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Xu-Chu Huang(黄旭初), Yi-Hua Song(宋艺华), and Yi Sun(孙毅)

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Exact solution of a topological spin ring with an impurity*

Xu-Chu Huang(黄旭初), Yi-Hua Song(宋艺华)†, and Yi Sun(孙毅)

Department of Physics, Changji University, Changji 830011, *China*

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The spin-1/2 Heisenberg chain coupled to a spin-S impurity moment with anti-periodic boundary condition is studied via the off-diagonal Bethe ansatz method. The twisted boundary breaks the $U(1)$ symmetry of the system, which leads to that the spin ring with impurity can not be solved by the conventional Bethe ansatz methods. By combining the properties of the R-matrix, the transfer matrix, and the quantum determinant, we derive the T–Q relation and the corresponding Bethe ansatz equations. The residual magnetizations of the ground states and the impurity specific heat are investigated. It is found that the residual magnetizations in this model strongly depend on the constraint of the topological boundary condition, the inhomogeneity of the impurity comparing with the hosts could depress the impurity specific heat in the thermodynamic limit. This method can be expand to other integrable impurity models without $U(1)$ symmetry.

Keywords: Bethe ansatz, impurity, topological spin ring

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1. Introduction

Recently, considerable attention has been drawn by the theory of impurities in both the Kondo problem and the topological state, and many new developments have been reported.[1–6] We know that the impurities play an important role in the strongly correlated electron systems, and even a small amount of defects may change the properties of the electron systems.[7–10] Then it is very important to construct the integrable systems including the impurities. Many impurity models with free end boundary conditions have been considered previously. Frahm and Zvyagin studied the effects of a boundary magnetic field and an impurity spin coupled to an open spin chain by means of Bethe ansatz method.[11] Wang proposed an open spin-1/2 Heisenberg chain coupled with two impurity spins sited at the ends, and exactly solved this model for arbitrary impurity spin and arbitrary exchange constants between the bulk and the impurities using Bethe ansatz method.[12] The integrable impurity problem of the Heisenberg chain with periodic boundary condition was first considered by Andrei and Johannesson.[13] They studied the integrable case of a spin $S > 1/2$ embedded in a spin-1/2 Heisenberg chain. Subsequently, the problem was generalized to arbitrary spins by Lee and Schlottmann.[14] In contrast to the periodic boundary conditions in the integrable impurity models, the anti-periodic boundary conditions are especially interesting, which are tightly related to the recent study on the topological states of matter.[15,16]

Since the Yang and Baxter's pioneering works,[17–19] the quantum Yang–Baxter equation, which defines the underlying algebraic structure, has become a cornerstone for constructing and solving the integrable models. The T–Q relation method and the algebraic Bethe ansatz method developed from the Yang–Baxter equation have become two very popular methods for dealing with the exact solutions of the known integrable models.[20] Although the algebraic Bethe ansatz method is a powerful tool exhibiting a rich mathematical structure, its implementation for models without $U(1)$ symmetry still has an obstacle. The main obstacle applying the algebraic Bethe ansatz to these models lies in the absence of a trivial reference state. Significant progress has been made recently for the integrable models without $U(1)$ symmetry. For example, a promising method for approaching such kind of problems is Sklyanin's separation variables method which has been applied to some integrable models.[21,22] Another important advance was made by Cao *et al.*,[23–25] who proposed the off-diagonal Bethe ansatz method to approach the exact solutions of generic integrable models either with or without $U(1)$ symmetry. The central step of this method lies in the construction of the T–Q ansatz with an extra off-diagonal term. For the integrable models with impurities, on one hand the twisted boundary breaks the $U(1)$ symmetry of the system, on the other hand the introduction of the impurity adds the freedom degree of the system, which make it difficult to resolve the impurity model without $U(1)$ symmetry. A systematic method is still absent to derive the Bethe ansatz equations for integrable impurity models without $U(1)$ symmetry.

