A Numerical Renormalization Group Study of a Kondo Hole in a One Dimensional Kondo Insulator

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Abstract

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. 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. The presence of the Kondo hole reduces RKKY interactions as can be seen in the staggered susceptibility.

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The onset of coherence in a Kondo lattice is associated with the opening of a gap in a Kondo insulator. Impurities can disrupt this coherence and produce midgap states. In this paper we will examine the effect of putting a Kondo hole in a one-dimensional Kondo insulator. A Kondo hole is a nonmagnetic impurity which has a conduction orbital but no f–orbital. Experimentally this is done by replacing Ce or U ions with La or Th ions. There is experimental evidence that these nonmagnetic impurities can behave as 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$_x$Pd$_3$, the resistivity below 50 K increases with decreasing temperature in a fashion reminiscent of Kondo impurities in a metal.

Sollie and Schlottmann 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 $\varepsilon_f$ on the other sites. They calculate the self–energy to second order perturbation in $U$ 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 in the vicinity of the hole site. However, this approach does not distinguish between the various types of gaps, e.g., spin and charge.

In this paper we use the density matrix renormalization group approach 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. The paper is organized as follows. In section II we present the Hamiltonian, which we study using the density matrix renormalization group approach. We present our results in section III. In section IIIa, 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 section IIIb, we present our results on the spin gap, charge gap, and neutral gap as 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. In section IIIc 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 $J$. In section IIId 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 section 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

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

where the conduction electron spin density on site $i$ is $\vec{S}_{ic} = \sum_{\alpha \beta} c_{i\alpha}^\dagger (\vec{\sigma}/2)_{\alpha \beta} c_{i\beta}$, and $\vec{\sigma}_{\alpha \beta}$ are Pauli matrices. On the host lattice the f-electron spin density is $\vec{S}_{if} = \sum_{\alpha \beta} f_{i\alpha}^\dagger (\vec{\sigma}/2)_{\alpha \beta} f_{i\beta}$, 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 $L=4, 6, 8, 16, \text{and } 24$. 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. The components of the pseudospin operator $\vec{I}$ are given by:

$$I_z = \frac{1}{2} \sum_i \left( c_{i \uparrow}^\dagger c_{i \uparrow} + c_{i \downarrow}^\dagger c_{i \downarrow} + f_{i \uparrow}^\dagger f_{i \uparrow} + f_{i \downarrow}^\dagger f_{i \downarrow} - 2 \right)$$
\[ I_+ = \sum_i (-1)^i (c_{i\uparrow}^\dagger c_{i\uparrow} - f_{i\uparrow}^\dagger f_{i\uparrow}) \]
\[ I_- = \sum_i (-1)^i (c_{i\downarrow} c_{i\uparrow} - f_{i\downarrow} f_{i\uparrow}) \]

The z–component of the pseudospin is the charge operator and is equal to \((N_{el}/2) - L\), where \(N_{el}\) 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 \(N_{el} = 2L - 1\)), 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 \(\Delta_S\) is defined as the energy difference between the lowest–lying excited spin state and the ground state:

\[ \Delta_S = E(S = \frac{3}{2}, I = 0) - E_0(S = \frac{1}{2}, I = 0) \]

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 \(\Delta_S \approx J\).

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 \(|n>\) with \(S = 1/2\) such that \(<0|\sum_q \rho_q|n> \neq 0\), where \(\rho_q\) is the q-component of the Fourier transformed charge density operator and \(|0>\) is the ground state. Notice that \(\rho_q\) is related to \(I_q^z\), where \(I_q\) is a Fourier transformed vector in pseudospin space given by

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

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

$$\Delta_C = E(S = \frac{1}{2}, I = 1) - E_0(S = \frac{1}{2}, I = 0)$$  \hspace{1cm} (5)

We also define a neutral gap $\Delta_N$ as the energy difference between the ground state and the lowest-lying excited neutral state with the same quantum numbers as the ground state ($S = 1/2, I = 0$):

$$\Delta_N = E(S = \frac{1}{2}, I = 0) - E_0(S = \frac{1}{2}, I = 0)$$  \hspace{1cm} (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. 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 2 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.

