Single magnetic impurity in a correlated electron system: Density-matrix renormalization group study

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We study a magnetic impurity embedded in a correlated electron system using the density-matrix renormalization group method. The correlated electron system is described by the one-dimensional Hubbard model. At half filling, we confirm that the binding energy of the singlet bound state increases exponentially in the weak-coupling regime and decreases inversely proportional to the correlation in the strong-coupling regime. The spin-spin correlation shows an exponential decay with distance from the impurity site. The correlation length becomes smaller with increasing the correlation strength. We find discontinuous reduction of the binding energy and of spin-spin correlations with hole doping. The binding energy is reduced by hole doping; however, it remains of the same order of magnitude as for the half-filled case.

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I. INTRODUCTION

Although more than 40 years have passed since the discovery of the Kondo effect, it is still one of the most interesting topics in condensed matter physics; it lies at the heart of understanding strongly correlated electron systems.[1] The Kondo effect, which leads to the quenching of an impurity spin, forms the basis of the physics of a single magnetic impurity embedded in a metal. In order to understand the Kondo effect, the Anderson model[2] has been applied with great success. In the theoretical studies, one generally assumes an impurity level to be embedded in a noninteracting conduction band.

In the past, a system of magnetic ions coupled to (strongly) correlated conduction electrons has attracted considerable interest in connection with the heavy-fermion behavior, namely, $Nd_{2-x}Ce_xCuO_4$.[3] This raised the question whether correlations among conduction electrons affect substantially the expected formation of heavy quasiparticles.[4] So far, a number of authors have studied models of a single magnetic impurity embedded in a host of correlated conduction electrons. Thereby, perturbation theory and other approximation schemes were applied.[5–10] For example, it was shown that the Kondo scale can increase exponentially in the weak-coupling regime with increasing interaction of the conduction electrons.[8,10] However, a quantitative theory is still missing. Moreover, the case of strongly correlated conduction electrons with band filling slightly less than one-half (hole doping) is still an open problem.

In this paper, we study a single magnetic impurity coupled to a correlated electron system. The latter is assumed to be one dimensional (1D) and described by a Hubbard Hamiltonian. Using the density-matrix renormalization group (DMRG) method, we calculate the binding energy of the impurity-induced bound state and spin-spin correlation functions between the impurity and the correlated electrons in the thermodynamic limit. Special attention is paid to the case of a nearly half-filled conduction band with repulsive electron-electron interactions. For a 1D correlated host, there has been a numerical study for similar models[11,12] as well as an analytical study for an integrable model.[13,14] We hope that the present investigation will contribute to better insights.

This paper is organized as follows. In Sec. II, we introduce our model, i.e., a magnetic impurity coupled to a Hubbard chain. In Sec. III, we give some numerical details of the DMRG method applied here. In Sec. IV, we first present calculated results for the binding energy and spin-spin correlation functions at half filling and discuss the effect of the host-band correlations on the Kondo physics. Then, we consider the evolution of the same quantities with hole doping. Section IV contains a summary of the results and the discussions.

II. MODEL

We study a magnetic impurity coupled to a 1D correlated electron system.[15] The Hamiltonian consists of three terms,

$$H = H_c + H_f + H_{cf}. \tag{1}$$

The first term H_c represents 1D correlated electrons. Here, we describe them by a Hubbard Hamiltonian,

$$H_c = t\sum_{i,\sigma}(c^\dagger_{i+1\sigma}c_{i\sigma} + \text{H.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{2}$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron with spin σ ($=\uparrow,\downarrow$) at site i, and $n_{i\sigma}=c^\dagger_{i\sigma}c_{i\sigma}$ is the number operator. Furthermore, t is the hopping integral between neighboring sites and U is the on-site Coulomb interaction. The second term H_f is the orbital energy of the magnetic impurity site. We assume that the impurity contains one orbital, e.g., $4f$, and the Coulomb repulsion on the orbital U_f is infinite. Since double occupancies are excluded, i.e., the f orbital is either empty or singly occupied, the impurity site is given by

$$H_f = \varepsilon_f\sum_\sigma \hat{f}^\dagger_\sigma\hat{f}_\sigma, \tag{3}$$

with $\hat{f}^\dagger_\sigma = f^\dagger_\sigma(1-f^\dagger_{\bar{\sigma}}f_{\bar{\sigma}})$, where $\bar{\sigma}=-\sigma$ and $\varepsilon_f<0$. For convenience, we define $r=-\varepsilon_f/U(>0)$ and label an electron on the impurity site as "f electron." The third term H_{cf} involves the interaction between the impurity site and the correlated electron system. The interaction is assumed to be local and described by a hybridization like in the Anderson model, i.e.,

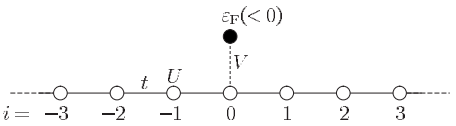

FIG. 1. Lattice structure of the system. Open and solid circles represent correlated electron system and impurity site, respectively. The bottom numbers i denote the site index of correlated electron system and $|i|$ corresponds to a distance between site i and the impurity site.

