Ghost spins and novel quantum critical behavior in a spin chain
with local bond-deformation

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Abstract

We study the boundary impurity-induced critical behavior in an integrable $SU(2)$-invariant model consisting of an open Heisenberg chain of arbitrary
spin-$S$ (Takhtajan-Babujian model) interacting with an impurity of spin $\vec{S}'$ located at one of the boundaries. For $S = 1/2$ or $S' = 1/2$, the impurity inter-
action has a very simple form $J\vec{S}_1 \cdot \vec{S}'$ which describes the deformed boundary
bond between the impurity $\vec{S}'$ and the first bulk spin $\vec{S}_1$ with an arbitrary
strength $J$. With a weak coupling $0 < J < J_0/[(S + S')^2 - 1/4]$, the impu-
rity is completely compensated, undercompensated, and overcompensated for
$S = S'$, $S > S'$ and $S < S'$ as in the usual Kondo problem. While for strong
coupling $J \geq J_0/[(S + S')^2 - 1/4]$, the impurity spin is split into two ghost
spins. Their cooperative effect leads to a variety of new critical behaviors
with different values of $|S' - S|$.

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I. INTRODUCTION

Quantum fluctuations induced by an impurity coupled to the one-dimensional Tomonaga-Luttinger liquid (TLL) play essential role in understanding the low temperature behavior of quasi-1D systems, such as quantum wires\cite{1}, fractional quantum Hall effect\cite{2}, carbon nanotubes\cite{3} or quasi-1D organic conductors\cite{4}. The problem of an impurity spin $\vec{S}'$ coupled with both of the neighboring sites of quantum chains was studied by a class of integrable $SU(2)$-invariant models\cite{5,6}. For the Heisenberg chain with ferromagnetic coupling, the impurity is locked into the critical behavior of the lattice, i.e., at low temperatures the specific heat is proportional to $T^{1/2}$ and the susceptibility diverges as $T^{-2}$ with logarithmic corrections\cite{7}. For a chain with antiferromagnetic coupling, the impurity spin is compensated by bulk spins with three different situations similar to the multichannel Kondo problem\cite{8}: for $S' = S$, it is the complete compensation and the impurity just corresponds to one more site in the chain; for $S' > S$, the partial compensation with Schottky anomaly when an external magnetic field $H$ is applied; and for $S' < S$, the overcompensation which gives rise to quantum critical behavior\cite{8}.

Meanwhile the effects of an impurity embedded in 1D TLL were extensively discussed recently. By renormalization group(RG) techniques, bosonization methods and boundary conformal field theories, many interesting results have been obtained, showing the unusual properties of TLL in the presence of a local potential barrier or a magnetic impurity\cite{9,10,11,12}. Generally speaking, these new findings indicate that the quantum impurity models renormalize to critical points corresponding to conformally invariant boundary conditions\cite{13,14,15}. The impurity-bulk coupling strength $J$ flows either to infinity when the impurity is screened, or to finite as if it is overscreened, no matter what the sign of $J$ is initially. In particular, numerical studies of the finite size spectrum support the picture that the fixed point corresponds to a chain disconnected at the impurity site for repulsive interaction\cite{17}. However, the low temperature impurity behavior described by previous Bethe ansatz integrable models do not correspond to the stable critical points mentioned above. For instance, at the critical
point the spin-$S$ impurity coupled to spin-1/2 antiferromagnetic Heisenberg chain has the effective screened spin $S_{\text{eff}} = S - 1/2$ rather than $S - 1$, despite the fact that it couples to the two neighboring 1/2-spin’s. In this respect, the critical point described by the impurity model is unstable, owing to the fact that these models have a fixed impurity coupling, a “fine tuned” impurity interaction term, and no backward scatterings. It is recalled that backward scattering is one of the essence of quantum impurity problem in 1D TLL. From the point of view of RG, electrons or spin waves moving in one-dimensional space will be largely scattered back by the impurity, while the tunneling effect could be perturbed. In the fixed point limit, they are completely scattered back after a phase shift due to interaction with the impurity, as long as transmission being plausibly neglected at sufficiently low temperature. Based on the fixed point observed by RG, some open boundary problems with the impurity located at the boundary were considered. By comparing the open boundary models and the periodic models, Zvyagin and co-author argued that the impurities in the integrable models could be generic. However, we remark either a transparent impurity or a boundary impurity in the integrable models considered earlier can not reveal a full picture of a generic impurity in the bulk since only one channel host is included in these models (for the transparent impurity, only forward scattering while for the boundary impurity, only one half-chain). To make the problem to be generic, one should consider two half-chains interacting symmetrically with the impurity. At low energy scales, the problem is effectively a two-channel one, as long as the interaction in the bulk is repulsive. Generally, tunneling through the impurity may exist. This causes hybridization, splitting and anisotropy of the two channels. However, the tunneling matrix is negligibly small comparing to the Kondo coupling or the impurity potential at low energy scales from the RG point of view. Therefore, these effects are not very harmful to the two-channel behavior.

