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RAPID COMMUNICATION

Exact ground state properties of the t–J model with open boundary conditions

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We develop a new method to study the ground state energy of the one-dimensional supersymmetric t–J model with open boundary conditions. The eigenvalues of the nested transfer matrix are characterized by the zero roots of corresponding polynomials instead of the T–Q relation and Bethe roots. The distribution of zero roots at the ground state is studied. We find that the zero roots form two-string pairs, finite pure real and pure imaginary boundary strings. Based on the distribution of zero roots, we obtain the ground state energy of the system in the thermodynamic limit.

Keywords: quantum spin chains, zero roots, ground state energy

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1. Introduction

The t–J model is of paramount importance in the investigation of strongly correlated electronic systems, particularly in elucidating the mechanisms underlying high-T_c superconductivity.[1,2] At the point $J = \pm 2t$, the one-dimensional t–J model exhibits supersymmetry and becomes exactly solvable. Through the application of the coordinate Bethe ansatz, Lai[3] and Sutherland[4] successfully derived the exact solution of the system under periodic boundary conditions.[5] Subsequently, the graded nested algebraic Bethe ansatz method was employed to analyze the one-dimensional supersymmetric t–J model.[6–9] Schlottmann investigated the distribution of Bethe roots for the ground state in the presence of an external magnetic field.[10] Bares *et al.* precisely determined the ground state and excitation spectrum of the system.[11] Moreover, a wide range of intriguing properties of the system have been extensively explored.[12–15] In recent years, numerical methods have also played an important role in the investigation of the t–J model.[16,17]

When the boundary fields are parallel, comprehensive investigations have been conducted regarding the exact physical properties of the system.[18–25] When the boundary fields are non-parallel, identifying suitable vacuum states becomes highly non-trivial, and the traditional Bethe ansatz approach fails. To address this challenge, the off-diagonal Bethe ansatz method has been developed.[26,27] The eigenvalues of the transfer matrix are characterized by inhomogeneous T–Q relations. Furthermore, the relevant physical properties have been investigated in the thermodynamic limit.[28,29]

In this work, we develop a new approach to study the ground state energy of the one-dimensional supersymmetric t–J model with open boundary conditions. The exact solution of the Hamiltonian can be expressed in terms of the eigenvalue of the nested transfer matrix. We express the eigenvalue of the nested transfer matrix in terms of zero roots. We demonstrate that, in the ground state, the zero roots exhibit a distinct distribution consisting of two-strings, pure real roots, and pure imaginary roots. Utilizing this distribution, we derive analytical expressions for the ground state energy at arbitrary filling factors and the surface energy at half-filling.

The paper is organized as follows. In Section 2, we present the Bethe ansatz solutions of the model. Section 3 provides a comparative analysis of the distributions of the zero roots of the nested transfer matrix. In Section 4, we calculate the ground state energy induced by the boundary fields in the thermodynamic limit. Finally, in Section 5 we summarize our findings and provide a discussion of the results.

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2. Exact solutions

The Hamiltonian of the system is given by

$$\begin{aligned} H &= -t\sum_{j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow}\mathbb{P}\left[c^{\dagger}_{j,\sigma}c_{j+1,\sigma}+c^{\dagger}_{j+1,\sigma}c_{j,\sigma}\right]\mathbb{P} \\ &\quad +J\sum_{j=1}^{L-1}\left[\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1}-\frac{1}{4}n_jn_{j+1}\right] \\ &\quad +\chi_1 n_1+2\boldsymbol{h}_1\cdot\boldsymbol{S}_1+\chi_L n_L+2\boldsymbol{h}_L\cdot\boldsymbol{S}_L, \end{aligned} \tag{1}$$

where $c^{\dagger}_{j,\sigma}$ and $c_{j,\sigma}$ are the creation and annihilation operators of electrons with spin $\sigma=\uparrow,\downarrow$ at j-th site, respectively. L is the total number of lattice sites. $n_j=\sum_\sigma n_{j\sigma}=\sum_\sigma c^{\dagger}_{j,\sigma}c_{j,\sigma}$ is the electron number operator. $\boldsymbol{S}_j$ is the spin operator of the electron on site j. $S_j=c^{\dagger}_{j,\uparrow}c_{j,\downarrow}$, $S^{\dagger}_j=c^{\dagger}_{j,\downarrow}c_{j,\uparrow}$ and $S^z_j=\frac{1}{2}(n_{j,\uparrow}-n_{j,\downarrow})$ are the generators of $su(2)$ symmetry in the spin sector. $\hat{N}=\sum_{j=1}^{L}n_j$ is the total number of electrons. $\mathbb{P}=\Pi_{j=1}^{L}(1-n_{j\uparrow}n_{j\downarrow})$ is the projector which is included to ensure the constraint of no double occupancy. $\boldsymbol{h}_1=(h_1^x,h_1^y,h_1^z)=(-\sin\theta\cos\varphi,-\sin\theta\sin\varphi,\cos\theta)/(2\xi)$ and $\boldsymbol{h}_L=(h_L^x,h_L^y,h_L^z)=(\sin\theta'\cos\varphi',\sin\theta'\sin\varphi',-\cos\theta')/[2(1-\xi')]$ are the boundary magnetic fields. $\chi_1=-1+1/(2\xi)$ and $\chi_L=-1+1/[2(1-\xi')]$ are the boundary chemical potentials. Here $\xi,\xi',\theta,\theta',\varphi$ and φ' are the boundary parameters, and we focus attention on the sector of $J=2t=2$.

