}
$$

and the $2N$ parameters $\{u_k|k=1,\cdots,2N\}$ in Q-function (23) are the Bethe roots. The singularity of eigenvalue $\Lambda(u)$ requires that the Bethe roots should satisfy the BAEs

$$a^{(1)}(u_k)Q(u_k-\eta)+d^{(1)}(u_k)Q(u_k+\eta)+c\,u_k(u_k+\eta)\,F^{(1)}(u_k)=0,\quad k=1,\cdots,2N. \qquad (24)$$

The eigenvalue of Hamiltonian (15) reads

$$E=\sum_{k=1}^{2N}\frac{4\eta}{(u_k+\frac{3\eta}{2})(u_k-\frac{\eta}{2})}+\frac{1}{\eta}3N+\frac{1}{\eta}E_0, \tag{25}$$

where $\{u_k\}$ should satisfy the BAEs (24) and

$$E_0=\frac{8}{3}+\frac{2\sqrt{1+\alpha_+^2}p_+\eta}{p_+^2-\frac{\eta^2}{4}(1+\alpha_+^2)}-\frac{2\sqrt{1+\alpha_-^2}p_-\eta}{p_-^2-\frac{\eta^2}{4}(1+\alpha_-^2)}. \tag{26}$$

3 Finite size scaling behavior

The present BAEs (24) are inhomogeneous, thus it is very hard to investigate the thermodynamic properties of the system by using the traditional thermodynamic Bethe ansatz. In order to overcome this difficulty, we first analyze the contribution of inhomogeneous term in the $T-Q$ relation (18).

Define the reduced $T-Q$ relation as

$$\Lambda_{hom}(u) = \Lambda_{hom}^{(\frac{1}{2},1)}(u+\frac{\eta}{2})\Lambda_{hom}^{(\frac{1}{2},1)}(u-\frac{\eta}{2})-\delta^{(1)}(u+\frac{\eta}{2}), \tag{27}$$

$$\Lambda_{hom}^{(\frac{1}{2},1)}(u) = a^{(1)}(u)\frac{Q(u-\eta)}{Q(u)}+d^{(1)}(u)\frac{Q(u+\eta)}{Q(u)}. \tag{28}$$

We should note that although all the non-diagonal boundary parameters are included in the above reduced $T-Q$ relation (28), the $\Lambda_{hom}(u)$ is not the eigenvalue $\Lambda(u)$. From the singularity analysis of the reduced $T-Q$ relation (28), we obtain following reduced BAEs

$$\frac{\frac{i}{2}-\mu_k}{\frac{i}{2}+\mu_k}\frac{pi-\mu_k}{pi+\mu_k}\frac{qi-\mu_k}{qi+\mu_k}\left(\frac{i-\mu_k}{i+\mu_k}\right)^{2N}=\prod_{l=1}^{M}\frac{i-(\mu_k-\mu_l)}{i+(\mu_k-\mu_l)}\frac{i-(\mu_k+\mu_l)}{i+(\mu_k+\mu_l)},\quad k=1,\cdots,M, \tag{29}$$

where $M=1,\cdots,2N$ and we have put $\eta=1$, $\mu_k=-iu_k-\frac{i}{2}$, $p=\frac{p_+}{\sqrt{1+\alpha_+^2}}-\frac{1}{2}$ and $q=-\frac{p_-}{\sqrt{1+\alpha_-^2}}-\frac{1}{2}$ for convenience. From the $\Lambda_{hom}(u)$ given by Eq.(27), we obtain the reduced energy which is defined as

$$E_{hom}=\partial_u\left\{\ln u(u+1)\Lambda_{hom}(u)\right\}\Big|_{u=0}=-\sum_{k=1}^{M}\frac{4}{\mu_k^2+1}+3N+E_0. \tag{30}$$

Solving the reduced BAEs (29), we could obtain the values of reduced Bethe roots $\{\mu_k\}$. Substituting the Bethe roots into Eq.(30), we obtain the values of E_{hom}.

Let us focus on the ground state. The reduced ground state energy can be calculated by the reduced BAEs (29). It is well-known that the even N and odd N give the same physical properties in the thermodynamic limit. Thus we set N is even. At the ground state, the number of Bethe roots in the reduced BAEs (29) is $M=N$. Without losing generality, we choose the boundary parameters as $p>0$ and $q\neq 0,-1$. We should note that at the points of $q=0,-1$, the boundary field is divergent due to the present parameterization of the Hamiltonian (15). The distribution of reduced Bethe roots at the ground state in the thermodynamic limit is shown in Figure 1. We see that the Bethe roots can be divided into six different regimes in the $p-q$ plane.

1) In the regime I, where $p \geq 1/2$, $q < -1$, $-1/2 \leq q < 0$ or $q \geq 1/2$, all the Bethe roots form 2-strings, i.e., $\mu_k = \lambda_k \pm \frac{i}{2} + \mathcal{O}(e^{-\delta N})$, where λ_k denotes the position of 2-string in the real axis, δ is a small positive number and $\mathcal{O}(e^{-\delta N})$ means the finite size correction.

2) In the regime II, where $p < 1/2$, $q < -1$, $-1/2 \leq q < 0$ or $q \geq 1/2$, besides $N-2$ 2-strings, there are two boundary strings, i.e., pi and $(p-1)i$. The boundary strings mean the pure imaginary Bethe roots which are related with the boundary parameters p and q [43].

3) In the regime III, where $p \geq 1/2$ and $0 < q < 1/2$, besides $N-2$ 2-strings, there are two boundary strings, qi and $(q-1)i$.

4) In the regime IV, where $0 < p < 1/2$ and $0 < q < 1/2$, besides $N-4$ 2-strings, there are four boundary strings, pi, $(p-1)i$, qi and $(q-1)i$.

5) In the regime V, where $p \geq 1/2$ and $-1 < q < -1/2$, besides $N-2$ 2-strings, only the boundary string qi survives and one real Bethe root λ_0 appears which is caused by the rearrangement of Fermi sea.

