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BRIEF REPORTS

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Absence of a magnetic-field-induced metal-insulator transition in Kondo insulators

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We investigate whether or not Kondo insulators undergo a magnetic-field-induced metal-insulator transition in one dimension at half filling using both a density matrix formulation of the numerical renormalization group and bosonization. Contrary to expectations, the quasiparticle gap never vanishes at any field and no metal-insulator transition is found. We discuss generalizing our result to the asymmetric Anderson lattice. [S0163-1829(96)06524-1]

In a strong magnetic field an ordinary narrow gap semiconductor becomes metallic when the field is comparable to the size of the gap. Is this also true for the class of rare earth compounds known as Kondo insulators, whose insulating gap is due to interactions between conduction electrons and localized f electrons?[1] Simple arguments[2–4] suggest that such a metal-insulator transition (MIT) should occur when the applied magnetic field h exceeds the exchange coupling J but is less than the conduction electron bandwidth. In this case, one expects the f spins to be completely polarized and decoupled from the conduction electrons, leaving an incompletely polarized band of metallic conduction electrons. This scenario is supported by mean field calculations such as those with slave bosons.[2,5] However, here we show that such expectations are not correct when spin fluctuations are taken into account.

We have studied the behavior of the insulating gap in a one-dimensional (1D) Kondo insulator as a function of magnetic field. We used bosonization and the density matrix formulation of the numerical renormalization group[6,7] to cover both the weak and strong coupling regimes. We find that the gap, while greatly reduced by the applied magnetic field, never vanishes at any value of h. This unexpected result is due to spin flip umklapp scattering across the Fermi surface, which removes degeneracies and keeps the gap open. We argue that this result also holds for the one-dimensional asymmetric Anderson lattice where there is no particle-hole symmetry.

The 1D Kondo lattice has spin-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

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

$$-h\sum_{i}\,(S^{z}_{ic}+S^{z}_{if}), \tag{1}$$

where the conduction electron spin density on site i is $\vec{S}_{ic}=\Sigma_{\alpha\beta}c^{\dagger}_{i\alpha}(\vec{\sigma}/2)_{\alpha\beta}c_{i\beta}$, the f-electron spin density is $\vec{S}_{if}=\Sigma_{\alpha\beta}f^{\dagger}_{i\alpha}(\vec{\sigma}/2)_{\alpha\beta}f_{i\beta}$, $\vec{\sigma}_{\alpha\beta}$ are Pauli matrices, and $h>0$ is the external magnetic field, chosen along the z axis. We set the hopping matrix element $t=1$ and choose J to favor antiferromagnetic ordering ($J>0$). 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.

In order to calculate the insulating gap over a broad range of J, we have used the density matrix renormalization group (DMRG) algorithm[6–8] to study the strong coupling regime ($J\gtrsim t$) and Abelian bosonization to study the weak coupling regime ($J<t$). We first describe the results of our numerical work.

The DMRG approach is a real space technique which has proven to be remarkably accurate for the Kondo lattice.[8] We used the finite system method[7] with open boundary conditions in which there is no hopping past the ends of the chain.

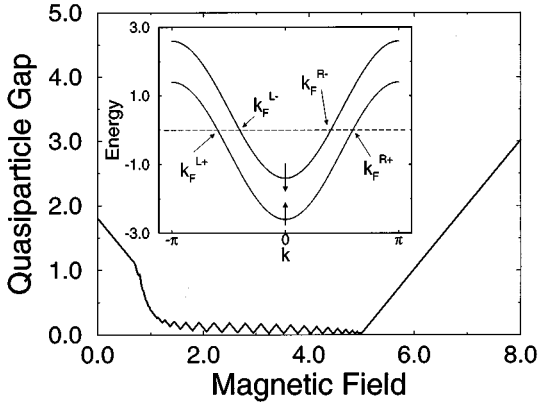

FIG. 1. Typical DMRG result for quasiparticle gap vs h. Here $J=2$ with $L=32$. Inset: Typical conduction electron band structure for $J=0$, $t=1$, and $h=2$.