The Hamiltonian (1) is obtained by taking the first order derivative of the logarithm of the transfer matrix $t(u)$, which is the the generating functional of all the conserved quantities of the system,

$$\begin{aligned} H &= -\frac{1}{2}\frac{\mathrm{d}\ln t(u)}{\mathrm{d}u}\bigg|_{u=0}+\frac{1}{2\xi}-\frac{1-2\xi'}{2(1-\xi')} \\ &\quad -2\hat{N}+L-1. \end{aligned} \tag{2}$$

The transfer matrix $t(u)$ is defined as

$$t(u)=\mathrm{str}_0\{K_0^{+}(u)\mathbb{T}_0(u)\}, \tag{3}$$

where u is the spectral parameter and str_0 is the super-partial-trace in the auxiliary space with the definition $\mathrm{str}_0 G=\sum_{\beta=1}^{3}(-1)^{p_\beta}G^{\beta}_{\beta}$, $p_1=0$, $p_2=1$, $p_3=1$ and G is an arbitrary matrix. $K_0^{+}(u)$ is the 3×3 boundary reflection matrix defined in the auxiliary space at one end of the chain

$$\begin{aligned} &K^{+}(u)=\begin{pmatrix} k^{+}_{11}(u) & 0 & 0 \\ 0 & k^{+}_{22}(u) & k^{+}_{23}(u) \\ 0 & k^{+}_{32}(u) & k^{+}_{33}(u) \end{pmatrix}, \\ &k^{+}_{11}(u)=\xi'-u,\ \ k^{+}_{22}(u)=\xi'-\frac{1}{2}-\frac{1-2u}{2}\cos\theta', \\ &k^{+}_{23}(u)=\frac{2u-1}{2}\sin\theta'\,\mathrm{e}^{\mathrm{i}\varphi'},\ \ k^{+}_{32}(u)=\frac{2u-1}{2}\sin\theta'\,\mathrm{e}^{-\mathrm{i}\varphi'}, \\ &k^{+}_{33}(u)=\xi'-\frac{1}{2}+\frac{1-2u}{2}\cos\theta'. \end{aligned} \tag{4}$$

The $\mathbb{T}_0(u)=T_0(u)K_0^{-}(u)\hat{T}_0(u)$ is the double-row monodromy matrix, where $T_0(u)$ and $\hat{T}_0(u)$ are the monodromy matrix and the reflecting one, respectively,

$$\begin{aligned} &T_0(u)=R_{0,L}(u)R_{0,L-1}(u)\cdots R_{0,1}(u), \\ &\hat{T}_0(u)=R_{1,0}(u)\cdots R_{L-1,0}(u)R_{L,0}(u), \\ &R_{0,j}(u)=u+\Pi_{0,j}, \end{aligned} \tag{5}$$

where $\Pi_{0,j}$ is the super permutation operator defined in the tensor space of the auxiliary and physical spaces. The boundary reflection of electrons at the other end is characterized by the 3×3 reflection matrix

$$\begin{aligned} &K^{-}(u)=\begin{pmatrix} k^{-}_{11}(u) & 0 & 0 \\ 0 & k^{-}_{22}(u) & k^{-}_{23}(u) \\ 0 & k^{-}_{32}(u) & k^{-}_{33}(u) \end{pmatrix}, \\ &k^{-}_{11}(u)=\xi+u,\ \ k^{-}_{22}(u)=\xi+\cos\theta u,\ \ k^{-}_{23}(u)=\sin\theta\,\mathrm{e}^{\mathrm{i}\varphi}u, \\ &k^{-}_{32}(u)=\sin\theta\,\mathrm{e}^{-\mathrm{i}\varphi}u,\ \ k^{-}_{33}(u)=\xi-\cos\theta u. \end{aligned} \tag{6}$$

According to Eq. (40), we know that the energy spectrum of the system can be obtained by the eigenvalues of the transfer matrix $t(u)$. The double-row monodromy matrix $\mathbb{T}_0(u)$ is a 3×3 matrix in the auxiliary space

$$\mathbb{T}_0(u)=\begin{pmatrix} A(u) & B_1(u) & B_2(u) \\ C_1(u) & D_{11}(u) & D_{12}(u) \\ C_2(u) & D_{21}(u) & D_{22}(u) \end{pmatrix}, \tag{7}$$

where the off-diagonal elements are used to construct the eigenstates of the system. Assume the eigenstates of the transfer matrix $t(u)$ are[29]

$$|\tilde{v}_1,\ldots,\tilde{v}_N;\mathcal{F}\rangle=B_{a_1}(\tilde{v}_1)\cdots B_{a_N}(\tilde{v}_N)|\Omega\rangle\mathcal{F}^{a_1\cdots a_N}, \tag{8}$$

where $\{\tilde{v}_j\}$ are the Bethe roots in the charge sector, $|\Omega\rangle=\otimes^{N}(1,0,0)^{\mathrm{T}}$ is the vacuum state, T means the transposition, and the coefficients $\{\mathcal{F}^{a_1\cdots a_N}\}$ are the vectors related to the nested eigenstate in the spin sector. In Eq. (8), the repeated indices should be summed. Acting the transfer matrix (3) on the Bethe state (8), we obtain

$$\begin{aligned} &t(u)|\tilde{v}_1,\ldots,\tilde{v}_N;\mathcal{F}\rangle \\ &=\Lambda(u)|\tilde{v}_1,\ldots,\tilde{v}_N;\mathcal{F}\rangle+\text{unwanted terms}. \end{aligned} \tag{9}$$

