Kondo effect in XXZ spin chains

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The Kondo effect in a one-dimensional spin-$\frac{1}{2}$ XXZ model in the gapless XY regime $(-1<\Delta\leqslant 1)$ is studied both analytically and numerically. In our model an impurity spin $(S=1/2)$ is coupled to a single spin in the XXZ spin chain. Perturbative renormalization-group (RG) analysis is performed for various limiting cases to deduce low-energy fixed points. It is shown that in the ground state the impurity spin is screened by forming a singlet with a spin in the host XXZ chain. In the antiferromagnetic side $(0<\Delta\leqslant 1)$ the host chain is cut into two semi-infinite chains by the singlet. In the ferromagnetic side $(-1<\Delta<0)$, on the other hand, the host XXZ chain remains as a single chain through ''healing'' of a weakened bond in the low-energy (long-distance) limit. The density-matrix renormalization-group method is used to study the size scaling of finite-size energy gaps and the power-law decay of correlation functions in the ground state. The numerical results are in good agreement with the predictions of the RG analysis. Low-temperature behaviors of specific heat and susceptibility are also discussed. [S0163-1829(98)04433-6]

I. INTRODUCTION

There has been a recent resurgence of interest in the Kondo effect[1] in one-dimensional (1D) strongly correlated systems. In 1D interacting systems belonging to the universality class of the Tomonaga-Luttinger (TL) liquids, a static impurity potential has a drastic effect and is renormalized to infinity or zero, depending on whether the interaction is repulsive or attractive.[2] This anomalous response to a static impurity of TL liquids has attracted a lot of attention and has led to further studies on the effects of a dynamic impurity (typically a magnetic impurity) in a TL liquid. A generalized Hubbard model with an impurity spin $(S=\frac{1}{2})$ and its variants have been studied by many authors. It was found that the Kondo temperature, which is a typical energy scale for host electrons to screen an impurity spin, has a power-law dependence on the Kondo exchange coupling.[3–5] Properties of low-energy fixed points have been discussed using perturbative renormalization-group analysis[4] and the boundary conformal field theory approach.[6–8] A recent Monte Carlo study[9] on the susceptibility of an impurity spin is consistent with anomalous power-law temperature dependence conjectured earlier.[4] In addition to the models with a simple Kondo coupling, there are some exactly solvable models in which an impurity spin is coupled to the spin density of electrons via special forms of the Kondo exchange coupling.[10,11] These solvable models, however, do not show the anomalous power-law behavior of the specific heat[10] because the operator responsible for this anomalous scaling is absent in the models constructed to be integrable. It seems that these solvable models do not represent a generic situation, and we will not address this issue further.

In this paper we consider a simplified model that we believe shares common features with the above-mentioned Kondo effect in 1D interacting electronic models like the Hubbard model. We here focus on the spin sector and discard the charge degree of freedom. This may correspond to the half-filled case in the original electronic models. The Hamiltonian of the system we discuss in this paper has the form $H=H_0+H_K$, where H_0 describes the host $S=\frac{1}{2}$ XXZ spin chain,

$$H_0=J\sum_{i=-\infty}^{\infty}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z),\tag{1}$$

and H_K the Kondo coupling,

$$H_K=J_K(S_0^xS_{\rm imp}^x+S_0^yS_{\rm imp}^y+\Delta S_0^zS_{\rm imp}^z).\tag{2}$$

The size of the impurity spin is also assumed to be 1/2. An important point of our model is the absence of SU(2) spin-rotation symmetry. We assume $|\Delta|<1$ to ensure that the host XXZ spin chain has gapless excitations. For simplicity we have used the same parameter Δ in H_0 and H_K. We note that Δ in H_0 is an important parameter controlling the power-law behavior of various correlations while Δ in H_K does not play any significant role in the following discussions. The Kondo coupling J_K can be either antiferromagnetic or ferromagnetic, but we will concentrate on the antiferromagnetic case $(J_K>0)$ in this paper. We will show in this paper that, when $0<\Delta<1$, the Kondo effect in the XXZ spin chain is very similar to the Kondo effect in TL liquids with $\frac{1}{2}<K_\rho<1$ and $K_\sigma=1$, where K_ρ and K_σ are parameters characterizing the TL liquids.[4] In this sense our model can be regarded as a toy model for the Kondo problem in 1D interacting electron systems.[12] We note that in Eq. (2) the impurity spin is coupled to a *single* spin located in the *middle* of the chain, unlike the model studied by Clarke *et al.*,[14] where an impurity spin is coupled to two spins symmetrically, and the model studied by Wang,[15] where an impurity spin is coupled to a boundary spin. This different form of Kondo coupling leads to different scaling behavior in both weak- and strong-coupling regimes.

Eggert and Affleck[16,17] studied, among various kinds of disorder, the model at the isotropic point ($\Delta=1$). They concluded that the impurity spin $\boldsymbol{S}_{\rm imp}$ forms a singlet with $\boldsymbol{S}_0$, and that the Heisenberg chain is decoupled into two semi-infinite chains in the low-energy limit. A leading irrelevant operator at the fixed point was identified and shown to have scaling dimension 2. It corresponds to exchange coupling between boundary spins of the two decoupled chains. In this paper we extend their analysis to the XXZ case ($|\Delta|<1$). We first bosonize the Hamiltonian and study its renormalization-group (RG) flows in the weak-coupling limit and in the strong-coupling limit. We will argue that the system is renormalized to stable low-energy fixed points where the impurity spin ($S=\frac{1}{2}$) is screened exactly. At the fixed points the boundary condition for the host XXZ spin chain depends on the parameter Δ of the host chain: For $0<\Delta\leqslant 1$ the spin chain is cut into two semi-infinite chains with open boundary condition at $i=\pm 1$. On the other hand, for $-1<\Delta<0$ the host spin chain is not affected much by the singlet and stays as a single chain. Leading irrelevant operators at these fixed points have noninteger scaling dimensions, yielding a noninteger power-law temperature dependence of the impurity contribution to specific heat and susceptibility. As evidence for this picture we will show finite-size scaling of the energy gap and spin-spin correlation functions in the ground state, both of which are obtained by using the density-matrix renormalization-group (DMRG) method. The numerical results are consistent with the picture drawn from the perturbative RG analysis. We note that our results are very different from a recent paper by Liu,[18] who studied the same model as ours and calculated various quantities near a strong-coupling fixed point. For example, he obtained super-linear temperature dependence (T^{α}, $\alpha>1$) for the impurity contribution to the specific heat and vanishing susceptibility at zero temperature, both of which cannot be correct on general grounds.

The plan of this paper is as follows. In Sec. II we discuss RG flows of our model using the standard Abelian bosonization method. Impurity contributions to specific heat and susceptibility are also discussed. We show results of numerical DMRG calculations in Sec. III and compare them with conclusions of the perturbative RG in Sec. II. For simplicity we set $J=1$ throughout this paper.

