Boundary Kondo problem in the integrable t-J model

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We study the problem of a boundary magnetic impurity coupled with the solvable t-J chain. This model provides a good starting point to understand the Kondo problem in a Luttinger liquid as well as in a strongly correlated host. As the Kondo coupling constant J_i may take arbitrary values without breaking the integrability, we can study the ferromagnetic and antiferromagnetic Kondo problems simultaneously. It is shown that the boundary coupling generally splits the impurity spin into two effective spins and induces the interaction-dependent residual entropy. The absence of Kondo screening in an antiferromagnetic Kondo coupling regime is found, which indicates a genuine competing effect between the Kondo coupling J_i and the impurity potential V_i. A local Landau-Luttinger liquid description is proposed to calculate the specific heat of the impurity.
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I. INTRODUCTION

With the development of nanofabrication techniques for quantum wires and the prediction of edge states in the fractional quantum Hall effect, the interest in one-dimensional (1D) quantum systems has been renewed in recent years.[1,2] In fact, much of the interest in 1D quantum systems is due to Anderson's observation[3] that the normal state properties of the quasi-2D high-T_c superconductors are strikingly different from all known metals (Fermi liquid) but are more similar to properties of 1D metals (Luttinger liquid). On the other hand, the impurity problem has been a current interest in the field of condensed matter physics. A well-known example is the Kondo problem, which stimulated a strong challenge to traditional perturbation theory and provided a possible ''laboratory'' to realize non-Fermi-liquid behavior. The local perturbation problem in a 1D Fermi system has been the subject of an intensive theoretical investigation in recent years, for both its interesting anomalies with respect to that of a higher-dimensional system and its relevance to a variety of physical situations such as the transport behavior of quantum wires[2,4] and the tunneling through a constriction in the quantum Hall regime.[5] Kane and Fisher[6] have argued that a single impurity in a 1D repulsive interacting system in fact corresponds to a chain disconnected at the impurity site at low-energy scales. Their observation was also justified in the framework of the renormalization group analysis of boundary conformal field theory,[7,8] which shows that the open boundary condition is indeed the stable fixed point for repulsive interactions. The Kondo problem in a 1D metal was considered by Lee and Toner,[9] who found the crossover of the Kondo temperature from the power-law dependence on the Kondo coupling constant to an exponential one, when the electron correlation goes from the strong limit to the weak limit. Subsequently, a poor man's scaling was performed by Furusaki and Nagaosa,[10] who addressed a conjecture that ferromagnetic Kondo screening may occur in 1D due to the special topology. Boundary conformal field theory[11] gave out a classification of critical behavior for the 1D Kondo problem (without impurity potential). It turns out that there are only two possibilities, a standard low-temperature thermodynamics or a non-Fermi-liquid observed by Furusaki and Nagaosa. It has been argued that the non-Fermi-liquid behavior is induced by the tunneling effect of conduction electrons through the impurity, which depends only on the bulk properties but not on the details of the impurity.[12]

Despite such important progress, the problem of a few impurities (potential, magnetic, especially both) embedded in a strongly correlated 1D system is still not very well understood. We note that the study of integrable models generally gives some useful information to understand a variety of physical situations in 1D. There are a few integrable models related to the impurity problem in 1D quantum systems: an impurity spin embedded in a spin-1/2 Heisenberg chain solved many years ago by Andrei and Johannesson[13] and an integrable impurity in the supersymmetric t-J or other related models.[14] The impurities in these models are exactly transparent due to the unphysical terms in the Hamiltonians and the results obtained from these models contradict the predictions of Kane and Fisher.[6] This shortcoming was overcome in some other integrable models[15–17] by introducing the open boundary condition at the impurity site. Unlike in 3D, the scalar potential[15] and the bond deformation[17] have significant effects on the low-temperature thermodynamics of the impurity.

In this paper, we consider a boundary magnetic impurity with arbitrary spin coupled with the integrable t-J chain.[19] The Hamiltonian we shall study reads

$$H = H_0 + H_i,$$

$$H_0=-t\sum_{j=1}^{L-1}\sum_{\sigma}\mathcal{P}(c_{j,\sigma}^{\dagger}c_{j+1,\sigma}+\text{H.c.})\mathcal{P}+\sum_{j=1}^{L-1}(J\mathbf{S}_j\cdot\mathbf{S}_{j+1}+Vn_jn_{j+1}),$$

$$H_i=2J_i\mathbf{S}_L\cdot\mathbf{S}+V_in_L, \tag{1}$$

where L is the length or site number of the system; $c_{j,\sigma}^{\dagger}$ ($c_{j,\sigma}$) are the creation (annihilation) operators of the conduction electrons, $\mathbf{S}_j=1/2\Sigma_{\sigma,\sigma'}c_{j,\sigma}^{\dagger}\tau_{\sigma,\sigma'}c_{j,\sigma'}$ are the spin operators of the conduction electrons (τ_j represent the Pauli matrices); $n_j=\Sigma_{\sigma}c_{j,\sigma}^{\dagger}c_{j,\sigma}$ is the number operator of the conduction electrons on site j; $\mathbf{S}$ is the impurity moment with spin S; t, J, V, J_i, and V_i are all constants; and $\mathcal{P}\cdots\mathcal{P}$ indicates the single occupation condition $n_j\leqslant 1$. In a previous paper,[15] we studied a model of two spin-1/2 boundary impurities coupled with an SU(3) t-J chain. We note that there is no genuine correlation between the two impurities and their physical effects are in fact additive: i.e., the problem is still in the single-impurity level. This is a common feature of the impurities in integrable models. In some sense, the present model is a generalization of the previous one but the boundary impurity has an arbitrary spin. We shall give a detailed description of our method and study the arbitrary c (definition see below) cases. As we shall show, the noninteger $2c$ generally induces secondary ''ghost spins'' and additional residual entropy (not considered in the previous work), which allows us to observe the quantum phase transitions at $2c=$integer. Without losing generality, we shall put $t=1$ in the following text.