We see that the assumed Bethe state (8) is indeed the eigenstate of the transfer matrix $t(u)$ if the unwanted terms in the above equation are zero roots, which give that the Bethe roots $\{\tilde{v}_j\}$ should satisfy the Bethe ansatz equations (BAEs),

$$\begin{aligned} &\left[k^{+}_{11}(\tilde{v}_j)-\frac{k^{+}_{22}(\tilde{v}_j)+k^{+}_{33}(\tilde{v}_j)}{2\tilde{v}_j+1}\right]k^{-}_{11}(\tilde{v}_j)\left(\frac{\tilde{v}_j+1}{\tilde{v}_j}\right)^{2L} \\ &\times\frac{\prod_{l=1}^{N}(\tilde{v}_j-\tilde{v}_l-1)(\tilde{v}_j+\tilde{v}_l)}{\hat{t}(\tilde{v}_j)}=1, \end{aligned} \tag{10}$$

where $\hat{t}(u)$ is the nested transfer matrix in the spin sector

$$\begin{aligned} \hat{t}(u) &= \frac{2u}{2u+1}\mathrm{tr}_{\bar{0}}\big[\bar{K}^{+}_{\bar{0}}(u)r_{\bar{0},1}(u+\tilde{v}_1+1)\cdots \\ &\quad\times r_{\bar{0},N}(u+\tilde{v}_N+1)\bar{K}^{-}_{\bar{0}}(u)r_{N,\bar{0}}(u-\tilde{v}_N)\cdots r_{1,\bar{0}}(u-\tilde{v}_1)\big], \end{aligned}$$

$$\bar{K}^+(u)=\begin{pmatrix} k_{22}^+(u) & k_{23}^+(u) \\ k_{32}^+(u) & k_{33}^+(u) \end{pmatrix},$$
$$\bar{K}^-(u)=\begin{pmatrix} \frac{(2u+1)k_{22}^-(u)-k_{11}^-(u)}{2u} & \frac{2u+1}{2u}k_{23}^-(u) \\ \frac{2u+1}{2u}k_{32}^-(u) & \frac{(2u+1)k_{33}^-(u)-k_{11}^-(u)}{2u} \end{pmatrix},$$
$$r_{\bar{0},j}(u)=u+P_{\bar{0},j},\quad [P_{\bar{0},j}]_{\beta_1,\beta_2}^{\alpha_1,\alpha_2}=-\delta_{\alpha_1,\beta_2}\delta_{\beta_1,\alpha_2}. \tag{11}$$

We should note that $\hat{t}(u)$ is still an operator. Then the eigenvalue of the transfer matrix $t(u)$ is

$$\begin{aligned}\Lambda(u) &= \left[k_{11}^+(u)-\frac{k_{22}^+(u)+k_{33}^+(u)}{2u+1}\right]k_{11}^-(u)(u+1)^{2L} \\ &\times\prod_{l=1}^{N}\frac{(u-\tilde{v}_l-1)(u+\tilde{v}_l)}{(u-\tilde{v}_l)(u+\tilde{v}_l+1)} \\ &-u^{2L}\prod_{l=1}^{N}\frac{1}{(u-\tilde{v}_l)(u+\tilde{v}_l+1)}\hat{t}(u).\end{aligned} \tag{12}$$

We see that now the eigenvalue problem is changed to the diagonalization of $\hat{t}(u)$. Due to the $U(1)$ symmetry breaking, the number of electrons with fixed spin is not conserved and the traditional Bethe ansatz does not work. We use the off-diagonal Bethe ansatz.

From the construction (11), we know that $\hat{t}(u)$ is an operator polynomial of u with degree $2N+2$, which can be completely determined by $2N+3$ constraints. By employing the fusion method, we obtain N operator product identities for the nested transfer matrix $\hat{t}(u)$ at the inhomogeneous points $\{\tilde{v}_j|j=1,\ldots,N\}$

$$\begin{aligned}&\hat{t}(\tilde{v}_j)\hat{t}(\tilde{v}_j+1) \\ &= \bar{a}(\tilde{v}_j)\bar{d}(\tilde{v}_j+1)\prod_{k=1}^{N}(\tilde{v}_j-\tilde{v}_k-1)(\tilde{v}_j+\tilde{v}_k) \\ &\times(\tilde{v}_j-\tilde{v}_k+1)(\tilde{v}_j+\tilde{v}_k+2),\quad j=1,\ldots,N,\end{aligned} \tag{13}$$

where

$$\begin{aligned}\bar{a}(u)&=\frac{u-\frac{1}{2}}{u+\frac{1}{2}}(u+\xi')(u+\xi), \\ \bar{d}(u)&=(u-\xi')(u-\xi).\end{aligned} \tag{14}$$

From the definition (11), we also obtain that $\hat{t}(u)$ satisfies the crossing relation

$$\left(\lambda+\frac{1}{2}\right)\hat{t}(\lambda)=\left(\lambda-\frac{1}{2}\right)\hat{t}(-\lambda). \tag{15}$$