II. PERTURBATIVE RENORMALIZATION-GROUP ANALYSIS

A. Weak-coupling limit

We follow Ref. 16 and bosonize the Hamiltonian H. Since the bosonization of the XXZ chain is a standard procedure, we do not repeat the derivation of a bosonized Hamiltonian here. After performing the Jordan-Wigner transformation and taking a continuum limit, we find that H_0 reduces to a free-boson model,

$$H_0^{(b)}=\frac{v}{2}\int_{-\infty}^{\infty}dx\left[\left(\frac{d\phi}{dx}\right)^2+\Pi^2\right], \tag{3}$$

where $\Pi(x)$ is a conjugate operator to the bosonic field $\phi(x)$: $[\phi(x),\Pi(y)]=i\delta(x-y)$. The spin-wave velocity v is known to be $v=(\pi/2\theta)\sin\theta$, where $\theta=\cos^{-1}\Delta$. The spins in the chain can be represented in terms of bosonic fields $\phi(x)$ and $\tilde{\phi}(x)$ ($\Pi=d\tilde{\phi}/dx$):[16,19]

$$S_j^z=\frac{1}{2\pi R}\frac{d\phi}{dx}+c_1(-1)^j\cos\frac{\phi}{R}, \tag{4a}$$

$$S_j^+=e^{i2\pi R\tilde{\phi}}\left[c_2\cos\frac{\phi}{R}+c_3(-1)^j\right], \tag{4b}$$

where $S_j^{\pm}=S_j^x\pm iS_j^y$. Here $x\approx j$ and the c_j's are numerical constants. The lattice spacing is assumed to be unity. The parameter R in Eqs. (4a) and (4b) is related to Δ in the original Hamiltonian (1) as

$$R=\left[\frac{1}{2\pi}\left(1-\frac{1}{\pi}\cos^{-1}\Delta\right)\right]^{1/2}. \tag{5}$$

With the Gaussian form of $H_0^{(b)}$, we can immediately find the scaling dimensions of operators $e^{ia\phi}$ and $e^{ia\tilde{\phi}}$, both of which are $a^2/4\pi$. Thus the dimensions of the staggered components of S_i^z and $S^{\pm}$ are $(4\pi R^2)^{-1}$ and πR^2, respectively.

From Eqs. (4a) and (4b) the Kondo interaction term H_K becomes

$$H_K^{(b)}=S_{\rm imp}^{+}e^{-i2\pi R\tilde{\phi}(0)}\left(\lambda_{F\perp}\cos\frac{\phi(0)}{R}+\lambda_{B\perp}\right)+\text{H.c.}$$
$$+S_{\rm imp}^{z}\left(\lambda_{Fz}\frac{d\phi(0)}{dx}+\lambda_{Bz}\cos\frac{\phi(0)}{R}\right), \tag{6}$$

where the couplings λ's are proportional to J_K. Since the impurity spin is coupled to a single spin $\boldsymbol{S}_0$ in our model, we have backward Kondo scattering terms proportional to λ_{Bz} and $\lambda_{B\perp}$. These terms do not appear in some models where $\boldsymbol{S}_{\rm imp}$ is coupled symmetrically to two neighboring spins, say $\boldsymbol{S}_0$ and $\boldsymbol{S}_1$.[20,21,14] These backscattering terms are important ingredients of our model. The backward spin-flip scattering term ($\propto\lambda_{B\perp}$) has scaling dimension πR^2 and is always a relevant operator. This should be contrasted with the conventional Kondo problem in 3D, where the Kondo interaction is a marginal operator of the form $d\phi/dx$. Therefore we conclude that the weak-coupling point ($J_K=0$) is unstable for $-1<\Delta\leqslant 1$ independent of the sign of J_K, and the system always flows to a strong-coupling regime. This situation is quite similar to the Kondo effect in a TL liquid.[4] To lowest order the scaling equation of the most divergent coupling $\lambda_{B\perp}$ is given by

$$\frac{d\lambda_{B\perp}}{d\ln L}=(1-\pi R^2)\lambda_{B\perp}, \tag{7}$$

where L is system size. We thus expect that the energy scale T_K at which the crossover from weak coupling to strong coupling occurs should be

$$T_K\propto|\lambda_{B\perp}|^{1/(1-\pi R^2)}\propto|J_K|^{1/(1-\pi R^2)} \tag{8}$$

for $|J_K|\ll J(=1)$. We identify this energy scale with the Kondo temperature.[22]

B. Strong-coupling limit for $0<\Delta\leqslant 1$

Let us consider the strong-coupling limit where $J_K \gg 1$. In this limit we first diagonalize H_K and treat the coupling between $\boldsymbol{S}_0$ and its neighbors ($\boldsymbol{S}_{\pm 1}$) as weak perturbations. The ground state of H_K is a spin singlet ($\boldsymbol{S}_0+\boldsymbol{S}_{\rm imp}=0$). In the limit $J_K\to\infty$ the system consists of the singlet and two decoupled semi-infinite chains (SIC's). With very large but finite J_K, we derive effective interactions acting on the subspace of the singlet plus the SIC's using $1/J_K$ expansion.[24] Second-order perturbation yields

$$H_2=-\frac{1}{2J_K(1+\Delta)}(S_1^+S_{-1}^-+S_1^-S_{-1}^+)-\frac{\Delta^2}{2J_K}S_1^zS_{-1}^z+\text{const.} \tag{9}$$

Higher-order calculations also give the same form of interactions (and irrelevant operators). We now need to know the bosonization of these operators $\boldsymbol{S}_{\pm 1}$ at the boundaries of the SIC's. This was discussed in detail by Eggert and Affleck[16] and we can simply borrow their results. The open-boundary condition implies that the phase field $\phi(x)$ is fixed to be some constant at $x=0$. To be specific, let us impose $\phi(0)=0$. The left-going field $\phi_L(x)=\sqrt{\pi}[\phi(x)+\tilde{\phi}(x)]$ and the right-going field $\phi_R(x)=\sqrt{\pi}[\phi(x)-\tilde{\phi}(x)]$ are no longer independent. From these chiral fields we introduce two left-going fields:

$$\phi_>(x)=\Theta(x)\phi_L(x)-\Theta(-x)\phi_R(-x), \tag{10a}$$

$$\phi_<(x)=\Theta(-x)\phi_L(x)-\Theta(x)\phi_R(-x), \tag{10b}$$

where $\Theta(x)$ is a Heaviside step function. The field $\phi_>(x)$ describes bosonic excitations in the SIC of the positive x region ($\boldsymbol{S}_i$: $i>0$), and the other field $\phi_<$ describes excitations in the negative x region. Their commutation relations are $[\phi_>(x),\phi_>(y)]=[\phi_<(x),\phi_<(y)]=-i\pi\,\text{sgn}(x-y)$ and $[\phi_>(x),\phi_<(y)]=0$. Their dynamics is governed by the Hamiltonian

$$H_{\rm SIC}=\frac{v}{4\pi}\int_{-\infty}^{\infty}dx\left[\left(\frac{d\phi_>}{dx}\right)^2+\left(\frac{d\phi_<}{dx}\right)^2\right]. \tag{11}$$

With these fields the boundary spins can be written as

$$S_1^{\pm}\propto\exp[\pm i2\sqrt{\pi}R\phi_>(0)],\quad S_1^z\propto\frac{d\phi_>(0)}{dx}, \tag{12a}$$

$$S_{-1}^{\pm}\propto\exp[\pm i2\sqrt{\pi}R\phi_<(0)],\quad S_{-1}^z\propto\frac{d\phi_<(0)}{dx}. \tag{12b}$$

The scaling dimension of $S_{\pm 1}^z$ is 1 and that of $S_{\pm 1}^{\pm}$ is $2\pi R^2$. In general, the vertex operators $e^{ia\phi_>}$ and $e^{ia\phi_<}$ have dimension $a^2/2$. We thus find that, among possible interactions generated by the $1/J_K$ expansions, $S_1^+S_{-1}^-+S_1^-S_{-1}^+$ is most dangerous and has dimension $4\pi R^2$. This operator is irrelevant when $0<\Delta\leqslant 1$. Therefore we may conclude that, when the anisotropy parameter Δ of the host XXZ spin chain is $0<\Delta\leqslant 1$, the infrared stable fixed point corresponds to the limit $J_K\to\infty$, where the system is decoupled into a singlet and two semi-infinite XXZ spin chains; see Fig. 1. The singlet acts like an infinitely high potential barrier for excitations in the spin chain and effectively cuts it into two SIC's. If the host spin chain is of finite length containing L spins and if we apply the periodic boundary condition, then its low-energy fixed point is an open spin chain consisting of $L-1$ spins, in addition to a decoupled spin singlet formed from the impurity spin and a spin originally in the host spin chain.[26] This strong-coupling fixed point is very similar to the one found for the Kondo effect in electronic TL liquids.[4]

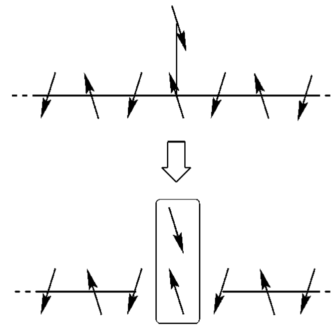

FIG. 1. Schematic picture of renormalization to the strong-coupling fixed point where the XXZ chain is cut by the singlet.