It is known that the behavior of a single magnetic impurity in the one-dimensional spin-1/2 Heisenberg model as well as the behavior of a single Kondo impurity in a three-dimensional free electron host is described by simi-

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†Corresponding author. E-mail: quantumage@163.com

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lar Bethe ansatz theories.[26] The spin-1/2 magnetic impurity manifests the total Kondo screening with Fermi liquids-like low temperature behavior of the magnetic susceptibility and specific heat.[27] The effects of impurity scattering on the surface of topological insulators have been investigated extensively.[28–30] A key issue is to determine the conditions for the stability of the current-carrying states at the edge of the sample,[31,32] as this is the feature that most directly impacts prospect for future applications in electronics and spintronics.[33] Therefore, it is worthwhile to investigate the effects of impurity when the impurity locates at the twisted boundary. In this paper, we consider the Heisenberg spin ring with a Möbius-like topological boundary condition coupled to a spin-S impurity. The Hamiltonian of the model is $H = H_0 + H_{\rm imp}$, which was first solved by Andrei and Johannesson,[13]

$$\begin{aligned} H_0 &= \frac{1}{2}J\sum_{i}^{N-1}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+1} + \frac{1}{2}J\left(\sigma_N^x\sigma_1^x - \sigma_N^y\sigma_1^y - \sigma_N^z\sigma_1^z\right), \\ H_{\rm imp} &= J\left(\frac{2}{2S+1}\right)^2\Big[\boldsymbol{\sigma}_N\cdot\boldsymbol{S} + \boldsymbol{\sigma}_{N+1}\cdot\boldsymbol{S} + \frac{1}{2}\{\boldsymbol{\sigma}_N\cdot\boldsymbol{S}, \boldsymbol{\sigma}_{N+1}\cdot\boldsymbol{S}\} \\ &\quad - S(S+1)\boldsymbol{\sigma}_N\cdot\boldsymbol{\sigma}_{N+1}\Big], \end{aligned} \tag{1}$$

where H_0 describes the host spin chain, $H_{\rm imp}$ is the interaction of the chain with the impurity, $\boldsymbol{\sigma}_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ are Pauli matrices, $\boldsymbol{S}$ is the spin operator of spin-S. The $\{,\}$ denotes an anticommutator. Here, we consider the anti-periodic boundary conditions $\sigma_{N+1}^\alpha = \sigma_1^x\sigma_1^\alpha\sigma_1^x$ ($\alpha = x, y, z$), that is, the spin on the N-th site connects with that on the first site after rotating a π angle along the x direction and forms a kink in the spin space. The impurity is assumed to be located on the kink (between the 1st and N-th sites), and interacts with both neighboring sites. We use the T–Q relation, together with some addition properties of the transfer matrix, to determine the complete set of the eigenvalues and Bethe ansatz equations of the transfer matrix associated with the Hamiltonian under certain constraint of the boundary parameters.[34] The aim of this paper is to expand the off-diagonal Bethe ansatz method, and investigate the impurity effects in the topological spin ring.

This paper is organized as follows. Section 2 serves as an introduction of our notations and some basic ingredients. We briefly describe the inhomogeneous topological spin ring with a spin-S simpurity. In Section 3, base on the properties of the transfer matrix and the quantum determinant, we drive the inhomogeneous T–Q relation for the eigenvalue of the transfer matrix and the corresponding Bethe ansatz equations. In Section 4, the impurity effects on the ground state and the thermodynamic limit for different impurity parameter c are discussed. Concluding remarks will be given in Section 5.

2. Transfer matrix

Let $\boldsymbol{V}_0, \boldsymbol{V}_1, \ldots, \boldsymbol{V}_N$ be 2D vector spaces over complex numbers $\boldsymbol{C}$. The $\boldsymbol{V}_0$ indicates the auxiliary space and the tensor product $\boldsymbol{V}_1 \otimes \cdots \otimes \boldsymbol{V}_N$ indicates the quantum space, where $\boldsymbol{V}_j$ corresponds to the j-th site of the spin chain with $j = 1, 2, \ldots, N$. On the tensor product $\boldsymbol{V}_0 \otimes \boldsymbol{V}_j$, we define the R-matrix

$$R_{0j}(u) = u + \frac{1}{2}\eta + \eta\boldsymbol{\sigma}_0\cdot\boldsymbol{S}_j, \tag{2}$$

where u is the spectral parameter, η is the crossing parameter (without loss of generality, we put $\eta = 1$). The $\boldsymbol{S}_j$ is either a spin-1/2 or an impurity spin-S at site j. Integrability requires that the R-matrix satisfies the following Yang–Baxter equation:

$$R_{12}(u)R_{13}(u+\mu)R_{23}(\mu) = R_{23}(\mu)R_{13}(u+\mu)R_{12}(u). \tag{3}$$