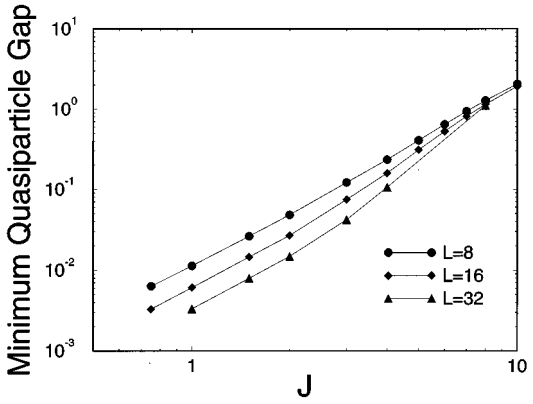

FIG. 2. DMRG results for minimum quasiparticle gap vs J with $L = 8$, 16, and 32. Solid lines are guides to the eye.

We studied lattices of size $L=6$, 8, 16, and 32, keeping up to 100 states. The energies were extremely accurate for $J \gg t$, with typical truncation errors of order 10^{-9} 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 $J=0.75$.

We consider a system to be insulating when the quasiparticle gap $\Delta_{\rm qp} \equiv \mu_{N+1} - \mu_N = 0$.[9] Here $\mu_N = E_N - E_{N-1}$ is the chemical potential and E_N is the ground-state energy with N electrons. To determine $\Delta_{\rm qp}$, we calculated the ground-state energies with $N=L$ and $N=L+1$ conduction electrons[10] for all possible values of the total S^z with $h=0$. Since the magnetic field term in the Hamiltonian commutes with the Hamiltonian, we can find the energies in the presence of a field by adding $-hS^z_{\rm tot}$ to the zero field energies. We then use the lowest energies $[E_N^{\rm min}(S^z_{\rm tot})$ and $E_{N+1}^{\rm min}(S^z_{\rm tot})]$ as a function of $S^z_{\rm tot}$ to calculate $\Delta_{\rm qp}$. In the presence of a field, finite size effects do not limit the size of the gap because the field can tune the levels E_N and E_{N+1} to be infinitesimally close. For example, for free electrons on an eight site lattice, the minimum $\Delta_{\rm qp}$ is zero to within the roundoff error of 10^{-15}. In Fig. 1 we show the quasiparticle gap as a function of h. The sawtooth oscillations occur as the ground states, E_N and E_{N+1}, change their polarizations with increasing h.

Notice that at high fields, the gap is proportional to h. This occurs when the spins of the half-filled lattice are completely polarized by the field. To calculate E_{N+1}, we add an electron whose spin is opposite to the field. The energy required to do this increases linearly in h, and hence $\Delta_{\rm qp}$ is proportional to h. This can also be understood in terms of splitting the up $(+)$ and down $(-)$ spin conduction electron bands. For fully polarized f spins, the conduction electron energies are $E_\pm = -2t\cos(k) \pm (J/4 - h/2)$. The two bands are completely separated at a field $h_a = J/2 + 4t$ and so, for $h > h_a$, $\Delta_{\rm qp} \sim h$. Our expression for h_a is only an estimate since the f spins are not fully polarized until the conduction bands separate.

For a given value of J, we can find the minimum quasiparticle gap, $\Delta_{\rm qp}^{\rm min}$, as a function of h from plots similar to Fig. 1. Roughly speaking, the minimum occurs at the largest field in which the up and down spin conduction bands are not completely separated. This field, $h_{\rm min}$, is of order the conduction electron bandwidth, i.e., $h_{\rm min} \sim h_a \sim 4t$. Notice that the minimum does not occur at $h \sim J$ or at $h \sim \Delta_{\rm qp}$ as one might expect. Figure 2 shows $\Delta_{\rm qp}^{\rm min}$ as a function of J. Fitting the curves for $J \leqslant 2$ to $\Delta_{\rm qp}^{\rm min} \sim J^b$, we find that b increases from 2.05 for $L=6$ to 2.16 for $L=32$. While the power law form indicates that the gap remains finite for $J>0$, we must turn to Abelian bosonization to draw definitive conclusions about the weak coupling regime $(J<t)$ in the thermodynamic limit.