the impurity site is hybridized with a single site (denoted as site 0) of the correlated electron system. Thus,

$$H_{cf} = V\sum_{\sigma} (c_{0\sigma}^{\dagger}\hat{f}_{\sigma} + \hat{f}_{\sigma}^{\dagger}c_{0\sigma}), \tag{4}$$

where V is the hopping integral between the impurity site and site 0. The lattice structure is shown in Fig. 1. Values of $|\varepsilon_f|=2-3$ eV and $V=0.1-0.2$ eV are typical for Ce^{3+} ions in metals. We will work in units where $t=1$ and take as values $|\varepsilon_f|=2-3$ and $V=0.1-0.2$, throughout.

III. METHOD

We employ the DMRG method, which is one of the most powerful numerical techniques for studying quantum lattice many-body systems including quantum impurity systems.[16] With the DMRG method, we can obtain ground-state and low-lying excited-state energies as well as expectation values of physical quantities quite accurately for very large finite-size systems.

In order to carry out our calculations, we consider N $(=N_{\uparrow}+N_{\downarrow})$ electrons (N: even) in a system consisting of a chain of L site correlated electron system (L: odd) and a single-impurity site. The electron density is defined as $n=N/(L+1)$. Note that the number of lattice sites must be taken as $L+1=4l-2$, with l (>1) being an integer to maintain the total spin of the ground state as $S=0$. If one chooses it as $L+1=4l$, the singlet and triplet states are degenerate. We now apply the open-end boundary conditions to the 1D correlated electron system and assume that the impurity site is hybridized with the central site of the 1D open chain. The latter corresponds to site 0, and sites i and $-i$ are equivalent. In this paper, we restrict ourselves to the half-filled and hole-doped cases $(N \leqslant L+1)$.

Regarding quantum impurity problems, it is generally complicated for finite-size calculations to obtain accurate results in the thermodynamic limit $L\to\infty$ because of finite-size effects. In our calculations, the most problematic finite-size effects are Friedel oscillations due to the open ends of the Hubbard chain. Mostly, the energy scale of the Kondo physics is exponentially small; nevertheless, Friedel oscillations can persist even at the center of the chain as they decay as a power law from the edge sites. Therefore, we study several long chains with sites $L+1=62$, 126, 190, 254, 318, 382, 446, and 510, and then perform the finite-size-scaling analysis based on the size-dependent quantities. All DMRG results in this paper are extrapolated to the thermodynamic limit $L\to\infty$. For precise calculations, we keep up to $m\approx 5000$ density-matrix eigenstates in the DMRG procedure. In this way, the maximum truncation error, i.e., the discarded weight, is 7×10^{-9}, while the maximum error in the ground-state energy is less than $10^{-8}-10^{-7}$.

IV. RESULTS

A. System at half filling ($n=1$)

1. Binding energy

We first study the binding energy between the f electron and the correlated electrons. It corresponds to an energy gain due to the formation of a Kondo (or local) singlet bound state. Hence, the binding energy is given by an energy difference between the first triplet excited state and the singlet ground state,

$$\Delta_B = \lim_{L\to\infty} \Delta_B(L), \tag{5}$$

with

$$\Delta_B(L) = E_0(L,N_{\uparrow}+1,N_{\downarrow}-1) - E_0(L,N_{\uparrow},N_{\downarrow}), \tag{6}$$

where $E_0(L,N_{\uparrow},N_{\downarrow})$ is the ground-state energy in a system of $L+1$ sites with $N_{\uparrow}$ up-spin and $N_{\downarrow}$ down-spin electrons. Note that, at half filling, the system is insulating for finite U. The bound state therefore may be from a local singlet rather than the Kondo singlet. Here and in the following, we will speak of a Kondo singlet only if it involves more than the central site of the correlated electrons.

In Fig. 2(a), we show the DMRG results of the binding energy Δ_B as a function of the Coulomb interaction U for various parameter sets. In total, the results for the different parameter sets are qualitatively the same; as U increases, the binding energy rises rapidly for small U, reaches a maximum around $U\approx 4$, and decreases gradually for large U. This behavior is similar to the dependence of the effective Heisenberg interaction on the Coulomb interaction in the half-filled Hubbard model.[21] Accordingly, the DMRG results show that for large values of U the binding energy is approximately proportional to the effective exchange coupling J_{cf}, between the impurity and site 0.[17] If we assume that the effective exchange coupling results from second-order perturbation, i.e., $J_{cf}=\frac{2V^2}{U-\varepsilon_f}$, we can explain why the results for $V=0.2$ are about four times larger than those for $V=0.1$. This estimation of the effective exchange coupling is also consistent with a slight decrease of the binding energy with increasing $|\varepsilon_f|$.