The structure of the present paper is the following: In the subsequent section, we derive the integrable conditions based on the reflection Yang-Baxter equation.[18] The Bethe ansatz equations (BAE's) and the eigenvalues of the Hamiltonian for the integrable cases will be given. In Sec. III, we study the ground state properties. The competing effect of J_i and V_i on the Kondo screening will be discussed in detail. Section IV is attributed to the derivation of the thermodynamics. A different method, i.e., the local Landau-Luttinger liquid description,[16,17] is used to study the low-temperature thermodynamics of the impurity. Such a method can also be applied to nonintegrable models and is thus general to the impurity problem in 1D quantum systems. Concluding remarks will be given in Sec. V. The Appendix is attributed to the eigenvalue problem of the nested Bethe ansatz.

II. BETHE ANSATZ

It is well known that H_0 is exactly solvable for $J=2$, $V=-1/2,3/2$.[19,20] By including the impurity, any electron impinging on the impurity will be completely reflected and suffer a reflection matrix R_j. The waves are therefore reflected at either end as

$$e^{ik_jx}\rightarrow -e^{-ik_jx},\quad x\sim 1,$$

$$e^{ik_jx}\rightarrow R_j^{-1}(k_j)e^{-ik_jx-2ik_jL},\quad x\sim L. \tag{2}$$

Let us consider the two-particle case. There are two ways from an initial state $(k_1,k_2,|)$ to a final state $(-k_1,-k_2,|)$:

$$\text{(I)}\quad (k_1,k_2,|)\rightarrow(k_2,k_1,|)\rightarrow(k_2,-k_1,|)\rightarrow(-k_1,k_2,|)\rightarrow(-k_1,-k_2,|),$$

$$\text{(II)}\quad (k_1,k_2,|)\rightarrow(k_1,-k_2,|)\rightarrow(-k_2,k_1,|)\rightarrow(-k_2,-k_1,|)\rightarrow(-k_1,-k_2,|),$$

where the symbol $|$ denotes the open boundary. Since the physical process is unique, the following equation must hold:

$$S_{12}(k_1,k_2)R_1(k_1)S_{12}(k_1,-k_2)R_2(k_2)=R_2(k_2)S_{12}(k_1,-k_2)R_1(k_1)S_{12}(k_1,k_2). \tag{3}$$

Above S_{12} is the two-electron scattering matrix. Equation (3) is just the reflection equation.[18] For the multiparticle cases, as long as the scattering matrix is factorizable or the two-body scattering matrix satisfies the Yang-Baxter relation[21]

$$S_{12}(k_1,k_2)S_{13}(k_1,k_3)S_{23}(k_2,k_3)=S_{23}(k_2,k_3)S_{13}(k_1,k_3)S_{12}(k_1,k_2), \tag{4}$$

Eq. (3) is the only restriction to the integrability of an open boundary system.[18] Generally, a c-number reflection matrix indicates either a boundary field in the spin-chain models or a scalar potential in a fermion system. However, in the present model, the boundary impurity has internal degrees of freedom and spin-exchange processes must be included when an electron is reflected by the boundary. That means that the reflection matrix R_j must be an operator one rather than a c-number one.

We consider first the $J=2$, $V=3/2$ case. Since the reflection process only consists of a one-electron effect, it is convenient to consider the single-particle eigenstate $|1\rangle=\Sigma_{x=1}^{L}\Psi(x)c_{x,\sigma}^{\dagger}|0\rangle$. With the Bethe-type wave function $\Psi(x)=A_+e^{ikx}+A_-e^{-ikx}$, we obtain

$$R(k)\equiv\frac{A_-}{A_+}e^{-2ikL}=-\frac{e^{ik}+(V_i+J_i\tau\cdot\mathbf{S})}{e^{-ik}+(V_i+J_i\tau\cdot\mathbf{S})}. \tag{5}$$

For arbitrary N-particle case, $R_j(k_j)$ must satisfy the reflection equation (3). It is known that the two-body scattering matrix takes the form[19,22]

$$S_{jl}(q_j-q_l)=-\frac{q_j-q_l+iP_{jl}}{q_j-q_l-i}, \tag{6}$$

where $q_j=\tan(k_j/2)/2$, and P_{jl} is the spin-exchange operator. Substituting Eqs. (5) and (6) into Eq. (3), we readily obtain the integrable condition for the present model as

$$J_i=\frac{1}{\left(S+\frac{1}{2}\right)^2-c^2},\quad V_i=\frac{S^2+S+1-\left(c-\frac{1}{2}\right)^2}{\left(S+\frac{1}{2}\right)^2-c^2}. \tag{7}$$