Besides, the values of $\hat{t}(u)$ at $u=0,\frac{1}{2}$ can be obtained directly

$$\begin{aligned}&\hat{t}(0)=0, \\ &\hat{t}\left(\frac{1}{2}\right)=\bar{d}\left(\frac{1}{2}\right)\prod_{k=1}^{N}(u-\tilde{v}_k)(u+\tilde{v}_k+1).\end{aligned} \tag{16}$$

The asymptotic behavior of $\hat{t}(u)$ reads

$$\lim_{u\to\infty}\hat{t}(u)=Cu^{2N+2}+\cdots,$$

$$C=2\cos\theta\cos\theta'+2\sin\theta\sin\theta'\cos(\phi'-\phi). \tag{17}$$

We express the eigenvalue $\hat{\Lambda}(u)$ of the nested transfer matrix $\hat{t}(u)$ in terms of the zero roots $\{z_j|j=1,\ldots,2N+3\}$ of the corresponding polynomial as

$$\left(u+\frac{1}{2}\right)\hat{\Lambda}(u)=C\prod_{j=1}^{2N+3}(u-z_j). \tag{18}$$

Then we conclude that the constraints (13)–(17) can completely determine the values of $\hat{\Lambda}(u)$ and the zero roots $\{z_j\}$ for a given set of inhomogeneity parameters $\{\tilde{v}_j\}$.

Replacing the operator $\hat{t}(u)$ by the eigenvalues $\hat{\Lambda}(u)$ in Eqs. (10) and (13), we obtain the constraints of zero roots $\{z_j\}$ and Bethe roots $\{\tilde{v}_j\}$. By solving these coupled equations, we obtain the values of $\{z_j\}$ and $\{\tilde{v}_j\}$. Substituting these values into Eqs. (12) and (18), we obtain the eigenvalues of the transfer matrices $t(u)$ and $\hat{t}(u)$. Then, according to Eq. (40), the energy spectrum of the Hamiltonian (1) can be obtained as

$$E=-\sum_{k=1}^{N}\frac{1}{\tilde{v}_k(\tilde{v}_k+1)}-2N. \tag{19}$$

It should be noted that the eigenvalues of the transfer matrix $\hat{\Lambda}(u)$ can also be parametrized in terms of the roots of the Bethe ansatz equations (BAEs). For diagonal boundary conditions, the Bethe ansatz solution can be constructed within the standard algebraic Bethe ansatz framework, whereas for generic non-diagonal boundaries the spectrum is characterized by an inhomogeneous T–Q relation and the Bethe roots satisfy inhomogeneous BAEs.[27] For the inhomogeneous BAEs, the distribution of Bethe roots is comparatively complicated, making traditional thermodynamic analysis extremely difficult. By instead focusing on zero roots, one can avoid direct treatment of the inhomogeneous BAEs.

3. Distribution of roots and numerical results

Now we determine the distribution of Bethe roots $\{\tilde{v}_j\}$ and zero roots $\{z_j\}$ in the thermodynamic limit. Substituting Eq. (18) into Eqs. (10) and (13), we obtain

$$\begin{aligned}&\left(\frac{\mu_j-\frac{1}{2}\mathrm{i}}{\mu_j+\frac{1}{2}\mathrm{i}}\right)^{2L}\left[\mu_j+\mathrm{i}\left(\xi'-\frac{1}{2}\right)\right] \\ &\times\left[\mu_j-\mathrm{i}\left(\xi-\frac{1}{2}\right)\right]\prod_{l=1}^{N}(\mu_j\pm\mu_l+\mathrm{i}) \\ &= C\frac{\prod_{k=1}^{2N+3}(\mu_j+\mathrm{i}\tilde{z}_k+\frac{\mathrm{i}}{2})}{\mu_j+\mathrm{i}}, \\ &C^2\prod_{k=1}^{2N+3}\frac{(\mu_j+\mathrm{i}z_k+\frac{\mathrm{i}}{2})(\mu_j+\mathrm{i}z_k-\frac{\mathrm{i}}{2})}{\mu_j(\mu_j-\mathrm{i})} \\ &=\bar{a}\left(\mathrm{i}\mu_j-\frac{1}{2}\right)\bar{d}\left(\mathrm{i}\mu_j+\frac{1}{2}\right)\end{aligned} \tag{20}$$

$$\times\prod_{l=1}^{N}(\mu_j\pm\mu_l+\mathrm{i})(\mu_j\pm\mu_l-\mathrm{i}), \tag{21}$$

where $\mu_j=-\mathrm{i}\tilde{\nu}_j-\frac{\mathrm{i}}{2}$, $j=1,\ldots,N$ and C is given by Eq. (17). Throughout this paper, the notation $F(\pm)$ means that these two functions should be multiplied, i.e., $F(\pm)=F(+)F(-)$.