Let us now consider the behavior in the limiting cases for weak and strong interaction strengths. A magnified view of the weak-coupling regime $(U<t)$ for $\varepsilon_f=-3$, $V=0.2$ is given in Fig. 2(b). When $U=0$, the system is metallic and essentially equivalent to the single-impurity Anderson model (SIAM) in the Kondo limit $(U_f/V=\infty)$ but asymmetric case $(\varepsilon \neq -U_f/2)$. The orbital energy of the impurity site is lower than the Fermi energy of the conduction band, so that the occupation number of the impurity site is always 1. The exchange interaction J_{cf} is estimated to be the order of V^2/ε_F and, therefore, the binding energy is expected to be very small but finite. We estimate it to be roughly $\Delta_B \simeq 10^{-7}-10^{-6}$. This value is compatible with the Kondo tem-

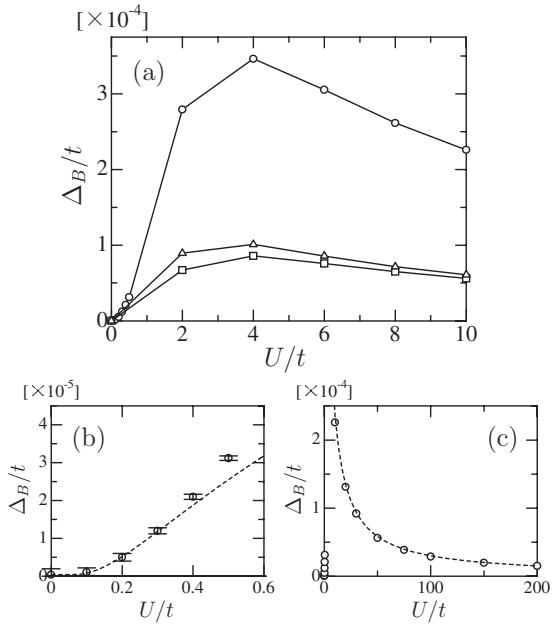

FIG. 2. (a) Binding energy Δ_B for $\varepsilon_f=-3$, $V=0.2$ (circles), $\varepsilon_f=-3$, $V=0.1$ (triangles), and $\varepsilon_f=-2$, $V=0.1$ (squares). (b) Magnified view of small U region for $\varepsilon_f=-3$, $V=0.2$. The data are fitted by a function $\Delta_B=\sqrt{\alpha U}\exp(-\beta/U)$ with $\alpha\simeq 2.5\times 10^{-4}$ and $\beta\simeq 0.4$. (c) Δ_B for $\varepsilon_f=-3$, $V=0.2$ in the strong-coupling regime ($U\gg t$). The data are fitted by a function $\Delta_B\simeq\frac{\lambda}{U-\varepsilon_F}$ with $\lambda\simeq 3.1\times 10^{-4}$.

perature T_K in the asymmetric SIAM.[18] The introduction of a finite Coulomb interaction makes the system insulating. With increasing U, Δ_B increases gradually when $U/t\lesssim 0.2$ and rapidly for $U/t\gtrsim 0.2$. There is a crossover from the Kondo singlet to a local singlet around $U/t=0.2$. Assuming an exponential behavior of Δ_B with U leads to a good fitting of the DMRG data, i.e., $\Delta_B=\sqrt{\alpha U}\exp(-\beta/U)$ with $\alpha\simeq 2.5\times 10^{-4}$ and $\beta\simeq 0.4$. Furthermore, Δ_B increases almost linearly in the regime $U/t=0.2-2$. We thus find that the binding energy of the local singlet can be a few orders of magnitude larger than that of the Kondo singlet.

The DMRG results for the strong-coupling regime ($U\gg t$) with $\varepsilon_f=-3$ and $V=0.2$ are plotted in Fig. 2(c). In this regime, the electrons are strongly localized at each site. Therefore, the system [Eq. (1)] can be reduced to the Heisenberg model with Hamiltonian,

$$H_{\text{eff}}=J\sum_i \mathbf{s}_i\cdot\mathbf{s}_{i+1}+J_{cf}\mathbf{S}_f\cdot\mathbf{s}_0, \tag{7}$$

with $J=\frac{4t^2}{U}$. The DMRG data can be fitted quite well by a function $\Delta_B=\frac{\lambda}{U-\varepsilon_F}$ with $\lambda\simeq 3.1\times 10^{-4}$. Despite the strong localization of the electrons, the binding energy is 2 orders of magnitude smaller than the cf exchange coupling. This is so because for $n=1$ a spin-density wave (SDW) is forming in the chain for any value of U (>0), which makes the formation of the local singlet state more difficult. This kind of behavior has already been observed before for $J>J_{cf}$.[19,20] We then note that the behavior of the binding energy for finite U is essentially the same as that of the Néel temperature in the half-filled Hubbard model.[21]