The reflection matrix in the integrable case can be rewritten as

$$R_j(q_j)=\frac{q_j-\frac{i}{2}}{q_j+\frac{i}{2}}\frac{q_j-ic+i(\tau\cdot\mathbf{S}+1)}{q_j+ic+i(S+1)}\frac{q_j+ic+i\tau\cdot\mathbf{S}}{q_j+ic+iS}. \quad (8)$$

For an N-particle system, suppose the wave function initially has an amplitude ζ_0. When the jth particle moves across another particle l, it suffers an S matrix $S_{jl}(q_j-q_l)$. At the right boundary, it is completely reflected back and suffers a factor $\exp(2ik_jL)R_j(q_j)$. Then it begins to move toward the left boundary. At the left boundary, it will be kicked back and suffers a factor -1. Finally it arrives at the initial site and finishes a periodic motion. Therefore we have the equation

$$-S^-_{jj-1}\cdots S^-_{j1}S^+_{j1}\cdots S^+_{jj-1}S^+_{jj+1}\cdots S^+_{jN}R_je^{2ik_jL}S^-_{jN}\cdots S^-_{jj+1}\zeta_0=\zeta_0 \quad (9)$$

or, more neatly,

$$S^-_{jj-1}\cdots S^-_{j1}S^+_{j1}\cdots S^+_{jj-1}S^+_{jj+1}\cdots S^+_{jN}R_jS^-_{jN}\cdots S^-_{jj+1}\zeta_0=-\left(\frac{q_j+\frac{i}{2}}{q_j-\frac{i}{2}}\right)^{2L}\zeta_0, \quad (10)$$

where $S^{\pm}_{jl}=S_{jl}(q_j\pm q_l)$. Equation (10) is just the reflection version of Yang's eigenvalue problem.[21] Its solution gives out the BAE's. To keep the continuity of the text, we consign the solution of Eq. (10) to the Appendix. The BAE's read

$$\left(\frac{q_j-\frac{i}{2}}{q_j+\frac{i}{2}}\right)^{2L+1}=-\frac{q_j-i(S+1-c)}{q_j+i(S+1-c)}\times\prod_{r=\pm}\prod_{l\neq j}^{N}\frac{q_j-rq_l-i}{q_j-rq_l+i}\times\prod_{\alpha=1}^{M}\frac{q_j-r\lambda_\alpha+\frac{i}{2}}{q_j-r\lambda_\alpha-\frac{i}{2}}, \quad (11)$$

$$\frac{\lambda_\alpha+i\left(S+\frac{1}{2}-c\right)}{\lambda_\alpha-i\left(S+\frac{1}{2}-c\right)}\frac{\lambda_\alpha+i\left(S-\frac{1}{2}+c\right)}{\lambda_\alpha-i\left(S-\frac{1}{2}+c\right)}\prod_{r=\pm}\prod_{j=1}^{N}\frac{\lambda_\alpha-rq_j+\frac{i}{2}}{\lambda_\alpha-rq_j-\frac{i}{2}}=\prod_{r=\pm}\prod_{\alpha\neq\beta}^{M}\frac{\lambda_\alpha-r\lambda_\beta+i}{\lambda_\alpha-r\lambda_\beta-i}, \quad (12)$$

where $M\leqslant N/2$ is the number of spin-down electrons and λ_α are the rapidities of the spinons. The eigenvalue of the Hamiltonian is given by

$$E=2N-\sum_{j=1}^{N}\frac{4}{4q_j^2+1}. \quad (13)$$

By following the same procedure, we can derive the integrable conditions for $J=2$, $V=-1/2$ as

$$J_i=\frac{1}{\left(S+\frac{1}{2}\right)^2-c^2},\quad V_i=\frac{S^2+S+1-\left(c+\frac{1}{2}\right)^2}{\left(S+\frac{1}{2}\right)^2-c^2}. \quad (14)$$

Since the physics of the two models are almost the same, we study only the $V=3/2$ case in the following text.

III. GROUND STATE PROPERTIES

As in most of many-body systems, the ground state properties reveal the main features of the fixed point physics. For the Kondo problem, the central point is the residual magnetization of the impurity, which measures the screening effect of the conduction electrons on the local moment. In the conventional Kondo system, one conduction electron is bounded by the impurity at low temperatures and reduces the residual magnetization from S to $S-1/2$. However, in the present model, the situation is more complicated. Both the bulk correlation and the scalar potential V_i may have significant effects on the Kondo screening. Especially, there is a competition between the Kondo coupling J_i and a repulsive V_i because J_i enhances the formation of the local composite (bound state of the local moment and a conduction electron) while a positive V_i prevents its formation. In the integrable case, J_i and V_i are not independent of each other but are parametrized by a unique real constant c. Even so, the competition effect can be shown exactly by varying c and analyzing the ground state configuration of the BAE's. The boundary coupling has two direct effects on the impurity. First, it splits the impurity spin into two effective spins with amplitudes $S+1/2-c$ and $S-1/2+c$, respectively, as we can read off from the BAE's (12). That means the in waves and the out waves of the conduction electrons ''see'' different values of the impurity spin. Notice that the mean value of the two effective spins is still S. Second, one of the conduction electrons may be pinned by the impurity in some c regions. The local bound state then behaves as an effective impurity and the effective spins will be further renormalized. From the BAE's (11) we can see that an imaginary mode $q=i(S+1-c)$ is a possible solution as long as $c<S+1$. However, such a mode is not always stable in the ground state. As we can read off from Eq. (13), the real modes form a band $-2\leqslant\epsilon(q)\leqslant 2$. The energy of the imaginary mode falls either below the band or above it. Therefore, the imaginary q mode defines a true bound state around the impurity.