In this paper, we consider the problem of an impurity spin interacting symmetrically with two half spin-chains. By mapping the problem to an open boundary one, we solve the related integrable model via Algebraic Bethe ansatz (ABA). The structure of the present paper is the following: In the subsequent section, we construct the model and derive the
Bethe ansatz equation. The ground state properties and the boundary bound states will be discussed in sect. III. In sect. IV, we discuss the thermodynamics of the open boundary as well as the impurity. It is found that the open boundary behaves as an overscreened spin and the impurity itself, may show different quantum critical behaviors, depending on the coupling constant $J$. Sect. V is attributed to the concluding remarks.

II. THE MODEL AND ITS BETHE ANSATZ

Let us start with the following Hamiltonian

$$H = J_0 \sum_{n=1}^{N-1} [\vec{S}_n \cdot \vec{S}_{n+1} + \vec{S}_{-n} \cdot \vec{S}_{-n-1}] + J S' \cdot (\vec{S}_1 + \vec{S}_{-1}),$$

(1)

where $J_0 > 0$ (antiferromagnetic coupling); $\vec{S}_n$ is the spin-1/2 operator, $\vec{S}'$ is the impurity spin operator. As long as $J_0 \neq J$ or $S' \neq 1/2$, back scattering off the impurity dominates over the forward scattering and the problem is effectively a two-channel one. No matter $J > 0$ (antiferromagnetic) or $J < 0$ (ferromagnetic), the second term in (1) causes ferromagnetic correlation between $\vec{S}_1$ and $\vec{S}_{-1}$. That means $\vec{S}_1$ and $\vec{S}_{-1}$ favors to form a spin-1 composite at low temperatures. In fact, there is a quasi-long-distance ferromagnetic correlation between $\vec{S}_n$ and $\vec{S}_{-n}$

$$< \vec{S}_n \cdot \vec{S}_{-n} > \sim (2n)^{-\theta},$$

(2)

where the exponents $\theta$ varies from 1 to 4, which can be derived from the boundary conformal field theory. Therefore, there is a tendency for $\vec{S}_n$ and $\vec{S}_{-n}$ to form a spin-1 composite and the problem could be mapped to a spin-1 chain coupled with a boundary impurity. We remark the composites far away from the impurity are not very tight and may lose sense as can be seen in (2), but this does not change very much the impurity behavior since the bulk-impurity interaction is local and very short-ranged. Hence, a spin-$S$ chain with a boundary impurity keeps the main feature of an impurity in a spin-$S/2$ chain. Caution should be taken when we construct the spin-$S$ open chain to avoid the Haldane gap since the original
Hamiltonian (1) is gapless. The formation of the high-spin composites is very similar to that in a multi-channel Kondo problem but with a different mechanism. Of course, the boundary impurity-induced critical behavior is quite generic.

Based on the above discussion, we study the low temperature behavior induced by an magnetic impurity $\vec{S}'$ coupled to an open antiferromagnetic Heisenberg chain of spin $S$ by use of Bethe ansatz exact solutions. It is well known that integrable generalization of isotropic $S = 1/2$ spin chain to arbitrary spin $S$ leads to the Hamiltonian

$$H_S = J_0 \sum_{j=1}^{N-1} Q_{2S}(\vec{S}_j \cdot \vec{S}_{j+1}),$$

where $Q_{2S}(x)$ is a polynomial of degree $2S$ of $SU(2)$ invariant quantities $x = \vec{S}_j \cdot \vec{S}_{j+1}$

$$Q_{2S}(x) = \sum_{j=1}^{2S} \sum_{k=1}^{j} \frac{1}{k} \prod_{l \neq j, l=0}^{2S} \frac{x - x_l}{x_j - x_l},$$

with $x_n = \frac{1}{2}n(n + 1) - S(S + 1), n = 0, 1, \cdots, 2S$. One recovers $H_{1/2} = J_0 \sum_{j=1}^{N-1} \vec{S}_j \cdot \vec{S}_{j+1}$, $H_1 = J_0 \sum_{j=1}^{N-1} [\vec{S}_j \cdot \vec{S}_{j+1} - (\vec{S}_j \cdot \vec{S}_{j+1})^2]$ as the usual Spin-1/2 Heisenberg model and the $S = 1$ Takhtajan-Babujian model respectively (up to an irrelevant constant). The construction of the model is based on the vertex weight operators $R(\lambda)$, represented by matrices acting on the tensor product spaces $V_1 \otimes V_2$ of two spins $\vec{S}_1, \vec{S}_2$, with a parameter $\lambda$ identified as spin rapidity. Its explicit form is

$$sR_{12}^{i j}(\lambda) = -\sum_{l=0}^{2S} \prod_{k=0}^{l} \frac{\lambda - k}{\lambda + k} P_l,$$

where $P_l$ is the projector selecting the states with total spin $l$ in the tensor product of the two spins involved, $P_l(x) = \prod_{n \neq 0}^{2S} \frac{x - x_n}{x_l - x_n}$. Owing to the Yang-Baxter equations satisfied by the $R$-matrix, we have the relationship $H_S \propto \frac{d}{dx} \ln t(\lambda)|_{\lambda=0}$, with $t(\lambda)$ being the transfer-matrix defined by

$$t(\lambda) = tr_A T(\lambda) = tr_A \{sR_A^{4N}(\lambda) \cdots sR_A^{41}(\lambda)\}.$$
Now, we put a magnetic impurity $\vec{S}'$ at one of the end of an open spin-$S$ Heisenberg chain, by considering the following integrable Hamiltonian

$$H = H_S + H_{imp},$$

(7)

$$H_{imp} = J_0 \sum_{l=|S-S'|+1}^{S+S'} \left( \sum_{k=|S-S'|+1}^{l} k \frac{k}{k^2 - c^2} \right) \prod_{n\neq l,n=|S-S'|}^{S+S'} \frac{y - y_n}{y_l - y_n},$$

