Numerical renormalization-group study of a Kondo hole in a one-dimensional Kondo insulator

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We have studied a Kondo hole in a one-dimensional Kondo insulator at half-filling using a density matrix formulation of the numerical renormalization group. The Kondo hole introduces midgap states. The spin density introduced by the hole is localized in the vicinity of the hole. It resides primarily in the f spins for small exchange coupling J and in the conduction spins for large J. We present results on the spin gap, charge gap, and neutral gap. The presence of the Kondo hole reduces the charge gap but not the spin gap relative to a Kondo insulator without defects. For small J, the spin gap is smaller than the charge gap, while for large J, the spin gap is larger than the charge gap. RKKY interactions are reduced by the Kondo hole as can be seen in the staggered susceptibility. [S0163-1829(96)05146-6]

I. INTRODUCTION

It is well known that a single Kondo impurity in a metal gives rise to a narrow resonance at the Fermi energy at low temperatures. In a Kondo lattice this resonance is replaced by a narrow renormalized f band that appears at the Fermi level at low temperatures and that is associated with the onset of coherence. Hybridization between this renormalized f band and a broadband of conduction electrons gives rise to a gap. If the electron filling puts the gap at the Fermi energy, the ground state is that of a narrow gap semiconductor and the result is a Kondo insulator. Kondo insulators have generated a great deal of interest both experimentally and theoretically.[1] Introducing disorder is one way to experimentally test whether the gap in materials believed to be Kondo insulators arises from many-body interactions and the onset of coherence. There are two ways in which impurities can have a deleterious effect on the gap. First they break translational invariance and disrupt the coherence that produced the gap. Second they produce midgap states. One common substitutional impurity is a Kondo hole. A Kondo hole is a nonmagnetic impurity which has a conduction orbital but no f orbital. Experimentally Kondo holes are made by replacing Ce ions with La ions. $Ce_3Bi_4Pt_3$ is a Kondo insulator. Measurements on $(Ce_{1-x}La_x)_3Bi_4Pt_3$ indicate that introducing Kondo holes reduces the charge[2,3] and spin[3,4] gaps. As the concentration of La ions increases, the specific heat, resistivity, and thermopower at low temperatures become that of a metal with a low carrier concentration.[2,3]

Let us briefly review the theoretical work that has been done on Kondo holes in Kondo insulators. Sollie and Schlottmann[5] have done calculations on a Kondo hole in an Anderson lattice with the energy of the f orbital, $\varepsilon_f=\infty$, on the Kondo hole site and a finite value of ε_f on the other sites. They calculate the self-energy to second-order perturbation in the Coulomb repulsion U about the Hartree-Fock solution, though they do not calculate the self-energy self-consistently and they neglect its momentum dependence. By examining the local f-electron density of states, they find midgap states localized in the vicinity of the hole site. Schlottmann[6] found that these midgap states have magnetic properties which result in a Curie susceptibility and a Schottky anomaly in the specific heat. He found that a finite concentration of Kondo holes does little to reduce the gap, but rather produces an impurity band inside the gap in the f-electron density of states. At very low temperatures this impurity band gives a metallic specific heat linear in temperature and a Pauli-like susceptibility. Doniach and Fazekas[7] used mean field theory to argue that magnetic interactions between Kondo holes could lead to antiferromagnetic ordering, though there is no experimental evidence for such ordering. Wermbter, Sabel, and Czycholl[8] studied the periodic Anderson model in infinite dimensions using self-consistent second-order perturbation theory in U. To calculate the resistivity they used the coherent potential approximation to treat the Kondo hole sites. Their resistivity has qualitatively the same temperature and concentration dependence as that found experimentally. In short, perturbation theory approaches are in qualitative agreement with experiment, though technically they are only valid for small U, while real materials have large U. In addition they do not distinguish between the various types of gaps, e.g., spin and charge.

In this paper we use the density matrix renormalization group approach[9] to study a Kondo hole in a one-dimensional Kondo lattice. To the best of our knowledge, this is the first numerical calculation of a Kondo hole in a Kondo lattice. Our approach is able to explore certain aspects of the problem that are difficult to access with perturbation theory. For example, we can go to larger values of U, i.e., smaller values of the spin exchange J. In addition, unlike analytic techniques used thus far, we can distinguish between various types of gaps, e.g., spin and charge. We can also study how Kondo holes can act like magnetic impurities. In our calculations we find that there is a spin density localized in the vicinity of the Kondo hole. There is experimental evidence that nonmagnetic Kondo holes can behave like Kondo impurities. For example, $CePd_3$ is a good metal whose resistivity decreases with decreasing temperature as T approaches zero. However, when nonmagnetic La ions are substituted for Ce ions in $Ce_{1-x}La_xPd_3$, the resistivity below 50 K increases with decreasing temperature in a fashion reminiscent of Kondo impurities in a metal.[10]