Using the R-matrix, we introduce the local transform matrix $L_{0j} = 1 \otimes \cdots \otimes R_{0j} \otimes \cdots 1$. Define the monodromy matrix of the system

$$\begin{aligned} T_0(u) &= L_{0N}^{(1/2)}(u-\theta_N)L_{0N-1}^{(1/2)}(u-\theta_{N-1})\cdots L_{01}^{(1/2)}(u-\theta_1 v)L_{0S}^{(S)}(u-c) \\ &= \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \end{aligned} \tag{4}$$

with $\{\theta_j | j = 1, \ldots, N\}$ being some generic site-dependent inhomogeneity parameters, and c a constant. The transfer matrix with anti-periodic boundary condition is given by

$$t(u) = {\rm tr}_0\,\sigma_0^x T_0(u) = B(u) + C(u), \tag{5}$$

where ${\rm tr}_0$ means tracing the auxiliary space 0. In order to construct the Hamiltonian describing the interaction of the chain with the impurity of spin S, we consider

$$T^\star = {\rm tr}_0\left[\sigma_0^x L_{0N}^{1/2}(u-\theta_N)L_{0S}^{(S)}(u-c)L_{01}^{1/2}(u-\theta_1)\right]. \tag{6}$$

Note that the impurity can interact only with the neighbour sites, and the couplings are different. The coupling between the N-th site and the impurity is the normal interaction, and the coupling between the 1st site and the impurity is the twisted interaction. The $H_{\rm imp}$ can be obtained via

$$H_{\rm imp} = J\frac{\partial \ln T^\star(u)}{\partial u}\,|_{u=0,\{\theta_j=0\}} - J(\sigma_N^x\sigma_1^x - \sigma_N^y\sigma_1^y - \sigma_N^z\sigma_1^z). \tag{7}$$

With the help of Eqs. (2), (4), and (5), the first order derivative of the logarithm of the transfer matrix gives the Hamiltonian

$$H = H_0 + H_{\rm imp} = J\frac{\partial \ln t(u)}{\partial u}\,|_{u=0,\{\theta_j=0\}}\,. \tag{8}$$

Both the Lax operator and monodromy matrix satisfy the Yang–Baxter relation

$$\begin{aligned} &R_{12}(u_1-u_2)L_{1j}^{(1/2)}(u_1)L_{2j}^{(1/2)}(u_2) \\ &\quad = L_{2j}^{(1/2)}(u_2)L_{1j}^{(1/2)}(u_1)R_{12}(u_1-u_2), \end{aligned} \tag{9}$$

$$R_{12}(u_1-u_2)L_{1j}^{(S)}(u_1)L_{2j}^{(S)}(u_2) = L_{2j}^{(S)}(u_2)L_{1j}^{(S)}(u_1)R_{12}(u_1-u_2), \tag{10}$$

$$R_{12}(u_1-u_2)T_1(u_1)T_2(u_2) = T_2(u_2)T_1(u_1)R_{12}(u_1-u_2). \tag{11}$$

It is easy to show that the R-matrix also satisfies the following relations:

$$\text{Initial condition:} \quad R_{12}(0) = P_{12}, \tag{12}$$

$$\text{Unitary relation:} \quad R_{12}(u)R_{21}(-u) = (1-u^2)\times \mathrm{i}d, \tag{13}$$

$$\text{Crossing relation:} \quad R_{12}(u) = V_1 R_{12}^{t_1}(-u-1)V_1, \quad V = -\mathrm{i}\sigma^y, \tag{14}$$

$$\text{PT-symmetry:} \quad R_{12}(u) = R_{21}(u) = R_{12}^{t_1 t_2}(u), \tag{15}$$

$$Z_2\text{-symmetry:} \quad \sigma_1^\alpha \sigma_2^\alpha R_{12}(u) = R_{12}(u)\sigma_1^\alpha \sigma_2^\alpha \quad \text{for} \quad \alpha = x,y,z, \tag{16}$$

$$\text{Fusion condition:} \quad R_{12}(\pm 1) = \pm 1 + P_{12}, \tag{17}$$

where P_{12} is the permutation operator and t_i denotes transposition in the i-th space.With the help of the Yang–Baxter relation, we can easily deduce the following commutation relations:

$$[A(u),A(v)] = [B(u),B(v)] = [C(u),C(v)] = [D(u),D(v)] = 0, \tag{18}$$

$$A(u)B(v) = \frac{u-v-1}{u-v}B(v)A(u) + \frac{1}{u-v}B(u)A(v), \tag{19}$$

$$D(u)B(v) = \frac{u-v+1}{u-v}B(v)D(u) - \frac{1}{u-v}B(u)D(v), \tag{20}$$

$$C(u)B(v) = B(v)C(u) + \frac{1}{u-v}\left[D(u)A(v) - D(v)A(u)\right]. \tag{21}$$

Define the pseudo vacuum state $|0\rangle$ as $\sigma_j^+|0\rangle = S^+|0\rangle = 0$, we obtain

$$C(u)|0\rangle = 0, \;\; A(u)|0\rangle = a(u)|0\rangle, \;\; D(u)|0\rangle = d(u)|0\rangle, \tag{22}$$

where $a(u) = \prod_{j=1}^N (u-\theta_j+1)(u-c+1/2+S)$, and $d(u) = \prod_{j=1}^N (u-\theta_j)(u-c+1/2-S)$. The Yang–Baxter relation of the R-mareix leads to the fact that the transfer matrices with different spectral parameters commute with each other: $[t(u),t(v)] = 0$. Then $t(u)$ serves as the generating function of the conserved quantities of the corresponding system, which ensures the integrability of the model.

3. Off-diagonal Bethe ansatz solutions

We suppose that $|\Psi\rangle$ is an eigenstate of $t(u)$ and independent of u, and has $t(u)|\Psi\rangle = \Lambda(u)|\Psi\rangle$. Base on the commutation relations Eqs. (18)–(21), the following useful formulas can be derived:[35]

$$\begin{aligned} &C(u)B(\mu_1)\cdots B(\mu_n)|0\rangle \\ &= \sum_{l=1}^n M_l \prod_{\substack{j=1\\ j\neq l}}^n B(\mu_j)|0\rangle + \sum_{k>l}^n M_{kl}B(u)\prod_{\substack{j=1\\ j\neq k,l}}^n B(\mu_j)|0\rangle, \end{aligned} \tag{23}$$

with

$$\begin{aligned} M_l = {}& g(u,\mu_l)a(u)d(\mu_l)\prod_{j\neq l} f(\mu_j,\mu_l)f(u,\mu_j) \\ &+ g(\mu_l,u)a(\mu_l)d(u)\prod_{j\neq l} f(\mu_j,u)f(\mu_l,\mu_j), \end{aligned}$$

$$\begin{aligned} M_{kl} = {}& d(\mu_k)a(\mu_l)g(u,\mu_k)g(\mu_l,u)f(\mu_l,\mu_k)\prod_{j\neq k,l} f(\mu_j,\mu_k)f(\mu_l,\mu_j) \\ &+ d(\mu_l)a(\mu_k)g(u,\mu_l)g(\mu_k,u)f(\mu_k,\mu_l) \\ &\times \prod_{j\neq k,l} f(\mu_j,\mu_l)f(\mu_k,\mu_j), \end{aligned} \tag{24}$$

where $f(u,\mu_j) = \frac{u-\mu_j-1}{u-\mu_j}$ and $g(u,\mu_j) = \frac{1}{u-\mu_j}$. We define $F_n(\{\mu_j\}) = \langle\Psi|\prod_{j=1}^n B(\mu_j)|0\rangle$ and set $F_0 = \langle\Psi|0\rangle = 1$. Using the define of the pseudo vacuum state, we have $\Lambda(u) = \langle\Psi|B(u)|0\rangle$. Obviously, the eigenvector $|\Psi\rangle$ is independent of the spectral parameter u, thus the eigenvalues of $t(u)$ can be determined by the relation between $\Lambda(u)$ and $F_n(\mu_j)$. From the following relation:

$$\begin{aligned} &F_1(u) = \Lambda(u), \\ &F_2(u,\mu_1) = \Lambda(u)\Lambda(\mu_1) - M_0, \\ &F_3(u,\mu_1,\mu_2) = \Lambda(u)\Lambda(\mu_1)\Lambda(\mu_2) - M_1\Lambda(\mu_2) - M_2\Lambda(\mu_1) - M_{21}\Lambda(u), \\ &\cdots\cdots, \\ &F_{n+1}(u,\{\mu_j\}_{j=1,\cdots,n}) = \Lambda(u)\prod_{j=1}^n \Lambda(\mu_j) - \sum_{l=1}^n M_l \prod_{\substack{j=1\\ j\neq l}}^n \Lambda(\mu_j) \\ &\qquad - \sum_{k>l}^n M_{kl}\Lambda(u)\prod_{\substack{j=1\\ j\neq k,l}}^n \Lambda(\mu_j), \end{aligned} \tag{25}$$

we note that the dependence of the functions $F_n(u)$ on u is solely determined by the operator $B(u)$, and $\Lambda(u)$ is a degree N polynomial of u. Hence $\Lambda(u)$ can be write as $\Lambda(u) = \Lambda_0\prod_{j=1}^N (u-z_j)$, where Λ_0 is a constant and z_j are roots of $\Lambda(u)$ with $\Lambda(z_j) = 0$. There are $N+1$ unknowns Λ_0 and $\{z_j|j=1,\ldots,N\}$. If there are $N+1$ equations, $\Lambda(u)$ can be determined completely. In order to get some function relations of the transfer matrix, we evaluate the transfer matrix $t(u)$ at the particular points θ_j and $\theta_j - 1$. Due to $a(\theta_j - 1) = d(\theta_j) = 0$ and $F_{N+1} = 0$, we have the following relation:

$$\Lambda(u) = \sum_{j=1}^N \frac{g(\theta_j,u)a(\theta_j)}{\Lambda(\theta_j)}d(u)\prod_{l\neq j}^N f(\theta_l,u)f(\theta_j,\theta_l). \tag{26}$$

Putting $u = \theta_j - 1$, we obtain the following relation:

$$\Lambda(\theta_j)\Lambda(\theta_j - 1) = -a(\theta_j)d(\theta_j - 1), \quad j = 1,\ldots,N. \tag{27}$$

The quantum determinant $\Delta_q(u) = -a(u)d(u-1)$ is independent of the representation basis, however it is related with the boundary conditions. Next we consider the transposition of the monodromy matrix in the auxiliary space

$$T_0^{t_0}(u) = L_{0N}^{t_0}(u-\theta_N)\cdots L_{01}^{t_0}(u-\theta_1)L_{0S}^{t_0}(u-c). \tag{28}$$

With the intrinsic properties of the R-matrix given in Eqs. (14) and (15), we deduce that

$$\begin{aligned} T_0^{t_0}(u) = {}& (-1)^{N+1}V_0^{-1}L_{0S}(-u+c-1) \\ &\times L_{01}(-u+\theta_1-1)\cdots L_{0N}(-u+\theta_N-1)V_0. \end{aligned} \tag{29}$$

Then we find

$$T_0^{t_1\cdots t_{N+1}t_0} = [L_{0N}(u-\theta_N)\cdots L_{01}(u-\theta_1)L_{0S}(u-c)]^{t_0t_1\cdots t_{N+1}} = (-1)^{N+1}L_{0S}(-u+c-1) \times L_{01}(-u+\theta_1-1)\cdots L_{0N}(-u+\theta_N-1). \quad (30)$$

For the anti-periodic boundary condition, the transfer matrix satisfies the relation

$$t^{t_1\cdots t_{N+1}}(u) = (-1)^N t(-u-1). \quad (31)$$

This relation Eq. (31) indicates that $\Lambda(u) = (-1)^N\Lambda(-u-1)$ for a finite site N, which has been proved by the direct diagonalization of $t(u)$.[36] The above relations Eqs. (25), (27), and (31) completely determine the eigenvalue $\Lambda(u)$, we propose the following T–Q relation for $\Lambda(u)$:

$$\Lambda(u) = \mathrm{e}^u a(u)\frac{Q_1(u-1)}{Q_2(u)} - \mathrm{e}^{-(u+1)}d(u)\frac{Q_2(u+1)}{Q_1(u)} - \xi(u)\frac{a(u)d(u)}{Q_1(u)Q_2(u)}, \quad (32)$$

where

$$Q_1(u) = \prod_{j=1}^{M}(u-\mu_j), \quad Q_2(u) = \prod_{j=1}^{M}(u-\nu_j). \quad (33)$$