(8)

where $y = \vec{S}_1 \cdot \vec{S}'$, $y_l = \frac{1}{2} [l(l+1) - S(S+1) - S'(S'+1)]$; $c$ is an arbitrary parameter describing the strength of the bulk-impurity interaction. The impurity is assumed to be sited at the left hand end of the chain, say the site $j = 0$, while its neighboring spin is $\vec{S}_1$. For $S = 1/2$, the model is reduced to that considered in Ref.[21]. Interestingly when $S = 1/2$ or $S' = 1/2$, the interaction term takes the simple form

$$H_{imp} = J \vec{S}_1 \cdot \vec{S},$$

(9)

with coupling constant $J = J_0/[(S' + S)^2 - c^2]$, which can range from negative infinity to positive one, and meet all the physical situations. So at least in these two cases, the Hamiltonian could be expected to properly describe the boundary bond effect in some real quasi-1D materials at very low temperature, such as the possible bond impurity $S' = 1/2$ in $S = 1$ Heisenberg antiferromagnet TMNIn$_2$.

To show the integrability of the Hamiltonian (7), let us first notice that the impurity term $H_{imp}$ could be more conveniently treated as the boundary operator, similar to the usual open boundary problem with an external field applied to the end. In addition to the Yang-Baxter equation (YBE) as the integrable condition of the bulk, there are some new consistent constraints (often called the reflect YBE ) for the same model to be integrable under the open boundary conditions, and the QISM is still available. A new $K$-operator is introduced corresponding to the boundary impurity. In most works, the $K$-operator is a $2 \times 2$ matrix with the elements being $c$-number describing the $S_z$-coupling to the applied field. The Sklyanin’s formalism can be extended to the generic representations of $K$-operator, which is written as a $2 \times 2$ matrix but with elements being operators rather than $c$-numbers. This operator-valued $K$ plays an useful role in constructing the boundary problem where
the quantum degrees of freedom of the boundary enter interactions. Of course generally, both $R, K$-vertices could be interpreted as the inhomogeneous vertices in a 2D lattice model. Our model corresponds to a very special one that the only “inhomogeneity” comes from the boundary row, leaving others uniform. It is built from

$$ K(\lambda) = S_{S'} R^{A0}(\lambda - ic) S_{S'} R^{A0}(\lambda + ic) $$

(10)

and $S_{S'} R(\lambda)^{A0}$ is given by

$$ S_{S'} R^{A0}(\lambda) = - \sum_{l=1}^{S' + S} \prod_{k=1}^{l} \frac{\lambda - k}{\lambda + k} \prod_{n \neq l, n = 1}^{S - S'} \frac{y - y_n}{y_l - y_n}. $$

(11)

It is straightforward to show that the doubled monodromy matrix

$$ \Theta(\lambda) = T(\lambda) K(\lambda) T^{-1}(-\lambda) $$

(12)

satisfies the reflection YB relations and its trace $\theta(\lambda) = tr_A \Theta(\lambda)$ satisfies $[\theta(\lambda), \theta(\mu)] = 0, \quad \forall \lambda, \mu$. Similarly, because $H \propto \frac{d}{d\theta} \ln \theta(\lambda)|_{\lambda=0}$, the Hamiltonian (7) is indeed integrable.

Its spectrum is uniquely determined by the following Bethe ansatz equations (BAE):

$$ \frac{\lambda_j + i(S' + c)}{\lambda_j - i(S' + c)} \cdot \frac{\lambda_j + i(S' - c)}{\lambda_j - i(S' - c)} \cdot [\frac{\lambda_j + iS}{\lambda_j - iS}]^{2N+1} = \prod_{i \neq j}^{M} \frac{\lambda_j - \lambda_i + i}{\lambda_j - \lambda_i - i} \cdot \frac{\lambda_j + \lambda_i + i}{\lambda_j + \lambda_i - i}. $$

(13)

The energy of the Hamiltonian (7) is

$$ E = -J_0 \sum_{j=1}^{M} \frac{S}{\lambda_j^2 + S^2} $$

(14)

up to a rapidity-independent constant. The magnetization is given by $S_z = NS + S' - M$ with $M$ being the number of down-spins. It is recalled that when $S' = S$, $c = 0$ (or $J = J_0$), the impurity is just the one more site of the chain. For convenience, we put $J_0 = 1$ in the following text.