The paper is organized as follows. In Sec. II we present the Hamiltonian, which we study using the density matrix

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renormalization group approach.[9] We present our results in Sec. III. In Sec. III A, we discuss the chemical potential as a function of electron filling. We find that the impurity introduces midgap states which lie in the center of the quasiparticle gap for large values of the exchange coupling J and move towards the edges of the gap as J decreases. In Sec. III B, we present our results on the spin gap, charge gap, and neutral gap as a function of J. For small J ($J \lesssim 3t$), the spin gap is smaller than the charge gap, while for large J ($J \gtrsim 3t$), the spin gap is larger than the charge gap. The presence of a Kondo hole reduces the charge gap but not the spin gap relative to the undoped Kondo insulator. In Sec. III C we find that the spin of the Kondo hole resides primarily in the conduction spins for large J and primarily in the f spins for small J. This crossover is an unexpected result. In Sec. III D we discuss the effect of the Kondo hole on the RKKY interactions. By examining the staggered susceptibility, we find that the RKKY oscillations are reduced when compared to a lattice with no Kondo hole. We state our conclusions in Sec. IV.

II. HAMILTONIAN

The standard one-dimensional Kondo lattice has spin-1/2 conduction electrons that hop from site to site with an on-site spin exchange $J(i)$ between the f electron and the conduction electron on that site. In the midst of this chain we place a Kondo hole which has no f orbital, and hence no on-site exchange. Thus the Hamiltonian is

$$H=-t\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+\text{H.c.})+\sum_{i}J(i)\vec{S}_{if}\cdot\vec{S}_{ic}, \tag{1}$$

where the conduction electron spin density on site i is $\vec{S}_{ic}=\Sigma_{\alpha\beta}c_{i\alpha}^{\dagger}(\vec{\sigma}/2)_{\alpha\beta}c_{i\beta}$, and $\vec{\sigma}_{\alpha\beta}$ are Pauli matrices. On the host lattice the f-electron spin density is $\vec{S}_{if}=\Sigma_{\alpha\beta}f_{i\alpha}^{\dagger}(\vec{\sigma}/2)_{\alpha\beta}f_{i\beta}$, while on the Kondo hole site $\vec{S}_{if}=0$ because there is no f electron. t is the hopping matrix element for the conduction electrons between neighboring sites. We set $t=1$. The on-site spin exchange $J(i)$ is zero for the Kondo hole and equal to J on the rest of the sites. We choose J to be antiferromagnetic ($J>0$). We place the Kondo hole in the middle of the lattice on site $i=L/2$, where L is the number of sites. We studied lattices of size $L=4$, 6, 8, 16, and 24. In the absence of a Kondo hole, the Kondo insulator corresponds to half-filling where the total number of conduction electrons, N, equals the number of sites, L.

Even with a Kondo hole, the Hamiltonian has SU(2) spin symmetry as well as SU(2) charge pseudospin symmetry.[11] The components of the pseudospin operator $\vec{I}$ are given by

$$I_z=\frac{1}{2}\sum_{i}(c_{i\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{i\downarrow}+f_{i\uparrow}^{\dagger}f_{i\uparrow}+f_{i\downarrow}^{\dagger}f_{i\downarrow}-2),$$

$$I_+=\sum_{i}(-1)^{i}(c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}-f_{i\uparrow}^{\dagger}f_{i\downarrow}^{\dagger}), \tag{2}$$

$$I_-=\sum_{i}(-1)^{i}(c_{i\downarrow}c_{i\uparrow}-f_{i\downarrow}f_{i\uparrow}).$$

The z component of the pseudospin is the charge operator and is equal to $(N_{\rm el}/2)-L$, where $N_{\rm el}$ is the total number of electrons including both conduction and f electrons. An $I_z=1$ state can be achieved by adding two electrons.

All the energy eigenstates have a definite value of S and I. At half-filling with one Kondo hole ($N=L$ and $N_{\rm el}=2L-1$), the ground state is a pseudospin singlet with total spin $S=1/2$ ($S=1/2$, $I=0$) for all values of J. The spin gap Δ_S is defined as the energy difference between the lowest-lying excited spin state and the ground state:

$$\Delta_S=E(S=\tfrac{3}{2},\ I=0)-E_0(S=\tfrac{1}{2},\ I=0), \tag{3}$$

where E_0 is the energy of the ground state. For $J\gg t$, the lowest spin excitation corresponds to forming a triplet between an f spin and a conduction spin on a site that is not a Kondo hole, with the remaining sites being the same as in the ground state. In this limit $\Delta_S\cong J$.