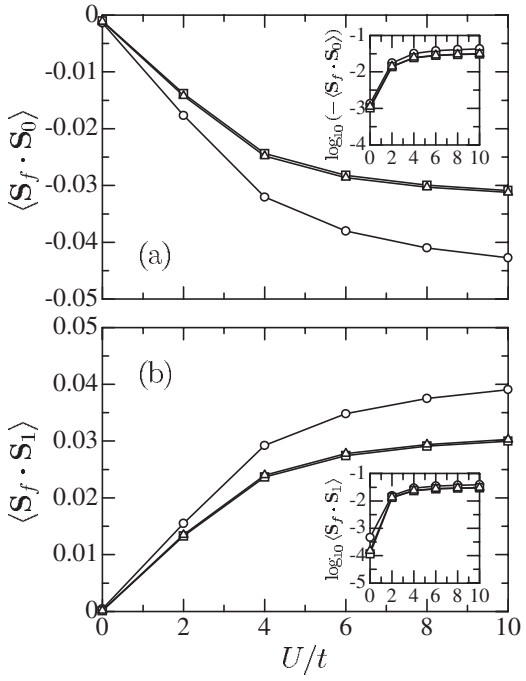

FIG. 3. Spin-spin correlation functions (a) $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$ and (b) $\langle\mathbf{S}_f\cdot\mathbf{s}_1\rangle$ as a function of the Coulomb interaction U for $\varepsilon_f=-3$, $V=0.2$ (circles), $\varepsilon_f=-3$, $V=0.1$ (triangles), and $\varepsilon_f=-2$, $V=0.1$ (squares). Inset: semilogarithmic plots of the magnitude of the spin-spin correlation functions.

2. Spin-spin correlations

In the Kondo problem, the spin degrees of freedom around the impurity play an essential role. Therefore, we investigate spin-spin correlations between the f electron and the correlated electrons. The correlated system is now described by the lattice model [Eq. (2)], so that we are allowed to study the distance r dependence of correlation functions, like $\langle\mathbf{S}_f\cdot\mathbf{s}_r\rangle$.

Let us first derive the spin-spin correlations between the spin on the impurity site and on the central site $i=0$, i.e., $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$. The DMRG results for various parameter sets are shown in Fig. 3(a) as function of the Coulomb interaction U. Since the antiferromagnetic correlation is derived from the cf exchange interaction, $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$ is negative for all parameter sets and Coulomb interaction strengths. The absolute value of $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$ increases with increasing V and with decreasing $|\varepsilon_F|$, as expected from the behavior of the binding energy. However, the influence of $|\varepsilon_F|$ is rather smaller. In the limit $U\to 0$, $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$ is antiferromagnetic but the magnitude is very small due to strong charge fluctuations, when the system is metallic [see inset of Fig. 3(a)]. It reflects the small binding energy around $U=0$. The magnitude of $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$ increases with increasing U and reaches its maximum value as $U\to\infty$, which means that one electron is localized on each site in that limit.

We consider next spin-spin correlations between a spin on the impurity site and on the next-nearest-neighbor site $i=1$, i.e., $\langle\mathbf{S}_f\cdot\mathbf{s}_1\rangle$. In Fig. 3(b), the DMRG results for $\langle\mathbf{S}_f\cdot\mathbf{s}_1\rangle$ are shown as a function of the Coulomb interaction U for vari-

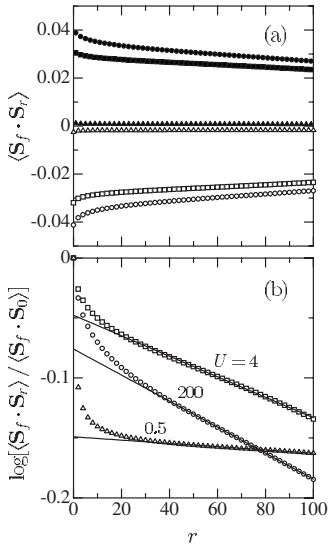

FIG. 4. (a) Spin-spin correlation functions $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ as a function of the distance r for $U=0.5$ (triangles), 4 (squares), and 200 (circles). (b) Semilogarithmic plot of the magnitude of the spin-spin correlation functions. The data are fitted by a function $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle \simeq \exp\left(-\frac{r}{\xi}\right)$ with $\xi=3184$, 508, 400 for $U=0.5$, 10, 200, respectively.

ous parameter sets. One expects ferromagnetic correlations from the effective Hamiltonian [Eq. (7)] for finite values of U, and indeed $\langle \mathbf{S}_f \cdot \mathbf{s}_1 \rangle$ has positive sign for all the parameter sets and Coulomb interaction strengths. Note that the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction induces ferromagnetic correlations, as substitute for the spin-spin interaction [Eq. (7)], in the weak-coupling ($U \sim 0$) and metallic regimes. However, it is difficult to separate the contribution from RKKY and the interaction [Eq. (7)]. The Coulomb interaction dependence of $\langle \mathbf{S}_f \cdot \mathbf{s}_1 \rangle$ is similar to that of $\langle \mathbf{S}_f \cdot \mathbf{s}_0 \rangle$. For the same parameter sets, the value of $\langle \mathbf{S}_f \cdot \mathbf{s}_1 \rangle$ is found to be slightly smaller than that of $|\langle \mathbf{S}_f \cdot \mathbf{s}_0 \rangle|$. This indicates a slow decay of the spin-spin correlation $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ with distance r. It implies that the spin of the f electron is hardly screened by the spin on site 0. In addition, the influence of V on the spin-spin correlations is rather small. Note that the binding energy depends strongly on the hybridization V.

