Numerical Renormalization Group Study of the One-Dimensional Kondo Insulator

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We have studied the one-dimensional Kondo chain at half filling using a density matrix formulation of the numerical renormalization group. The charge gap is larger than the spin gap for all antiferromagnetic values of the exchange coupling J. A new type of excitation, a neutral spin singlet, consists of a particle and a hole which are repulsive for $J \gtrsim 5t$ and attractive for $J \lesssim 5t$. As $J \to 0$, RKKY interactions become more important and the staggered susceptibility $\chi(q=2k_F)$ diverges. We have also studied $\chi(q)$ and the dispersion of the low-lying spin excitations as a function of wave vector q.

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Strongly correlated electrons play a key role in our understanding of a wide variety of phenomena such as superconductivity, magnetism, and heavy fermion behavior. Simple models containing the essential physics of these systems have challenged theorists for decades. The need for a general method capable of calculating low-lying energy levels with well-controlled approximations was recently answered by the development of the density matrix formulation of the numerical renormalization group [1,2]. In this paper we demonstrate the power of this technique using the one-dimensional Kondo lattice at half filling. Our choice of the "Kondo insulator" problem reflects interest stimulated by recent experiments exploring the semiconducting behavior of materials such as CeNiSn and $Ce_3Bi_4Pt_3$ [3].

Our results elucidate the nature of the excitations and the interplay between Kondo and RKKY interactions. The one-dimensional Kondo lattice at half filling is an insulator with a gap to both spin and charge excitations. Our work confirms that the charge gap is larger than the spin gap for all nonzero values of the exchange coupling J [4,5]. In addition to charge and spin excitations, we find a new type of excitation, a neutral spin singlet. The lowest such state consists of a particle and a hole which are repulsive for $J \gtrsim 5t$ and attractive for $J \lesssim 5t$, where t is the hopping matrix element. We also find that RKKY interactions increase in importance as J decreases [6], leading to a staggered susceptibility $\chi(q=2k_F)$ that diverges as $J \to 0$. To the best of our knowledge, this is the first time this divergence has been seen for the Kondo lattice.

Previous theoretical approaches have suffered from various limitations that do not hamper our renormalization group technique. For example, perturbation theory is restricted to unphysically large exchange coupling [7]; mean field theory neglects quantum fluctuations [8]; variational solutions cannot cover the myriad of possible wave functions [9]; quantum Monte Carlo simulation [10] has difficulty attaining low temperatures; and exact diagonalization [4] is confined to small lattice sizes (≤ 10 sites).

The one-dimensional Kondo lattice has spin-$\frac{1}{2}$ conduction electrons that hop from site to site with an on-site spin exchange between a local f electron and the conduction electron on that site. Thus the Hamiltonian is

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

where the conduction electron spin density on site i is $\mathbf{S}_{ic} = \sum_{\alpha\beta} c^\dagger_{i\alpha}(\boldsymbol{\sigma}/2)_{\alpha\beta}c_{i\beta}$, the f-electron spin density is $\mathbf{S}_{if} = \sum_{\alpha\beta} f^\dagger_{i\alpha}(\boldsymbol{\sigma}/2)_{\alpha\beta}f_{i\beta}$, and $\boldsymbol{\sigma}_{\alpha\beta}$ are Pauli matrices. The Hamiltonian has SU(2) spin symmetry as well as SU(2) charge pseudospin symmetry [11]. The pseudospin operators are $I^+ = \sum_i (-1)^i (c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} - f^\dagger_{i\uparrow}f^\dagger_{i\downarrow})$, $I^- = (I^+)^\dagger$, and $I^z = \sum_{i\sigma}(c^\dagger_{i\sigma}c_{i\sigma} + f^\dagger_{i\sigma}f_{i\sigma} - 1)/2$. Notice that I^z is simply the charge operator. We set $t=1$, and we choose J to be antiferromagnetic ($J>0$). To study the Kondo insulator we restrict ourselves to half filling where the total number of conduction electrons N equals the number of sites L.