6) In the regime VI, where $0 < p < 1/2$ and $-1 < q < -1/2$, besides $N-4$ 2-strings, there are three boundary strings qi, $(q-1)i$, pi and one real root λ_0.

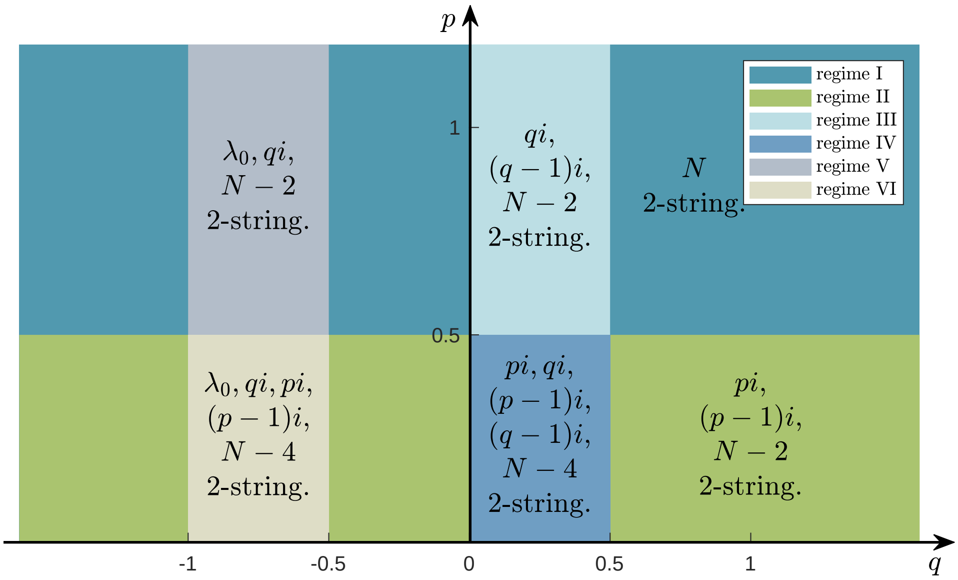

Figure 1: The distribution of reduced Bethe roots at the ground states with different boundary parameters p and q.

Because the Bethe roots are different in the different regimes of boundary parameters, we shall discuss them separately. In the regime I, where all the Bethe roots are the 2-strings. Substituting the 2-string solutions into the reduced BAEs (29), omitting the exponentially small corrections and taking the product of all the string solutions, we readily obtain

$$\begin{aligned}
&-\frac{i-\lambda_j}{i+\lambda_j}\,\frac{(p-\frac{1}{2})i-\lambda_j}{(p-\frac{1}{2})i+\lambda_j}\,\frac{(p+\frac{1}{2})i-\lambda_j}{(p+\frac{1}{2})i+\lambda_j}\,\frac{(q-\frac{1}{2})i-\lambda_j}{(q-\frac{1}{2})i+\lambda_j}\,\frac{(q+\frac{1}{2})i-\lambda_j}{(q+\frac{1}{2})i+\lambda_j} \\
&\times\left(\frac{\frac{1}{2}i-\lambda_j}{\frac{1}{2}i+\lambda_j}\,\frac{\frac{3}{2}i-\lambda_j}{\frac{3}{2}i+\lambda_j}\right)^{2N} = \prod_{l=1}^{M_1}\left[\frac{i-(\lambda_j-\lambda_l)}{i+(\lambda_j-\lambda_l)}\right]^2\left[\frac{i-(\lambda_j+\lambda_l)}{i+(\lambda_j+\lambda_l)}\right]^2 \\
&\times\frac{2i-(\lambda_j-\lambda_l)}{2i+(\lambda_j-\lambda_l)}\,\frac{2i-(\lambda_j+\lambda_l)}{2i+(\lambda_j+\lambda_l)}, \quad j=1,\cdots,M_1. \qquad (31)
\end{aligned}$$

Taking the logarithm of above Eq.(31), we obtain

$$2\pi I_j = W(\lambda_j; M_1) + \theta_{2p-1}(\lambda_j) + \theta_{2p+1}(\lambda_j) + \theta_{2q-1}(\lambda_j) + \theta_{2q+1}(\lambda_j), \ j = 1, \cdots, M_1, \quad (32)$$

where

$$W(\lambda_j; M_1) = \theta_2(\lambda_j) + 2N\left[\theta_1(\lambda_j) + \theta_3(\lambda_j)\right] - \sum_{l=1}^{M_1}\left[2\theta_2(\lambda_j - \lambda_l) + 2\theta_2(\lambda_j + \lambda_l) + \theta_4(\lambda_j - \lambda_l) + \theta_4(\lambda_j + \lambda_l)\right], \quad (33)$$

I_j is the quantum number, $\theta_n(x) = 2\arctan(2x/n)$ and $M_1 = N/2$. The ground state is characterized by the set of quantum numbers

$$\{I_j\} = \{1, 2, \cdots, M_1\}. \quad (34)$$

Solving the reduced BAEs (32) and substituting the values of Bethe roots into Eq.(30), we obtain the reduced ground state energy as

$$E_{hom} = -2\sum_{j=1}^{M_1} \frac{1}{\lambda_j^2 + \frac{1}{4}} + \frac{3}{\lambda_j^2 + \frac{9}{4}} + 3N + E_0 \equiv G(\lambda_j; M_1). \quad (35)$$

Now, we are ready to characterize the contribution of inhomogeneous term in the $T-Q$ relation (18) at the ground state by the quantity

$$E_{inh} = E_{hom} - E_g, \quad (36)$$

where E_{hom} is the reduced ground state energy given by (35) and E_g is the actual ground state energy (25) of the Hamiltonian (15). The ground state energy E_g can be obtained by two methods. One is solving the inhomogeneous BAEs (24) directly and the other is density matrix renormalization group (DMRG) [44–46]. We have checked that the ground state energy E obtained by these two methods are the same.