The $\xi(u)$ is an adjust function, and $\xi(u) = \mathrm{e}^u - \mathrm{e}^{-u-1}$ for odd N, $M = (N+1)/2$ (for even N, $M = N/2+1$). The corresponding Bethe ansatz equations can be obtained as

$$a(\mu_j) = -\frac{\mathrm{e}^{-\mu_j-1}}{\xi(\mu_j)}Q_2(\mu_j+1)Q_2(\mu_j), \quad (34)$$

$$d(\nu_j) = \frac{\mathrm{e}^{\nu_j}}{\xi(\nu_j)}Q_1(\nu_j-1)Q_1(\nu_j). \quad (35)$$

Generally, the Bethe roots distribute in the whole complex plane with the selection rules $\mu_j \neq \mu_l$, $\mu_j \neq \nu_l$, and $\mu_j \neq \nu_l+1$, which ensure the simplicity of "poles" in the T–Q ansatz. The eigenvalues of the Hamiltonian (1) take the following form:

$$E = -J\sum_{j=1}^{M}\left(\frac{1}{\mu_j+1} - \frac{1}{\nu_j}\right) + \frac{2SJ}{(S+1/2)^2-c^2}. \quad (36)$$

4. Ground state and impurity specific hetat

The interaction between the impurity and the spin ring depends on the parameter c, and c could be real or imaginary values. Therefore, we discuss the ground state properties for different c values with the standard method proposed by Yang and Yang.[17] Note that the distributions of the roots $\{\mu_j\}$ and $\{\nu_j\}$ are not independent, which essentially are decided by the selection rules of elementary excitation at the anti-periodic boundary condition of the system. In the homogeneous limits $\theta_j \to 0$, with the help of Eqs. (34) and (35), we obtain the following Betha ansatz equations:

$$\left(\frac{\mu_j+1}{\widetilde{\mu}_j+1}\right)^N\left[\frac{c-\mu_j-(S+\frac{1}{2})}{c+\widetilde{\mu}_j+(S+\frac{1}{2})}\right] = \mathrm{e}^{-2\mathrm{i}\mathrm{Im}(\mu_j)}\prod_{l=1}^{M}\left(\frac{\mu_j+\widetilde{\mu}_l+2}{\widetilde{\mu}_j+\mu_l+2}\right)\left(\frac{\mu_j+\widetilde{\mu}_l+1}{\widetilde{\mu}_j+\mu_l+1}\right), \quad (37)$$

and the energy eigenvalues

$$E = -J\sum_{j=1}^{M}\left(\frac{1}{\mu_j+1}+\frac{1}{\widetilde{\mu}_j+1}\right) + \frac{2SJ}{(S+1/2)^2-c^2}, \quad (38)$$

where $\widetilde{\mu}_j$ indicates the conjugate of μ_j.

First, we consider the case of imaginary $c = \mathrm{i}\zeta$. The exchange interaction between the impurity and the spin ring is always positive corresponding to antiferromagnetic coupling. All the modes of $\{\mu_j\}$ take imaginary values in the ground state to minimize the energy. We set $\mu_j = \lambda_j + \mathrm{i}\gamma_j$, and introduce the following function:

$$\theta\left(\frac{\lambda}{n}\right) = \frac{1}{\mathrm{i}}\ln\frac{\lambda-\mathrm{i}n}{\lambda+\mathrm{i}n} - \pi. \quad (39)$$

Taking the logarithm of Eq. (37), we obtain

$$\frac{I_j}{N} = \frac{1}{2\pi}\left\{\theta\left(\frac{\gamma_j}{\lambda_j+1}\right) + \frac{1}{N}\theta\left(\frac{\gamma_j-\zeta}{\lambda_j+S+1/2}\right) + \frac{2\gamma_j}{N} - \frac{1}{N}\sum_{l=1}^{M}\theta\left(\frac{\gamma_j-\gamma_l}{\lambda_j+\lambda_l+2}\right) + \theta\left(\frac{\gamma_j-\gamma_l}{\lambda_j+\lambda_l+1}\right)\right\}, \quad (40)$$

where I_j are some integers (or half-integers). Define

$$Z_N(\lambda,\gamma) = \frac{1}{2\pi}\left\{\theta\left(\frac{\gamma}{\lambda+1}\right) + \frac{1}{N}\theta\left(\frac{\gamma-\zeta}{\lambda+S+1/2}\right) + \frac{2\gamma}{N} - \frac{1}{N}\sum_{l=1}^{M}\theta\left(\frac{\gamma-\gamma_l}{\lambda+\lambda_l+2}\right) + \theta\left(\frac{\gamma-\gamma_l}{\lambda+\lambda_l+1}\right)\right\}. \quad (41)$$