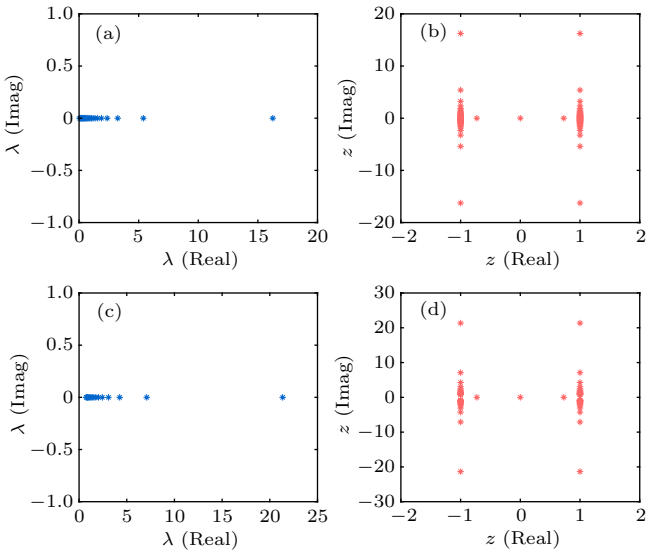


Fig. 1. (a) The distribution of roots $\{\mu_j\}$ on the complex plane for $N=L=48$ in the ground state. (b) The patterns of zero roots $\{z_j\}$ with $N=L=48$. (c) The distribution of roots $\{\mu_j\}$ with $N=2/3L=32$. (d) The patterns of zero roots $\{z_j\}$ with $N=2/3L=32$. Here, $\xi=1.9$, $\xi'=0.3$ and $\theta=\phi=\theta'=\phi'=0$.

The distribution of roots $\{\mu_j\}$ and zero roots $\{z_l\}$ can be obtained by solving the Eqs. (20) and (21) for the finite system size.[30] The numerical results of roots and zero roots at the ground state with $L=48$ at filling $n=1$ and $n=2/3$ are shown in Fig. 1. Next, we check the correctness of these results. The ground state energy can also be computed by the DMRG method[31] and the results are shown in Table 1, where some other filling cases are also given. We see that they are highly consistent with each other.

From the expression of the non-parallel boundary magnetic fields, we know that the singular points of the boundary parameters are $\xi=0$ and $\xi'=1$. According to them, we divide the boundary parameters into four regimes: (I) $\xi>0$, $\xi'<1$, (II) $\xi>0$, $\xi'>1$, (III) $\xi<0$, $\xi'<1$ and (IV) $\xi<0$, $\xi'>1$. In these regimes, the physical properties of the system are different. Thus, we should consider them separately.

Table 1. The ground state energies E_{DMRG} obtained by using the DMRG method and E_{R} obtained by the roots. Here $\xi=1.9$, $\xi'=0.3$ and $\theta=\phi=\theta'=\phi'=0$.

L	N	E_{DMRG}	E_{R}	n
48	48	–67.1002	–67.0940	1
48	40	–61.5918	–61.5971	5/6
48	32	–53.9162	–53.9118	2/3
48	24	–43.5365	–43.5332	1/2
48	16	–30.6370	–30.6349	1/3
48	8	–15.8286	–15.8278	1/6

From the exact numerical calculation with finite L and the singularity analysis with infinite L, we obtain the patterns of roots and zero roots at the ground state for different boundary parameters regimes. We should note that boundary strings can lower the energy when the system size L becomes infinite. After some calculations, we summarize the results in Table 2. It should be noted that the values of the pure real zero roots (z_{01} and z_{02}) and pure imaginary zero roots ($\mathrm{i}z_{03}$) are not required for our analysis. In the following section, we prove that the values of the paired roots do not appear in the final expression of the ground state energy.

Table 2. The patterns of Bethe roots and zero roots in the ground state for different regimes. It should be note that the zero roots form the pairs and the imaginary parts are denoted as $\{\pm\mathrm{i}\tilde{z}_j\}$, which means that if there is a zero root $\mathrm{i}\tilde{z}_j$, there must exist another zero root $-\mathrm{i}\tilde{z}_j$.

Regime	$\{\mu_k\|k=1,\ldots,N\}$	$\{z_j\|j=1,\ldots,2N+3\}$
I	$\lambda_j\pm\frac{\mathrm{i}}{2},\lambda_j\in\boldsymbol{R}$, $j=1,\ldots,\frac{N}{2}$	$1+\tilde{z}_j,-1-\mathrm{i}\tilde{z}_j,\pm z_{01},0$, $j=1,\ldots,N$
II	$v_j\pm\frac{\mathrm{i}}{2},v_j\in\boldsymbol{R}$, $j=1,\ldots,\frac{N}{2}-1$, $\mu_{N-1}\in\boldsymbol{R}$, $\mu_N=\mathrm{i}(\xi'-\frac{1}{2})$	$1+\tilde{z}_j,-1-\mathrm{i}\tilde{z}_j,\pm z_{01},\pm z_{02},\pm\mathrm{i}z_{03},0$, $j=1,\ldots,N-2$
III	$v_j\pm\frac{\mathrm{i}}{2}$, $v_j\in\boldsymbol{R}$, $j=1,\ldots,\frac{N}{2}-1$, $\mu_{N-1}\in\boldsymbol{R}$, $\mu_N=\mathrm{i}(\frac{1}{2}-\xi)$	$1+\tilde{z}_j,-1-\mathrm{i}\tilde{z}_j,\pm z_{01},\pm z_{02},\pm\mathrm{i}z_{03},0$, $j=1,\ldots,N-2$
IV	$\lambda_j\pm\frac{\mathrm{i}}{2},\lambda_j\in\boldsymbol{R}$, $j=1,\ldots,\frac{N}{2}-1$, $\mu_{N-1}=\mathrm{i}(\xi'-\frac{1}{2})$, $\mu_N=-\mathrm{i}(\xi-\frac{1}{2})$	$1+\tilde{z}_j,-1-\mathrm{i}\tilde{z}_j,\pm z_{01},\pm z_{02},\pm\xi',0$, $j=1,\ldots,N-2$

4. Ground state energy

Based on the obtained distribution of roots, we are ready to calculate the ground state energy in the thermodynamic limit by combining Eqs. (10), (13) and (18).