To find the charge gap, we note that optical experiments measure the charge gap by measuring the conductivity which is determined by the current-current correlation function. The current is related to the charge density through the continuity equation. Thus the lowest-lying charge excitation is the lowest excited state $|n\rangle$ with $S=1/2$ such that $\langle 0|\Sigma_q\rho_q|n\rangle\neq 0$, where ρ_q is the q component of the Fourier-transformed charge density operator and $|0\rangle$ is the ground state.[12] Notice that ρ_q is related to $\vec{I}_q^{z}$ where $\vec{I}_q$ is a Fourier-transformed vector in pseudospin space given by

$$I_q^z=\frac{1}{2}\sum_{i}e^{-i\vec{q}\cdot\vec{r}_i}(c_{i\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{i\downarrow}+f_{i\uparrow}^{\dagger}f_{i\uparrow}+f_{i\downarrow}^{\dagger}f_{i\downarrow}-2),$$

$$I_q^+=\sum_{i}e^{-i\vec{q}\cdot\vec{r}_i}(-1)^{i}(c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}-f_{i\uparrow}^{\dagger}f_{i\downarrow}^{\dagger}), \tag{4}$$

$$I_q^-=\sum_{i}e^{-i\vec{q}\cdot\vec{r}_i}(-1)^{i}(c_{i\downarrow}c_{i\uparrow}-f_{i\downarrow}f_{i\uparrow}).$$

Using the Wigner-Eckart theorem, one can show that the ($S=1/2$, $I=1$) states are the only states $|n\rangle$ for which the charge density ρ_q has finite matrix elements $\langle n|\rho_q|0\rangle$ with the ground state $|0\rangle$. Thus the charge gap Δ_C is the energy difference between the ground state and the lowest pseudospin triplet state:[11,12]

$$\Delta_C=E(S=\tfrac{1}{2},\ I=1)-E_0(S=\tfrac{1}{2},\ I=0). \tag{5}$$

For a half-filled Kondo insulator without a Kondo hole, the ground state is a pseudospin and spin singlet ($S=0$, $I=0$). We can define a neutral singlet gap as the energy difference between the ground state and the lowest-lying excited neutral spin singlet state, i.e., $\Delta_{NS}=E(S=0,\ I=0)-E_g(S=0,\ I=0)$.[13] When a Kondo hole is present, we can define a neutral gap Δ_N as the energy difference between the ground state and the lowest-lying excited neutral state with the same quantum numbers as the ground state ($S=1/2$, $I=0$):

$$\Delta_N=E(S=\tfrac{1}{2},\ I=0)-E_0(S=\tfrac{1}{2},\ I=0). \tag{6}$$

For the half-filled Kondo lattice without a Kondo hole, the neutral singlet has been found to be an elementary excitation consisting of a ''particle'' and a ''hole,'' which are ($S=1/2$, $I=1/2$) excitations.[13] In a single-site basis, a ''hole'' is a site with one f electron and no conduction electrons with quantum numbers ($S=1/2$, $I=1/2$, $I_z=-1/2$); this hole is different from a Kondo hole. A ''particle'' is a site with one f electron and two conduction electrons with ($S=1/2$, $I=1/2$, $I_z=+1/2$). A particle and a hole can be combined to form a charge excitation ($S=0, I=1$) or a neutral singlet excitation ($S=0$, $I=0$). (Other combinations are also possible.) When a Kondo hole is added to the lattice, one can think in terms of a hole or a particle on the Kondo hole site. A hole on the Kondo hole site has no conduction electrons, no f electrons, and quantum numbers ($S=0$, $I=1/2, I_z=-1/2$). A particle on the Kondo hole site has two conduction electrons, no f electrons, and quantum numbers ($S=0, I=1/2, I_z=+1/2$). A particle (hole) on a Kondo hole site can be combined with a hole (particle) on an ordinary Kondo site to form a charge excitation ($S=1/2$, $I=1$) or a neutral excitation ($S=1/2$, $I=0$). These are the excitations associated with the charge gap and the neutral gap. [Because the spin is 1/2 and not zero, we do not call the particle-hole excitation ($S=1/2$, $I=0$) a neutral singlet, but rather just a neutral excitation.]

We use the density matrix renormalization group (DMRG) algorithm[9] to calculate the ground state and the first few excited states of the Kondo lattice. This real-space technique has proved to be remarkably accurate for one-dimensional systems such as the Kondo and Anderson lattices.[12,14] We used the finite system method[9] with open boundary conditions in which there is no hopping past the ends of the chain. We kept up to 140 states per block. The results were extremely accurate for $J \gg t$, with typical truncation errors of order 10^{-10} for $J=10$. For $J \lesssim t$, the f-spin degrees of freedom lead to a large number of nearly degenerate energy levels. As a result, the accuracy was significantly reduced, with truncation errors of order 10^{-4} for $J=0.5$.