In Figure 2(a), we give the values of E_{inh} versus the system size N in the regime I. The red circles are the data calculated from Eq.(36) and the blue solid line is the fitted curve. From the fitted curve, we find that E_{inh} and N satisfy the power law relation $E_{inh} = \gamma N^{\beta}$. Due to the fact that $\beta < 0$, the value of E_{inh} tends to zero when the system size N tends to infinity. Therefore, in the thermodynamic limit, the inhomogeneous term in the $T-Q$ relation (18) can be neglected at the ground state and $E_{hom} = E_g$. The subfigure shows the distribution of Bethe roots with $N = 10$.

In the regime II, substituting the $N-2$ 2-strings, two boundary strings $\mu_{M-1} = pi$ and $\mu_M = (p-1)i$ into the reduced BAEs (29) and taking the logarithm, we have

$$2\pi I_j = W(\lambda_j; M_2) + \theta_{2q-1}(\lambda_j) + \theta_{2q+1}(\lambda_j) - \theta_{1-2p}(\lambda_j) - \theta_{2p+1}(\lambda_j) - \theta_{3+2p}(\lambda_j) - \theta_{5-2p}(\lambda_j) - 2\theta_{3-2p}(\lambda_j), \quad j = 1, 2, \cdots, M_2, \quad (37)$$

where $W(\lambda_j; M_2)$ is given by Eq.(33) with the replacing of M_1 by M_2, $M_2 = N/2 - 1$ and the quantum numbers are

$$\{I_j\} = \{1, 2, \cdots, M_2\}. \quad (38)$$

The corresponding reduced ground state energy reads

$$E_{hom} = G(\lambda_j; M_2) + \frac{4}{p^2 - 1} + \frac{4}{(p-1)^2 - 1}, \quad (39)$$

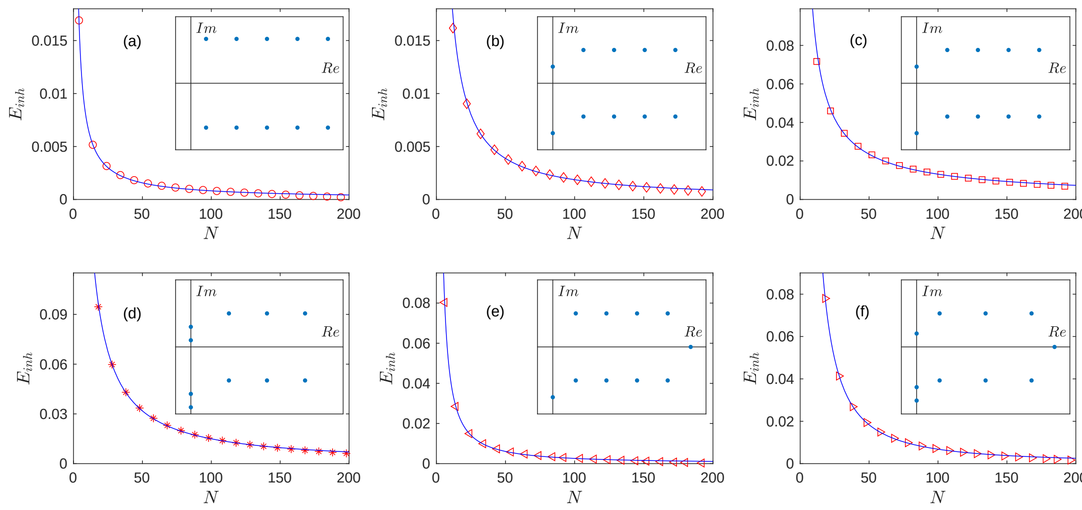

Figure 2: The values of E_{inh} versus the system size N. The data can be fitted as $E_{inh} = \gamma N^{\beta}$. Due to the fact $\beta < 0$, when the size of system $N \to \infty$, the contribution of the inhomogeneous term tends to zero. Here (a) $p = 1.1370, q = -1.0821, \gamma = 0.06203$ and $\beta = -0.9407$ in regime I; (b) $p = 0.3263, q = -1.8931, \gamma = 0.2371$ and $\beta = -1.052$ in regime II; (c) $p = 0.2428, q = 2.3735, \gamma = 0.6236$ and $\beta = -0.8384$ in regime III; (d) $p = 0.4453, q = 0.3789, \gamma = 2.234$ and $\beta = -1.087$ in regime IV; (e) $p = 0.8410, q = -0.6990, \gamma = 0.715$ and $\beta = -1.219$ in regime V; (f) $p = 0.3971, q = -0.7985, \gamma = 4.912$ and $\beta = -1.429$ in regime VI. The subfigures show the distribution of Bethe roots with $N = 10$.

where $G(\lambda_j; M_2)$ is given by Eq.(35) with the replacing of M_1 by M_2.

The procedure in the regime III is similar and reduced ground state energy is

$$E_{hom} = G(\lambda_j; M_2) + \frac{4}{q^2-1} + \frac{4}{(q-1)^2-1}. \tag{40}$$

In the regime IV, substituting the string solutions including four boundary strings into Eq.(29) and taking the logarithm, we have

$$\begin{aligned}2\pi I_j = W(\lambda_j; M_3) - \theta_{1-2p}(\lambda_j) - \theta_{2p+1}(\lambda_j) - \theta_{3+2p}(\lambda_j) - \theta_{5-2p}(\lambda_j) - 2\theta_{3-2p}(\lambda_j)\\ -\theta_{1-2q}(\lambda_j) - \theta_{2q+1}(\lambda_j) - \theta_{3+2q}(\lambda_j) - \theta_{5-2q}(\lambda_j) - 2\theta_{3-2q}(\lambda_j), \quad j = 1, 2, \cdots, M_3,\end{aligned} \tag{41}$$

where $M_3 = N/2 - 2$ and the quantum numbers are

$$\{I_j\} = \{1, 2, \cdots, M_3\}. \tag{42}$$

The reduced ground state energy is

$$E_{hom} = G(\lambda_j; M_3) + \frac{4}{p^2-1} + \frac{4}{(p-1)^2-1} + \frac{4}{q^2-1} + \frac{4}{(q-1)^2-1}. \tag{43}$$