The above result is a natural generalization of the conclusion of Eggert and Affleck to the case $0<\Delta<1$. In their case the low-energy fixed point is a singlet plus decoupled two semi-infinite Heisenberg spin chains, and the leading irrelevant operator at the fixed point is a dimension 2 operator, $\boldsymbol{S}_1\cdot\boldsymbol{S}_{-1}$. In our case the operator $S_1^+S_{-1}^-+S_1^-S_{-1}^+$ has a smaller scaling dimension than $S_1^zS_{-1}^z$ because of the absence of the SU(2) symmetry. Since its dimension $4\pi R^2$ is in general noninteger, we may expect that it should give anomalous power-law temperature dependence to various quantities.

The coupling to the Kondo impurity gives rise to an extra contribution to the specific heat and the spin susceptibility, which we denote as δC and $\delta\chi$. Their temperature dependence near the strong-coupling fixed point is determined by the leading irrelevant operator, $\hat{O}_1=g_1(S_1^+S_{-1}^-+S_1^-S_{-1}^+)$, where g_1 is a coupling constant. To obtain leading temperature dependence we may use a perturbation expansion in $\hat{O}_1$.[27]

We first estimate δC. Up to second order, the change in the free energy is given by

$$\delta F=-\int_0^{\beta/2}d\tau\langle\hat{O}_1(\tau)\hat{O}_1(0)\rangle\propto-\int_{\tau_c}^{\beta/2}d\tau\left(\frac{\pi T\tau_c}{\sin\,\pi T\tau}\right)^{2d}, \tag{13}$$

where $d=4\pi R^2$, β is inverse of the temperature T, $\hat{O}_1(\tau)\equiv e^{\tau H_{\rm SIC}}\hat{O}e^{-\tau H_{\rm SIC}}$, and τ_c is a cutoff to regularize the integral. Note that there is no first-order contribution of $\hat{O}_1$ to δF. The low-temperature expansion of the integral in Eq. (13) for general d reads

$$\int_{\tau_c}^{\beta/2}\left(\frac{\pi T\tau_c}{\sin\,\pi T\tau}\right)^{2d}d\tau-\frac{\tau_c}{2d-1}$$

$$=\begin{cases}-\frac{\tau_c}{3}(\pi T\tau_c)^2, & d=1\\ \frac{\tau_c(d-1)}{2d-1}(\pi T\tau_c)^{2d-1}B\left(\frac{1}{2},\frac{3}{2}-d\right), & 1<d<\frac{3}{2}\\ \frac{\tau_c}{2}(\pi T\tau_c)^2\ln(1/\pi T\tau_c), & d=\frac{3}{2}\\ \frac{\tau_c d(\pi T\tau_c)^2}{3(2d-3)}, & \frac{3}{2}<d<\frac{5}{2},\end{cases} \tag{14}$$

where $B(a,b)$ is the beta function. Note that any irrelevant operator with dimension $d>3/2$ generates a positive T^2 term. From these equations we get

$$\delta C\propto\begin{cases}(d-1)^2T^{2d-2}/(3-2d), & 1<d<\frac{3}{2}\\ T\ln(1/\pi T\tau_c), & d=\frac{3}{2}\\ T/(2d-3), & \frac{3}{2}<d<\frac{5}{2},\end{cases} \tag{15}$$

in the low-temperature limit. Since $d=4\pi R^2$, the boundary case $d=\frac{3}{2}$ corresponds to $\Delta=1/\sqrt{2}$. When $0<\Delta<1/\sqrt{2}$, δC is proportional to $T^{8\pi R^2-2}$ with the exponent changing from 0 to 1 as Δ varying from 0 to $1/\sqrt{2}$. This anomalous power-law behavior is reminiscent of the Kondo effect in TL liquids.[4] The logarithmic correction appears at $\Delta=1/\sqrt{2}$ when the dimension of the leading irrelevant operator becomes 3/2. This is mathematically the same as in the two-channel Kondo problem.[27] When $1/\sqrt{2}<\Delta\leqslant 1$, the leading term of δC is proportional to T.

We next consider $\delta\chi$. Here we need to distinguish two kinds of spin susceptibilities: one responding to a magnetic field applied in the z direction and the other responding to the one in the xy plane. We shall call them $\delta\chi_z$ and $\delta\chi_\perp$, respectively. Suppose we apply a magnetic field locally[28] only to $\boldsymbol{S}_{\rm imp}$ such that the perturbation,

$$H_h=h_zS^z_{\rm imp}+h_xS^x_{\rm imp}, \tag{16}$$

is added to the Hamiltonian. Using the $1/J_K$ expansion again, we can generate effective interactions induced by H_h in the Hilbert space of the singlet plus the SIC's (Fig. 1). From the symmetry we expect to have the following operators in addition to other less relevant ones: $\hat{O}_{h1}=h_z(S^z_1+S^z_{-1})$, $\hat{O}_{h2}=h_z^2(S^+_1S^-_{-1}+S^-_1S^+_{-1})$, and $\hat{O}_{h3}=h_x(S^x_1+S^x_{-1})$. In terms of the bosonic fields they may be written as $\hat{O}_{h1}\propto h_z[\partial_x\phi_>(0)+\partial_x\phi_<(0)]$, $\hat{O}_{h2}\propto h_z^2\cos\{2\sqrt{\pi}R[\phi_>(0)-\phi_<(0)]\}$, and $\hat{O}_{h3}\propto h_x\{\cos[2\sqrt{\pi}R\phi_>(0)]+\cos[2\sqrt{\pi}R\phi_<(0)]\}$, whose scaling dimensions are 1, $4\pi R^2$, and $2\pi R^2$. We can now estimate δF induced by these operators using Eq. (14) and obtain $\delta\chi_\alpha=-\partial^2\delta F/\partial h_\alpha^2|_{h=0}$. One point to be mentioned is that products of $\hat{O}_1$ and $\hat{O}_{h2}$ can contribute a term $h_z^2T^{8\pi R^2-1}$ to δF, leading to a term proportional to $T^{8\pi R^2-1}$ in $\delta\chi_z$. From these considerations, we conclude that in the low-temperature limit $\delta\chi$ has the following form:

$$\delta\chi_z(T)-\delta\chi_z(0)\propto\begin{cases}\frac{4\pi R^2-1}{8\pi R^2-3}T^{8\pi R^2-1}, & 0<\Delta<1/\sqrt{2}\\ T^2\ln(1/T), & \Delta=1/\sqrt{2}\\ T^2, & 1/\sqrt{2}<\Delta\leqslant 1,\end{cases} \tag{17a}$$

$$\delta\chi_\perp(T)-\delta\chi_\perp(0)\propto T^{4\pi R^2-1},\quad 0<\Delta\leqslant 1. \tag{17b}$$

We note that there is always a contribution proportional to T^2 coming from irrelevant operators. When $0<\Delta\ll 1$, the term $T^{8\pi R^2-1}$ might be difficult to observe, because of its small coefficient ($\propto 4\pi R^2-1$), compared with the T^2 term. We also note that in general the zero-temperature limit of the susceptibility $\delta\chi(0)$ is of order $1/T_K$.