III. RESULTS

A. Chemical potential vs filling

We study how the chemical potential varies with electron filling. We consider a 16-site Kondo lattice with the Kondo hole on site 8. We vary the electron filling and define the chemical potential by

$$\mu(N)=E_0(N)-E_0(N-1), \tag{7}$$

where $E_0(N)$ is the ground state energy with N electrons. Our results are shown in Fig. 1, where we have scaled the chemical potential by J. When the Kondo hole is absent, there is a jump in the chemical potential that is centered about half-filling ($N=16$). This is the quasiparticle gap which is defined as the difference of chemical potentials

$$\Delta_{\mathrm{QP}}=\mu(N+1)-\mu(N). \tag{8}$$

From Fig. 1, we see that the Kondo hole introduces states in the gap for large J. The chemical potential of these midgap states corresponds to the energy of adding a particle or a hole to the half-filled system. To understand why these midgap states have a chemical potential so close to zero, note that for $J \gg t$, an on-site spin singlet forms between the f spin and the conduction electron spin on each host lattice site. (''Host lattice site'' refers to an ordinary Kondo site which does not have a Kondo hole.) When we put zero, one, or two conduction electrons on the Kondo hole site, the associated electrons or holes will be localized in the vicinity of the impurity, and the energies of these three states will be nearly degenerate. This means that the chemical potential corresponding to adding a particle or a hole to a half-filled system is close to zero. This is indeed what we see for $J=10$. As J decreases, these midgap states move toward the edges of the gap as the associated states become less localized.

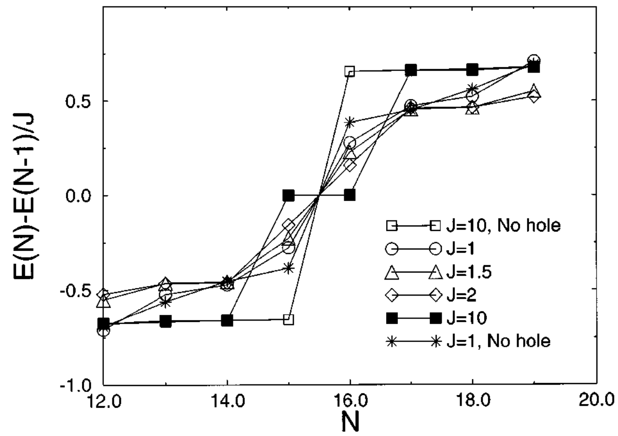

FIG. 1. Chemical potential scaled by J vs number of conduction electrons, N. The scaled chemical potential is defined by $\mu=[E(N)-E(N-1)]/J$. $t=1$, $L=16$, and the Kondo hole is on site $i=8$. Open boundary conditions are used. The midgap states associated with large J move toward the edges of the gap as J decreases. For comparison, we show the chemical potential for the case of no Kondo hole with $J=1$ and $J=10$. The solid lines are guides to the eye.

B. Gaps

We have calculated the spin, charge, and neutral gaps as a function of J for $L=8$, 16, and 24 at half-filling ($N=L$). Our results are shown in Fig. 2. For comparison we show the corresponding values of the gaps when there is no Kondo hole.[13] The value of the spin gap is not affected much by the presence of the Kondo hole. However, the Kondo hole reduces the charge gap and the neutral gap by roughly a factor of 2 for large J.

Without a Kondo hole the spin gap is smaller than the charge gap for all values of J. However, when there is a Kondo hole, the spin gap is larger than the charge gap for $J \gtrsim 3$ and smaller than the charge gap for $J \lesssim 3$. To understand this behavior for small J, note that the midgap states move to the edges of the gap as J decreases and the charge excitations become less localized. As a result, the Kondo hole has less of an effect on the system and it behaves much like the unperturbed Kondo insulator with the spin gap less than the charge gap. To understand the large J behavior, note that when $J \gg t$, we can describe the eigenstates in terms of simple on-site states. Each ordinary Kondo site can be in a singlet state involving the f electron and a conduction electron with an energy of $-3J/4$, a spin-triplet state with energy