(i) $c\geqslant S+1$. In this case, the Kondo coupling is ferromagnetic and the boundary coupling cannot induce any stable bound state. In the ground state, all the modes $\{q_j\}$ and $\{\lambda_\alpha\}$ take real values. Define the quantities

$$Z_L^c(q)=\frac{1}{2L}\left\{\sum_{r=\pm}\sum_{\alpha=1}^{M}\theta_1(q-r\lambda_\alpha)-\sum_{r=\pm}\sum_{j=1}^{N}\theta_2(q-rq_j)+\phi_c^e(q)+\phi_c^i(q)\right\}+\theta_1(q),$$

$$Z_L^s(\lambda)=\frac{1}{2L}\left\{\sum_{r=\pm}\sum_{j=1}^{N}\theta_1(\lambda-rq_j)-\sum_{r=\pm}\sum_{\beta=1}^{M}\theta_2(\lambda-r\lambda_\beta)+\phi_s^e(\lambda)+\phi_s^i(\lambda)\right\}, \tag{15}$$

where $\theta_n(q)=2\arctan(2q/n)$ and

$$\phi_c^e(q)=2\theta_1(q),\quad \phi_c^i(q)=\theta_{2(c-S-1)}(q), \tag{16}$$

$$\phi_s^e(\lambda)=\theta_2(\lambda),\quad \phi_s^i(\lambda)=\theta_{(2c+2S-1)}(\lambda)-\theta_{(2c-2S-1)}(\lambda). \tag{17}$$

Notice that the zero modes are forbidden in an open boundary system.[23] Obviously, $Z_L^c(q_j)=\pi I_j/L$ and $Z_L^s(\lambda_\alpha)=\pi J_\alpha/L$ give the logarithmic version of the BAE's, where I_j and J_α are integers. In the ground state, both $\{I_j\}$ and $\{J_\alpha\}$ are closely packed numbers from 1 up to N and M, respectively. The cutoffs of q and λ are defined as $Z_L^c(Q)=\pi(N+1/2)/L$ and $Z_L^s(\Lambda)=\pi(M+1/2)/L$. Define the density functions as

$$\rho_L^c(q)=\frac{1}{2\pi}\frac{dZ_L^c(q)}{dq}-\frac{1}{2L}\delta(q),$$
$$\rho_L^s(\lambda)=\frac{1}{2\pi}\frac{dZ_L^s(\lambda)}{d\lambda}-\frac{1}{2L}\delta(\lambda). \tag{18}$$

We have the relations

$$\int_{-Q}^{Q}\rho_L^c(q)dq=\frac{1}{L}N,\quad \int_{-\Lambda}^{\Lambda}\rho_L^s(\lambda)d\lambda=\frac{1}{L}M. \tag{19}$$

As demonstrated by many authors,[24] $\Lambda\to\infty$ for the ground state in the thermodynamic limit $L\to\infty$, since any hole in the real λ axis induces an excited state.[25] Substituting Eq. (18) into the second equation of Eq. (19), we deduce that $N=2M$, which means the residual magnetization is

$$M_s=S+\frac{1}{2}N-M=S. \tag{20}$$

Therefore, the impurity moment cannot be screened anymore in this case.

(ii) $S+1/2<c<S+1$. In this case, the Kondo coupling is still ferromagnetic. Due to the strong Kondo coupling and the weak impurity potential, one boundary bound state occurs with $q=i(S+1-c)$. Since $|q|<1/2$, we can see that the energy level of this mode,

$$\epsilon(q)=2-\frac{4}{1-4(S+1-c)^2}<-2, \tag{21}$$

is below the conduction band. Therefore this state is a stable bound state. Taking the local bound state into account, the two effective spins become $S_\pm=S+1/2\pm(1-c)$. This leads to $N=2M$ and $M_s=S$. It seems that the local spin is still unscreened. However, we note that the localized electron and the impurity form a spin-$(S+1/2)$ composite due to the ferromagnetic Kondo coupling J_i. When $c\to S+1/2+0^+$, $J_i,V_i\to-\infty$. Both J_i and V_i enhance the formation of the local composite and the composite behaves as a perfect local moment with spin $(S+1/2)$. It is the composite rather than the original impurity interacting with the host effectively. In such a sense, we can say that the local moment is partially screened because the residual magnetization is only S. If we include another half chain interacting with the impurity, the problem becomes a two-channel Kondo problem[26,27] and we expect the realization of Furusaki-Nagaosa's conjecture $(M_s=S-1/2)$.

(iii) $-(S-1/2)<c<S+1/2$. The Kondo coupling is antiferromagnetic. The boundary bound state $q=i(S+1-c)$ is no longer a stable state since it has much higher energy. The ground state is still described by closely packed real q modes and λ modes. The residual magnetization is $S-1/2$, indicating an usual Kondo screening as in conventional Kondo systems.[28] Such a result suggests that the Kondo coupling $J_i>0$ is dominant over V_i even in the strong coupling limit $c\to S+1/2+0^-(J_i,V_i\to+\infty)$.