III. GROUND STATE, BOUNDARY CORRELATOR AND BOUNDARY STRINGS

Due to the reflection symmetry of the model and its Bethe ansatz equation, there is a restriction on the rapidities: $\lambda_j \neq \pm \lambda_l$, for $j \neq l$. Therefore, $\lambda_j = 0$ is forbidden in this
system. Generally, the bulk solutions of (13) can be described by the following strings in the thermodynamic limit

$$\lambda^n_{j,\gamma} = \lambda^n_{\gamma} + \frac{i}{2}(n - 2j + 1), \quad j = 1, 2, \cdots, n$$

(15)

with \(\lambda^n_{\gamma}\) a positive real number. Since \(c\) and \(-c\) give the same Hamiltonian, not losing generality, we consider only \(c > 0\) (\(c\) real) or \(Im \ c > 0\) (\(c\) imaginary) cases. For \(c < S'\) and or imaginary \(c\), (15) are the only possible solutions of the Bethe ansatz equation (13).

For each class of states classified by \(n\)-strings, we introduce the usual density distribution function \(\rho_n(\lambda)\) and \(\rho_{n,h}(\lambda)\), representing occupied states (particles) and missing states (holes) respectively. The Bethe ansatz equation of the \(n\)-strings reads:

$$\rho_{n,h}(\lambda) + \sum_{l=1}^{\infty} A_{nl} \rho_l(\lambda) = a_{n,2S}(\lambda) + \frac{1}{2N} [\phi_{n}^{imp}(\lambda) + \phi_{n}^{edg}(\lambda)],$$

(16)

where \(a_n(\lambda) = n/2\pi(\lambda^2 + n^2/4), a_{n,l}(\lambda) = \sum_{k=1}^{\min(n,l)} a_{n+l-1-2k}(\lambda); A_{nl}\) is an integral operator with the kernel

$$A_{nl}(\lambda) = a_{|n+l|}(\lambda) + 2 \sum_{k=1}^{\min(n,l)-1} a_{n+l-2k}(\lambda) + a_{|n-l|}(\lambda),$$

\(\phi_n^{imp}(\lambda) = a_{n,2S'}(\lambda - ic) + a_{n,2S'}(\lambda + ic)\) is the impurity contribution; \(\phi_n^{edg}(\lambda) = a_n(\lambda) + a_{n+1}(\lambda) + a_{n-1}(\lambda)(1 - \delta_{1,n})\) is the surface or edge term, which is independent of the magnetic impurity. Notice \(\delta(\lambda)\) in \(\phi_n^{edg}\) is included to cancel the \(\lambda^n_{\gamma} = 0\) term, which is the solution of the Bethe ansatz equation but corresponds to a zero wave function (a direct result of the restriction \(\lambda_j \neq \lambda_l\)). In the ground state, only \(2S\)-strings exist\(^2\) and (16) is reduced to

$$A_{2S,2S} \rho_{2S}(\lambda) = a_{2S,2S}(\lambda) + \frac{1}{2N} [\phi_{2S}^{imp}(\lambda) + \phi_{2S}^{edg}(\lambda)],$$

(17)

By Fourier transforming (17), we readily obtain

$$\rho_{2S}(\lambda) = \rho_{2S}^0(\lambda) + \frac{1}{2N} [\rho_{2S}^{imp}(\lambda) + \rho_{2S}^{edg}(\lambda)],$$

(18)

$$\rho_{2S}^0(\lambda) = \frac{1}{2\cosh(\pi\lambda)};$$

(19)

$$\rho_{2S}^{imp}(\lambda) = \frac{1}{2\pi} \int \frac{\sinh(S'\omega) \cosh(c\omega)}{\cosh(S\omega)} e^{-i\omega\lambda} d\omega, \quad \text{for} \ S > S'$$

(20)
\[ \rho_{2S}^{\text{imp}}(\lambda) = \frac{1}{2\pi} \int \frac{e^{-(S-S')|\omega|} \cosh(c\omega)}{\cosh \frac{\omega}{2}} e^{-i\omega \lambda} d\omega, \quad \text{for } S < S' \]  

\[ \rho_{2S}^{\text{edg}}(\lambda) = \frac{1}{2\pi} \int \frac{\tanh \frac{\omega}{2}(1 - e^{S|\omega|})}{2 \sinh(S\omega)} e^{-i\lambda \omega} d\omega + \rho_{2S}(\lambda). \]  