Let us now consider the distance dependence of the spin-spin correlation functions. In Fig. 4(a), we plot the DMRG results for $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ as a function of distance r ($=|i|$). We choose three Coulomb interactions: (i) $U=0.5$ in the Kondo-singlet regime, (ii) $U=200$ in the limit of the local singlet regime, and (iii) $U=4$ in the intermediate regime where a maximal binding energy is obtained. The results for different distances are extrapolated to the thermodynamic limit $L \to \infty$. We find that $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ decays slowly and the sign changes alternately with r, i.e., $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ has a positive (negative) sign for odd (even) r, denoted by solid (empty) symbols in Fig. 4(a). The interaction [Eq. (7)] and/or the RKKY interactions cause ferromagnetic (antiferromagnetic) correlations between the spin of the f electron and that of the odd (even) site r. The absolute value of $\langle \mathbf{S}_f \cdot \mathbf{s}_i \rangle$ increases with increasing U because larger Coulomb interactions stabilize the $2k_F$-SDW oscillation which accompanies charge localization.

Since the system is in a spin-gapped ground state, an exponential decay of the spin-spin correlation with distance must be expected. In Fig. 4(b), we present a semilogarithmic plot of $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ as a function of distance r. For a convenient comparison, we have normalized $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ with respect to its value at $r=0$. The results can be fitted with a function $\exp\left(-\frac{r}{\xi}\right)$ and thus the exponential decay of the correlation functions is confirmed for all values of U. The correlation lengths are estimated as $\xi=3184$, 508, 400 for $U=0.5$, 4, 200, respectively. They seem to be much longer than those of other standard spin-gapped systems, e.g., $\xi=3.19$ in the two-leg isotropic Heisenberg system. However, it has been found that in the zigzag Heisenberg chain, the correlation lengths increase rapidly with decreasing binding energy.[22] Thus, the very large values of ξ reflect exponentially small binding energies. This also means that spin-polarized electrons are widely spread around the impurity site, i.e., the Kondo screening effect is quite weak. Furthermore, we note that the correlation functions decay rapidly around $r \simeq 0$. The decay rate is dependent on the magnitude of the cf exchange interaction.

B. Less than half filling ($n<1$)

We are also interested in doped systems, which are metallic even if $U>0$. We thus investigate the properties of the model [Eq. (1)] with $\varepsilon_f=-3$ for various hole concentrations $n=1-N_h/L$, where N_h is the number of doped holes ($N_h>0$). For this choice of ε_f, the occupation number of the impurity site is near unity because the Fermi level lies well above ε_f. In the strong-coupling limit ($U \gg t$), doubly occupied sites are excluded and therefore we can derive an effective model [Eq. (1)] by applying degenerate perturbation theory.[5] The effective Hamiltonian is written as

$$H = H_t + H_J + H_p + H_K + H'. \tag{8}$$

Here, H_t is the kinetic-energy term of the conduction electrons,

$$H_t = \sum_{i\sigma} t_i (\hat{c}^\dagger_{i+1\sigma} \hat{c}_{i\sigma} + \hat{c}^\dagger_{i\sigma} \hat{c}_{i+1\sigma}),$$

$$t_i = -\frac{t}{2}\left[1 - \frac{V^2(2+2r+r^2)}{2\varepsilon_f^2(1+r)^2}\delta_{i0}\right], \tag{9}$$

with $\hat{c}^\dagger_{i\sigma} = c^\dagger_{i\sigma}(1-n_{i\sigma})$. Furthermore, H_J is a spin-coupling term between the conduction electrons, which is of the Heisenberg type,

$$H_J = J_i \sum_i \mathbf{s}_i \cdot \mathbf{s}_{i+1},$$

$$J_i = \frac{2t^2}{U}\left[1 - \frac{V^2}{\varepsilon_f(U-\varepsilon_f)}\delta_{i0}\right]. \tag{10}$$

The sum of these two terms defines the 1D correlated electron system. It is essentially equivalent to a t-J model except for small modifications around site 0 due to the impurity. The term H_p corresponds to the one-particle potential around the impurity site, which is given by

$$H_p = -\frac{\eta V^2}{2\varepsilon_f(1+r)}(1-n_0) + \frac{V^2 t^2}{\varepsilon_f^2 U(1+r)^2}\sum_{i=\pm 1}(1-n_i),$$

$$\eta = 2 + r + \frac{2t^2}{\varepsilon_f^2(1+r)^2}(2+7r+7r^2+r^3). \quad (11)$$