In the regime V, the logarithm form of the BAEs are

$$\begin{aligned}2\pi I_j = W(\lambda_j; M_4) + \theta_{2p-1}(\lambda_j) + \theta_{2p+1}(\lambda_j) - \theta_{3+2q}(\lambda_j) - \theta_{3-2q}(\lambda_j) - 2\theta_{1-2q}(\lambda_j)\\ -\theta_1(\lambda_j - \lambda_0) - \theta_1(\lambda_j + \lambda_0) - \theta_3(\lambda_j - \lambda_0) - \theta_3(\lambda_j + \lambda_0), \quad j = 1, 2, \cdots, M_4,\end{aligned} \tag{44}$$

where $M_4 = N/2 - 1$ and the quantum numbers are $\{I_j\} = \{1, 2, \cdots, M_4\}$. We shall note that the quantum number corresponding to the real Bethe root λ_0 is 0. The reduced ground state energy reads

$$E_{hom} = G(\lambda_j; M_4) + \frac{4}{q^2-1} - \frac{4}{\lambda_0^2+1}. \tag{45}$$

Similarly, the reduced ground state energy in the regime VI is

$$E_{hom} = G(\lambda_j; M_5) + \frac{4}{p^2-1} + \frac{4}{(p-1)^2-1} + \frac{4}{q^2-1} - \frac{4}{\lambda_0^2+1}, \tag{46}$$

where $M_5 = N/2 - 2$.

Substituting the reduced ground state energies in different regimes into Eq.(36), we obtain the values of E_{inh}, which are shown in Figures 2(b)-(f). According to the finite size scaling analysis, we see that the inhomogeneous term indeed can be neglected at the ground state in the thermodynamic limit.

4 Boundary energy

In this section, we study the physical effects induced by the unparallel boundary magnetic fields and compute the boundary energy [47–49]. The values of Bethe roots at the ground state are determined by the quantum numbers $\{I_j\}$. Thus we define the counting function as $Z(\lambda_j) = \frac{I_j}{2N}$. In the thermodynamic limit, the Bethe roots can take the continuous values and we have $Z(\lambda_j) \to Z(u)$. Taking the derivative of $Z(u)$ with respect to u, we obtain

$$\frac{dZ(u)}{du} = \rho(u) + \rho^h(u), \tag{47}$$

where $\rho(u)$ is the density of Bethe roots and $\rho^h(u)$ means the density of holes in the real axis. Again, the distribution of Bethe roots in different regimes are different. We should consider them separately. In regime I, from the BAEs (32) with the constraint $N \to \infty$ and using Eq.(47), we obtain the density of states as

$$\begin{aligned}\rho(u) &= \frac{dZ(u)}{du} - \frac{1}{2N}[\rho^h(u) + \delta(u)] \\ &= a_1(u) + a_3(u) + \frac{1}{2N}\left[a_2(u) + a_{2p-1}(u) + a_{2p+1}(u) + a_{2q-1}(u) + a_{2q+1}(u)\right] \\ &\quad - \frac{1}{2N}[\rho^h(u) + \delta(u)] - \int_{-\infty}^{\infty} \left[2a_2(u-v) + a_4(u+v)\right]\rho(v)dv,\end{aligned} \tag{48}$$

where

$$\begin{aligned}a_n(u) &= \frac{1}{2\pi}\frac{n}{u^2+\frac{n^2}{4}}, \\ \rho^h(u) &= \frac{1}{2N}\left[\delta\left(u-\lambda_1^h\right) + \delta\left(u+\lambda_1^h\right) + \delta\left(u-\lambda_2^h\right) + \delta\left(u+\lambda_2^h\right)\right].\end{aligned} \tag{49}$$

We should note that the presence of delta-function in Eq.(48) is due to that $\lambda_j = 0$ is the solution of BAEs (32), which should be excluded because it makes the wavefunction vanish identically [50]. Meanwhile, two holes λ_1^h and λ_2^h should be introduced to ensure the magnetization satisfying

$$\frac{M}{N} = 2\int_{-\infty}^{\infty} \rho(u)du = 1. \tag{50}$$

Thus the holes are located at the infinities in the real axis.

With the help of Fourier transformation

$$\tilde{F}(\omega)=\int_{-\infty}^{\infty}e^{i\omega u}F(u)du,\qquad F(u)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i\omega u}\tilde{F}(\omega)d\omega, \tag{51}$$

from Eq.(48), we obtain

$$\tilde{\rho}(\omega)=\tilde{\rho}_g(\omega)+\tilde{\rho}_0(\omega)+\tilde{\rho}_1(\omega)+\tilde{\rho}_2(\omega), \tag{52}$$

where

$$\begin{aligned}
\tilde{a}_n(\omega) &= e^{-\frac{n|\omega|}{2}},\quad \tilde{\rho}_g(\omega)=\frac{\tilde{a}_1(\omega)+\tilde{a}_3(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)},\quad \tilde{\rho}_0(\omega)=\frac{1}{2N}\frac{\tilde{a}_2(\omega)-1}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)},\\
\tilde{\rho}_1(\omega) &= \begin{cases}\frac{1}{2N}\frac{\tilde{a}_{2p+1}(\omega)-\tilde{a}_{1-2p}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}, & 0<p<\frac{1}{2},\\ \frac{1}{2N}\frac{\tilde{a}_{2p-1}(\omega)+\tilde{a}_{2p+1}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}, & p>\frac{1}{2},\end{cases}\\
\tilde{\rho}_2(\omega) &= \begin{cases}-\frac{1}{2N}\frac{\tilde{a}_{1-2q}(\omega)+\tilde{a}_{-2q-1}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}, & q<-\frac{1}{2},\\ \frac{1}{2N}\frac{\tilde{a}_{2q+1}(\omega)-\tilde{a}_{1-2q}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}, & -\frac{1}{2}<q<\frac{1}{2},\\ \frac{1}{2N}\frac{\tilde{a}_{2q-1}(\omega)+\tilde{a}_{2q+1}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}, & q>\frac{1}{2}.\end{cases}
\end{aligned} \tag{53}$$