4.1. Regime (I): $\xi>0$ and $\xi'<1$

In regime (I), according to the patterns of zero roots, we express the eigenvalue $\hat{\Lambda}(u)$ as

$$(u+\frac{1}{2})\hat{\Lambda}(u)=C(u-z_{01})(u+z_{01})u$$
$$\times\prod_{j=1}^{N}(u-\mathrm{i}\tilde{z}_j-1)(u+\mathrm{i}\tilde{z}_j+1). \tag{22}$$

Substituting (22) into BAEs (10) and (13), we obtain

$$\left(\frac{\mu_j-\frac{1}{2}\mathrm{i}}{\mu_j+\frac{1}{2}\mathrm{i}}\right)^{2L}\left(\mu_j+\mathrm{i}\left(\xi'-\frac{1}{2}\right)\right)\left(\mu_j-\mathrm{i}\left(\xi-\frac{1}{2}\right)\right)$$
$$\times\prod_{l=1}^{N}(\mu_j-\mu_l+\mathrm{i})(\mu_j+\mu_l+\mathrm{i})$$
$$=C\frac{\mu_j+\frac{1}{2}\mathrm{i}}{\mu_j+\mathrm{i}}\left(\mu_j+\frac{\mathrm{i}}{2}+\mathrm{i}z_{01}\right)\left(\mu_j+\frac{\mathrm{i}}{2}-\mathrm{i}z_{01}\right)$$

$$\times\prod_{k=1}^{N}\left(\mu_j-\tilde{z}_k+\frac{3}{2}\mathrm{i}\right)\left(\mu_j+\tilde{z}_k-\frac{1}{2}\mathrm{i}\right), \tag{23}$$

$$\frac{\mu_j+\mathrm{i}}{\mu_j+\frac{1}{2}\mathrm{i}}\frac{\mu_j-\mathrm{i}}{\mu_j-\frac{1}{2}\mathrm{i}}\left(\mu_j\pm\mathrm{i}\left(\frac{1}{2}-\xi'\right)\right)\left(\mu_j\pm\mathrm{i}\left(\frac{1}{2}-\xi\right)\right)$$

$$\times\prod_{l=1}^{N}(\mu_j\pm\mu_l+\mathrm{i})(\mu_j\pm\mu_l-\mathrm{i})$$

$$=C^2\left(\mu_j\pm\mathrm{i}\left(\frac{1}{2}+z_{01}\right)\right)\left(\mu_j\pm\mathrm{i}\left(\frac{1}{2}-z_{01}\right)\right)$$

$$\times\prod_{k=1}^{N}\left(\mu_j\pm\left(\tilde{z}_k-\frac{3}{2}\mathrm{i}\right)\right)\left(\mu_j\pm\left(\tilde{z}_k-\frac{1}{2}\mathrm{i}\right)\right). \tag{24}$$

Because Bethe roots $\{\mu_k\}$ form the two-strings at the ground state, we parameterize these complex conjugate pairs as

$$(\mu_{k_1},\mu_{k_2})=\left(\lambda_k+\frac{\mathrm{i}}{2}+\mathrm{o}(\mathrm{e}^{-\varepsilon L}),\lambda_k-\frac{\mathrm{i}}{2}+\mathrm{o}(\mathrm{e}^{-\varepsilon L})\right),$$
$$k=1,\ldots,M,\quad M=N/2, \tag{25}$$

where λ_k is the position of the two-string on the real axis, and $\mathrm{o}(\mathrm{e}^{-\varepsilon L})$ means the finite size correction which can be neglected if $L\to\infty$. Because we focus on the thermodynamic limit, N is set to be even without loss of generality.

Substituting $\mu_{k_1}=\lambda_j+\frac{\mathrm{i}}{2}$ and $\mu_{k_2}=\lambda_j-\frac{\mathrm{i}}{2}$ into Eq. (23) respectively, and multiplying the two obtained equations, we have

$$\left(\frac{\lambda_j-\mathrm{i}}{\lambda_j+\mathrm{i}}\right)^{2L}\frac{\lambda_j+\frac{3}{2}\mathrm{i}}{\lambda_j+\mathrm{i}}\frac{\lambda_j+\frac{1}{2}\mathrm{i}}{\lambda_j}(\lambda_j+\mathrm{i}\xi')\left(\lambda_j+\mathrm{i}(\xi'-1)\right)$$

$$\times(\lambda_j-\mathrm{i}\xi)\left(\lambda_j-\mathrm{i}(\xi-1)\right)\prod_{l=1}^{N/2}(\lambda_j-\lambda_l+\mathrm{i})^2(\lambda_j+\lambda_l)$$

$$\times(\lambda_j+\lambda_l+2\mathrm{i})=C^2(\lambda_j+\mathrm{i}(1\pm z_{01}))(\lambda_j\pm\mathrm{i}z_{01})$$

$$\times\prod_{k=1}^{N}(\lambda_j\pm(\tilde{z}_k-\mathrm{i}))(\lambda_j-\tilde{z}_k+2\mathrm{i})(\lambda_j+\tilde{z}_k). \tag{26}$$