It describes the attraction (repulsion) of a hole at site 0 (1) by the f electron. Furthermore, H_K is a spin-spin interaction term in analogy to the cf exchange interaction,

$$H_K = \frac{2\gamma V^2}{U-\varepsilon_f}\mathbf{S}_f\cdot\mathbf{s}_0 + \frac{tV^2(2+r)}{U\varepsilon_f(1+r)^2}\mathbf{S}_f\cdot\sum_{i=\pm 1}(\hat{\mathbf{s}}_{i0}+\hat{\mathbf{s}}_{0i}), \quad (12)$$

with $\hat{\mathbf{s}}_{ii'}=(1/2)\Sigma_{\alpha\beta}\hat{c}^\dagger_{i\alpha}\sigma_{\alpha\beta}\hat{c}^\dagger_{i'\beta}$, where $\sigma_{\alpha\beta}$ are the Pauli matrices. Furthermore, $\gamma=1+2t^2/(U-\varepsilon)^2$. The last term H' gives a correction to the effective model,

$$H' = \frac{2V^2t^2}{U\varepsilon_f^2(1+r)^2}\sum_{i=\pm 1}\mathbf{S}_f\cdot[\mathbf{s}_i(1-n_0)-\mathbf{s}_0(1-n_i)]. \quad (13)$$

The first term of Eq. (13) implies an antiferromagnetic interaction between the impurity site and site ±1 if there is a hole at site 0; on the other hand, the second term gives a correction to the Kondo-type interaction, i.e., the first term of Eq. (12), and the antiferromagnetic spin exchange between the impurity site and site 0 may be reduced.

1. Binding energy

Of particular interest is the evolution of the binding energy of the impurity-induced bound state upon hole doping. We can easily imagine that the binding energy is suppressed by hole doping due to the enhancement of charge fluctuation. Thus, away from half filling, the 1D correlated system is metallic and the bound state changes from a local singlet to the Kondo singlet. If the bound state survives with hole doping, it has a much larger energy than the standard Kondo singlet. In Fig. 5, we show the binding energy Δ_B as a function of band filling n ($\leqslant 1$) at (a) $V=0.2$ and (b) $V=0.1$ with $\varepsilon_f=-3$ for various values of U. Filled (empty) symbols refer to the data for $n=1$ ($n<1$) and empty symbols at $n=1$ represent the values for infinitesimally doped systems (see below). Roughly speaking, Δ_B is discontinuously reduced at $n=1$ and decreases with increasing hole doping for all cases except $U=0$. We find, however, that Δ_B remains of the same order of magnitude as in the half-filled case even at doping level up to a few percent. Also, the dependence of Δ_B on U is weaker for higher doping concentrations.

More precisely, there are two differences in behavior on the hybridization strength V. One is that in the vicinity of $n=1$, the binding energy for $V=0.2$ decreases more rapidly than that for $V=0.1$ despite larger cf exchange coupling [Eq. (12)]. It must be associated with the attraction between doped holes and the f electron, which is described in detail in the next paragraph. The other is that the binding energy disappears at lower doping levels for small values of V; Δ_B for $V=0.2$ maintains its value at $n\lesssim 0.9$ and that for $V=0.1$ goes to zero around $n\simeq 0.8-0.9$. It results from the size of the cf exchange coupling J_{cf}, and thus the critical doping concentration is highest at $U\approx 4$, giving a maximal value of J_{cf}.

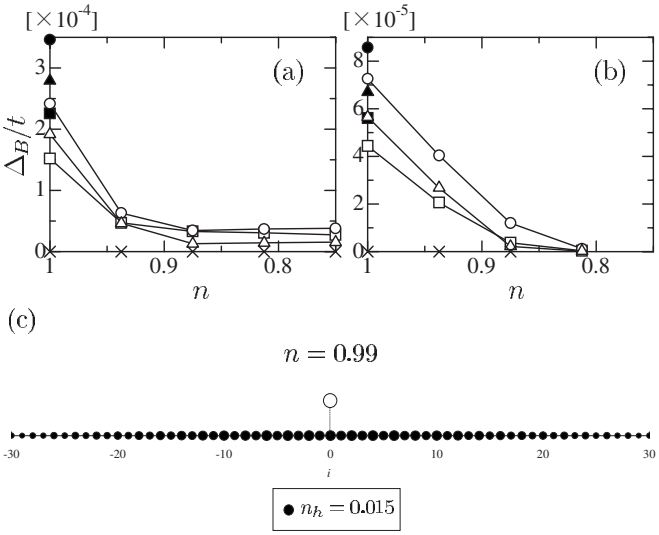

FIG. 5. Binding energy Δ_B for (a) $V=0.2$ and (b) $V=0.1$ with $\varepsilon_f=-3$ as a function of the band filling n. The Coulomb interaction strengths are $U=0$ (crosses), 2 (triangles), 4 (circles), and 10 (squares). Filled (empty) symbols correspond to the data for $n=1$ ($n<1$), and empty symbols at $n=1$ represent the values for infinitesimally doped systems. (c) Calculated hole density $n_{hi}=1-n_i$ for $V=0.2$, $U=4$, and $n=0.99$. The size of a dot is proportional to the hole density and is explicitly shown for $h=0.015$.