Our strategy for the weak coupling regime is as follows. We start with the partition function $\exp(-\beta H)$ and integrate out the f spins to obtain an effective action for the conduction electrons. After dropping irrelevant terms,[12] we bosonize the effective Hamiltonian and look for gaps in the excitation spectrum. We find that spin excitations are gapless, while charge excitations have a gap. To see why the charge gap remains open, note that for $h \leqslant h_a$, the f spins are not completely polarized because there are zero energy excitations in which an f spin, which initially points up in the field, flips down and then back up. This is accompanied by the spin flip umklapp scattering of conduction electrons across the Fermi surface, which removes degeneracies at the Fermi energy and prevents the charge gap from closing.

We write the partition function as a functional integral over Grassman variables $\underline{c}$ and $\underline{f}$ where $\overline{c} = (\overline{c_+}, \overline{c_-})$ (i.e., spin up, spin down) and $f = (f_+, f_-)$:

$$\mathcal{Z} \sim \int \mathcal{D}\overline{c}\mathcal{D}c\mathcal{D}\overline{f}\mathcal{D}f e^{-S} \tag{2}$$

with the action S given by

$$S = \sum_i \int_0^\beta d\tau \{\overline{c_i}(\partial_\tau - \mu)c_i + \overline{f_i}(\partial_\tau - \mu_f)f_i\} \tag{3}$$

$$+ \int_0^\beta d\tau H\{\overline{c}, c, \overline{f}, f\}. \tag{4}$$

Here H is the Hamiltonian (1) with the fermion operators replaced by their corresponding Grassman variables and β is the inverse temperature. We enforce the constraint of one f

electron per site by introducing an imaginary chemical potential $\mu_f = i\pi/2\beta$ which eliminates the states with zero or two f electrons.[11]

We can write $S = S_c + S_{cf}$ with

$$S_c = \sum_i \int_0^\beta d\tau \left\{ \overline{c_i} \left(\partial_\tau - \mu - \frac{h}{2}\sigma^z \right) c_i - t(\overline{c_i} c_{i+1} + \text{H.c.}) \right\},$$

$$S_{fc} = \sum_i \int_0^\beta d\tau \overline{f_i}(M_0 + M_1) f_i, \tag{5}$$

where the matrices M_0 and M_1 are given by

$$M_0 = \partial_\tau - \mu_f - \frac{h}{2}\sigma^z, \tag{6}$$

$$M_1 = \frac{J}{4}(\overline{c_i}\sigma^z c_i)\sigma^z + \frac{J}{2}\{(\overline{c_i}\sigma^- c_i)\sigma^+ + \text{H.c.}\}. \tag{7}$$

Since the action is quadratic in the f states, they can be integrated out to yield an effective action for the conduction electrons:

$$\mathcal{Z} \sim \int \mathcal{D}\overline{c}\mathcal{D}c e^{-S_c + \mathrm{Tr}\ln(M_0 + M_1)}. \tag{8}$$

We can expand $\ln(M_0+M_1)$ around M_0 to get terms with 2, 4, 6,...,n fermion fields. If we scale to longer length scales and lower energy scales, dimensional analysis indicates that, when $h > J$, the nth order vertex scales like $L^{(n/2)-2}$, where L is a unit of length. This means that all terms with more than four fields are irrelevant[13] in the RG sense, and that the fourth order vertex can be approximated by a constant. In the limit $\beta \gg h > J$, we can write (in a Fourier representation)

$$\mathcal{Z} \sim \int \mathcal{D}\overline{c}\mathcal{D}c e^{-S_2 - S_4}, \tag{9}$$

$$S_2 = \frac{1}{\beta}\sum_{\omega,s} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \overline{c_s}(k\omega) \left\{ i\omega - \mu + s\left(\frac{J}{4} - \frac{h}{2}\right) - 2t\cos(k) \right\} c_s(k\omega), \tag{10}$$

$$S_4 = -\frac{u_0}{\beta^3} \sum_{\omega\omega_1\omega_2} \int_{-2\pi}^{2\pi} \frac{dq}{2\pi} \times \int_{-\pi}^{\pi} \frac{dk_1 dk_2}{(2\pi)^2} \overline{c_+}(k_1\omega_1)\overline{c_-}(k_2\omega_2) c_+ \times (k_2 - q, \omega_2 - \omega) c_-(k_1 + q, \omega_1 + \omega). \tag{11}$$