C. Strong-coupling limit for $-1<\Delta<0$

When the parameter Δ in the host spin chain is in the range $-1<\Delta<0$, the dimension of the operator $S^+_1S^-_{-1}+S^-_1S^+_{-1}$ is smaller than 1 and is relevant. This means that the open-boundary fixed point discussed in the previous subsection cannot be a low-energy fixed point when $-1<\Delta<0$. Both limits $J_K\to 0$ and $J_K\to\infty$ in the original Hamiltonian H_0+H_K are unstable. We thus need to find a nontrivial fixed point.

Let us for the moment forget the singlet of $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_0$, and concentrate on the rest of the spins. That is, we consider the two semi-infinite spin chains weakly coupled by a ferromagnetic exchange interaction H_2:

$$H_\lambda=\sum_{i=1}^{\infty}(S^x_iS^x_{i+1}+S^y_iS^y_{i+1}+\Delta S^z_iS^z_{i+1})+\sum_{i=1}^{\infty}(S^x_{-i}S^x_{-i-1}+S^y_{-i}S^y_{-i-1}+\Delta S^z_{-i}S^z_{-i-1})-\lambda(S^x_1S^x_{-1}+S^y_1S^y_{-1}), \tag{18}$$

where $0<\lambda\ll 1$. We have dropped the irrelevant $S^z_1S^z_{-1}$ term. Since the term $\lambda(S^x_1S^x_{-1}+S^y_1S^y_{-1})$ is a relevant perturbation (dimension $=4\pi R^2$), the fixed point $\lambda=0$ is unstable. On the other hand, in the strong-coupling limit $\lambda\gg 1$, the two spins $\boldsymbol{S}_1$ and $\boldsymbol{S}_{-1}$ are in one of the triplet state, $S=1$ and $S^z=0$. Virtual transitions from this state to excited states generate a residual ferromagnetic exchange coupling between $\boldsymbol{S}_2$ and $\boldsymbol{S}_{-2}$, of the form similar to H_2, which is again a relevant perturbation. Thus, the fixed point $\lambda=\infty$ is also unstable, and we expect that there should be an intermediate-coupling fixed point. We will argue that this nontrivial fixed point is simply a pure XXZ spin chain where the spins $\boldsymbol{S}_i$ ($i>0$) are rotated by π around the z axis. The argument goes as follows. The rotation of $\boldsymbol{S}_i$ ($i>0$) around the z axis by π changes the sign of λ ($-\lambda\to\lambda$) in H_λ. Since $S^x_1S^x_{-1}+S^y_1S^y_{-1}$ is relevant, the coupling λ grows as the energy scale decreases. The $S^z_1S^z_{-1}$ term is also generated in the course of the RG transformation. Thus, the two chains get coupled stronger at a lower energy scale. We next consider

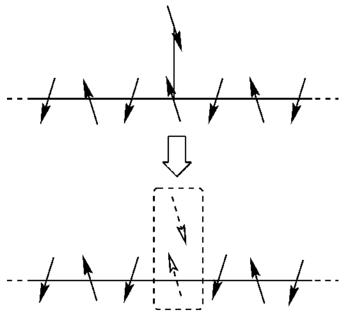

FIG. 2. Schematic picture of renormalization to the stable fixed point consisting of a singlet weakly coupled to a spin chain. The singlet looks ''transparent'' for low-energy excitations in the chain.

the opposite limit where the two chains are well connected but one bond is slightly disturbed. This is described by the Hamiltonian,

$$H_\varepsilon=\sum_{i=1}^{\infty}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z)+\sum_{i=1}^{\infty}(S_{-i}^xS_{-i-1}^x+S_{-i}^yS_{-i-1}^y+\Delta S_{-i}^zS_{-i-1}^z)+(1-\varepsilon_\perp)(S_1^xS_{-1}^x+S_1^yS_{-1}^y)+(1-\varepsilon_z)\Delta S_1^zS_{-1}^z, \tag{19}$$

where $0<\varepsilon_\perp,\ \varepsilon_z\ll 1$. Bosonizing this Hamiltonian as in Sec. II A, we find that the perturbations ($\propto\varepsilon$) give the spin-Peierls operator $\sin[\phi(0)/R]$ of dimension $(4\pi R^2)^{-1}$ and dimension 2 operators like $(\partial\phi/\partial x)^2$. Since they are irrelevant ($\varepsilon_\perp,\varepsilon_z\to 0$ in the low-energy limit), we recover the pure XXZ spin chain. It is tempting to assume that the RG trajectories starting from the unstable point describing two weakly coupled chains [Eq. (18)] continuously flow to the stable fixed point of the pure XXZ chain. Although we cannot prove it, we believe this is what actually happens. We note that this phenomenon is closely related to the well-known result that a backward-scattering potential is renormalized to zero for fermions interacting with mutual attractive interactions.[2] It is also similar to the ''healing'' of weak bonds that Eggert and Affleck found for the isotropic Heisenberg chain with two symmetrically perturbed bonds.[16] Coming back to the Hamiltonian H_λ, we conclude that its low-energy fixed point is a pure XXZ spin chain with the spins $\boldsymbol{S}_i$ ($i>0$) rotated around the z axis by π.

We now return to our Kondo problem. What we have found so far is that (i) the Kondo coupling is a relevant operator at the weak-coupling point and leads to a singlet formation and that (ii) weakly coupled spin chains are renormalized to a strongly coupled single chain. Combining these two observations together, we propose the model schematically shown in Fig. 2 as a candidate for the low-energy fixed point. The model consists of the singlet of $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_0$ on top of the pure XXZ chain where spins are rotated as discussed in the last paragraph. An important point is that low-energy excitations are spin-density fluctuations of long wavelength in the chain, and that for these low-energy excitations the singlet has essentially no effect. In other words, the singlet is ''transparent'' for them. At short-length scale there is a coupling between $\boldsymbol{S}_0$ and its neighbors ($\boldsymbol{S}_1+\boldsymbol{S}_{-1}$). We assume that, as far as low-energy physics is concerned, the singlet is rigid and can be broken only virtually by the weak coupling of $\boldsymbol{S}_0$ to the spin chain. Thus, the stable fixed point may also be represented schematically as in Fig. 3. From the assumption of the rigid singlet, we can integrate it out to get effective interactions $\hat{O}_2=S_1^xS_{-1}^x+S_1^yS_{-1}^y$ and $\hat{O}_3=S_1^zS_{-1}^z$ for the low-energy excitations in the spin chain. In the boson representation they are linear combinations of $\sin(\phi/R)$, $(\partial\phi/\partial x)^2$, and $(\partial\phi/\partial t)^2$, which are irrelevant operators for the spin chain with the parameter Δ in the range $-1<\Delta<0$. Hence the model is stable against weak perturbations, and we conjecture that the above model gives a correct picture of the strong-coupling fixed point for the case $-1<\Delta<0$. Although it is impossible to show analytically that the RG trajectories leaving from the unstable weak-coupling point reach this fixed point (Figs. 2 and 3), the numerical results we show in the next section provide good evidence for our picture.

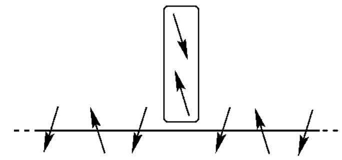

FIG. 3. Schematic picture of the low-energy fixed point.