Substituting $\mu_{k_1}=\lambda_j+\frac{\mathrm{i}}{2}$ and $\mu_{k_2}=\lambda_j-\frac{\mathrm{i}}{2}$ into Eq. (24) respectively, and multiplying the obtained equations, we have

$$\frac{\lambda_j+\frac{3}{2}\mathrm{i}}{\lambda_j-\frac{3}{2}\mathrm{i}}\frac{\lambda_j-\mathrm{i}}{\lambda_j+\mathrm{i}}\frac{\lambda_j-\frac{1}{2}\mathrm{i}}{\lambda_j+\frac{1}{2}\mathrm{i}}\frac{\lambda_j+\mathrm{i}(1-\xi')}{\lambda_j-\mathrm{i}(1-\xi')}\frac{\lambda_j+\mathrm{i}(1-\xi)}{\lambda_j-\mathrm{i}(1-\xi)}$$

$$\times\frac{\lambda_j+\mathrm{i}\xi'}{\lambda_j-\mathrm{i}\xi'}\frac{\lambda_j+\mathrm{i}\xi}{\lambda_j-\mathrm{i}\xi}\frac{\lambda_j-\mathrm{i}(1-z_{01})}{\lambda_j+\mathrm{i}(1-z_{01})}\frac{\lambda_j-\mathrm{i}(1+z_{01})}{\lambda_j+\mathrm{i}(1+z_{01})}$$

$$\times\prod_{k=1}^{N}\frac{\lambda_j+\tilde{z}_k-2\mathrm{i}}{\lambda_j-\tilde{z}_k+2\mathrm{i}}\prod_{l=1}^{N/2}\frac{\lambda_j+\lambda_l+2\mathrm{i}}{\lambda_j+\lambda_l-2\mathrm{i}}=1. \tag{27}$$

Dividing Eq. (26) by its complex conjugate and considering (27), we obtain

$$\left(\frac{\lambda_j-\mathrm{i}}{\lambda_j+\mathrm{i}}\right)^{2L}=-\frac{\lambda_j-\frac{\mathrm{i}}{2}}{\lambda_j+\frac{\mathrm{i}}{2}}\frac{\lambda_j+\mathrm{i}(1-\xi')}{\lambda_j-\mathrm{i}(1-\xi')}\frac{\lambda_j+\mathrm{i}\xi}{\lambda_j-\mathrm{i}\xi}$$
$$\times\prod_{l=1}^{N/2}\frac{\lambda_j-\lambda_l-\mathrm{i}}{\lambda_j-\lambda_l+\mathrm{i}}\frac{\lambda_j+\lambda_l-\mathrm{i}}{\lambda_j+\lambda_l+\mathrm{i}},$$
$$j=1,\ldots,N/2. \tag{28}$$

Taking the logarithm of Eq. (28), we have

$$2L\theta_2(\lambda_j)=2\pi I_j+\theta_1(\lambda_j)-\theta_{2(1-\xi')}(\lambda_j)-\theta_{2\xi}(\lambda_j)$$
$$+\sum_{l=1}^{N/2}\theta_2(\lambda_j-\lambda_l)+\theta_2(\lambda_j+\lambda_l),$$
$$j=1,\ldots,N/2, \tag{29}$$

where $\{I_j\}$ are the quantum numbers characterizing the ground state and take the values

$$\{I_j\}=\{L-N+1,\ldots,L-N/2\}, \tag{30}$$

the function $\theta_m(\lambda)$ is given by

$$\theta_m(\lambda)=2\arctan(2\lambda/m). \tag{31}$$

At half-filling, from the distribution of the Bethe roots in Fig. 1, we know that $\lambda_j\in(0,\infty)$. If the filling factor $n=N/L<1$, we will have $\lambda_j\in(Q_0,\infty)$, and the lowest energy can be achieved by choosing Q_0 as large as possible. Q_0 is the Bethe root closest to the origin, i.e., $|Q_0|=\min_j|\lambda_j|$.

Thus in the thermodynamic limit, the distribution of Bethe roots becomes continuous and we can define the density $\rho_1(\lambda)$ of Bethe roots, which can be calculated by taking the derivative of Eq. (29) as

$$\rho_1(\lambda)=a_2(\lambda)-\frac{1}{2L}\left[a_1(\lambda)-a_{2(1-\xi')}(\lambda)-a_{2\xi}(\lambda)\right]$$
$$-\left[\int_{-\infty}^{-Q_0}+\int_{Q_0}^{\infty}\right]a_2(\lambda-\mu)\rho_1(\mu)\,\mathrm{d}\mu, \tag{32}$$

where the function $a_m(\lambda)$ is

$$a_m(\lambda)=\frac{1}{2\pi}\frac{m}{\lambda^2+m^2/4}, \tag{33}$$

and Q_0 is determined by the constraint

$$\left[\int_{-\infty}^{-Q_0}+\int_{Q_0}^{\infty}\right]\rho_1(\lambda)\,\mathrm{d}\lambda=\frac{N}{2L}=\frac{n}{2}. \tag{34}$$

Then, we obtain the ground state energy as

$$E_1=-2L\left[\int_{-\infty}^{-Q_0}+\int_{Q_0}^{\infty}\right]\mathrm{d}\lambda\rho_1(\lambda)\left[2-\frac{1}{1+\lambda^2}\right]. \tag{35}$$