The ground state energy can be readily calculated as

\[ E_0/N = f_{\text{bulk}}^0 + \frac{1}{N} (F_{\text{imp}}^0 + F_{\text{edg}}^0 + \frac{1}{2} f_{\text{bulk}}^0), \]  

\[ f_{\text{bulk}}^0 = \frac{1}{2}[\Psi(\frac{1}{2}) - \Psi(\frac{1}{2} + S)], \]  

\[ F_{\text{imp}}^0 = \frac{1}{4} \sum_{r=\pm} [\Psi(\frac{1}{2} + \frac{1}{2}|S - S'| + irc) - \Psi(\frac{1}{2} + \frac{1}{2}(S + S') + irc)], \]  

\[ F_{\text{edg}}^0 = \frac{1}{4} [\Psi(\frac{1}{2} + \frac{1}{2}(S - \frac{1}{2})) - \Psi(\frac{1}{2} + \frac{1}{2}(S + \frac{1}{2})) + \Psi(\frac{1}{2} + \frac{1}{2}|S - 1|) - \Psi(\frac{1}{2} + \frac{1}{2}(S + 1))]. \]  

where \( \Psi \) is the digamma function. As a byproduct, the correlator of \( \vec{S}' \) and \( \vec{S}_1 \) can be exactly derived for the present model. When \( S = 1/2 \) or \( S' = 1/2 \) we have

\[ < \vec{S}' \cdot \vec{S}_1 > = \frac{\partial}{\partial J} E_0. \]  

Since \( c \) (and therefore \( J \)) is only included in \( \rho_{2S}^{\text{imp}}(\lambda) \), we need only the impurity energy \( F_{\text{imp}}^0 \). The boundary correlator can be calculated as

\[ < \vec{S}' \cdot \vec{S}_1 > = J^{-2} \frac{\partial}{\partial c^2} F_{\text{imp}}^0. \]  

Now we turn to \( c > S' \) case. In addition to the \( n \)-string solutions (15), an imaginary mode \( \lambda = i(c - S') \) appears to be a solution of the Bethe ansatz equation (13). In fact, in this case a so-called boundary \( n-k \)-string is possible solution of the BAE

\[ \lambda_{bs}^{n-k,m} = i(c - S') + im, \quad m = k, k + 1, \cdots, n, \]  

where \( k < S' - c \) or \( k = 0 \). Generally, there is no restriction for \( n \) in the spin chain with a boundary field. However, in our case, \( \lambda = \pm i(S' + c) \) are not solutions as we can see from the Bethe ansatz equation. That means \( n < 2S' \). In addition, for \( 2c = \text{integer case} \), \( k \) must be zero due to the restriction \( \lambda_j \neq \lambda_l, j \neq l \). Suppose there is an \( n - k \) boundary string in
the ground state configuration. The change of the $2S$-string distribution $\rho_{bs}(\lambda)/2N$ can be readily derived from the following equation

$$A_{2S,2S}\rho_{bs}(\lambda) = -\sum_{l=k}^{n}\left\{a_{2S,2S}[\lambda - i(c - S') + l] + a_{2S,2S}[\lambda + i(c - S') + l]\right\}. \quad (30)$$

The energy carried by the boundary string is

$$\epsilon_{bs} = -\frac{\pi}{2} \int a_{2S,2S}(\lambda)\rho_{bs}(\lambda) - \sum_{l=k}^{n}\frac{S}{S^2 - (c - S' + l)^2}. \quad (31)$$

By solving (30) via Fourier transformation and submitting $\rho_{bs}$ into (31), we find $\epsilon_{bs} = 0$. That means the boundary string contributes nothing to the total energy in the thermodynamic limit. It corresponds to a charged vacuum in the sine-Gordon theory\textsuperscript{29}. We remark that some boundary string will be stabilized with a finite magnetization. Such a situation is much like those of the fermion systems with boundary potential\textsuperscript{29} or Kondo impurity\textsuperscript{20,22}.

**IV. THERMODYNAMICS**

In this section, we consider the thermodynamics of $c \leq S'$ (antiferromagnetic) case. The thermodynamic Bethe ansatz equations can be derived by following the standard method\textsuperscript{10,24}. At finite temperatures, the solutions of BAE are described by (15). The energy of the system takes the form

$$\frac{E}{N} = -\pi \sum_{n=1}^{\infty} \int a_{n,2S}(\lambda)\rho_n(\lambda)d\lambda + \sum_{n=1}^{\infty} nH \int \rho_n(\lambda)d\lambda, \quad (32)$$

where $H$ is the external magnetic field. The entropy of the system reads

$$S/N = \sum_{n=1}^{\infty} \int \{(\rho_n + \rho_{n,h}) \ln(\rho_n + \rho_{n,h}) - \rho_n \ln \rho_n - \rho_{n,h} \ln \rho_{n,h}\}d\lambda. \quad (33)$$

By minimizing the free energy $F = E - TS$ we readily obtain the following equation

$$\ln(1 + \eta_n) = \frac{nH - \pi a_{n,2S}}{T} + \sum_{l=1}^{\infty} A_{n,l} \ln(1 + \eta_l^{-1}), \quad (34)$$

where $\eta_n(\lambda) \equiv \rho_{n,h}(\lambda)/\rho_n(\lambda)$ and $\eta_0(\lambda) \equiv 0$. With the identities
\[ A_{n,m} - G(A_{n-1,m} + A_{n+1,m}) = \delta_{n,m}, \quad A_{1,m} - GA_{2,m} = \delta_{1,m}, \quad (35) \]

\[ B_{n,m} - G(B_{n-1,m} + B_{n+1,m}) = \delta_{n,m}, \quad B_{1,m} - GB_{2,m} = \delta_{1,m}. \quad (36) \]

where \( B_{n,m} \) and \( G \) are integral operators with the kernels \( a_{n,m}(\lambda) \) and \( \frac{1}{2} \cosh(\pi \lambda) \) respectively, (34) can be reduced to

\[ \ln \eta_n = - \frac{\pi}{2T \cosh(\pi \lambda)} \delta_{n,2S} + G[\ln(1 + \eta_{n-1}) + \ln(1 + \eta_{n+1})], \quad (37) \]

with the boundary condition

\[ \lim_{n \to \infty} \frac{\ln \eta_n}{n} = \frac{H}{T}. \quad (38) \]