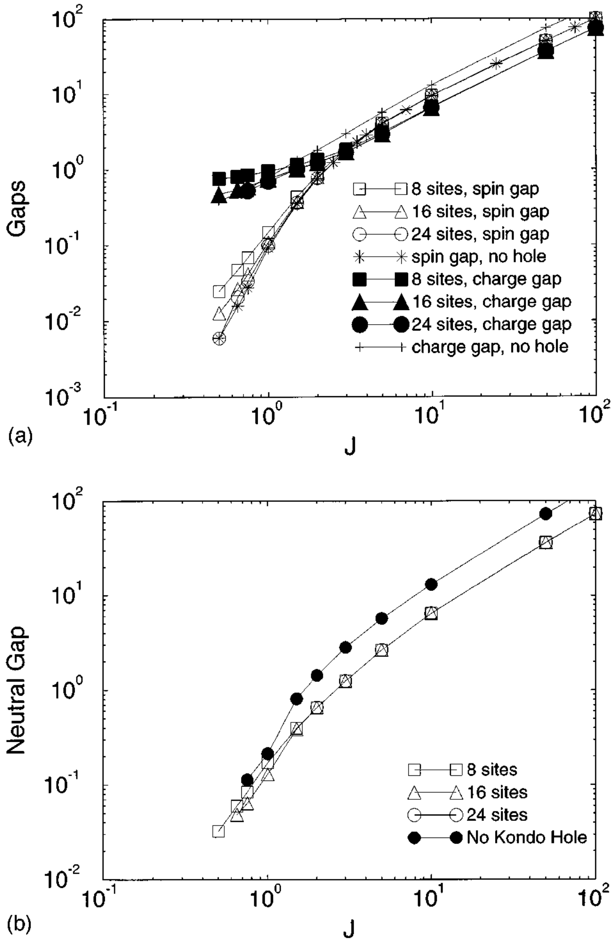

FIG. 2. (a) Spin and charge gaps vs J for $L=8$, 16, and 24 sites with open boundary conditions. The Kondo hole is on site $i=L/2$. $t=1$. For comparison, we show the spin and charge gaps without a Kondo hole for $L=24$. (b) Neutral gap vs J for $L=8$, 16, and 24 sites with open boundary conditions. The Kondo hole is on site $i=L/2$. $t=1$. For comparison, we show the neutral singlet gap for a Kondo insulator without a Kondo hole for $L=24$. The solid lines are guides to the eye.

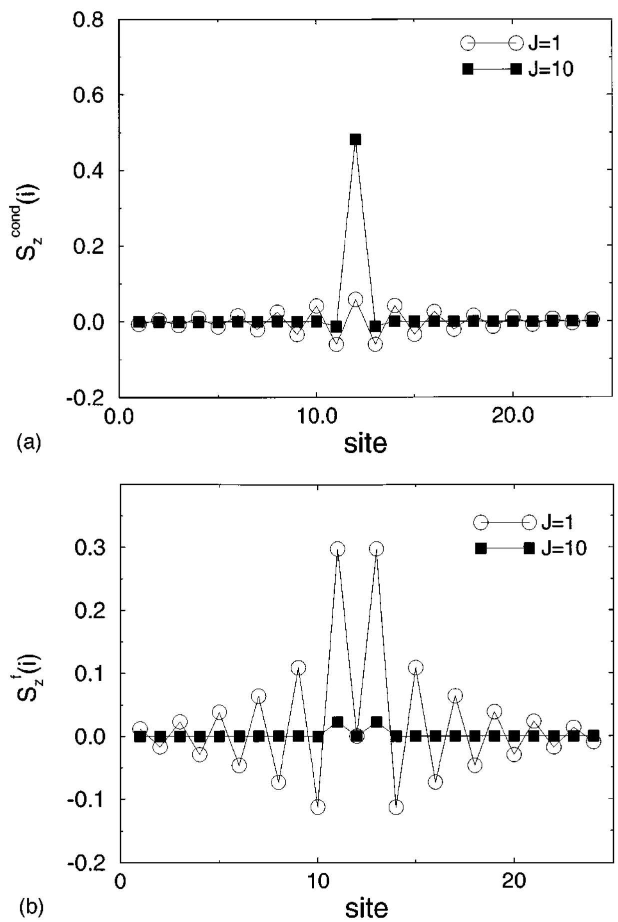

FIG. 3. (a) z component of the conduction spin vs site for $J=1$ and $J=10$ for a 24-site lattice with the Kondo hole on site $i=12$. (b) z component of the f spin vs site for $J=1$ and $J=10$ for a 24-site lattice with the Kondo hole on site $i=12$. Notice that the amplitude of the RKKY oscillations fall off exponentially for $J=1$. The solid lines are guides to the eye.