Assuming that our Kondo model is indeed renormalized to the strong-coupling fixed point of Fig. 2, we can obtain leading temperature dependences of δC and $\delta\chi$ as in the last subsection. Since we know that a leading irrelevant operator at the fixed point is among the operators $\sin[\phi(0)/R]$, $[\partial\phi(0)/\partial x]^2$, and $[\partial\phi(0)/\partial t]^2$, we find that the low-temperature behavior of δC is given by Eq. (15) with $d=(4\pi R^2)^{-1}$. We thus get

$$\delta C\propto\begin{cases} T, & -1<\Delta<-1/2\\ T\ln(1/T), & \Delta=-1/2\\ T^{1/(2\pi R^2)-2}, & -1/2<\Delta<0.\end{cases} \tag{20}$$

When a weak magnetic field is applied to $\boldsymbol{S}_{\rm imp}$, we obtain the operators $\hat{O}_{h1}=h_z(S_1^z+S_{-1}^z)$, $\hat{O}_{h2}=h_z^2(S_1^+S_{-1}^-+S_1^-S_{-1}^+)$, and $\hat{O}_{h3}=h_x(S_1^x+S_{-1}^x)$ after integrating out the singlet. Since these operators are not boundary operators at the fixed point of our interest, the scaling dimensions of $\hat{O}_{h2}$ and $\hat{O}_{h3}$ are different from the open-boundary case. Here we use the bosonization formulas (4a) and (4b) and find that the dimensions of $\hat{O}_{h2}$ and $\hat{O}_{h3}$ are $(4\pi R^2)^{-1}$ and πR^2, respectively. We then obtain the following low-temperature behavior:

$$\delta\chi_z(T)-\delta\chi_z(0)\propto\begin{cases}\dfrac{1-4\pi R^2}{6\pi R^2-1}T^{(1/2\pi R^2)-1}, & -\dfrac{1}{2}<\Delta<0\\ T^2\ln(1/T), & \Delta=-\dfrac{1}{2}\\ T^2/(1-6\pi R^2), & -1<\Delta<-\dfrac{1}{2}.\end{cases} \tag{21a}$$

$$\delta\chi_\perp \propto T^{2\pi R^2-1}. \tag{21b}$$

D. Strong-coupling limit of the XY case ($\Delta=0$)

We briefly comment on the low-energy fixed point for the XY case. Since this is exactly on the border of the two cases discussed in Secs. II B and II C, we naturally expect that a picture for the fixed point of the $\Delta=0$ case should be something in between Figs. 1 and 2. That is, the singlet of $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_0$ does not completely cut the host XXZ spin chain into two pieces. The weakened connection between $\boldsymbol{S}_1$ and $\boldsymbol{S}_{-1}$ is not healed as in the negative Δ case. This is because at the open-boundary fixed point ($J_K=\infty$) the operator $S_1^+S_{-1}^- + S_1^-S_{-1}^+$ is a marginal operator. We expect that the impurity contribution to the specific heat and the susceptibilities have the following low-temperature limit:

$$\delta C \propto T, \tag{22a}$$

$$\delta\chi_z(T) - \delta\chi_z(0) \propto T^2, \tag{22b}$$

$$\delta\chi_\perp(T) \propto \log(1/T). \tag{22c}$$

III. RESULTS OF DMRG CALCULATIONS

A. Numerical methods

In this section we present our numerical results for finite chains. The Hamiltonian we studied is H_0+H_K, Eqs. (1) and (2). The site index i in Eq. (1) runs from $-l$ to $l-1$, and the total number of spins in the host XXZ chain is $L=2l+1$. We impose the open boundary condition at the left and right ends of the host XXZ chain. Using the DMRG method proposed by White,[29] we calculated lowest energy gap and spin-correlation functions in the ground state. In order to accelerate the numerical calculation, we employed the improved algorithm proposed by White.[30] We also used the finite-system method to achieve high accuracy. Up to 100 states were kept for each block and the truncation error is typically 10^{-8}. This error is directly related to the accuracy of energy.

As we mention in Introduction, our model may be regarded as a toy model for the Kondo effect in 1D electron systems that have charge degrees of freedom as well as spin. In this context we note that it is much easier to apply the DMRG method to the spin chains than to electronic models like the Hubbard model away from half filling, because the Hilbert space is smaller and the DMRG converges faster for spin chains. We can thus treat large spin systems to reach scaling regime. It seems that for the Kondo effect of electronic models the application of Monte Carlo methods[9] is more successful than the DMRG method.[31]

B. Numerical results for $\Delta=0.5$

As a typical case of $0<\Delta<1$ we have chosen $\Delta=0.5$. In this case $R=1/\sqrt{3\pi}$ and $v=3\sqrt{3}/4$. With this choice we have computed the lowest energy gap E_g for chains of $L=1$ (mod4). Numerical results of the finite-size gap are shown in Fig. 4. The energy gap is the difference between the lowest energy in the sector $S^z_{\rm tot}=0$ and that in the sector $S^z_{\rm tot}=1$. According to the RG analysis in Sec. II B, the ground state of a sufficiently long chain is described as two decoupled

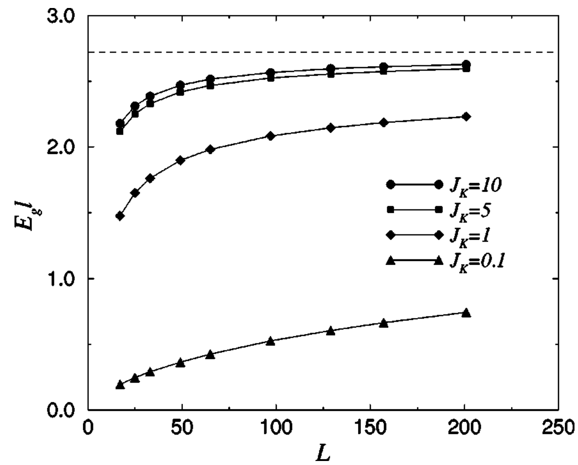

FIG. 4. Energy gap E_g as a function of system size L for $\Delta=0.5$. The data points are the gap computed for $L=17$, 25, 33, 49, 65, 94, 129, 157, and 201 [$L=1$ (mod4)]. The dashed line represents the infinite-L limit, $E_g l=\sqrt{3}\pi/2$.

chains, each having $(L-1)/2$ spins, plus a rigid spin singlet of $\boldsymbol{S}_0$ and $\boldsymbol{S}_{\rm imp}$ in between them. Note that $(L-1)/2=l$ is an even integer.

To interpret finite-size scaling of the data, let us bosonize the two open XXZ chains of length l, following Refs. 16 and 32. The mode expansions of the phase fields are given by

$$\phi_\mu(x,t)=\pi R+\hat{Q}_\mu\frac{x}{l}+\sum_{n>0}\frac{\sin k_n x}{\sqrt{\pi n}} \times(a_{n\mu}e^{-ik_n vt}+a^\dagger_{n\mu}e^{ik_n vt}), \tag{23}$$

$$\tilde\phi_\mu(x,t)=\tilde\phi_{0\mu}+\hat{Q}_\mu\frac{vt}{l}+i\sum_{n>0}\frac{\cos k_n x}{\sqrt{\pi n}} \times(a_{n\mu}e^{-ik_n vt}-a^\dagger_{n\mu}e^{ik_n vt}), \tag{24}$$

where $k_n=\pi n/l$ and the operators obey the commutation relations $[\tilde\phi_{0\mu},\hat{Q}_\nu]=i\delta_{\mu,\nu}$ and $[a_{m\mu},a^\dagger_{n\nu}]=\delta_{m,n}\delta_{\mu,\nu}$ ($\mu,\nu=l$ or r). The suffixes l and r stand for the left ($\boldsymbol{S}_i$: $i<0$) and right ($\boldsymbol{S}_i$: $i>0$) spin chains, respectively. The fields ϕ_l and $\tilde\phi_l$ (ϕ_r and $\tilde\phi_r$) are therefore defined in the negative (positive) x region, and $\phi_l+\phi_r$ and $\tilde\phi_l+\tilde\phi_r$ correspond to ϕ and $\tilde\phi$ in Eq. (3). Note that ϕ_l and ϕ_r are different from $\phi_<$ and $\phi_>$. Substituting Eqs. (23) and (24) into Eq. (3) yields the Hamiltonian of the μ chain

$$H_\mu=\frac{\pi v}{l}\left(\frac{\hat{Q}^2_\mu}{2\pi}+\sum_{n>0}na^\dagger_{n\mu}a_{n\mu}-\frac{1}{24}\right). \tag{25}$$