Then the ground state energy (35) can be expressed as

$$E_g=-2N\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\tilde{\rho}(\omega)d\omega+3N+E_0=Ne_g+e_s, \tag{54}$$

where e_g is the ground state energy density which is the same as that for the periodic boundary condition [9],

$$e_g=-2\int_{-\infty}^{\infty}\frac{[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)]^2}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}d\omega+3=-1, \tag{55}$$

and e_s is boundary energy

$$e_s = 2\pi-4+E_0+e_1+e_2, \tag{56}$$

$$e_1 = \begin{cases}-\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\frac{\tilde{a}_{2p-1}(\omega)+\tilde{a}_{2p+1}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}d\omega, & p>\frac{1}{2},\\ -\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\frac{\tilde{a}_{2p+1}(\omega)-\tilde{a}_{1-2p}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}d\omega, & 0<p<\frac{1}{2},\end{cases} \tag{57}$$

$$e_2 = \begin{cases}\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\frac{\tilde{a}_{-2q-1}(\omega)+\tilde{a}_{1-2q}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}d\omega, & q<-\frac{1}{2},\\ -\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\frac{\tilde{a}_{2q+1}(\omega)-\tilde{a}_{1-2q}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}d\omega, & -\frac{1}{2}<q<\frac{1}{2},\\ -\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\frac{\tilde{a}_{2q-1}(\omega)+\tilde{a}_{2q+1}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}d\omega, & q>\frac{1}{2}.\end{cases} \tag{58}$$

Now, we consider the regime II. The boundary strings pi and $(p-1)i$ can give rise to the rearrangement of Bethe roots in Fermi sea. From BAEs (37), the density of states

$\rho_p(u)$ is obtained as

$$\begin{aligned}\rho_p(u) &= a_1(u)+a_3(u)-\int_{-\infty}^{\infty}\left[2a_2(u-v)+a_4(u-v)\right]\rho_p(v)dv \\ &+\frac{1}{2N}\left[a_2(u)-a_{1-2p}(u)+a_{2p+1}(u)+a_{2q-1}(u)+a_{2q+1}(u)-\delta(u)\right] \\ &-\frac{1}{2N}\left[2a_{2p+1}(u)+2a_{3-2p}(u)+a_{3+2p}(u)+a_{5-2p}(u)\right]. \end{aligned} \tag{59}$$

In order to show that there exist the stable boundary bound states, we denote the deviation between $\rho_p(u)$ and $\rho(u)$ as $\delta\rho_p(u)=\rho_p(u)-\rho(u)$. From Eqs.(48) and (59), we obtain

$$\begin{aligned}\delta\rho_p(u) &= -\frac{1}{2N}\left[2a_{2p+1}(u)+2a_{3-2p}(u)+a_{3+2p}(u)+a_{5-2p}(u)\right] \\ &-\int_{-\infty}^{\infty}\left[2a_2(u-v)+a_4(u-v)\right]\delta\rho_p(v)dv. \end{aligned} \tag{60}$$

Taking the Fourier transformation of Eq.(60), we have

$$\delta\tilde{\rho}_p(\omega)=-\frac{1}{2N}\frac{2\tilde{a}_{2p+1}(\omega)+2\tilde{a}_{3-2p}(\omega)+\tilde{a}_{3+2p}(\omega)+\tilde{a}_{5-2p}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)}. \tag{61}$$

The energy deviation δe_p induced by the density deviation $\delta\tilde{\rho}_p(\omega)$ can be expressed as

$$\begin{aligned}\delta e_p &= -2N\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\delta\tilde{\rho}_p(\omega)d\omega+\frac{4}{p^2-1}+\frac{4}{(p-1)^2-1} \\ &= 2\int_0^{\infty}\frac{e^{-(p+1)\omega}}{1+e^{-\omega}}dw+2\int_0^{\infty}\frac{e^{-(2-p)\omega}}{1+e^{-\omega}}d\omega+\frac{2}{p(p-1)}<0. \end{aligned} \tag{62}$$

Because of $\delta e_p<0$, the boundary strings are stable. Then we conclude that in this regime, the ground state energy of the system is $E_g=Ne_g+e_s+\delta e_p$. The total spin long z-direction is $S_z=-\int_{-\infty}^{\infty}\delta\rho_p(u)=3/4$.

Next, we consider the regime III where boundary strings are qi and $(q-1)i$. Similarly, the energy deviation δe_q between this case and that without boundary strings is

$$\begin{aligned}\delta e_q &= -2N\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\delta\tilde{\rho}_q(\omega)d\omega+\frac{4}{p^2-1}+\frac{4}{(p-1)^2-1} \\ &= 2\int_0^{\infty}\frac{e^{-(q+1)\omega}}{1+e^{-\omega}}dw+2\int_0^{\infty}\frac{e^{-(2-q)\omega}}{1+e^{-\omega}}d\omega+\frac{2}{q(q-1)}<0. \end{aligned} \tag{63}$$

Due to the fact $\delta e_q<0$, we know that the ground state energy is $E_g=Ne_g+e_s+\delta e_q$ and the total spin long z-direction is $S_z=3/4$.

In the regime IV, we combine the results (62) and (63), and conclude that the ground state energy with boundary strings pi, $(p-1)i$, qi and $(q-1)i$ equals to $E_g=Ne_g+e_s+\delta e_p+\delta e_q$.

Then, we consider the regime V where besides the $N-2$ 2-string, there also exist one real Bethe root λ_0 and a single boundary string qi. Taking the thermodynamic limit of BAEs (44), we obtain the density of states $\rho_{\lambda q}(u)$ as

$$\begin{aligned}\rho_{\lambda q}(u) &= a_1(u)+a_3(u)-\frac{1}{2N}\left[a_1(u-\lambda_0)+a_1(u+\lambda_0)+a_3(u-\lambda_0)+a_3(u+\lambda_0)\right] \\ &+\frac{1}{2N}\left[a_2(u)+a_{2p-1}(u)+a_{2p+1}(u)-2a_{1-2q}(u)-a_{3+2q}(u)-a_{3-2q}(u)-\delta(u)\right] \\ &-\int_{-\infty}^{\infty}\left[2a_2(u-v)+a_4(u-v)\right]\rho_{\lambda q}(v)dv. \end{aligned} \tag{64}$$