(37) is almost the same equation to that of the 2S-channel Kondo problem with only a different driving term. The free energy reads

\[ \frac{F}{N} = f_{\text{bulk}} + \frac{1}{N} F_{\text{imp}} + \frac{1}{N} F_{\text{edg}}, \quad (39) \]

\[ f_{\text{bulk}} = f_{\text{bulk}}^0 - T \int [2 \cosh(\pi \lambda)]^{-1} \ln[1 + \eta_{2S}(\lambda)] d\lambda, \quad (40) \]

\[ F_{\text{edg}} = \frac{1}{4} H - \frac{1}{2} T \int [2 \cosh(\pi \lambda)]^{-1} \{ \ln[1 + \eta_{1}(\lambda)] + \ln[1 + \eta_{2}(\lambda)] \} d\lambda, \quad (41) \]

\[ F_{\text{imp}} = -(S' - \frac{1}{2}) H - \frac{1}{2} T \sum_{n=1}^{\infty} \int \Phi_{n}^{\text{imp}}(\lambda) \ln[1 + \eta_{n}^{-1}(\lambda)] d\lambda, \quad (42) \]

It is not easy to reduce further \( F_{\text{imp}} \) for arbitrary real \( c \). The boundary behaves always as a spin-1/4 (in fact one half of a spin-1/2) and its critical effect in the XXZ spin-1/2 chain has been discussed in a previous work. In our case, the “boundary spin” shows overscreened critical behavior as will be discussed in the following text.

**A. High Temperature Limit**

When \( T \to \infty \), the driving term tends to zero. Therefore in this limit the functions \( \eta_n(\lambda) \) tend to constants \( \eta^-_n \) satisfying the algebraic equation

\[ \eta_n^- = (1 + \eta^-_{n-1})(1 + \eta^-_{n+1}), \quad (43) \]

with the boundary conditions
\[ \eta_0^- \equiv 0, \quad \lim_{n \to \infty} \frac{\ln \eta_n^-}{n} = \frac{H}{T} \equiv 2x_0. \quad (44) \]

The solutions of (43) are
\[ \eta_n^- = \frac{\sinh^2(n + 1)x_0}{\sinh^2 x_0} - 1. \quad (45) \]

Substituting (45) into (41) we get
\[ F_{edg} \sim -\frac{1}{2} T \ln(2 \cosh x_0). \quad (46) \]

Notice that only the pure boundary term is given in the above expression. Obviously, the open boundary’s contribution to the free energy is one half of a spin-1/2. The entropy of the open boundary is \( \ln \sqrt{2} \). To calculate the impurity free energy, we note that the integral kernel \( \Phi_{imp}^n \) in (42) can be written with real variable as
\[ \Phi_{imp}^n(\lambda) = \sum_{r=\pm} \sum_{k=1}^{n} a_{n+1+2S'+2rc-2k}(\lambda) \epsilon(n + 1 + 2S' + 2rc - 2k), \quad (47) \]
where \( \epsilon(x) = \text{sign}(x) \) and \( \epsilon(0) = 0 \). Since all \( a_n(\lambda) \) are equivalent to \( \delta(\lambda) \) in \( T \to \infty \) limit, we can replace (47) by
\[ \Phi_{imp}^n(\lambda) \to a_{n,2S'-cI}(\lambda) + a_{n,2S'+cI}(\lambda), \quad \text{for} \quad c_I = 2c \quad (48) \]
\[ \Phi_{imp}^n(\lambda) \to a_{n,2S'-cI}(\lambda) + a_{n,2S'+cI}(\lambda) + \delta(\lambda) \sum_{l=1}^{c_I} \delta_{n,2S'-cI+2l-1}, \quad \text{for} \quad c_I \neq 2c, \quad (49) \]
where \( c_I \) is the integer part of \( 2c \). Therefore, the impurity free energy reads
\[ F_{imp} \sim -\frac{1}{4} T [\ln(1 + \eta_{2S'-cI}) + \ln(1 + \eta_{2S'+cI})], \quad \text{for} \quad c_I = 2c, \quad (50) \]
\[ F_{imp} \sim -\frac{1}{4} T [\ln(1 + \eta_{2S'-cI}) + \ln(1 + \eta_{2S'+cI})] \]
\[ + \frac{1}{2} T \sum_{l=1}^{c_I} [\ln(1 + \eta_{2S'-cI+2l-1}) - \ln \eta_{2S'-cI+2l-1}], \quad \text{for} \quad c_I \neq 2c. \quad (51) \]