Its energy eigenvalue and eigenfunctions are

$$E_\mu=\frac{\pi v}{l}\left[2\pi R^2(S^z_\mu)^2+\sum_{n>0}nm_{n\mu}-\frac{1}{24}\right], \tag{26}$$

$$|S^z_\mu,\{m_{n\mu}\}\rangle=\exp(i2\pi RS^z_\mu\tilde\phi_{0\mu})\prod_{n>0}\frac{(a^\dagger_{n\mu})^{m_{n\mu}}}{m_{n\mu}!}|0\rangle, \tag{27}$$

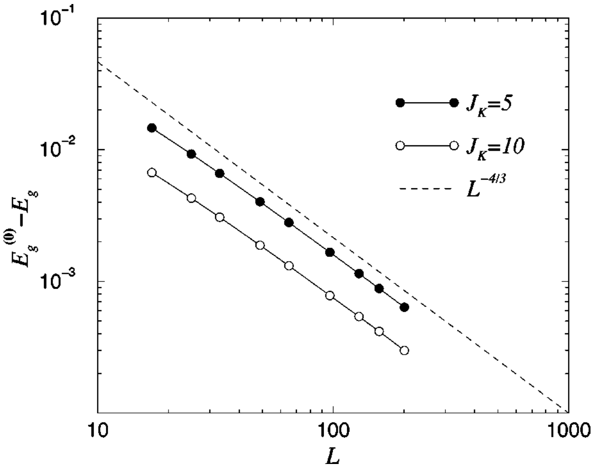

FIG. 5. Size dependence of the correction to the energy gap $E_g^{(0)}$, which is the gap calculated in the limit $J_K=\infty$. The dashed line represents the theoretically predicted $L^{-4/3}$ dependence.

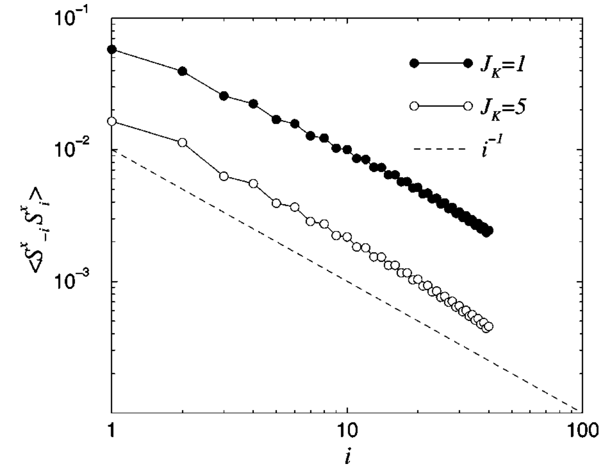

FIG. 6. Correlation between S^x_{-i} and S^x_i calculated for $\Delta=0.5$ and $L=201$. The dashed line corresponds to the $1/i$ decay obtained from the perturbative calculation.

where $|0\rangle$ is a vacuum $(a_{n\mu}|0\rangle=0)$. The constant S^z_μ is nothing but a quantum number of total S^z of each chain. Since l is an even integer, S^z_μ can take integer values only. Therefore, in the limit $J_K\to\infty$, the ground state of the total system is the state with $S^z_\mu=m_{n\mu}=0$ for $\mu=l$ and r. The first excited states are fourfold degenerate and correspond to $(S^z_l,S^z_r)=(\pm1,0),(0,\pm1)$ and $m_{n\mu}=0$. The energy gap in this limit is then given by

$$E_g=\frac{\pi v}{l}\,2\pi R^2, \tag{28}$$

which equals $\sqrt{3}\pi/2l$ at $\Delta=1/2$. This gap value is shown as a dashed line in Fig. 4. It is clear that all the curves in Fig. 4 are gradually approaching the dashed line as L increases. How the curves finally approach it in the $L\to\infty$ limit is determined by the leading irrelevant operator $\hat{O}_1$, whose explicit form we may take:

$$\hat{O}_1\propto\cos\{i2\pi R[\tilde{\phi}_r(0,0)-\tilde{\phi}_l(0,0)]\}. \tag{29}$$

The correction to Eq. (28) due to the operator $\hat{O}_1$ can be obtained from a lowest-order perturbation expansion.[33] Since the degenerate first excited states $|S^z_l=1,S^z_r=0\rangle$ and $|S^z_l=0,S^z_r=1\rangle$ have a nonzero matrix element,

$$\begin{aligned}&\langle S^z_l=1,S^z_r=0|\hat{O}_1|S^z_l=0,S^z_r=1\rangle\\ &\quad\propto\left\langle 0\left|\exp\left[-2\pi R\sum_{n=1}^{l}\frac{1}{\sqrt{\pi n}}(a_{nr}-a^\dagger_{nr}-a_{nl}+a^\dagger_{nl})\right]\right|0\right\rangle\\ &\quad\propto L^{-4\pi R^2},\end{aligned} \tag{30}$$

the degeneracy of these two states is lifted by an amount which scales as $L^{-4\pi R^2}$. The same is true for the other two degenerate states $|S^z_l=-1,S^z_r=0\rangle$ and $|S^z_l=0,S^z_r=-1\rangle$. On the other hand, the ground-state energy does not change in first-order perturbation. Hence we may expect that the leading correction to the energy gap should be proportional to $L^{-4\pi R^2}$, which goes to zero faster than the finite-size gap ($\propto L^{-1}$). This L dependence is indeed observed in our numerical data shown in Fig. 5. The data show very clear power-law behavior with the exponent $4/3=4\pi R^2$, in perfect agreement with the theory. This can be regarded as a numerical proof of the presence of the leading irrelevant operator with the scaling dimension $4\pi R^2$ at the strong-coupling fixed point we discussed in Sec. II B. We note that the energy gap $E_g^{(0)}$ used in Fig. 5 is the one at $J_K=\infty$, or equivalently, the finite-size gap of an *XXZ* spin chain containing l spins under the open-boundary condition. The reason why we have used $E_g^{(0)}$ rather than Eq. (28) is to reduce the effect of a bulk irrelevant operator $\cos(2\phi/R)$ of dimension $1/\pi R^2=3$.

Using the DMRG method, we have also calculated an equal-time two-point spin correlation function $\langle S^x_i S^x_j\rangle$ in the ground state for $L=201$ ($S^z_{\rm tot}=0$). According to our picture of the strong-coupling fixed point, the host *XXZ* spin chain is effectively cut by a singlet in the low-energy limit (Fig. 1). We naturally expect that correlations across the singlet should be much weaker than correlations within one of the decoupled chains. Our numerical results shown in Figs. 6 and 7 support this idea: A correlation function across the singlet shows power-law dependence on i with an exponent larger than that for a pure *XXZ* chain ($J_K=0$), $2\pi R^2$.