(iv) $-S<c<-(S-1/2)$. The Kondo coupling is antiferromagnetic and no stable bound state exists in the ground state. By following the same procedure, we derive that the residual magnetization is S, indicating the absence of Kondo screening. Though the Kondo coupling $J_i>0$, it seems V_i is dominant over J_i and prevents the conduction electrons from screening the impurity. In the conventional Kondo problem, the impurity potential does not change the fixed point and only induces the renormalization of the Kondo coupling constant.[28] However, in the present case, the strong coupling fixed point predicted in 3D is no longer stable. Such a phenomenon strongly suggests that the charge-spin cooperation plays an important role in the 1D Kondo problem and gives a typical example of the competition between J_i and V_i.

(v) $-(S+1/2)<c<-S$. In this case, the system is still in the regime of antiferromagnetic Kondo coupling. From the BAE's (11) and (12) we can see that an imaginary spin mode $\lambda=i(S-1/2+c)$ may assist the formation of a boundary bound state with $q=i(S+c)$. This mode carries much lower energy than those of the real modes and is therefore stable in the ground state. Taking these bound states into account, the two effective spins read $S_\pm=S-1/2\pm(1-c)$. In the thermodynamic limit, a direct calculation gives $N=2M-1$ in the ground state. Therefore, the residual magnetization takes the value of $S-1/2$, which indicates a typical Kondo screening. In fact, both the positive J_i and negative V_i assist one conduction electron to form tight-bonding pair with the local moment. The bounded spin mode is a signal of the formation of the local spin $(S-1/2)$ bound state.

(vi) $c<-(S+1/2)$. In this case, both the ferromagnetic Kondo coupling $(J_i<0)$ and the repulsive impurity potential prevent the conduction electrons screening the impurity. The residual magnetization is S and no Kondo screening occurs.

The above discussion shows that the boundary coupling does have a significant effect on the Kondo screening. The central point is the spin splitting. By taking the stable bound states into account, suppose we have two effective spins $S_\pm$. The Kondo effect on these effective spins is as usual. The only difference is that if $S_-<0$, its residual magnetization is $-(|S_-|-1/2)$ rather than $S_- -1/2$. Therefore, the total residual magnetization of the impurity is $M_s=S_++S_-+[\mathrm{sgn}(S_+)+\mathrm{sgn}(S_-)]/2$. Since $S_\pm$ are interaction dependent, we naturally get two results: i.e., the impurity is either screened ($M_s=S-1/2$) or unscreened ($M_s=S$).

IV. THERMODYNAMICS

In this section, we derive the thermodynamic equations of the present model via the thermal Bethe ansatz.[29,32] We shall omit the excitations which break the stable boundary bound states since these excitations are accompanied by finite energy gaps and their contributions to the low-temperature thermodynamic quantities are exponentially small.

A. Thermodynamic Bethe ansatz

At finite temperatures, the solution of the BAE's is described by a sequence of real $\{q_j\}$ and a variety of $\{\lambda_\alpha\}$ strings. From the Bethe ansatz equations we obtain

$$\rho_c(q)+\rho_c^h(q)=a_1(q)+\frac{1}{4\pi L}\phi_c'(q)-\frac{1}{2L}\delta(q)-[2]\rho_c(q)+\sum_{m=1}^{\infty}[m]\rho_{s,m}(q), \tag{22}$$

$$\rho_{s,m}^h(\lambda)=\frac{1}{4\pi L}\phi_{s,m}'(\lambda)-\frac{1}{2L}\delta(\lambda)+[m]\rho_c(\lambda)-\sum_{n=1}^{\infty}A_{mn}\rho_{s,n}(\lambda), \tag{23}$$

where $\rho_{s,m}$ ($\rho_{s,m}^h$) are the densities of the m-string (holes), $[n]$ is an integral operator with the kernel $a_n(q)=n/\{2\pi[q^2+(n/2)^2]\}$, $A_{mn}=[m+n]+2[m+n-2]+\cdots+[|m-n|+1]$, and $\phi_{s,m}=\sum_{j=1}^{m}\phi_s^i\{\lambda+i[(m+1)/2-j]\}$. In a magnetic field H, the free energy of the system can be written as

$$\begin{aligned}F/L=&\int\left[\epsilon_0(q)-\mu-\frac{H}{2}\right]\rho_c(q)dq+\sum_{n=1}^{\infty}nH\int\rho_{s,n}(\lambda)d\lambda\\&-T\int[(\rho_c+\rho_c^h)\ln(\rho_c+\rho_c^h)-\rho_c\ln\rho_c-\rho_c^h\ln\rho_c^h]dq\\&-T\sum_{n=1}^{\infty}\int[(\rho_{s,n}+\rho_{s,n}^h)\ln(\rho_{s,n}+\rho_{s,n}^h)-\rho_{s,n}\ln\rho_{s,n}\\&-\rho_{s,n}^h\ln\rho_{s,n}^h]d\lambda,\end{aligned} \tag{24}$$

where $\epsilon_0(q)=-2\pi a_1(q)+2$ and μ is the chemical potential. At the equilibrium state, by minimizing the free energy we obtain

$$\ln\eta=\frac{\epsilon_0-\mu}{T}+\{[2]-[1]G\}\ln(1+\eta^{-1})-G\ln(1+\zeta_1), \tag{25}$$

$$\ln\zeta_n=G[\ln(1+\zeta_{n-1})+\ln(1+\zeta_{n+1})],\quad n>1, \tag{26}$$

$$\ln\zeta_1=-G\ln(1+\eta^{-1})+G\ln(1+\zeta_2), \tag{27}$$

where $\eta(q)=\rho_c^h(q)/\rho_c(q)$, $\zeta_n(\lambda)=\rho_{s,n}^h(\lambda)/\rho_{s,n}(\lambda)$, and G is an integral operator with the kernel $[2\cosh(\pi\lambda)]^{-1}$. Since we are only interested in the Kondo effect, we consider here the spin part of the impurity free energy, which reads

$$F_{imp}^s=-\frac{T}{4\pi}\sum_{n=1}^{\infty}\int\phi_{s,n}'(\lambda)\ln[1+\zeta_n^{-1}(\lambda)]d\lambda. \tag{28}$$