We use the density matrix renormalization group (DMRG) algorithm to calculate the ground state and the first few excited states of the Kondo lattice. This real-space technique has proven to be remarkably accurate for one dimensional systems such as the Kondo and Anderson lattices. We used the finite system method 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 Versus 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

$$\mu(N) = E_0(N) - E_0(N-1)$$  \hspace{1cm} (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

$$\Delta_{QP} = \mu(N+1) - \mu(N)$$  \hspace{1cm} (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 0, 1, or 2 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.

**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. 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, 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 $J/4$, a “hole” state with no conduction electrons ($S = 1/2, I = 1/2, I_z = -1/2$), or a “particle” state with two 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 2 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 $\Delta_S \approx J/4$. 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 $\Delta N \approx \Delta C \approx 74.0$, and for $J = 10$ and $L = 24$ we find $\Delta S = 9.40$ and $\Delta N \approx \Delta C \approx 6.57$.

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. 3a 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. 3b shows, the z–component of the f–spins on the nearest neighbor sites are polarized and have most of the spin. The f–spins on neighboring sites further 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 $|<0|S_z^f(0)|0>|$ of the f–spins to the form $\exp(-r/\xi)$, where $r$ is the distance from the Kondo hole and $\xi$ is the localization length. In Fig. 5 we plot the localization length $\xi$ versus $J$.

This crossover from conduction spins to f–spins as $J$ decreases is shown in Fig. 4 where we plot the total conduction spin $\sum_i S_{z}^{\text{cond}}$ and the total f–spin $\sum_i S_{z}^{f}$ of the lattice versus $J$. The crossover occurs around $J \approx 4t$. 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 the hopping of the down spin electrons. So the spin–1/2 resides primarily in the f–spins. Polarizing the f–spins costs exchange energy but that is less important than the kinetic energy for $J \lesssim 4t$. To see why the crossover
occurs at $J \approx 4t$, note that we can write the Hamiltonian as

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

where we sum over repeated Greek indices. The hopping term and the exchange term are comparable when $J \approx 4t$.

**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 $\chi(q = 0) = -\partial^2 E/\partial H^2 = 0$.

However, the staggered susceptibility $\chi(q)$ is finite. To calculate the susceptibility $\chi(q)$, we apply a small staggered magnetic field $h_z = h_o \cos(qr)$ which couples to both the f–spins and the conduction spins. The magnitude $h_o$ lies between $10^{-6}t$ and $5 \cdot 10^{-4}t$. When $h_o$ is this small, the plot of $S(q)$ versus $h_o$ is a straight line whose slope is the susceptibility $\chi(q)$. ($S(q)$ is the Fourier transform of $<0|S_z(i)|0>$.) 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 wavevector of the noninteracting conduction electrons.) At half–filling $2k_F a = \pi$ 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 wavevectors other than the wavevectors of the staggered field. This will also reduce $\chi(q = 2k_F)$ relative to its value in lattice 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 (4 and 6 sites) which we can diagonalize exactly. In Fig. 6 we plot the staggered susceptibility $\chi(qa = 2k_Fa = \pi)$ versus $J$ for lattices with and without a Kondo hole at half–filling. 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 a pristine lattice.

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 $J \to \infty$, the chemical potential of these midgap states goes to zero which corresponds to the degeneracy of states with 0, 1, and 2 conduction electrons on the Kondo hole site. 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. 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 $\Delta_C \sim 3J/4$. 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. However, having a finite concentration of Kondo holes introduces effects that we have not considered here such as
impurity bands and interactions between the Kondo holes.