At the half-filling, $Q_0=0$ and the ground state energy is

$$E_1=E_\mathrm{p}+E_\mathrm{b1}, \tag{36}$$

$$E_\mathrm{p}=-2N+L\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-2|w|}}{1+\mathrm{e}^{-|w|}}\,\mathrm{d}w=-2L\ln 2, \tag{37}$$

$$E_\mathrm{b1}=-\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-|w|}}{2(1+\mathrm{e}^{-|w|})}$$
$$\times\left[\mathrm{e}^{-\frac{|w|}{2}}-\mathrm{e}^{-\xi|w|}-\mathrm{e}^{-(1-\xi')|w|}+1\right]\mathrm{d}w, \tag{38}$$

where E_p is the ground state energy of the corresponding periodic spin chain,[11] which is consistent with fact that the boundary fields are only applied in the spin sector, and E_b1 is the surface energy of the system (1).

4.2. Other regimes

By using the similar process, we can study the ground state energy in the regimes (II)–(IV). We should note that distributions of Bethe roots and zero roots in these regimes are different from those in the regime (I), care should be taken with some calculating details. Here, we only list the final results.

According to the results shown in Table 1, the eigenvalue $\hat{\Lambda}(u)$ can be expressed as

$$\begin{aligned}(u+\frac{1}{2})\hat{\Lambda}(u) &= C(u-z_{01})(u-z_{02})(u-\mathrm{i}z_{03})\\ &\times(u+z_{01})(u+z_{02})(u+\mathrm{i}z_{03})u\\ &\times\prod_{j=1}^{N-2}(u-\mathrm{i}\tilde{z}_j-1)(u+\mathrm{i}\tilde{z}_j+1),\end{aligned}\tag{39}$$

in regimes (II) and (III), and

$$\begin{aligned}(u+\frac{1}{2})\hat{\Lambda}(u) &= C(u-z_{01})(u-z_{02})(u-\xi')\\ &\times(u+z_{01})(u+z_{02})(u+\xi')u\\ &\times\prod_{j=1}^{N-2}(u-\mathrm{i}\tilde{z}_j-1)(u+\mathrm{i}\tilde{z}_j+1),\end{aligned}\tag{40}$$

in regime (IV). Combining Eqs. (1), (40) and BAEs (10), (13), we obtain the density of Bethe roots at the ground state in the thermodynamic limit

$$\begin{aligned}\rho_1(\lambda) &= a_2(\lambda)-\frac{1}{2L}[a_1(\lambda)+b(\lambda)]\\ &-\left[\int_{-\infty}^{-Q_0}+\int_{Q_0}^{\infty}\right]a_2(\lambda-\mu)\rho(\mu)\mathrm{d}\mu,\end{aligned}\tag{41}$$

where the integration limit Q_0 is determined by the constraint

$$\left[\int_{-\infty}^{-Q_0}+\int_{Q_0}^{\infty}\right]\rho(\lambda)\mathrm{d}\lambda=\frac{N-2}{2L}=\frac{n}{2}-\frac{1}{L},\tag{42}$$

and the function $b(\lambda)$ in different regimes is different

$$b(\lambda)=\begin{cases}-a_{2\xi}(\lambda)+a_{2\xi'}(\lambda), & \text{(II)}\\ -a_{2(1-\xi')}(\lambda)+a_{2(1-\xi)}(\lambda), & \text{(III)}\\ a_{2(1-\xi)}(\lambda)+a_{2\xi'}(\lambda). & \text{(IV)}\end{cases}$$

Substituting the density (41) into the energy expression, we obtain the ground state energy as

$$E_1=2L\pi\left[\int_{-\infty}^{-Q_0}+\int_{Q_0}^{\infty}\right]a_2(\lambda)\rho(\lambda)\mathrm{d}\lambda-2N+e_{\mathrm{b}},$$

where $e_{\mathrm{b}}=(\xi'-\xi'^2)^{-1}$ in regime (II), $e_{\mathrm{b}}=(\xi-\xi^2)^{-1}$ in regime (III) and $e_{\mathrm{b}}=(\xi'-\xi'^2)^{-1}+(\xi-\xi^2)^{-1}$ in regime (IV).

5. Conclusion

In this paper, we study the ground state energy of the integrable 1D t–J model with boundary magnetic fields. Different from the previous studies, where the inhomogeneous T–Q relation and inhomogeneous Bethe ansatz equations should be considered, we develop a new method, that is the thermodynamic limit results can be obtained by using the zeros properties of the corresponding algebraic polynomial, where the related equations are homogeneous.

By analyzing the distribution of the zero roots of the transfer matrix, the boundary energy has been obtained for the Heisenberg and XXZ spin[32] chains with generic boundary conditions, as well as for the antiperiodic XXZ spin chain.[33] They present a universal procedure to calculate the surface energy of the 1D spin chain with generic non-diagonal boundary fields. In addition, the finite-temperature free energy of the periodic Heisenberg spin chain has been obtained from the distribution of the zero roots, since the free energy per site can be determined by the largest eigenvalue of the quantum transfer matrix. And this method is free from any approximations. It would be interesting to extend the present analysis to the finite temperature and study the free energy, specific heat and magnetic susceptibility of the system.

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