ω, ω_1, and ω_2 are fermion Matsubara frequencies, $s = \pm 1$ denotes spin, and $u_0 = J^2/16h$.

When $J < t$ and $h > J$, then $u_0 \ll t$; this defines the weak coupling regime. In this case the important wave vectors are centered around the four Fermi points $\pm k_{F\pm}$ (see inset to Fig. 1). Because of this we introduce right and left movers according to $[\chi = +1(R), (-1)(L)]$

$$c_{\chi s}(k,\omega) = \begin{cases} c_s(\chi k_{Fs} + k, \omega), & |k| \leqslant \Gamma \\ 0 \quad \text{otherwise}, \end{cases} \tag{12}$$

where Γ is some cutoff $\ll k_F$ that restricts excitations to the vicinity of the Fermi surface. The Fermi points are determined by the relation

$$-s\left(\frac{h}{2} - \frac{J}{4}\right) = 2t\cos(k_{Fs}) \tag{13}$$

and around the Fermi points the dispersion relation is linear in k:

$$-2t\cos(\chi k_{F\pm} + k) \approx -2t\cos(k_{F\pm}) + 2t\sin(k_{F\pm})k. \tag{14}$$

Using (13), one can show that $2t\sin(k_{F\pm}) \equiv v_F$ is independent of the spin index. Linear bands around the Fermi points are a good approximation as long as the magnetic field is somewhat smaller than $4t + J/2$ (where the free electron bands split). With linear bands we can apply bosonization. In preparation for this we write the real space Hamiltonian corresponding to Eqs. (9)–(11) as follows:

$$H = -v_F \sum_{\chi s} \int dx \psi^\dagger_{\chi s}(x) \chi i \partial_x \psi_{\chi s}(x) + u_0 \sum_\chi \int dx \{ \rho_{\chi,+}(x)\rho_{\chi,-}(x) + 2\rho_{\chi,+}(x)\rho_{(-\chi),-}(x) - 2\psi^\dagger_{\chi,+}(x)\psi^\dagger_{\chi,-}(x)\psi_{(-\chi),+}(x)\psi_{(-\chi),-}(x) \}, \tag{15}$$

where $\psi_{\chi s}$ are fermion operators corresponding to $c_{\chi s}$ and $\rho_{\chi,s} = \psi^\dagger_{\chi s}\psi_{\chi s}$. We note two important aspects of Hamiltonian (15): (i) A backward scattering term, which normally opens a spin gap,[14,15] is absent. This term is present when $h = 0$, but is destroyed by the magnetic field, yielding gapless spin excitations. (ii) Umklapp scattering across the Fermi surface, described by the last term, is not eliminated by the magnetic field. These scattering events survive the magnetic field because the Fermi points satisfy $k_F^{R+} - k_F^{L-} = \pi$ and $k_F^{R-} - k_F^{L+} = \pi$ for $h \leqslant h_a$ (see inset of Fig. 1). These umklapp processes are responsible for keeping the charge gap open.