For the limit $n\to 1$, we have extrapolated the finite-size binding energy $\Delta_B(L)$ to the thermodynamic limit $L\to\infty$ for the four-hole-doped system by going up to $L+1=510$. One notices that the value of the binding energy in the limit $n\to 1$ differs from the $n=1$ undoped value. It reflects the fact that the binding energy of the Kondo singlet in the infinitesimally doped system is less than that of the local singlet in the undoped system. The reason being that, when the system is doped by a hole, the carrier tends to move onto site 0 due to the attraction from the impurity site [Eq. (11)] and thus a spin-singlet formation is prevented. In Fig. 5(c), we show the hole density $n_{hi}=1-n_i$ for $V=0.2$ and $U=4$ for the 1% hole-doped case. One can see that the doped holes concentrate around the impurity site. The discontinuity is higher for $V=0.2$ than for $V=0.1$ because the attractive interaction is enhanced by the hybridization V. Such a discontinuity of the spin-excitation energy has also been found in studies of ladder systems.[23,24] Note that in the hole-doped case, the V dependence of the binding energy is not simple because V enhances two competing effects: (i) the attraction between doped holes and the f electron and (ii) the cf exchange coupling between conduction electrons and the f electron.

2. Spin-spin correlations

Finally, we study the hole-doping dependence of spin-spin correlations between the f and conduction electrons. The correlation is expected to be weakened by hole doping due to an increase of charge fluctuations. In Fig. 6, we show the spin-spin correlation functions $\langle\mathbf{S}_f\cdot\mathbf{s}_0\rangle$ and $\langle\mathbf{S}_f\cdot\mathbf{s}_1\rangle$ as a function of band filling n ($\leqslant 1$) when (a) $V=0.2$ and (b) $V=0.1$ with $\varepsilon_f=-3$ for various Coulomb interaction strengths. The properties are fundamentally linked to those of the binding energy

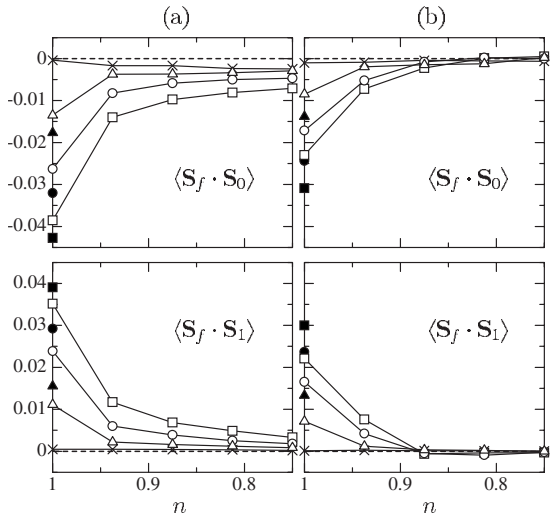

FIG. 6. Spin-spin correlation functions $\langle \mathbf{S}_f \cdot \mathbf{s}_0 \rangle$ and $\langle \mathbf{S}_f \cdot \mathbf{s}_1 \rangle$ for (a) $V=0.2$ and (b) $V=0.1$ with $\varepsilon_f=-3$ as a function of the band filling n. The Coulomb interaction strengths are $U=0$ (crosses), 2 (squares), 4 (triangles), and 10 (circles). Filled (empty) symbols correspond to the data for $n=1$ ($n<1$) and empty symbols at $n=1$ represent the values for infinitesimally doped systems.

as follows: (i) correlations are suppressed by hole doping and (ii) there exists a discontinuity at $n=1$.

Let us now investigate the DMRG results for the two V values. When $V=0.2$, all the correlation functions for finite U decrease rapidly close to $n=1$ and decay slowly when $n \lesssim 0.9$. This behavior is quite similar to that of the binding energy. It is seen that $|\langle \mathbf{S}_f \cdot \mathbf{s}_1 \rangle / \langle \mathbf{S}_f \cdot \mathbf{s}_0 \rangle|$ decreases with decreasing n. The small value corresponds to a rapid decay of $\langle \mathbf{S}_f \cdot \mathbf{s}_r \rangle$ around $r=0$, as seen in Fig. 4, e.g., for $U=0.5$ and $n=1$. It is accompanied by a transfer from the local singlet to the Kondo singlet. It also suggests a reduction of the RKKY interaction with doping. In addition, it is surprising that $\langle \mathbf{S}_f \cdot \mathbf{s}_0 \rangle$ seems to be enlarged by hole doping for small values of U ($\lesssim 2$). The "exchange hole" around the impurity is as a consequence of the Pauli principle. When $V=0.1$, all the correlation functions decrease monotonously and go to zero around $n \simeq 0.9$, which is accompanied by a vanishing of the binding energy. For $n \lesssim 0.8-0.9$, $|\langle \mathbf{S}_f \cdot \mathbf{s}_1 \rangle|$ has small negative values for large values of U, which indicates antiferromagnetic correlations between the f electron and the spin at site 1. It is derived from the first term of Eq. (13) and was previously suggested in Ref. 5.