$J/4$, a ''hole'' state with no conduction electrons ($S=1/2$, $I=1/2$, $I_z=-1/2$), or a ''particle'' state with 2 conduction electrons ($S=1/2$, $I=1/2$, $I_z=1/2$). The particle and hole states have zero energy. The Kondo hole can have one conduction electron ($S=1/2, I=0$), be in a ''hole'' state with no electrons ($S=0$, $I=1/2$, $I=-1/2$), or be in a ''particle'' state with two conduction electrons ($S=0$, $I=1/2$, $I_z=1/2$). These three Kondo hole states have zero energy. In the ground state, the Kondo hole has one conduction electron and every site of the host lattice is a singlet when $J \gg t$. The lowest spin excitation consists of a single host site with a spin triplet, with the remaining sites being in their ground state configuration; this gives $\Delta_S \approx J$.[13,15,16] The lowest charge excitation ($S=1/2$, $I=1$) consists of a hole (particle) on the Kondo hole site and a particle (hole) on a host site. Since one singlet is destroyed, this results in $\Delta_C \approx 3J/4$. Notice that these estimates indicate that the spin gap is greater than the charge gap for large J. The low-lying eigenstates consist of linear combinations of these local excitations. These simple estimates of the gaps work very well for $J \gg t$; e.g., for $J=100$ and $L=24$ we find numerically that $\Delta_S = 99.9$ and $\Delta_N \cong \Delta_C \cong 74.0$, and for $J=10$ and $L=24$ we find $\Delta_S = 9.40$ and $\Delta_N \cong \Delta_C \cong 6.57$.

C. Where the spin resides

At half-filling ($N=L$) a Kondo lattice with a single Kondo hole has a total spin $S=1/2$. When $J \gg t$, the Kondo hole has one conduction electron and every site of the host lattice is a singlet in the ground state. Thus the spin-1/2 resides in the conduction orbital of the Kondo hole. This can be seen in Fig. 3(a) where we plot the z component of the conduction spin versus site. As J decreases, the spin 1/2 is no longer predominantly in the conduction orbitals. Rather it is primarily in the f orbitals of the sites neighboring the Kondo hole. For $J=1$, as Fig. 3(b) shows, the z components of the f spins on the nearest-neighbor sites are polarized and have most of the spin. The f spins on neighboring sites farther away from the Kondo hole have RKKY oscillations with an envelope that decays exponentially, indicating that the spin is localized in the f orbitals for small J. Notice that for large J, e.g., $J=10$, the spin density has very little amplitude in the f spins. We can fit the absolute value of the z component

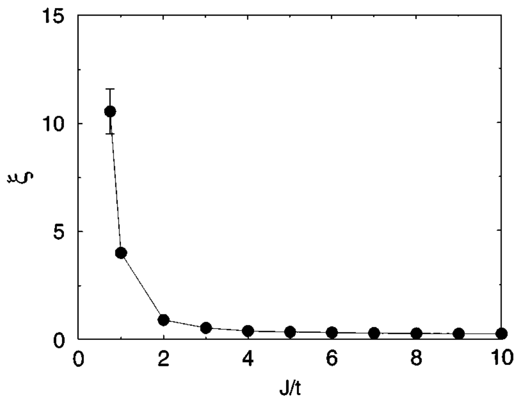

FIG. 4. Spin localization length ξ vs J for a 24-site lattice with open boundary conditions. ξ is deduced by fitting $|\langle 0|S_z^f(r)|0\rangle|$ to the form $\exp(-r/\xi)$ where r is the distance from the hole. The error bars are the standard deviation of the fit. The error bars are smaller than the size of the points for all J except $J=0.75$. The solid line is a guide to the eye. $t=1$.

$|\langle 0|S_z^f(r)|0\rangle|$ of the f spins to the form $\exp(-r/\xi)$, where r is the distance from the Kondo hole and ξ is the localization length. In Fig. 4 we plot the localization length ξ versus J.

This crossover from conduction spins to f spins as J decreases is shown in Fig. 5 where we plot the total conduction spin $\Sigma_i S_z^{\rm cond}$ and the total f spin $\Sigma_i S_z^f$ of the lattice versus J. The crossover occurs around $J\approx 4t$. This is not a finite-size effect because the curves for an 8-site lattice are indistinguishable from those shown for a 24-site lattice. We can understand why this crossover occurs in the following way. As we discussed earlier, for large J, the spin is primarily in the conduction orbital of the Kondo hole. For $J\lesssim 4t$, it is energetically favorable for both up and down spin conduction electrons to hop freely. Putting the spin-1/2 in the conduction spins would polarize the conduction electrons and impede their hopping due to the Pauli exclusion principle.