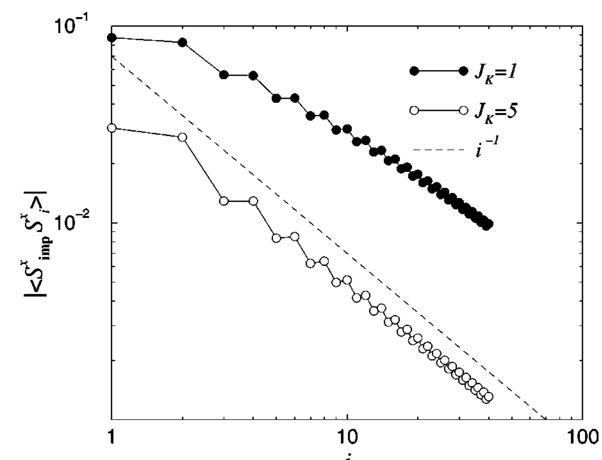

FIG. 7. Correlation between $S^x_{\rm imp}$ and S^x_i calculated for $\Delta=0.5$ and $L=201$. The dashed line represents the expected i^{-1} behavior.

The exponents for $\langle S^x_{-i}S^x_i\rangle$ and $\langle S^x_{\rm imp}S^x_i\rangle$ can be obtained from the following argument. First we consider $\langle S^+_{-i}S^-_i\rangle$, which is equivalent to $\langle S^x_{-i}S^x_i\rangle$. Since it vanishes when the XXZ chain is completely decoupled, the nonzero contribution is due to the leading irrelevant operator $S^+_1S^-_{-1}+S^-_1S^+_{-1}$. To first order in $\hat{O}_1$ the correlator is

$$\langle S^+_{-i}S^-_i\rangle \propto \int dt \langle S^-_{-1}(t)S^+_{-i}(0)\rangle_l \langle S^+_1(t)S^-_i(0)\rangle_r, \quad (31)$$

where the averages $\langle\ \rangle_l$ and $\langle\ \rangle_r$ are evaluated for the ground state of each decoupled chain. Since the scaling dimension of the boundary operator $S^\pm_{\mp 1}$ is $2\pi R^2$ and that of $S^\mp_{\pm i}$ is πR^2, we expect the correlator to scale as

$$\langle S^+_{-i}S^-_i\rangle \propto i^{-6\pi R^2+1}, \quad (32)$$

from which we get $\langle S^x_{-i}S^x_i\rangle \propto 1/i$ for $\Delta=1/2$. The results in Fig. 6 are consistent with this perturbative calculation.

The correlation between $S^x_{\rm imp}$ and S^x_i can be calculated using the $1/J_K$ expansion, which can be justified in the low-energy limit. At $J_K=\infty$ the ground state of the whole system is a direct product of $|S\rangle$, which is the singlet wave function of $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_0$, and the ground states of the left and right decoupled spin chains, which we denote as $|l\rangle$ and $|r\rangle$. We calculate the correlation function $\langle S^+_{\rm imp}S^-_i\rangle$ to lowest order in the coupling between $\boldsymbol{S}_0$ and its neighboring spin $S^-_0S^+_1$:

$$\langle S^+_{\rm imp}S^-_i\rangle \sim \frac{1}{J_K}\langle S|S^+_{\rm imp}|T\rangle\langle T|S^-_0|S\rangle\langle r|S^+_1S^-_i|r\rangle$$
$$\propto (-1)^i i^{-3\pi R^2}, \quad (33)$$

where $|T\rangle$ is a triplet state of $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_0$ having excitation energy of order J_K. The exponent $3\pi R^2(=1)$ is a sum of the dimensions of S^+_1 and S^-_i. The data for $J_K=5$ in Fig. 7 are in excellent agreement with the above calculation, although the data for $J_K=1$ is curving, which we think is due to a crossover to the true scaling regime.

C. Numerical results for $\Delta=-0.5$

Here we present the numerical results for negative Δ. Using the DMRG method, we have calculated finite-size gap and spin-correlation functions for $\Delta=-0.5$, where $R=1/\sqrt{6\pi}$ and $v=3\sqrt{3}/8$.

Figure 8 shows the finite-size energy gap as a function of the system size for $L=1$ (mod4). As in the last section, the gap is defined as the difference between the lowest energy in the sector $S^z_{\rm tot}=0$ and that in the sector $S^z_{\rm tot}=1$. We find that the normalized gap E_gL increases for small J_K, while it decreases for large J_K. This is consistent with our picture of the renormalization flows (Fig. 2). For small J_K the excitation gap is due to fluctuations of $\boldsymbol{S}_{\rm imp}$ weakly coupled to the host spin chain. This coupling is renormalized and becomes stronger as we saw in Sec. II A. For large J_K, on the other hand, the host XXZ chain is almost cut by a singlet, and the finite-size gap roughly corresponds to the singlet-to-triplet excitation energy in half chains. As L increases, or equivalently, as the energy scale decreases, the renormalized coupling between the almost decoupled chains becomes larger (''healing''), leading to the decrease of the normalized finite-size gap. It is clear that all the curves in Fig. 8 approach the dashed line $E_gL=\sqrt{3}\pi/8=0.680\ldots$, which is the value one expects for a single XXZ chain of length L. Unlike in the case of $\Delta=0.5$, however, we have not been able to obtain information on the scaling dimension of a leading irrelevant operator from the numerical data. A log-log plot of $|E_g-E^{(0)}_g|$ versus L did not give straight lines corresponding to power-law scaling. This would mean that the systems we have studied ($L\sim 200$) are not large enough.

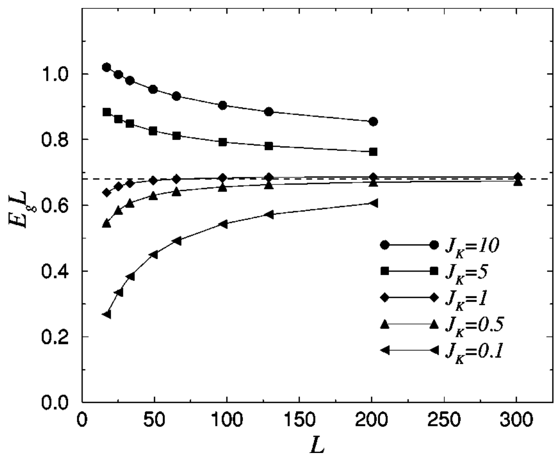

FIG. 8. Energy gap E_g as a function of system size L for $\Delta=-0.5$. The data are taken for $L=17$, 25, 33, 49, 65, 97, 129, 201, and 301. The dashed line represents the infinite-L limit, $E_gL=\sqrt{3}\pi/8$.