The above considerations can be made explicit by bosonizing[14,15] the Hamiltonian (15) which, in this case, separates into commuting spin and charge parts. These are expressed in terms of Bose fields $[\phi_\mu(x), \Pi_\nu(y)] = i\delta_{\mu\nu}\delta(x-y)$, where μ, ν stand for sp (spin) or c (charge). The spin component is ($\tilde{u}_0 \equiv u_0/2\pi$)

$$H_{\mathrm{sp}} = \frac{1}{2} v_{\mathrm{sp}} \int dx \left\{ \lambda_{\mathrm{sp}} (\partial_x \phi_{\mathrm{sp}}(x))^2 + \frac{1}{\lambda_{\mathrm{sp}}} \Pi^2_{\mathrm{sp}}(x) \right\}, \tag{16}$$

where

$$v_{\mathrm{sp}} = \sqrt{(v_F - 3\tilde{u}_0)(v_F + \tilde{u}_0)}, \quad \lambda_{\mathrm{sp}} \equiv \sqrt{\frac{v_F - 3\tilde{u}_0}{v_F + \tilde{u}_0}}. \tag{17}$$

Diagonalizing H_{sp} by a canonical transformation leads to a linear gapless spectrum for the spin excitations:

$$\epsilon(k) = \sqrt{(v_f - 3\tilde{u}_0)(v_F + \tilde{u}_0)}|k|. \tag{18}$$

On the other hand, the Hamiltonian H_c for the charge sector has a cosine term arising from spin-flip umklapp scattering across the Fermi surface:

$$H_c=\frac{v_c}{2}\int dx\{(\partial_x\varphi_c(x))^2+\pi_c^2(x)\}$$
$$+\frac{2u_0}{(2\pi\alpha)^2}\int dx\cos(\sqrt{8\pi}\lambda_c^{-1/4}\varphi_c(x)), \quad (19)$$

where α is a cutoff related to the lattice spacing and

$$v_c=\sqrt{(v_F+3\tilde{u}_0)(v_F-\tilde{u}_0)}, \quad \lambda_c\equiv\sqrt{\frac{v_F+3\tilde{u}_0}{v_F-\tilde{u}_0}}. \quad (20)$$

Since $\tilde{u}_0=J^2/32\pi h$ is always positive, the coefficient of $\varphi_c(x)$ in the argument of the cosine term is always smaller than $\sqrt{8\pi}$. In this regime,[16] the cosine term is relevant and opens a gap Δ for the charge excitations. No broken symmetry is associated with this charge gap. Following the renormalization group procedure in Ref. 14, we find that for $h>J$ (and $J<t$), the gap goes as $\Delta\sim\exp(-Av_Fh/J^2)$, where A is a real positive constant. The factor J^{-2} in the exponent shows that pairs of spin flips dominate, e.g., an f spin, which initially points up in the field, flips down, and then back up.

As already noted, when $h\sim 4t$, i.e., right before the two conduction bands separate, the spectrum is quadratic and bosonization no longer applies. The charge gap should increase in this case because the processes responsible for the opening of the gap (umklapp spin flip scattering across the Fermi surface) are enhanced by the increased density of states at the band edges. Thus we conclude that an external magnetic field, however strong, fails to induce a MIT.

The Kondo Hamiltonian (1) has particle-hole symmetry. However, we argue that there is also no field-induced MIT for the half-filled one-dimensional asymmetric Anderson lattice, which lacks particle-hole symmetry. If we start in the mixed valence regime, the external field Zeeman splits the f band away from the Fermi energy and into the Kondo regime, where our Kondo lattice calculations are valid. This can be shown using the Schrieffer-Wolff transformation. DMRG calculations on small asymmetric Anderson lattices ($L\leqslant 8$) also do not find a MIT.[17]

Although our calculations were done in one dimension, it is interesting to note that recent resistivity and Hall measurements on $Ce_3Bi_4Pt_3$ in pulsed fields up to 61 T do not see the signatures expected for a transition from a semiconductor to a good metal.[18] This material acts like a semimetal or a dirty metal at the lowest temperatures ($T<5$ K) and highest fields ($h>50$ T), even though the field exceeds the experimentally deduced value of the gap ($\Delta\sim 37$ K).[19]

To summarize, 1D Kondo insulators do not undergo a magnetic-field-induced MIT due to strong spin flip scattering across the Fermi surface. A large field can significantly reduce but not close the insulating gap. We suggest that the absence of a field-induced MIT applies also to the 1D asymmetric Anderson model.

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