Denote the deviation between $\rho_{\lambda q}(u)$ and $\rho(u)$ as $\delta\rho_{\lambda q}(u) = \rho_{\lambda q}(u) - \rho(u)$. From Eqs.(48) and (64), the value of $\delta\rho_{\lambda q}(u)$ reads

$$\begin{aligned}\delta\rho_{\lambda q}(u) &= -\frac{1}{2N}\left[a_1(u-\lambda_0)+a_1(u+\lambda_0)+a_3(u-\lambda_0)+a_3(u+\lambda_0)\right] \\ &\quad -\frac{1}{2N}\left[a_{1-2q}(u)-a_{-1-2q}(u)+a_{3-2q}(u)+a_{3+2q}(u)\right] \\ &\quad -\int_{-\infty}^{\infty}\left[2a_2(u)+a_4(u)\right]\delta\rho_{\lambda q}(v)dv. \end{aligned} \tag{65}$$

Taking the Fourier transformation of Eq.(65), we obtain

$$\delta\tilde{\rho}_{\lambda q}(\omega) = -\frac{1}{2N}\frac{\tilde{a}_{1-2q}(\omega)-\tilde{a}_{-1-2q}(\omega)+\tilde{a}_{3-2q}(\omega)+\tilde{a}_{3+2q}(\omega)}{1+2\tilde{a}_2(\omega)+\tilde{a}_4(\omega)} - \frac{1}{N}\frac{\cos(\omega\lambda_0)e^{-\frac{|\omega|}{2}}}{1+e^{-|\omega|}}. \tag{66}$$

Then the deviation of energy $\delta e_{\lambda q}$ induced by $\delta\tilde{\rho}_{\lambda q}(\omega)$ is given by

$$\begin{aligned}\delta e_{\lambda q} &= -2N\int_{-\infty}^{\infty}\left[\tilde{a}_1(\omega)+\tilde{a}_3(\omega)\right]\delta\tilde{\rho}_{\lambda q}(\omega)d\omega + \frac{4}{q^2-1} - \frac{4}{\lambda_0^2+1} \\ &= 2\int_0^{\infty}\frac{e^{-(2+q)\omega}}{1+e^{-\omega}}d\omega - 2\int_0^{\infty}\frac{e^{q\omega}}{1+e^{-\omega}}d\omega - \frac{2}{1+q} < 0. \end{aligned} \tag{67}$$

Due to $\delta e_{\lambda q} < 0$, the ground state energy in this regime is $E_g = Ne_g + e_s + \delta e_{\lambda q}$ and the total spin long z-direction is $S_z = 3/4$.

In the regime VI, there are $N-4$ 2-string, one real Bethe root λ_0 and three boundary strings qi, pi and $(p-1)i$. Combining the results (62) and (67), we obtain the ground state energy as $E_g = Ne_g + e_s + \delta e_p + \delta e_{\lambda q}$.

After tedious calculation, we find that the boundary energy e_b for all the regimes in Figure 1 can be expressed as

$$e_b = \begin{cases} -\dfrac{2}{p} - \dfrac{2}{q} + 2\pi - 4 + E_0, & p > 0,\ q > 0 \text{ or } q < -1, \\ -\dfrac{2}{p} - \dfrac{2}{q} + 2\pi\csc(q\pi) + 2\pi - 4 + E_0, & p > 0,\ -1 < q < 0. \end{cases} \tag{68}$$

The numerical check is shown in Figure 3, where the coloured solid lines are the boundary energies calculated by the expression (68) and the red points are those obtained by using the DMRG. Specifically, for each red point, we first compute the boundary energies with $N = 4, 14, \cdots, 194$ based on the DMRG results. Then from the finite size scaling analysis of these data, we obtain the corresponding results in the thermodynamic limit. As shown in Figure 3, the analytical and numerical results agree with each other very well.

5 Conclusions

In this paper, we have studied the thermodynamic limit and boundary energy of the isotropic spin-1 Heisenberg chain with generic integrable non-diagonal boundary reflections. We find that the ground state configurations of Bethe roots of the reduced BAEs with different model parameters are different. We show that the contribution of inhomogeneous term in the associated $T-Q$ relation can be neglected in the thermodynamic limit. This fact allows us to calculate the boundary energy induced by the unparallel boundary magnetic fields. The method provided in this paper can be used to study the thermodynamic properties of other quantum integrable models with certain interesting symmetries.

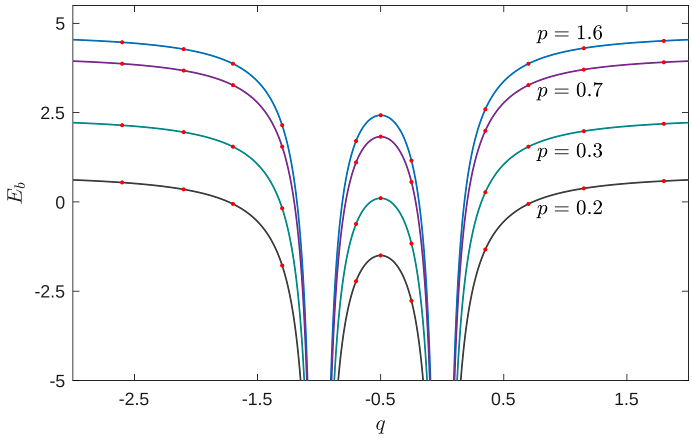

Figure 3: Boundary energies versus the boundary parameters p and q. The coloured curves are those calculated from the analytical expression (68) pand the red points are those obtained from the DMRG. The values of q at the red points are $q = -2.6, -2.1, -1.7, -1.3, -0.7, -0.5, -0.25, 0.35, 0.7, 1.15$ and 1.8.

Acknowledgments

Financial support from the National Natural Science Foundation of China (Grant Nos. 12074410, 12047502, 11934015, 11975183, 11947301, 11775177, 11775178 and 11774397), the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB33000000), the Major Basic Research Program of Natural Science of Shaanxi Province (Grant Nos. 2017KCT-12 and 2017ZDJC-32), and the Double First-Class University Construction Project of Northwest University is gratefully acknowledged. One of the authors, Zhihan Zheng would like to thank Dr. Yangyang Chen, Dr. Fakai Wen and Dr. Yi Qiao for their helpful discussions.