We use the density matrix renormalization group algorithm [1,2] 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 Heisenberg spin chains [12]. Although the Kondo lattice includes fermion degrees of freedom in addition to spin, the differences in the algorithms are small; for example, states of a block are labeled by N as well as by total S_z. We primarily used the finite system method [2] with open boundary conditions in which there is no hopping past the ends of the chain. We studied lattices of size $L=4$, 6, 8, 16, and 24, keeping up to 180 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 $J=0.5$.

In agreement with previous work, we find that the ground state is a singlet [13] and the lowest excited state is a spin triplet [4] for all values of J. The energy difference between these two states is the spin gap $\Delta_S = E(S=1,I=0) - E_g(S=0,I=0)$ where $E_g(S=0,I=0)$ is the ground state. The charge gap Δ_C is the energy difference between the ground state and the lowest pseudospin triplet state, i.e., $\Delta_C = E(S=0,I=1) - E_g(S=0,I=0)$. Us-

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ing the Wigner-Eckert theorem, one can show that the $(I=1,S=0)$ 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 $|0\rangle$. Figure 1 shows Δ_S and Δ_C for $0.5 \leq J \leq 100$. Since the density of states ρ at the Fermi energy for free electrons with open boundary conditions is given by $\rho=2/\pi^2 t$, $0.5 \leq J \leq 100$ roughly corresponds to $0.1 \leq J\rho \leq 20$. Notice that the charge gap is larger than the spin gap for all nonzero values of J, confirming the conclusion of previous calculations [4,5]. We also define a neutral singlet gap as the energy difference between the ground state and the lowest-lying excited neutral spin singlet state, i.e., $\Delta_{NS}=E(S=0,I=0)-E_g(S=0,I=0)$. The quasiparticle gap is defined by $\Delta_{QP}=\mu_{N+1}-\mu_N$ where the chemical potential is $\mu_N=E_g(N)-E_g(N-1)$, and $N=L$ for half filling. We find that Δ_{QP} is slightly less than Δ_C for all J. Notice that $\Delta_{QP}>0$ for $J>0$, indicating that the half-filled Kondo lattice is an insulator, since Δ_{QP} is much larger at half filling than away from half filling.

When $J \gg t$, we can describe the eigenstates in terms of simple on-site states. Each 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 $(S=\frac{1}{2}, I=\frac{1}{2}, I_z=-\frac{1}{2})$, or a "particle" state with two conduction electrons $(S=\frac{1}{2}, I=\frac{1}{2}, I_z=\frac{1}{2})$. The particle and hole states have zero energy. In the ground state every site is a singlet when $J \gg t$. The lowest excitation consists of a single site with a spin triplet, with the remaining sites having singlets, and has $\Delta_S \approx J$ [5,7]. The lowest-lying excited spin singlet states with $I=0$ and $I=1$ have a site in a hole state and another site in a particle state, with $\Delta_C \approx 3J/2$ [5,7]. Since the particle and hole are $I=\frac{1}{2}$ states, they can combine to form $I=0$ or $I=1$ states. In either case, the f electrons on these two sites form a spin singlet. The low-lying eigenstates consist of linear combinations of these local excitations, e.g., they have a well-defined wave vector q in the case of periodic boundary conditions. These simple estimates of the gaps work very well for $J \gg t$; e.g., for $J=100$ we find numerically that $\Delta_S=99.9$ and $\Delta_{NS} \cong \Delta_C \cong 148$, and for $J=10$ we find $\Delta_S=9.39$ and $\Delta_{NS} \cong \Delta_C \cong 13.1$.