The entropy of the impurity is
\[ S_{imp} = \ln \sqrt{(2S' + 1)^2 - c_I^2}, \quad \text{for} \quad c_I = 2c, \quad (52) \]
\[ S_{imp} = \ln \sqrt{(2S' + 1)^2 - c_I^2} \]
\[ - \sum_{l=1}^{c_I} \ln \frac{2S' - c_I + 2l}{\sqrt{(2S' - c_I + 2l - 1)(2S' - c_I + 2l + 1)}}, \quad \text{for} \quad c_I \neq 2c. \quad (53) \]
¿From (52-53) we see that even at high temperature limit, the impurity spin is split into ghost spins via the boundary bond deformation. Though the magnetization of the impurity is almost the same to that of a free spin $\vec{S}'$, the entropy is strongly interaction-dependent.

**B. Low Temperature Limit**

When $T \to 0$, the driving term in (37) diverges. That means $\eta_{2S} \to 0$ and all other $\eta_n$ tend to constant $\eta_n^+$ which satisfy the same equation of $\eta_n^-$ but with a different boundary condition. Since the equation is decoupled at $n = 2S$, we have different solutions for $n > 2S$ and $n \leq 2S$

$$\eta_n^+ = \frac{\sinh^2(n - 2S + 1)x_0}{\sinh^2 x_0} - 1, \quad \text{for} \quad n \geq 2S,$$

$$\eta_n^+ = \frac{\sin^2 \frac{n \pi}{2(S+1)}}{\sin^2 \frac{n \pi}{2(S+1)}} - 1, \quad \text{for} \quad n < 2S.$$  

The residual entropy of the open boundary is

$$S_{\text{edg}} = \frac{1}{2} \ln[2 \cos \frac{\pi}{2(S + 1)}].$$ 

For $2c = c_I$, the impurity behaves still as two ghost spins $S' + c_I/2$ and $S' - c_I/2$. The entropy of a ghost spin $\bar{S}$ reads

$$S_{\text{ghost}} = \frac{1}{2} \ln[2(\bar{S} - S) + 1], \quad \text{for} \quad |\bar{S}| > S,$$

$$S_{\text{ghost}} = \frac{1}{2} \ln \frac{\sin \frac{\pi 2S + 1}{2(S+1)}}{\sin \frac{\pi}{2(S+1)}}, \quad \text{for} \quad |\bar{S}| \leq S.$$ 

The summation of the two ghost spins’ entropy gives that of the whole impurity. When $c_I \neq 2c$, the difference between the residual entropies for $c_I \neq 2c$ and $c_I = 2c$, i.e., $\Delta S_{\text{imp}}$ reads

$$\Delta S_{\text{imp}} = -\frac{1}{2} \sum_{l=1}^{c_I} [\ln(1 + f_{2S' - c_I + 2l - 1}) - \ln f_{2S' - c_I + 2l - 1}],$$

with $f_n = \lim_{x_0 \to 0} \eta_n^+$. This result shows that the spin configuration of the ground state is very complicated and strongly depends on the impurity-bulk coupling. It would be plausible
to coin it as a local spin glass. In fact, the residual entropy has jumps at \( c = c_I/2 \). That means quantum phase transition occurs for \( c \) across a half integer or an integer.

To obtain the leading order of some thermodynamic quantities such as the specific heat and the susceptibility, we need the low temperature (\( T << T_k \)) expansion. This can be done by following the standard method developed for the multi-channel Kondo problem. For \( T \to 0 \), only the excitations near the Fermi surface (\( \lambda \to \pm \infty \)) are important. The driving term in (37) can be approximately replaced by \( -(\pi/T)exp(-\pi|\lambda|) \). We introduce the new variables \( \zeta_\pm = \pm \pi \lambda + \ln(\pi/T) \), then \( \eta_n \) take the following asymptotic form

\[
\eta_n(\zeta_\pm) \sim \eta_n^+ + (\alpha_n + \beta_n x_0^2)e^{-\zeta_\pm}, \quad \text{for} \quad n \geq 2S, \tag{60}
\]

\[
\eta_n(\zeta_\pm) \sim \eta_n^+ + (\alpha_n + \beta_n x_0^2)e^{-\tau \zeta_\pm}, \quad \text{for} \quad n < 2S. \tag{61}
\]

Here \( \alpha_n \) and \( \beta_n \) are constants, \( \tau = 2/(S+1) \) and \( \pm \) denotes the two Fermi points. For imaginary \( c = ib \), the free energy of the impurity reads

\[
F_{\text{imp}} \sim F_{\text{imp}}^0 - T \int \left[ \frac{1}{2 \cosh(\zeta + \pi b - \ln \frac{\pi}{T})} + \frac{1}{2 \cosh(\zeta - \pi b - \ln \frac{\pi}{T})} \right] \ln(1 + \eta_{2S'})d\zeta. \tag{62}
\]

Notice that we have replaced \( \zeta_\pm \) by \( \zeta \) in the integral. In this case, the bond deformation does not change the effective strength of the impurity but the energy scale \( T_k \) (Kondo temperature)

\[
T_k \sim \pi \cosh^{-1}(\pi b). \tag{63}
\]