References

[1] X.-W. Guan, M. T. Batchelor and C. Lee, *Fermi gases in one dimension: From Bethe ansatz to experiments*, Rev. Mod. Phys. **85**, 1633 (2013), doi:10.1103/RevModPhys.85.1633.

[2] M. Takahashi, *Thermodynamics of one-dimensional solvable models*, Cambridge University Press, (1999), doi:10.1017/CBO9780511524332.

[3] L. Dolan, C. R. Nappi and E. Witten, *A relation between approaches to integrability in superconformal Yang-Mills theory*, J. High Energ. Phys. **10**, 017 (2003), doi:10.1088/1126-6708/2003/10/017.

[4] J. Sirker, R. G. Pereira, and I. Affleck, *Diffusion and ballistic transport in one-dimensional quantum systems*, Phys. Rev. Lett. **103**, 216602 (2009), doi:10.1103/PhysRevLett.103.216602.

[5] J. de Gier and F. H. L. Essler, *Bethe ansatz solution of the asymmetric exclusion process with open boundaries*, Phys. Rev. Lett. **95**, 240601 (2005), doi:10.1103/PhysRevLett.95.240601.

[6] H. A. Bethe, *Zur Theorie der Metalle. i. Eigenwerte und eigenfunktionen der linearen atomkette*, Zeit. für Phys. **71**, 205 (1931), doi:10.1007%2FBF01341708.

[7] A. B. Zamolodchikov and V. A. Fateev, *Model factorized s matrix and an integrable heisenberg chain with spin 1., in russian*, Sov. J. Nucl. Phys. **32**, 298 (1980).

[8] L. A. Takhtajan, *The picture of low-lying excitations in the isotropic Heisenberg chain of arbitrary spins*, Phys. Lett. A 87, 479 (1982), doi:10.1016/0375-9601(82)90764-2.

[9] H. M. Babujian, *Exact solution of the isotropic Heisenberg chain with arbitrary spins: Thermodynamics of the model*, Nucl. Phys. B **215**, 217 (1983), doi:10.1016/0550-3213(83)90668-5.

[10] H. M. Babujian, *Exact solution of the one-dimensional isotropic Heisenberg chain with arbitrary spins s*, Phys. Lett. A **90**, 479 (1982), doi:10.1016/0375-9601(82)90403-0.

[11] F. D. M. Haldane, *Continuum dynamics of the 1-D Heisenberg antiferromagnet: I-dentification with the $O(3)$ nonlinear sigma model*, Phys. Lett. **93A**, 464 (1983), doi:10.1016/0375-9601(83)90631-X.

[12] F. D. M. Haldane, *Nonlinear field theory of large-spin Heisenberg antiferromagnets: Semiclassically quantized solitons of the one-dimensional easy-axis Neel state*, Phys. Rev. Lett. **50**, 1153 (1983), doi:10.1103/PhysRevLett.50.1153.

[13] I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, *Rigorous results on valence-bond ground states in antiferromagnets*, Phys. Rev. Lett. **59**, 799 (1987), doi:10.1103/PhysRevLett.59.799.

[14] I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, *Valence bond ground states in isotropic quantum antiferromagnets*, Commun. Math. Phys. **115**, 477 (1988), doi:10.1007/BF01218021.

[15] M. N. Barber and M. T. Batchelor, *Spectrum of the biquadratic spin-1 antiferromagnetic chain*, Phys. Rev. B **40**, 4621 (1989), doi:10.1103/PhysRevB.40.4621.

[16] A. Klümper, *The spectra of q-state vertex models and related antiferromagnetic quantum spin chains*, J. Phys. A: Math. Gen. **23**, 809 (1990), doi:10.1088/0305-4470/23/5/023.

[17] K.-J.-B. Lee and P. Schlottmann, *Integrable spin-1 Heisenberg chain with impurity*, Phys. Rev. B **37**, 379 (1988), doi:10.1103/PhysRevB.37.379.

[18] F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter and G. R. W. Quispel, *Surface exponents of the quantum XXZ, Ashkin-Teller and Potts models*, J. Phys. A **20**, 6397 (1987), doi:10.1088/0305-4470/20/18/038.

[19] E. K. Sklyanin, *Boundary conditions for integrable quantum systems*, J. Phys. A **21**, 2375 (1988), doi:10.1088/0305-4470/21/10/015.

[20] P. P. Kulish and E. K. Sklyanin, *Quantum spectral transform method recent developments*, Lect. Notes in Phys. **151**, 61 (1982), doi:10.1007/3-540-11190-5_8.

[21] P. P. Kulish, N. Yu. Reshetikhin and E. K. Sklyanin, *Yand-Baxter equatuon and representation theory: 1*, Lett. Math. Phys. **5**, 393 (1981), doi:10.1142/9789812798336_0027.

[22] P. P. Kulish and N. Yu. Reshetikhin, *Quantum linear problem for the sine-Gordon equation and higher representations*, J. Sov. Math. **23**, 2435 (1983), doi:10.1007/BF01084171.

[23] A. N. Kirillov and N. Yu. Reshetikhin, *Exact solution of the Heisenberg XXZ model of spin s*, J. Sov. Math. **35**, 2627 (1986), doi:10.1007/BF01083768.

[24] A. N. Kirillov and N. Yu. Reshetikhin, *Exact solution of the integrable XXZ Heisenberg model with arbitrary spin. I. The ground state and the excitation spectrum*, J. Phys. A **20**, 1565 (1987), doi:10.1088/0305-4470/20/6/038.

[25] L. A. Takhtajan, *The picture of low-lying excitations in the isotropic Heisenberg chain of arbitrary spins*, Phys. Lett. A **87**, 479 (1982), doi:10.1016/0375-9601(82)90764-2.

[26] L. Mezincescu, R.I. Nepomechie and V. Rittenberg, *Bethe ansatz solution of the Fateev-Zamolodchikov quantum spin chain with boundary terms*, Phys. Lett. A **147**, 70 (1990), doi:10.1016/0375-9601(90)90016-H.