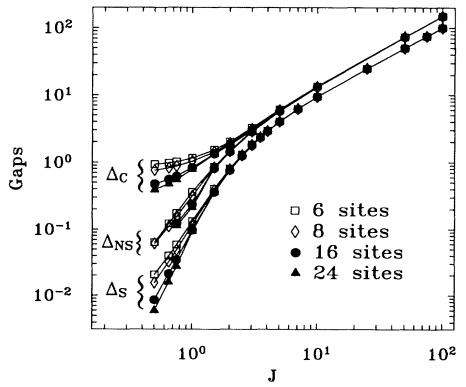

FIG. 1. The spin gap, neutral singlet gap, and charge gap versus J with open boundary conditions. To avoid cluttering the figure, Δ_{QP} is not shown since Δ_{QP} overlaps with Δ_C.

Given that the system is in a certain state, how do we know what state a site is in? One way is to examine the eigenstate directly, which we can do for $L=4$. Another way is to study the single-site reduced density matrix. Let i label the eight possible states of a single site, and j label the basis states of the rest of the lattice. Then if the system is in a state with wave function ψ, the single-site density matrix is

$$\rho_{ii'}=\sum_j \psi_{ij}\psi^*_{i'j}, \tag{2}$$

where $i,i'=1,\ldots,8$. For this system the eigenstates of ρ are the eigenstates of a single-site Hamiltonian, and the eigenvalues of ρ are the probabilities of those states when the system is in the state ψ. For example, for the ground state of a large lattice, the probability of a site being in a singlet state is unity for $J \to \infty$ and is 99.1% for $J=10$. For $J=1$, however, it is only 44.9%, with probabilities of 5.5% for each of the three spin triplet states, and 9.7% for each of the four particle and hole states. Clearly the strong-coupling picture is no longer valid for $J \lesssim t$, where the eigenstates are a complicated linear combination of on-site singlet, triplet, hole, and particle states.

We have studied the dispersion of the lowest $S=1$ $(I=0)$ state for $L=4$, 6, and 8 with periodic boundary conditions. The dispersion curves have their maximum at $q=0$ and their minimum at $q=\pi$, in agreement with the hybridization gap picture in which the lowest energy spin-flip excitation involves taking an electron from the lower band $q=\pi$ and putting it in the upper band at $q=0$ [5,8]. In the large J regime, we expect the spin excitation bandwidth W_S to be approximately $8t^2/J$ from perturbation theory in t/J [4,14]. This agrees well with our numerical results, e.g., $W_S \simeq 0.75$ for $J=10$. As J decreases, W_S initially increases, though less rapidly than $8t^2/J$, and then falls rapidly. For example, $W_S \simeq 1.4$ for $J=4$ and $W_S \simeq 0.23$ for $J=1$. These values are less than the free electron bandwidth of $4t$ and are roughly comparable to the spin gap, e.g., for $L=6$ with periodic boundary conditions $\Delta_S \simeq 2.87$ for $J=4$ and $\Delta_S \simeq 0.089$ for $J=1$. For $J \lesssim 1$, other bands drop below the top of the lowest $S=1$ band. Of course, as $J \to 0$, all the bands become degenerate and the conduction electrons become free.

The lowest-lying $S=2$ state consists of two $S=1$ elementary excitations. For $t/J \ll 1$, perturbation theory [7] indicates that the two triplet excitations will repel each other [5]. Numerically we find this repulsion exists for all J since $E(S=2)-E_g > 2[E(S=1)-E_g]$. Note that two $S=1$ elementary excitations can also form an $S=0$ state. The fact that the lowest $S=2$ state lies below the first excited $S=0$ state for $J \lesssim 1$ implies that the triplet

excitations have ferromagnetic interactions for small J.

By comparing the Kondo and RKKY energy scales, Varma and Doniach [6] have argued that RKKY interactions will dominate as J decreases, eventually leading to antiferromagnetic ordering of the localized f spins with wave vector $q=2k_F$. We have looked for this crossover in the ground state by calculating both the f-spin–f-spin correlation function and the staggered susceptibility as a function of J. Since $2k_Fa=\pi$ for one dimension at half filling (a is the lattice constant), the f-f correlation function oscillates in sign from site to site with an amplitude that decays exponentially with distance (see Fig. 2 inset) [15]. Exponential decay is characteristic of a system with gaps in its energy spectrum, though the fit to $\exp(-r/\xi)$ is much more approximate for $J<1$ where the gaps are smaller and the correlation length ξ becomes comparable to the lattice size. The correlation length ξ decreases rapidly as J increases, but not in a simple power law or exponential fashion. Typical numbers are $\xi/a\sim 6\pm 2$ for $J=0.75$ and $\xi/a\sim 0.35\pm 0.001$ for $J=5$.