B. Residual entropy

To give further information of the ground state, we study the residual entropy of the impurity. When $T\to0$, $\eta\to\exp[(\epsilon_c-\mu)/T]$, for $\epsilon_c<\mu$. Therefore the driving term in Eq. (27) tends to $-\infty$. That means $\zeta_1\to0$ and all the other ζ_n take constant values[28,30] ζ_n^+ with

$$\zeta_n^+(x_0)=\frac{\sinh^2(nx_0)}{\sinh^2x_0}-1,\quad x_0=\frac{H}{2T}. \tag{29}$$

From Eq. (28) we deduce the residual entropy as

$$S_{res}=\frac{1}{4\pi}\sum_{n=1}^{\infty}\int\phi_{s,n}'(\lambda)\ln\left[1+\frac{1}{\zeta_n^+(0)}\right]d\lambda. \tag{30}$$

For simplicity, we consider the $c>S+1$ case. Other cases can be studied by following the same method without any difficulty. The only little difference is that when the boundary bound state occurs, its contribution to $\phi_{s,n}$ should be taken into account. Since at zero temperature ζ_n are variable independent, the integral operators $[n]$ are equivalent to unity and $a_n(\lambda)$ are equivalent to $\delta(\lambda)$ under integration. This makes the calculations very simple. When $2c=$integer, the impurity spin is split into two effective spins $S_\pm=S\pm(c-1/2)$. Notice $S_-<0$ and contributes a negative value to $\phi_{s,n}'$. Therefore, its contribution to the entropy is also negative. The total entropy of the impurity is just the mean value of the two effective spins, which is always positive:

$$S_{res}=\frac{1}{2}\ln(2S_+)-\frac{1}{2}\ln(2|S_-|)=\frac{1}{2}\ln\frac{2c+2S-1}{2c-2S-1}. \tag{31}$$

When $2c\neq$integer, the situation is somewhat complicated. In this case, the effective spins take noninteger and non-half-integer values and there is a mismatch between the impurity and the conduction electrons. Put $2c_I=$integer part of $2c$ and $\alpha=2(c-c_I)$. We have

$$\frac{1}{2\pi}\phi_{s,n}'(\lambda)\to a_{n,2c_I+2S-1}(\lambda)-a_{n,2c_I-2S-1}(\lambda)-a_\alpha(\lambda)\sum_{l=1}^{2S}\delta_{n,2c_I-2S+2l-2}, \tag{32}$$

where $a_{n,m}=\sum_{k=1}^{min(m,n)}a_{n+1+m-2k}$. Obviously, c_I splits the impurity spin into two effective spins $S_\pm=S\pm(c_I-1/2)$ and the nonzero α induces secondary ‘‘ghost spins’’ with values between $2c_I-2S$ and $2c_I+2S-2$, which reveals a local diffraction effect in the spin sector. By substituting Eq. (32) into Eq. (30), we obtain

$$S_{res}=\frac{1}{2}\ln\frac{2c_I+2S-1}{2c_I-2S-1}-\sum_{l=1}^{2S}\ \ln\frac{2(c_I-S-1+l)}{\sqrt{4(c_I-S-1+l)^2-1}}. \tag{33}$$

Obviously, there is a finite jump of the residual entropy at $c=c_I(>S+1)$:

$$\Delta S_{res}=\lim_{\delta\to 0}[S_{res}(c_I+\delta)-S_{res}(c_I-\delta)]$$
$$=\ln\left[\frac{(c_I+S-1/2)(c_I-S-1)}{(c_I-S-1/2)(c_I+S-1)}\right]. \tag{34}$$

The discontinuity of the residual entropy at $c=c_I$ indicates a first-order quantum phase transition. Such a behavior shows that the local spin configuration is strongly interaction dependent rather than simply screened or decoupled as understood in the conventional Kondo problem. This strongly suggests that both the bulk correlation and the scalar potential have nontrivial effects on the ground state configuration of the impurity.

C. Local Landau-Luttinger liquid description

Despite the finite residual entropy in the ground state, the temperature dependence of the impurity specific heat should not be affected in its leading order since there are no extra degrees of freedom to induce the overscreening effect. Therefore, Nozières' local Fermi liquid theory[31] can be used with a slight modification. Consider a noninteracting 1D open chain. The ''momenta'' k' is quantized as

$$k'=k+\frac{1}{2L}\delta_0(k), \tag{35}$$

where $k=\pi n/L$ (n positive integer) are the ''momenta'' of the pure open boundary system and $\delta_0(k)$ is the phase shift due to the particle-impurity scattering. The change of the density of states is therefore