[27] E. C. Fireman, A. Lima-Santos and W. Utiel, *Bethe ansatz solution for quantum spin-1 chains with boundary terms*, Nucl. Phys. B **626**, 435 (2002), doi:10.1016/S0550-3213(02)00027-5.

[28] A. Doikou, *Fused integrable lattice models with quantum impurities and open boundaries*, Nucl. Phys. B **668**, 447 (2003), doi:10.1016/j.nuclphysb.2003.07.001.

[29] C.S. Melo, G.A.P. Ribeiro and M.J. Martins, *Bethe ansatz for the XXX-S chain with non-diagonal open boundaries*, Nucl. Phys. B **711**, 565 (2005), doi:10.1016/j.nuclphysb.2004.12.008.

[30] L. Frappat, R.I. Nepomechie and É. Ragoucy, *Complete Bethe ansatz solution of the open spin-s XXZ chain with general integrable boundary terms*, J. Stat. Mech. **0709**, P09009 (2007), doi:10.1088/1742-5468/2007/09/P09009.

[31] R. Baiyasi and R. Murgan, *Generalized $T-Q$ relations and the open spin-s XXZ chain with nondiagonal boundary terms*, J. Stat. Mech. **1210**, P10003 (2012), doi:10.1088/1742-5468/2012/10/P10003.

[32] R. Murgan, *Bethe ansatz of the open spin-s XXZ chain with nondiagonal boundary terms*, J. High Energ. Phys. **04**, 076 (2009), doi:10.1088/1126-6708/2009/04/076.

[33] J. Cao, W.-L. Yang, K. Shi and Y. Wang, *Off-diagonal Bethe ansatz and exact solution of a topological spin ring*, Phys. Rev. Lett. **111**, 137201 (2013), doi:10.1103/PhysRevLett.111.137201.

[34] Y. Wang, W.-L. Yang, J. Cao and K. Shi, *Off-diagonal Bethe ansatz for exactly solvable models*, Springer Press, (2015), doi:10.1007/978-3-662-46756-5.

[35] Y.-Y. Li, J. Cao, W.-L. Yang, K. Shi and Y. Wang, *Thermodynamic limit and surface energy of the XXZ spin chain with arbitrary boundary fields*, Nucl. Phys. B **884**, 17 (2014), doi:10.1016/j.nuclphysb.2014.04.010.

[36] P. Sun, Z.-R. Xin, Y. Qiao, K. Hao, L. Cao, J. Cao, T. Yang and W.-L. Yang, *Surface energy and elementary excitations of the XXZ spin chain with arbitrary boundary fields*, J. Phys. A: Math. Theor. **52**, 265201 (2019), doi:10.1088/1751-8121/ab2259.

[37] Z. Xin, Y. Qiao, K. Hao, J. Cao, W.-L. Yang, K. Shi and Y. Wang, *Thermodynamic limit and twisted boundary energy of the XXZ spin chain with antiperiodic boundary condition*, Nucl. Phys. B **936**, 501 (2018), doi:10.1016/j.nuclphysb.2018.10.002.

[38] Y. Qiao, Z. Xin, K. Hao, J. Cao, W.-L. Yang, K. Shi, Y. Wang, *Twisted boundary energy and low energy excitation of the XXZ spin torus at the ferromagnetic region*, New J. Phys **20**, 073046 (2018), doi:10.1088/1367-2630/aad35c.

[39] F. Wen, T. Yang, Z.-Y. Yang, J. Cao, K. Hao and W.-L. Yang, *Thermodynamic limit and boundary energy of the su(3) spin chain with non-diagonal boundary fields*, Nucl. Phys. B **915**, 119 (2017), doi:10.1016/j.nuclphysb.2016.12.003.

[40] J. Cao, S. Cui, W.-L. Yang, K. Shi, Y. Wang, *Exact spectrum of the spin-s Heisenberg chain with generic non-diagonal boundaries*, J. High Energ. Phys. **02**, 036 (2015), doi:10.1007/JHEP02(2015)036.

[41] C.-N. Yang, *Some exact results for the many-body problem in one dimension with repulsive delta-function interaction*, Phys. Rev. Lett. **19**, 1312 (1967), doi:10.1103/PhysRevLett.19.1312.

[42] R. J. Baxter, *Exactly solved models in statistical mechanics*, Academic Press, London, (1982), doi:10.1142/9789814415255_0002.

[43] A. Kapustin, S. Skorik, *Surface excitations and surface energy of the antiferromagnetic XXZ chain by the Bethe ansatz approach*, J. Phys. A **29**, 1629 (1996), doi:10.1088/0305-4470/29/8/011.

[44] S. R. White, *Density matrix formulation for quantum renormalization groups*, Phys. Rev. Lett. **69**, 2863 (1992), doi:10.1103/PhysRevLett.69.2863.

[45] S. R. White, *Density-matrix algorithms for quantum renormalization groups*, Phys. Rev. B **48**, 10345 (1993), doi:10.1103/PhysRevB.48.10345.

[46] U. Schollwöck, *The density-matrix renormalization group*, Rev. Mod. Phys. **77**, 259 (2005), doi:10.1103/RevModPhys.77.259.

[47] M. Gaudin, *Boundary energy of a Bose gas in one dimension*, Phys. Rev. A **4**, 386 (1971), doi:10.1103/PhysRevA.4.386.

[48] C. J. Hamer, G.R.W. Quispel and M. T. Batchelor, *Conformal anomaly and surface energy for Potts and Ashkin-Teller quantum chains*, J. Phys. A **20**, 5677 (1987), doi:10.1088/0305-4470/20/16/040.

[49] M. T. Batchelor and C. J. Hamer, *Surface energy of integrable quantum spin chains*, J. Phys. A **23**, 671 (1990), doi:10.1088/0305-4470/23/5/019.

[50] P. Fendley and H. Saleur, *Deriving boundary S matrices*, Nucl. Phys. B **428**, 681 (1994), doi:10.1016/0550-3213(94)90369-7.