V. CONCLUSION

Using the DMRG method, we have studied a magnetic impurity embedded in a correlated electron system, which is assumed to be the 1D Hubbard chain. At half filling, we confirm that the binding energy increases exponentially in the weak-coupling regime. There is a crossover from the Kondo singlet to the local singlet. The former state involves a wider spread of spin-polarized electrons around the impurity than the latter one. With increasing values of U, the binding energy has a maximum around $U \approx 4$ and afterward decreases inversely proportional to the Coulomb interaction. Due to the formation of a singlet bound state, the spin-spin correlation function decays exponentially with distance from the impurity site for all values of U (>0). The correlation length is quite long when the binding energy is small. It becomes shorter with increasing Coulomb interaction. For infinitesimally hole doping, we find a discontinuous reduction of the binding energy and of the spin-spin correlations from the values at half filling. For further doping, the binding energy is reduced but remains of the same order of magnitude as in the half-filled case even for doping concentration of a few percent. The electron-doped case is not studied here, but we expect qualitatively similar properties as for hole doping. When U becomes very large, the effective repulsion of electrons at site 0 is somewhat enlarged and the probability for double occupancy is correspondingly reduced due to the presence of the impurity.[5] However, there is no discontinuity at half filling. This is so because when an electron is added to the half-filled system, it is distributed almost uniformly over the 1D chain.

Possible further extensions of this work include the computation of the specific heat away from half filling. This is of interest because of available experiments on Ce doped Nd_2CuO_4. However, sufficiently accurate calculations are not simple and will require considerble efforts. A simple extension is the computation of spectral densities.

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[1] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
[2] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[3] T. Brugger, T. Schreiner, G. Roth, P. Adelmann, and G. Czjzek, Phys. Rev. Lett. **71**, 2481 (1993).
[4] P. Fulde, V. Zevin, and G. Zwicknagl, Z. Phys. B: Condens. Matter **92**, 133 (1993).
[5] T. Schork and P. Fulde, Phys. Rev. B **50**, 1345 (1994).
[6] D. Poilblanc, D. J. Scalapino, and W. Hanke, Phys. Rev. Lett. **72**, 884 (1993).
[7] J. Igarashi, K. Murayama, and P. Fulde, Phys. Rev. B **52**, 15966 (1995).
[8] G. Khaliullin and P. Fulde, Phys. Rev. B **52**, 9514 (1995).
[9] T. Schork, Phys. Rev. B **53**, 5626 (1996).
[10] W. Hofstetter, R. Bulla, and D. Vollhardt, Phys. Rev. Lett. **84**, 4417 (2000).
[11] K. A. Hallberg and C. A. Balseiro, Phys. Rev. B **52**, 374 (1995).
[12] S. Costamagna, C. J. Gazza, M. E. Torio, and J. A. Riera, Phys. Rev. B **74**, 195103 (2006).
[13] P. Phillips and N. Sandler, Phys. Rev. B **53**, R468 (1996).

[14] A. A. Zvyagin, Phys. Rev. Lett. **79**, 4641 (1997); P. Schlottmann and A. A. Zvyagin, Phys. Rev. B **56**, 13989 (1997).
[15] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993).
[16] *Density Matrix Renormalization*, Lecture Notes in Physics, edited by I. Peschel, X. Wang, M. Kaulke, and K. Hallberg (Springer, Berlin, 1999).
[17] K. Yosida, Phys. Rev. **147**, 223 (1966).
[18] D. Meyer, T. Wegner, M. Potthoff, and W. Nolting, Physica B **270**, 225 (1999).
[19] J. Igarashi, T. Tonegawa, M. Kaburagi, and P. Fulde, Phys. Rev. B **51**, 5814 (1995).
[20] W. Zhang, J. Igarashi, and P. Fulde, Phys. Rev. B **56**, 654 (1997).
[21] Y. H. Szczech, M. A. Tusch, and D. E. Logan, Phys. Rev. Lett. **74**, 2804 (1995).
[22] S. R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996).
[23] D. Poilblanc, O. Chiappa, J. Riera, S. R. White, and D. J. Scalapino, Phys. Rev. B **62**, R14633 (2000).
[24] S. Nishimoto, E. Jeckelmann, and D. J. Scalapino, Phys. Rev. B **66**, 245109 (2002).