$$\delta D(k)=\frac{1}{\pi}\frac{\delta_0'(k)}{\epsilon'(k)}, \tag{36}$$

where $\epsilon(k)$ is the single-particle energy. For the interacting 1D electron systems, the quasiparticles can be defined in the charge and spin sectors, respectively.[32] The phase shifts are generally functionals of the distributions of the quasiparticles $n_c(q)$ and $n_s(\lambda)$ and can be expressed as

$$\delta_c(q)=\delta_{c,0}(q)+\sum_{r=\pm}\sum_{q'\neq q}\theta_{cc}(q,rq')\,\delta n_c(q')$$
$$+\sum_{r=\pm}\sum_{\lambda}\theta_{cs}(q,r\lambda)\,\delta n_s(\lambda), \tag{37}$$

$$\delta_s(\lambda)=\delta_{s,0}(\lambda)+\sum_{r=\pm}\sum_{q}\theta_{sc}(\lambda,rq)\,\delta n_c(q)$$
$$+\sum_{r=\pm}\sum_{\lambda'\neq\lambda}\theta_{ss}(\lambda,r\lambda')\,\delta n_s(\lambda'), \tag{38}$$

where $\delta_{c,0}$ and $\delta_{s,0}$ are the bare phase shifts induced by the impurity, θ's are the phase shifts of the particle-particle scattering, and $\delta n_{c,s}=n_{c,s}-n_{c,s}^0$ is the change of the quasiparticle distributions induced by the impurity. On the other hand, $\delta n_{c,s}$ in the ground state take the form

$$\delta n_c(q)=\frac{\delta_c'(q)}{2L},\quad \delta n_c(\lambda)=\frac{\delta_s'(\lambda)}{2L}. \tag{39}$$

Equations (37) and (38) are thus reduced in the thermodynamic limit $L\to\infty$ to

$$\delta_c'(q)=\delta_{c,0}'(q)+\frac{1}{2\pi}\int_{-q_F}^{q_F}\theta_{cc}'(q,q')\,\delta_c'(q')dq'$$
$$+\frac{1}{2\pi}\int_{-\lambda_F}^{\lambda_F}\theta_{cs}'(q,\lambda)\,\delta_s'(\lambda)d\lambda, \tag{40}$$

$$\delta_s'(\lambda)=\delta_{s,0}'(\lambda)+\frac{1}{2\pi}\int_{-q_F}^{q_F}\theta_{sc}'(\lambda,q)\,\delta_c'(q)dq$$
$$+\frac{1}{2\pi}\int_{-\lambda_F}^{\lambda_F}\theta_{ss}'(\lambda,\lambda')\,\delta_s'(\lambda')d\lambda', \tag{41}$$

where q_F and λ_F are the Fermi ''momenta.'' Notice $o(1/L)$ terms have been omitted in the above equations. The low-temperature thermodynamics of the impurity is therefore characterized by two constants

$$\delta D_c(q_F)=\frac{1}{\pi}\frac{\delta'(q_F)}{\epsilon_c'(q_F)},\quad \delta D_s(\lambda_F)=\frac{1}{\pi}\frac{\delta_s'(\lambda_F)}{\epsilon_s'(\lambda_F)}, \tag{42}$$

where $\epsilon_{c,s}$ are the quasiparticle energies.

In our case,

$$\delta_{c,0}(q)=\phi_c(q),\quad \delta_{s,0}(\lambda)=\phi_s(\lambda), \tag{43}$$

$$\theta_{sc}'(\lambda,q)=\theta_{cs}'(q,\lambda)=2\pi a_1(q-\lambda), \tag{44}$$

$$\theta_{cc}'(q,q')=\theta_{ss}'(q,q')=-2\pi a_2(q-q'). \tag{45}$$

As the low-temperature specific heat is proportional to the densities of states, the following relation holds:

$$\frac{\delta C}{C_0}=\frac{\delta_c'(Q)}{\rho_c(Q)}+\frac{\delta_s'(\Lambda)}{\rho_s(\Lambda)}, \tag{46}$$

where δC is the specific heat induced by the impurity and the open boundaries and C_0 is the specific heat of the bulk (per unit length); $\rho_c(q)$ and $\rho_s(\lambda)$ are the quasiparticle distributions in the ground state. We note that this method is not applicable to the susceptibility for $S>1/2$ since the residual magnetization is finite and the low-temperature susceptibility is Curie type. However, when $S=1/2$ and $0<c<1$ or $-1<c<-1/2$, $M_s=0$, the leading order of the impurity susceptibility is Pauli type and the present method works.

V. CONCLUDING REMARKS

In conclusion, we propose an integrable model of a boundary impurity spin coupled with the integrable open t-J chain. In our model, The ''fine-tuned'' effect in the periodic integrable models is overcome and the interaction term takes a very simple form. The coupling constant J_i can take an arbitrary value with a proper boundary potential V_i without destroying the integrability of the Hamiltonian. This allows us to study the antiferromagnetic and ferromagnetic Kondo problem simultaneously. Some new phenomena driven by the boundary coupling have been found, which can never appear in the periodic models as well as in the conventional Kondo problems: (i) The boundary coupling splits the impurity spin into two effective ''ghost spins'' $S-c+1/2$ and $S+c-1/2$. That means the coupling not only changes the energy scales (Kondo temperature) as in the conventional Kondo problem but also renormalizes the effective strength of the impurity spin. Such a phenomenon reveals a pure correlation effect. (ii) Depending on the strength of the coupling, the system may show behavior differing from those of the conventional Kondo problems. A typical example is that the scalar potential may destruct the Kondo screening even in the antiferromagnetic Kondo coupling regime. (iii) The residual entropy is strongly coupling dependent which indicates that the local spin configuration near the impurity is very complicated rather than simply screened or decoupled as understood in the conventional Kondo problem. The mismatch between the effective spins and the conduction electrons drives a series of quantum phase transitions at $2c$ $=$integes.