The system behaves as a 2\( S \)-channel Kondo system with an impurity \( \vec{S}' \). For real \( c \) and \( c_I = 2c \), the free energy of the impurity can be rewritten as

\[
F_{\text{imp}} \sim F_{\text{imp}}^0 - T \sum_{\pm} \int G_\pm \left[ \frac{1}{\pi(\zeta - \ln \frac{\pi}{T})} \right] \ln(1 + \eta_{2S'\pm\epsilon I})d\zeta. \tag{64}
\]

For \( c_I \neq 2c \),

\[
F_{\text{imp}} \sim F_{\text{imp}}^0 - T \sum_{\pm} \int G_\pm \left[ \frac{1}{\pi(\zeta - \ln \frac{\pi}{T})} \right] \ln(1 + \eta_{2S'\pm\epsilon I})d\zeta - \frac{T}{2\pi} \sum_{l=1}^{c_I} \int \left[ \frac{1}{\pi(\zeta - \ln \frac{\pi}{T})} \right]^2 + \left( c - \frac{1}{2} \epsilon I \right)^2 \ln(1 + \eta_{2S'\pm\epsilon I + 2l - 1})d\zeta, \tag{65}
\]
where

\[ G_{\pm}(\lambda) = \int \frac{e^{\mp(c-\frac{1}{2}c_I)\omega}}{4\pi \cosh \frac{\omega}{2}} e^{-i\lambda \omega} d\omega. \] (66)

Notice \( G_{\pm}(\lambda) \) are convergent in the real axis since \( c - c_I/2 < 1/2 \). The specific heat and the susceptibility can be easily derived from the free energy. With different values of \( c \), different quantum critical behavior may appear. (i) For \( S \pm c_I/2 \geq S \), both the ghost spins are underscreened and the leading terms in the specific heat and the susceptibility are the Schottky term and the Curie term respectively. (ii) For \( S' - c_I/2 < S < S' + c_I/2 \), no matter how large \( S' \) is,

\[ C_{\text{imp}} \sim T, \quad \chi_{\text{imp}} \sim T^{-1} + O(T^{r-1}), \] (67)

which indicate a novel critical behavior. (iii) For \( S' \pm c_I/2 < S \), the system behaves as a conventional overscreened Kondo system. The above results show that the bond deformation has two effects: The half integer part of \( c (c_I/2) \) renormalizes the impurity spin and the rest \( (c - c_I/2) \) renormalizes the effective energy scale \( T_k \) (Kondo temperature).

V. CONCLUDING REMARKS

In conclusion, we propose an integrable model of a boundary impurity spin \( \vec{S}' \) coupled with an open Takhatajian-Babujian spin-\( S \) chain. The relation between the present model and the bulk impurity problem in a spin chain is discussed. In our model, when \( S \) or \( S' \) is one half, The “fine tuned” effect in the periodic integrable models is overcome and the interaction term in our case takes a very simple form. The coupling constant \( J \) can take arbitrary value without destroying the integrability of the Hamiltonian, while in the periodic models, there is a constraint to \( J \). Though a similar \( s's R^0(\lambda - c) \) can be introduced in the periodic models, the parameter \( c \) must be real (imaginary in our case) which describes a weak-linked impurity to the bulk. The interaction only affects the energy scale (Kondo temperature) but does not change the fixed point of the system. With an imaginary \( c \), the
model Hamiltonians constructed for bulk impurities are non-Hermitian and their spectra generally lie in the complex plane rather than in the real axis completely. In our model, both real $c$ and imaginary $c$ define a Hermitian Hamiltonian due to the reflection symmetry, and the coupling constant $J$ meets all physical situations. Some new quantum critical phenomena driven by the impurity-bulk coupling have been found, which can never appear in the periodic models: (i) The stronger coupling $J$ may split the impurity spin into effective “ghost spins” $S' - c_I/2$ and $S' + c_I/2$. That means the coupling not only change the energy scales (Kondo temperature) as in the conventional Kondo problem but also renormalizes the effective strength of the impurity spin. It seems that the strength of these ghost spins does not change via temperature. Such a phenomenon reveals a pure correlation effect. We remark a similar effect can be induced by the impurity potential in the Luttinger-Kondo problems. (ii) Depending on the strength of the coupling, the system may show a variety of critical behavior differing from those of the conventional Kondo problems. A typical example is that when $S' - c_I/2 < S < S' + c_I/2$, the leading term in the susceptibility is Curie type, while that of the specific heat is overscreened $2S$-channel Kondo type. Such a fascinating non-Fermi liquid behavior has never been found in the conventional impurity problem (notice these are induced by the same impurity). (iii) The open boundary, which can be produced by either an impurity (no matter magnetic or non-magnetic) or bond deformation, shows overscreened multi-channel behavior as long as the bulk spin $S > 1/2$. Such an effect is caused by the self-avoiding of the scattering of each spin-wave with its reflection counterpart and is common to the multi-channel systems in 1D. Our results strongly suggests that some new intermediate fixed point may exist for the Kondo problem in a strongly correlated host.

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