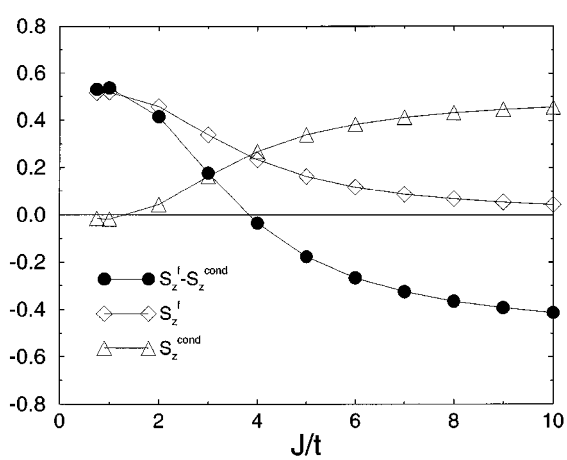

FIG. 5. Total f spin $[S_z^f=\Sigma_i S_z^f(i)]$, total conduction spin $[S_z^{\rm cond}=\Sigma_i S_z^{\rm cond}(i)]$, and the difference $(S_z^f-S_z^{\rm cond})$ vs J/t for a 24-site lattice. Corresponding curves for an 8-site lattice are indistinguishable from those shown. Notice that where the spin 1/2 resides crosses over from f spins to conduction spins as J increases. The solid lines are guides to the eye.

For example, suppose the spin-1/2 is entirely in the conduction orbital on the Kondo hole site with $S_z=1/2$. Then another spin-up electron cannot hop onto or past the Kondo hole. If the polarization were spread over many sites, then the kinetic energy cost would be reduced. We might hope to reduce the hopping energy cost to zero in an infinite lattice by spreading the spin polarization over the conduction orbitals of the entire lattice. However, because of the gaps, the polarization is localized in the vicinity of the Kondo hole and therefore costs a finite amount of energy. In fact, this energy cost is greater than the spin gap for small J. The evidence for this is in the lowest-lying spin excitation ($S=3/2$, $I=0$) which defines the upper edge of the spin gap. In this state the f electrons contain slightly more than all of the spin ($\Sigma_i S_z^f=1.58$ and $\Sigma_i S_z^{\rm cond}=-0.08$ for $J=1$) which implies that the energy cost to polarize the conduction electrons in the spin-up direction is greater than the spin gap. On the other hand, polarizing the f electrons just costs exchange energy which is less important than the kinetic energy for $J\lesssim 4t$. So the spin 1/2 resides primarily in the f spins. To see why the crossover occurs at $J\approx 4t$, note that we can write the Hamiltonian as

$$H=-t\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+\text{H.c.})+\sum_i\frac{J(i)}{4}(\vec{\sigma}_{if})_{\alpha\beta}\cdot(\vec{\sigma}_{ic})_{\gamma\delta}\times f_{i\alpha}^{\dagger}f_{i\beta}c_{i\gamma}^{\dagger}c_{i\delta}, \tag{9}$$

where we sum over repeated Greek indices. The hopping term and the exchange term are comparable when $J\approx 4t$. For $J\lesssim 4t$, the exchange energy dominates and singlets form on every site of the host lattice, leaving the spin 1/2 in the conduction orbital of the Kondo hole.

D. Susceptibility

At zero temperature the uniform susceptibility $\chi(q=0)$ is zero because there is a spin gap between the ground state and the lowest spin excitations. The ground state is an $S=1/2$ doublet whose energy is linear in a uniform magnetic field due to Zeeman splitting. Thus $\chi(q=0)=-\partial^2E/\partial H^2=0$.

However, the staggered susceptibility $\chi(q)$ is finite. To calculate the susceptibility $\chi(q)$, we apply a small staggered magnetic field $h_z=h_0\cos(qr)$ which couples to both the f spins and the conduction spins. The magnitude h_0 lies between $10^{-6}t$ and $(5\times 10^{-4})t$. When h_0 is this small, the plot of $S(q)$ versus h_0 is a straight line whose slope is the susceptibility $\chi(q)$. [$S(q)$ is the Fourier transform of $\langle 0|S_z(i)|0\rangle$.] We use periodic boundary conditions with $q_n=2\pi n/L$.

The staggered susceptibility $\chi(q=2k_F)$ is a measure of the RKKY coupling between f spins. (k_F is the Fermi wave vector of the noninteracting conduction electrons.) At half-filling $2k_Fa=\pi$ and the RKKY coupling favors antiferromagnetic alignment of the f spins. Since the Kondo hole is missing an f spin, we expect the RKKY oscillations, and hence $\chi(q=2k_F)$, to be diminished by the presence of a Kondo hole. In addition the Kondo hole breaks translational invariance and allows the system to respond at wave vectors other than the wave vectors of the staggered field. This will also reduce $\chi(q=2k_F)$ relative to its value in lattice without a Kondo hole.