Next we show the results of correlation functions that we computed for the ground state of the $L=201$ system ($S^z_{\rm tot}=0$). Figures 9 and 10 show the correlation functions of $\boldsymbol{S}_{-i}$ and $\boldsymbol{S}_i$. The correlator $\langle S^x_{-i}S^x_i\rangle$ is positive and decays like $i^{-1/3}$, while $\langle S^z_{-i}S^z_i\rangle$ is negative and decays much faster like i^{-2}. These features are exactly what we expect from our picture of the low-energy fixed point (Figs. 2 and 3). Since the spin chain is well connected, the correlation functions $\langle S^\alpha_{-i}S^\alpha_i\rangle$ should behave as in a pure XXZ chain without an impurity spin. That is, exponents of power-law decays should be the same as those in the pure chain, although amplitudes of the correlators will depend on J_K. From Eqs. (4a) and (4b) we see that at long distance $S^z_i\sim d\phi/dx$ and S^+_i

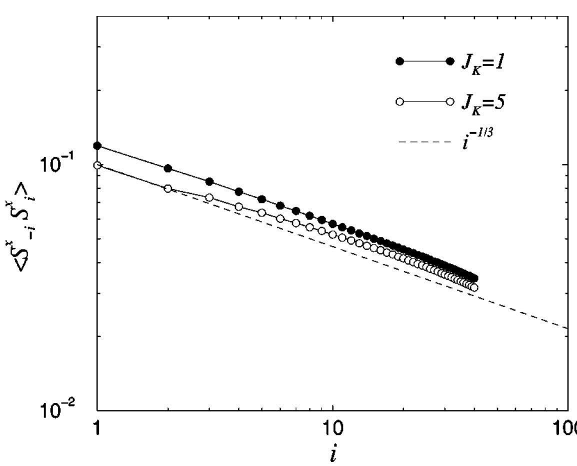

FIG. 9. Correlation function $\langle S^x_{-i}S^x_i\rangle$ for $\Delta=-0.5$ and $L=201$. The dashed line corresponds to the $i^{-1/3}$ decay.

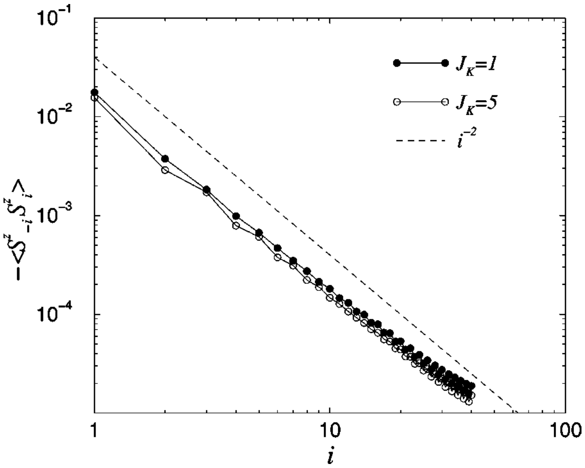

FIG. 10. Correlation function $\langle S^z_{-i} S^z_i \rangle$ for $\Delta = -0.5$ and $L = 201$. The dashed line corresponds to the i^{-2} behavior.

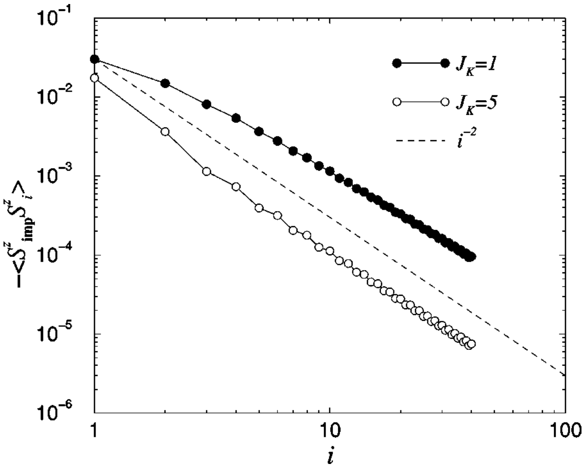

FIG. 12. Correlation between $S^z_{\rm imp}$ and S^z_i for $\Delta = -0.5$ and $L = 201$. The dashed line corresponds to the expected i^{-2} decay.

$\sim(-1)^i e^{i2\pi R\tilde{\phi}}$, whose scaling dimensions are 1 and $\pi R^2 = 1/6$. Hence $\langle S^z_{-i} S^z_i \rangle$ should decay as i^{-2} and $\langle S^x_{-i} S^x_i \rangle \propto i^{-1/3}$, in agreement with the numerical result.[34]

We next discuss correlations between $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_i$. Since there is always a short-distance correlation between $\boldsymbol{S}_{\rm imp}$ and $\boldsymbol{S}_1 + \boldsymbol{S}_{-1}$, we expect $\langle S^\alpha_{\rm imp} S^\alpha_i \rangle \propto \langle (S^\alpha_1 + S^\alpha_{-1}) S^\alpha_i \rangle$ with a smaller constant of proportion for larger J_K. Noting that $S^x_1 + S^x_{-1}$ corresponds to the staggered component in a pure *XXZ* chain without the spin rotation of $\boldsymbol{S}_i$ $(i>0)$, we conclude that $\langle S^x_{\rm imp} S^x_i \rangle \propto i^{-1/3}$ and $\langle S^z_{\rm imp} S^z_i \rangle \propto i^{-2}$ for large i. Our numerical results shown in Figs. 11 and 12 show exactly the feature discussed above. Hence we conclude that the numerical results support our picture of the low-energy fixed point.

IV. CONCLUSIONS

In this paper we have studied the Kondo effect due to an extra spin coupled to a gapless *XXZ* spin chain. In our model the backward spin-flip scattering is always a relevant perturbation. At low energy the impurity spin is screened by a spin in the host chain, and the characteristic energy scale, the Kondo temperature T_K, has a power-law dependence on the Kondo coupling. From the perturbative RG analysis for various limits, we have deduced properties of strong-coupling, low-energy fixed points. In the antiferromagnetic side $(0<\Delta\leqslant 1)$ the host *XXZ* chain is cut by the singlet into two separate chains. On the other hand, in the ferromagnetic side $(-1<\Delta<0)$ the singlet does not harm the host spin chain in the low-energy limit. This may be understood qualitatively by mapping the problem to a spinless fermionic system using the Jordan-Wigner transformation. The fermions have mutual repulsive (attractive) interactions in the antiferromagnetic (ferromagnetic) region. The singlet may then be viewed as an impurity potential for the fermions, which can be a relevant or irrelevant perturbation, depending on the sign of the mutual interactions. Employing the known result for the spinless fermion system,[2] we can argue that the host spin chain is cut into two pieces in the antiferromagnetic case whereas in the other case the singlet does not affect the low-energy properties of the spin chain.

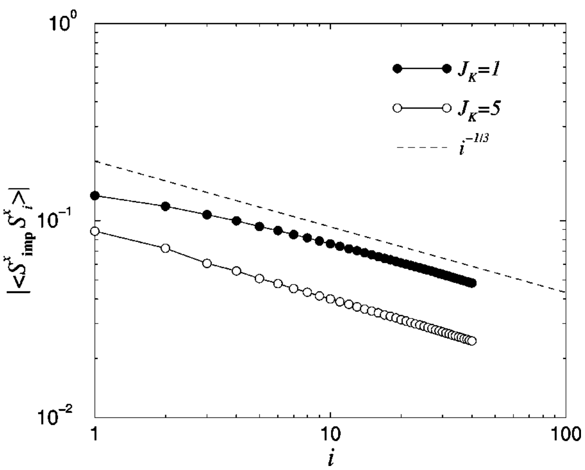

FIG. 11. Correlation between $S^x_{\rm imp}$ and S^x_i for $\Delta = -0.5$ and $L = 201$. The dashed line corresponds to the $i^{-1/3}$ behavior.

We have used the powerful DMRG method to numerically compute finite-size energy gaps and correlation functions. The numerical results are consistent with the RG analysis. For $\Delta = 0.5$, the normalized gap approaches the value for a chain of half length, and the correlation function across $\boldsymbol{S}_0$ decays much faster than in a pure spin chain $(J_K = 0)$. These results are explained successfully based on the RG analysis of the strong-coupling fixed point (Fig. 1). For $\Delta = -0.5$ we have found that the normalized gap approaches the value for a spin chain without the Kondo impurity. The correlation functions also show the same power-law behavior as in the pure spin chain. These results are consistent with our picture of the fixed point where the host spin chain remains as a single chain through the healing of a coupling weakened by the singlet formation (Figs. 2 and 3).

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