Then $Z_N(\lambda_j,\gamma_j) = I_j/N$ gives the Bethe ansatz equation (37). Note that I_j are related to not only the parity of N and M but also the distribution of the roots, which are decided by the topological boundary. For the ground state, I_j must take consecutive numbers around zero symmetrically. In principle, each possible I_j may correspond to a solution $\{\mu_j\}$ of the Bethe ansatz equations. However, those solutions may not be occupied. We treat the occupied solutions as "particles" and the unoccupied solutions as "holes", and define a density function for the ground state $\rho_N(x) = \mathrm{d}Z_N(x)/\mathrm{d}x = \rho(x) + \rho^{\mathrm{h}}(x)$, where $\rho(x)$ and $\rho^{\mathrm{h}}(x)$ are the densities of the particles and holes, respectively. From the selection rules, we know that the distribution of the Bethe roots in the ground state is on a straight line, which means that all the imaginary modes have the same value. Therefore, we can take γ as a constant in the ground state, and only consider the distribution of λ. The density function can be written as

$$\rho_N(\lambda) = \phi_\gamma(\lambda+1) + \frac{1}{N}\phi_{\gamma-\zeta}(\lambda+S+1/2) - \frac{1}{N}\sum_{l=1}^{M}\phi_{\gamma-\gamma_l}(\lambda+\lambda_l+2) + \phi_{\gamma-\gamma_l}(\lambda+\lambda_l+1), \quad (42)$$

where $\phi_n(x) = \frac{1}{2\pi}\frac{2n}{x^2+n^2}$. The density function at the ground state satisfies $\int_{-\Lambda}^{\Lambda}\rho_N(\lambda)\mathrm{d}\lambda = M/N$, where Λ is the cutoff

of the λ modes. Normally, Λ is decided by the dressed energy $\varepsilon(\pm\Lambda) = 0$, and indicates the boundary of the Fermi sphere.[35] Here we only consider the case $\Lambda = \infty$. Following the standard procedure outline elsewhere,[37] we obtain the residual magnetization of the ground state $M_{\rm g} = S$, which means that the impurity can not be screened.[38]

For the case of real value c, the coupling between the impurity and the spin ring can be ferromagnetic or antiferromagnetic for $|c| < S+1/2$ and $S+1/2 < |c|$, respectively. Obviously, there exists a critical point $|c| = S+1/2$, which corresponds to a quantum phase transition to a non-Fermi liquid quantum critical region. When $S+1/2 < |c|$, the real modes of μ at $\mathrm{Re}\{\mu_j\} = c-(S+1/2)$ can exist in the ground state. With a similar discuss, the self magnetization of the ground state is $M_{\rm g} = S$, which means that the impurity can not be screened. When $S+1/2 > |c|$, the exchange interaction between the impurity and the bulk is in the antiferromagnetic region, and no bound state can exist in the ground state. In this case, the residual magnetization of the ground state $M_{\rm g} = S-1/2$, which means that the impurity moment is partially screened (for $S > 1/2$).

In order to investigate the impurity effects in the thermodynamic limit, we consider a special case of $c = \mathrm{i}\zeta$ and $\mu_j = \mathrm{i}\gamma_j$ to investigate the thermodynamic of the present model. In the thermodynamic limit, in the leading order of $O(N^{-1})$, equation (40) takes the form

$$\rho_N(\gamma) = \phi_1(\gamma) - \int \left[2\phi_2(\gamma-\gamma')+\phi_1(\gamma-\gamma')\right]\rho_N(\gamma')\,\mathrm{d}\gamma'. \quad (43)$$