We expect the staggered magnetic susceptibility $\chi(q=2k_F)$ to diverge at the transition between magnetic and nonmagnetic ground states at the critical coupling $J=J_c$. To calculate $\chi(q)$, we apply a very small staggered magnetic field ($10^{-7}t\le h\le 10^{-4}t$), observe the magnetic response $S_z(q)$, and use $S_z(q)=\chi(q)h_z(q)$. We can apply the field to either the f spin or the total spin (f spin+conduction spin) on each site. As shown in Fig. 2 for $L=4$ and 6 with $0.05\le J\le 2$, $\chi(q=2k_F)$ diverges as $J\to J_c=0$. We know that $\chi(q)$ is infinite for $J=0$ since the f electrons are completely isolated in that case. However, as $J\to 0$, the divergence is most pronounced for $q=2k_F$ due to RKKY oscillations. Our results for $L=4$ and 6 are exact since we are able to keep all the states. For small J, the system is so close to an instability that the numerical inaccuracy associated with larger lattice sizes was enough to result in spontaneous magnetization even for very small fields. For $L=4$ and 6, we find that for both the f spin and total spin susceptibility $\chi(q=2k_F)\to J^{-2}$ as $J\to 0$. We caution that the dependence on J may change for larger lattice sizes.

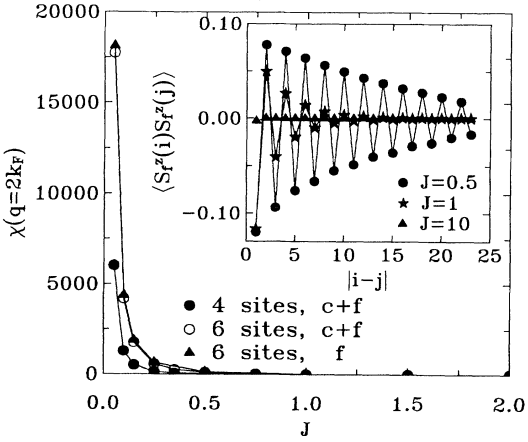

FIG. 2. The staggered susceptibility $\chi(q=2k_F)$ versus J for the ground state with periodic boundary conditions. $0.05\le J\le 2$. The susceptibilities are shown for both the total spin as well as the f spins. The divergence is due to RKKY interactions. Inset: Ground state f-spin–f-spin correlation function versus distance for various values of J with open boundary conditions. RKKY oscillations dominate for small J.

Recent neutron scattering experiments on the Kondo insulator CeNiSn found that $\chi(q)$ was independent of q [16]. However, our results as well as general considerations indicate that for the Kondo lattice the behavior of $\chi(q)$ versus q depends on the value of J/t. Since the ground state is a singlet with a gap to spin excitation, $\chi(q=0)=0$ for all values of J/t. On the other hand, $\chi(q=2k_F)$ diverges as $J\to J_c$, but is quite small for large J. This implies that the curve $\chi(q)$ versus q will vary strongly for small J, but will be flat for large J/t. Since real materials such as CeNiSn have small J/t, as indicated by the small energy gaps seen experimentally, our results do not explain the neutron scattering experiments [16].