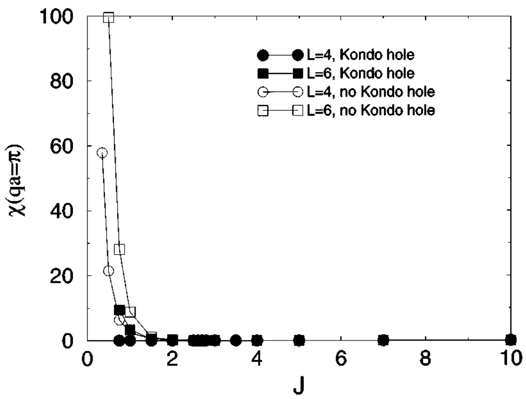

FIG. 6. Staggered susceptibility $\chi(qa=2k_F a=\pi)$ vs J for $L=4$ and 6 at half-filling with periodic boundary conditions. The Kondo hole is on site $i=L/2$. For comparison we also show $\chi(qa=2k_F a=\pi)$ for lattices without a Kondo hole.

As J approaches zero, numerical noise can induce spurious antiferromagnetic ordering of the lattice because the states with and without long range order are very close in energy. Because of this, we only study short chains (four and six sites) which we can diagonalize exactly. In Fig. 6 we plot the staggered susceptibility $\chi(qa=2k_F a=\pi)$ versus J for lattices with and without a Kondo hole at half-filling.[17] As expected, our results show that the staggered susceptibility is greatly reduced by the presence of a Kondo hole. This reflects the suppression of RKKY oscillations. As the lattice gets longer, we expect that the effect of a single Kondo hole will be diluted and $\chi(q)$ will approach the value of an undoped Kondo insulator.

IV. CONCLUSIONS

We have studied a Kondo hole in the middle of a one-dimensional Kondo lattice at half-filling using the density matrix renormalization group technique. The Kondo hole introduces midgap states which move from the middle of the quasiparticle gap to the edges as the exchange coupling J goes from large values to small values. As $J\rightarrow\infty$, the chemical potential of these midgap states goes to zero which corresponds to the degeneracy of states with zero, one, and two conduction electrons on the Kondo hole site. We presented results on the spin gap, charge gap, and neutral gap as a function of J. For small J the spin gap is smaller than the charge gap. However, for large J, the spin gap is larger than the charge gap because the energy to change a singlet into a triplet is $\Delta_S\sim J$ while the energy to transfer an electron or a hole from the Kondo hole to another site which had a singlet is $\Delta_C\sim 3J/4$. We found that the Kondo hole reduced the size of the charge gap relative to the charge gap of a Kondo insulator without defects. This agrees qualitatively with experiment.[2,3] However, we found that the Kondo hole did not reduce the size of the spin gap relative to an undoped Kondo insulator, whereas neutron scattering and susceptibility measurements indicate a reduction of the spin gap.[3,4] This indicates that a finite concentration of interacting Kondo holes is needed to reduce the spin gap. One possible scenario is that magnetic interactions between the Kondo holes lead to low-energy spin excitations that would reduce the spin gap. If there are enough Kondo holes, they could have antiferromagnetic[7] or spin glass order. In these cases there would be no spin gap.

At half-filling there are an odd number of spins and the ground state has $S=1/2$. This spin 1/2 is localized in the vicinity of the Kondo hole. It is primarily in the f spins for small J and in the conduction spins for large J. The crossover occurs at $J\approx 4t$ where the kinetic energy is comparable to the exchange energy. The presence of the Kondo hole reduces RKKY oscillations as can be seen in the staggered susceptibility $\chi(qa=2k_F=\pi)$.

Putting Kondo holes into Kondo insulators can be done experimentally by replacing Ce ions with La ions. It should be possible to look in real materials for some of the effects listed above, e.g., midgap states and reduced RKKY oscillations. Our results are valid for a dilute concentration of noninteracting Kondo holes, i.e., for Kondo holes whose separation is much greater than the localization length of excitations in the vicinity of the Kondo holes. However, having a larger concentration of Kondo holes introduces effects that we have not considered here such as impurity bands and interactions between the Kondo holes.[6–8]

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[17] When we applied a staggered field ($q=\pi$) to a four-site lattice with a Kondo hole on site $i=2$, the field pointed up at the Kondo hole and down on the nearest-neighbor sites. Since the net spin $S=1/2$ is in the conduction orbital on the Kondo hole for large J, the ground state has $S_z=+1/2$ for $J\geqslant 2.7$. For small J the net spin resides primarily in the f spins near the Kondo hole. To align with the staggered field, the f spins on the nearest neighbors to the Kondo hole point down. So the ground state has $S_z=-1/2$ for $J\leqslant 2.6$. A similar crossover in the z component of the spin of the ground state occurs for $L=6$.