Equation (43) can be resolved by the Fourier transformation, and the contributions of the impurity and the anti-periodic boundary to the density are

$$\rho_S(\gamma) = \frac{1}{\cosh(\frac{\gamma-\zeta}{S+1/2})},$$

$$\rho_a(\gamma) = \frac{1}{2\cosh(\pi\gamma)} + \frac{1}{4\pi}\int \frac{\mathrm{e}^{-\mathrm{i}\gamma\omega}}{1+2\mathrm{e}^{-\omega}+\mathrm{e}^{\omega}}\,\mathrm{d}\omega. \quad (44)$$

Therefore, the impurity contribution to the low temperature specific heat reads

$$C_s = \frac{1}{4}T^{-2}\int \frac{1}{\cosh(\pi\gamma)}\frac{\epsilon_S^2(\gamma)\,\mathrm{e}^{\epsilon_S(\gamma)/T}}{(1+\mathrm{e}^{\epsilon_S(\gamma)/T})^2}\,\mathrm{d}\gamma, \quad (45)$$

where $\epsilon_S(\gamma) = \dfrac{-4(S+1)J}{(\gamma-\zeta)^2+(2S+1)^2}$. It is hard to obtain the analytically expression of temperature specific heat for normal ζ and S, however, we can give some numerical results by applying the approximate calculations (see Fig. 1).

From the above discussion, we conclude that the impurity can not be screened for the antiferromagnetic cases. The impurity moments only can be partially screened for the ferromagnetic case. The coupling interaction of the impurity is different to that in the one-dimensional quantum system with $U(1)$ system.[12] The topological boundary condition will produce a finite boundary energy described by a phase factor, which constraints the interaction between the impurity and the spin kink. The screen behaviors of the impurity strongly depend on the competition between the quantum fluctuation and the constraint of the topological boundary condition. When the impurity parameter c is a pure imaginary value, the contribution of the impurity on the specific heat mainly depends on the impurity spin, and the effects of the anti-periodic boundary are depressed in the thermodynamic limit. From Fig. 1, we note that the peak of specific heat moves down gradually with the increase of ζ, which means that the inhomogeneity of the impurity comparing with the hosts could depress the contribution of the impurity on the specific heat. These results are similar to the situation for the Kondo problem in a Luttinger liquid predicted by Furysaki and Nagaosa.[39] The Kondo coupling in this model indicates the topological nature of the system.

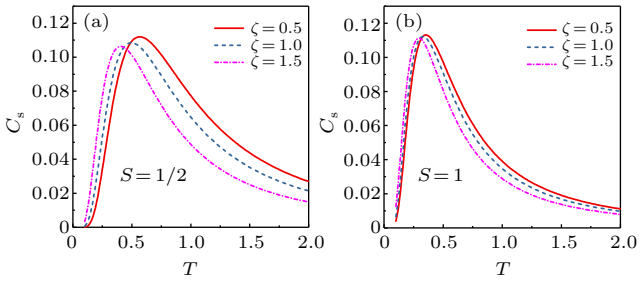


Fig. 1. The impurity specific heat $C_{\rm s}$ as a function of temperature T for the system with the impurity spin-1/2 (a) and the impurity spin-1 (b), where the impurity parameter $\zeta = 0.5, 1, 1.5$.

5. Conclusion

The spin-1/2 Heisenberg chain described by the Hamiltonian (1) with anti-periodic boundary condition is studied via the off-diagonal Bethe ansatz method. The crucial ideal of the off-diagonal Bethe ansatz method is to construct the function relations between the eigenvalues of the transfer matrix and the elements of the monodromy matrix. The eigenvalues of the transfer matrix are given in terms of the T–Q relations, and the Bethe ansatz equations are given by the regularity of the eigenvalue. Based on the Bethe ansatz equations, we investigate the distribution of roots and the residual magnetization in the ground states by the usual method.[35] It is found that the screen behavior of the impurity strongly depends on the topological boundary condition, the anti-periodic boundary condition contributes a finite boundary energy described by a phase factor. The selection rules of Bethe roots decide the properties of the ground states and the elementary excitation of the topological spin ring, which indicates the topological nature of the system. In the thermodynamic limit, the impurity contribution to the specific heat is also investigated, and the results indicate that the thermodynamic properties can be adjusted by the impurity parameters. When the impurity does not interact with the boundary fields, the function relation between the

eigenvalue and the quantum determinant still holds via some properties of the R-matrix and K-matrices. In this case, this method can also deal with the impurity integrable models with arbitrary boundary conditions, which will be investigated in our next work.

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