In strong coupling, the lowest-lying excited spin singlet states with $I=0$ and $I=1$ consist of a particle-hole pair. We have verified this picture in a number of ways: (1) direct examination of the eigenstate for $L=4$; (2) finding the eigenvalues of the density matrix in Eq. (2); and (3) noting that the f-spin–f-spin correlation function has qualitatively the same spatial dependence as the conduction electron density-density correlation function for large J. (For small J, the f-spin–f-spin correlation function acquires RKKY oscillations which do not appear in the density-density correlation function.) To determine whether or not the particle and hole attract or repel each other, we can compare Δ_C and Δ_{NS} to the quasiparticle gap Δ_{QP} which gives the energy of the particle and hole infinitely far apart. If the particle and hole attract, $\Delta_{QP}-\Delta_{C,NS}>0$. In this case, the particle and hole prefer to be nearest neighbors, and the binding energy $\Delta_{QP}-\Delta_{C,NS}$ should be independent of the lattice size. On the other hand, if the interaction is repulsive, $\Delta_{QP}-\Delta_{C,NS}<0$. In this case the particle and hole prefer to be far apart and the magnitude of the repulsive energy $|\Delta_{QP}-\Delta_{C,NS}|$ decreases as L increases. Figure 3 is a plot of $\Delta_{QP}-\Delta_{C,NS}$ versus J. For the $I=1$ state, which determines Δ_C, the particle and hole are repulsive for all J. However, for the $I=0$ state, which determines Δ_{NS}, the particle and hole are repulsive for $J\gtrsim 5$ and attractive for $J\lesssim 5$. The curves show the expected L dependence for $J\gtrsim 1$. For $J\lesssim 1$, finite size effects separate the curves. Further confirmation of this interpretation for the $I=0$ state comes from the conduction electron density-density correlation functions shown in the inset to Fig. 3. (The f-spin–f-spin correlation functions look similar.) In the attractive regime, the magnitude of the correlation function has a maximum for nearest neighbor distances, while in the repulsive regime the maximum occurs at greater

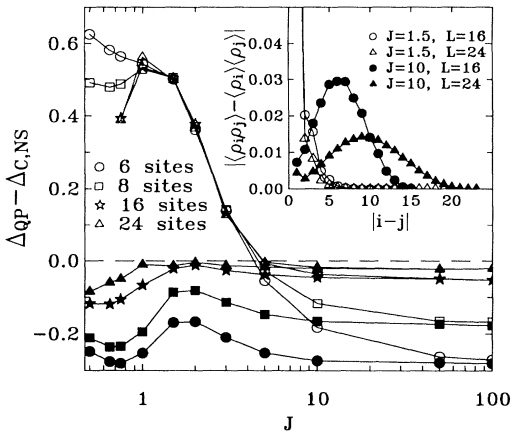

FIG. 3. $\Delta_{QP}-\Delta_{C,NS}$ versus J with open boundary conditions. Open symbols refer to the Δ_{NS} and filled symbols to Δ_C. $\Delta_{QP}-\Delta_{C,NS}>0$ indicates that the particle and hole attract while $\Delta_{QP}-\Delta_{C,NS}<0$ implies that they repel. Inset: Conduction electron density-density correlation function of the lowest excited ($I=0$, $S=0$) state versus distance. For $J=1.5$ (attractive regime), the particle and hole have their largest correlation on nearest neighbor sites. For $J=10$ (repulsive regime), the particle and hole move farther apart as L increases. Open boundary conditions were used.

separations as L increases [17].

To understand this behavior for $J\lesssim 5$, note that the particle and hole have a hard core repulsion as well as RKKY interactions that grow as J decreases. Since $2k_F$ is π/a, we expect the RKKY interaction between a particle and a hole with opposite f spins to have maximum attraction between nearest neighbor sites. For the case of the pseudospin triplet, this attraction is overcome by the hard core repulsion because the spatial wave function is symmetric. However, for the singlet state, the antisymmetric spatial wave function ignores the hard core repulsion, and the particle and hole attract. For $J\gtrsim 5$, RKKY interactions are very weak, and the particle and hole separate in both cases.

To conclude, we have shown that a recently developed renormalization group technique enables us to uncover the physics of strongly correlated electron systems by calculating the low-lying energy levels. For the one-dimensional Kondo insulator, we examined the nature of the excitations, and we studied how RKKY interactions increase as J decreases.

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