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APPENDIX

In dealing with the open boundary integrable models, we often encounter the following eigenvalue problem:

$$S_{jj-1}^{-}\cdots S_{j1}^{-}S_{j1}^{+}\cdots S_{jj-1}^{+}S_{jj+1}^{+}\cdots S_{jN}^{+}R_jS_{jN}^{-}\cdots S_{jj+1}^{-}\psi_0 \equiv X_j\Psi_0=\epsilon(q_j)\psi_0, \tag{A1}$$

where $S_{jl}^{\pm}$ and R_j are the scattering matrix and the reflection matrix, respectively. In our case, up to constant factors they take the forms

$$S_{jl}^{\pm}=\frac{q_j\pm q_l+i\gamma P_{jl}}{q_j\pm q_l+i\gamma}, \tag{A2}$$

$$R_j=\frac{q_j-ic\gamma+i\gamma(\tau_j\cdot\mathbf{S}+1)}{q_j-ic\gamma+i\gamma(S+1)}\,\frac{q_j+ic\gamma+i\gamma\tau_j\cdot\mathbf{S}}{q_j+ic\gamma+i\gamma S}, \tag{A3}$$

where $\gamma=\pm1$. Define $\overline{\psi_0}=(S_{jj-1}^{-}\cdots S_{j1}^{-})^{-1}\psi_0$. Equation (A1) can be rewritten as

$$S_{j1}^{+}\cdots S_{jj-1}^{+}S_{jj+1}^{+}\cdots S_{jN}^{+}R_jS_{jN}^{-}\cdots S_{jj+1}^{-}S_{jj-1}^{-}\cdots S_{j1}^{-}\overline{\psi_0} \equiv X_j'\overline{\psi_0}=\epsilon(q_j)\overline{\psi_0}. \tag{A4}$$

For convenience, we introduce an auxiliary space τ and define

$$U_\tau(q) =S_{\tau j}^{+}S_{\tau 1}^{+}\cdots S_{\tau j-1}^{+}\cdots S_{\tau N}^{+}R_{\tau 0}S_{\tau N}^{-}\cdots S_{\tau j+1}^{-}S_{\tau j-1}^{-}\cdots S_{\tau 1}^{-}S_{\tau j}^{-}, \tag{A5}$$

with $q_\tau=q$. Obviously, $S_{\tau j}^{-}(q_j)=P_{\tau j}$ and

$$\mathrm{tr}_\tau\, U_\tau(q_j)=\frac{2q_j+2i\gamma}{2q_j+i\gamma}X_j'. \tag{A6}$$

Since $S_{\tau l}^{\pm}$ satisfy the Yang-Baxter relation

$$S_{\tau\tau'}^{-}(q-q')S_{\tau j}^{\pm}(q\pm q_j)S_{\tau' j}^{\pm}(q'\pm q_j) =S_{\tau' j}^{\pm}(q'\pm q_j)S_{\tau j}^{\pm}(q\pm q_j)S_{\tau\tau'}^{-}(q-q'), \tag{A7}$$

from Eq. (3) we can easily show that $U_\tau(q)$ satisfies the reflection equation

$$S_{\tau\tau'}^{-}(q-q')U_\tau(q)S_{\tau\tau'}^{+}(q+q')U_{\tau'}(q') =U_{\tau'}(q')S_{\tau\tau'}^{+}(q+q')U_\tau(q)S_{\tau\tau'}^{-}(q-q'). \tag{A8}$$

Therefore, the eigenvalue problem (A3) is reduced to Sklyanin's eigenvalue problem.[18] By following the same procedure introduced in Ref. 18, we obtain the eigenvalue of $X_j'(q_j)$ as

$$\epsilon(q_j)=\prod_{\alpha=1}^{M}\frac{q_j+\Lambda_\alpha}{q_j-\Lambda_\alpha}\,\frac{q_j-\Lambda_\alpha-i\gamma}{q_j+\Lambda_\alpha+i\gamma}. \tag{A9}$$

The parameters Λ_α are determined by

$$\frac{\Lambda_\alpha-i\gamma(S+c-1)}{\Lambda_\alpha+i\gamma(S+c)}\,\frac{\Lambda_\alpha-i\gamma(S-c)}{\Lambda_\alpha+i\gamma(S-c+1)} \times\prod_{j=1}^{N}\frac{(\Lambda_\alpha+q_j)(\Lambda_\alpha-q_j)}{(\Lambda_\alpha+q_j+i\gamma)(\Lambda_\alpha-q_j+i\gamma)} =\prod_{\beta\neq\alpha}\frac{(\Lambda_\alpha+\Lambda_\beta)(\Lambda_\alpha-\Lambda_\beta-i\gamma)}{(\Lambda_\alpha+\Lambda_\beta+2i\gamma)(\Lambda_\alpha-\Lambda_\beta+i\gamma)}. \tag{A10}$$

By replacing Λ_α with $\lambda_\alpha-i\gamma/2$ in Eqs. (A9) and (A10), we readily obtain the BAE's.

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