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REFERENCES

1 J. M. Lawrence, J. D. Thompson, and Y. –Y. Chen, Phys. Rev. Lett. 54, 2537 (1985).

2 R. Sollie and P. Schlottmann, J. Appl. Phys. 69, 5478 (1991); R. Sollie and P. Schlottmann, J. Appl. Phys. 70, 5803 (1991); and P. Schlottmann, J. Appl. Phys. 75, 7045 (1994) and references therein.

3 S. R. White, Phys. Rev. Lett. 68, 3487 (1992); Phys. Rev. B 48,10345 (1993); R.M. Noack, S.R. White and D.J. Scalapino, in Computer Simulations in Condensed Matter Physics VII, Eds. D.P. Landau, K.K. Mon, and H.B. Schützler (Springer Verlag, Heidelberg, Berlin, 1994), p. 85-98.

4 T. Nishino and K. Ueda, Phys. Rev. B 47, 12451 (1993); B. A. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. 61, 125 (1988).

5 M. Guerrero and C. C. Yu, Phys. Rev. B. 51, 10301 (1995).

6 C. C. Yu and S. R. White, Phys. Rev. Lett. 71, 3866 (1993).

7 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.

8 M. Guerrero and R. M. Noack, Phys. Rev. B. 53, 3707 (1996).

9 Z. Wang, X.-P. Li, and D-H. Lee, Phys. Rev. B 47, 11935 (1993).

10 M. Sigrist, et al., Phys. Rev. B 46, 13838 (1992).

11 When we applied a staggered field ($q = \pi$) to a 4 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 $J \geq 2.7$. 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 $J \leq 2.6$. 
A similar crossover in the $z$–component of the spin of the ground state occurs for $L = 6$.

\textsuperscript{12} P. Schlottmann, Phys. Rev. B \textbf{46}, 998 (1992); P. Schlottmann, Physica B \textbf{206& 207}, 816 (1995); S. Doniach and P. Fazekas, Phil. Mag. \textbf{65}, 1171 (1992).
FIGURES

FIG. 1. Chemical potential scaled by $J$ versus 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 $J = 10$. The solid lines are guides to the eye.

FIG. 2. (a) Spin and charge gaps versus $J$ for $L = 8, 16, 24$ 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 versus $J$ for $L = 8, 16, 24$ sites with open boundary conditions. The Kondo hole is on site $i = L/2$. $t = 1$. The solid lines are guides to the eye.

FIG. 3. (a) $z$–component of the conduction spin versus 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 versus 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.

FIG. 4. Total f–spin ($S_f^z = \sum_i S_f^z(i)$), total conduction spin ($S_{\text{cond}}^z = \sum_i S_{\text{cond}}^z(i)$), and the difference ($S_f^z - S_{\text{cond}}^z$) versus $J/t$. 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.

FIG. 5. Spin localization length $\xi$ versus $J$ for a 24 site lattice with open boundary conditions. $\xi$ is deduced by fitting $<0|S_f^z(r)|0>$ 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. $t = 1$. 

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FIG. 6. Staggered susceptibility $\chi(qa = 2k_Fa = \pi)$ versus $J$ 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 $\chi(qa = 2k_Fa = \pi)$ for lattices without a Kondo hole.
Figure 1

$\frac{E(N) - E(N-1)}{J}$

- $J=10$, No hole
- $J=1$
- $J=1.5$
- $J=2$
- $J=10$
Figure 2a

- 8 sites, spin gap
- 16 sites, spin gap
- 24 sites, spin gap
- Spin gap, no hole
- 8 sites, charge gap
- 16 sites, charge gap
- 24 sites, charge gap
- Charge gap, no hole
Figure 2b

Neutral Gap vs. $J$ for different site numbers:
- 8 sites
- 16 sites
- 24 sites
Figure 3b

$S_z^f(i)$

site

$J=1$

$J=10$
Figure 4
Figure 6

$\chi(qa=\pi)$ vs $J$

- $L=4$, Kondo hole
- $L=6$, Kondo hole
- $L=4$, no Kondo hole
- $L=6$, no Kondo hole