Two-impurity Kondo problem for correlated electrons

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The behavior of two magnetic impurities coupled to correlated electrons in one dimension is studied using the DMRG technique for several fillings. On-site Coulomb interactions among the electrons lead to a small Kondo screening cloud and an overall suppression of magnetic order. For arbitrary electronic correlations and large inter-impurity distances \( R \), we find a \( 1/R^2 \) decay of magnetic correlations.

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The almost complete understanding of the behavior of magnetic impurities interacting with conduction electrons in metals is one of the major achievements of modern condensed matter theory. The impurity magnetism is mainly affected by two distinct mechanisms, namely Kondo screening and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. While the RKKY interaction typically favors magnetic ordering of the impurities, the Kondo effect works against order since it tends to quench individual impurity spins. This competition characterizes the magnetism in many heavy-fermion compounds, where one essentially deals with a Kondo lattice of rare-earth impurities carrying a local moment due to inner \( f \)-electrons. As emphasized by Varma, the basic features of the interplay between the Kondo effect and the RKKY interaction are already contained in the two-impurity Kondo problem which has attracted much attention lately.

So far all studies of the two-impurity Kondo problem have ignored correlations among the conduction electrons. While this is certainly a reasonable assumption in most conventional metals, it breaks down if deviations from Fermi liquid theory become important. For instance, Brugger et al. reported experimental evidence for heavy-fermion behavior in the strongly correlated material \( \text{Nd}_{2−x}\text{Ce}_x\text{CuO}_4 \). This behavior has been modeled by considering a lattice of \( 4f \) Nd ions interacting with strongly correlated conduction electrons in the copper-oxide planes. Furthermore, experimental studies of magnetic impurities in one-dimensional (1D) quantum wires (which are described by the strongly correlated Luttinger liquid state) are coming into reach due to recent fabrication advances.

In this paper, as a prototypical example for the effects of correlations among conduction electrons, we employ the density matrix renormalization group (DMRG) method to study the case of 1D interacting electrons. Recent DMRG studies for the Kondo lattice model have investigated the influence of electronic correlations on charge or spin gaps. Here we present results for the simpler and physically more transparent two-impurity Kondo model, with main focus on the impurity spin-spin correlations.

In the absence of spin or lattice instabilities, 1D interacting electrons form a Luttinger liquid characterized by a dimensionless interaction strength \( g \). Generally, for repulsive interactions, one has \( 0 < g < 1 \), and \( g = 1 \) is the noninteracting (Fermi liquid) value. While the Luttinger liquid has been thoroughly studied for the clean case and in the presence of elastic potential scattering, the implications of magnetic impurities are only beginning to emerge.

On the one hand, the Kondo effect in a Luttinger liquid leads to the formation of a ground-state many-body singlet. The impurity spin is screened by the electrons like in the conventional single-channel Kondo effect for noninteracting electrons, albeit with a larger Kondo temperature. One finds \( T_K \sim (\rho_0 J)^{2/(1−g)} \) instead of the uncorrelated result \( T_K \sim \exp(−1/\rho_0 J) \), where \( J > 0 \) is the antiferromagnetic exchange coupling and \( \rho_0 \) the electronic density of states at the Fermi energy. On the other hand, the RKKY interaction becomes quasi-long-ranged in a Luttinger liquid. For two spin-\( \frac{1}{2} \) impurities described by spin operators \( S_1 \) and \( S_2 \), one finds the effective RKKY Hamiltonian

\[
H_{\text{eff}} = K S_1 S_2 , \quad \text{where} \quad K \sim J^2 R^{−g} \cos(2k_F R) . \tag{1}
\]

The \( 2k_F \)-oscillatory RKKY indirect exchange coupling \( K \) is defined by second-order perturbation theory in the exchange coupling \( J \). Higher-order terms (which are also responsible for the Kondo effect) cannot be written in the simple form. As a function of inter-impurity distance \( R \), the RKKY coupling decays slower than the conventional \( 1/R \) Fermi liquid result, which is recovered by putting \( g = 1 \).

The competition between the RKKY interaction and the Kondo effect shows up in the magnetic correlations between the impurities, \( \langle S_1 S_2 \rangle \). From Eq. (1), one would...
Due to higher-order contributions in the exchange coupling $J$, this expression is expected to saturate for temperatures below the Kondo temperature $T_K$. Therefore the ratio between the relevant energy scales, $\mathcal{K}/T_K$, is crucial for the ground-state value of $\langle S_1 S_2 \rangle$. The sign of $\langle S_1 S_2 \rangle$ depends on the sign of $\mathcal{K}$ in Eq. (1), and therefore $\langle S_1 S_2 \rangle$ is also $2k_F$-oscillatory. For very small $J$, the RKKY interaction dominates such that $\langle S_1 S_2 \rangle$ takes its maximum (singlet or triplet) value. For very large $J$, Kondo screening is effective in quenching the impurity spins and magnetic order disappears, i.e., $\langle S_1 S_2 \rangle \to 0$. In order to describe the crossover from RKKY to Kondo-dominated behavior, a non-perturbative approach is mandatory. We note that the unstable fixed point separating these behaviors (see Ref. [3]) is absent in the correlated case since the electron-hole symmetry required for its presence is broken.

We have studied two spin-$1/2$ impurities $S_i$ $(i = 1, 2)$ coupled to the electron spin density $s(x_1)$ at the respective impurity location by the standard exchange term $J s(x_1) S_i$. The 1D correlated electrons are modelled as a Hubbard chain, with nearest-neighbor hopping $t = 1$ and repulsive on-site Coulomb interaction $U \geq 0$. The low-temperature behavior of the Hubbard chain away from half-filling is equivalent to a Luttinger liquid, and the appropriate values for $g$ as a function of $U$ and the filling factor can be found in Ref. [4]. Directly at half-filling, a finite $U$ causes a charge gap leading to a Mott insulator instead of the metallic Luttinger liquid state. However, since the spin sector remains gapless, the magnetic properties of the Hubbard chain still follow the Luttinger liquid predictions, but with $g = 0$. Away from half-filling, one has $1/2 \leq g \leq 1$. We have primarily studied the half-filled case, for which $\langle S_1 S_2 \rangle$ has been calculated. We included $m \approx 200$ states of the reduced density matrix to study chains of even length $N \approx 80$, with an accuracy better than 1% for $\langle S_1 S_2 \rangle$ even in unfavorable cases (small $U$ and quarter-filling). The two impurities are arranged symmetrically around the center of the chain. In units of the lattice spacing, their distance $R$ takes odd values varying between 1 (impurities at the chain center) and $N - 1$ (impurities at opposite chain ends). This geometry is shown in Fig. 2. The bulk behavior is then reproduced in the limit of large $N$ and $R \ll N/2$.

In Fig. 3, DMRG results for $\langle S_1 S_2 \rangle$ are shown for $J = 1$ and various $U$. Since the data were obtained for half-filling and $R$ is odd, RKKY correlations are always antiferromagnetic such that $\langle S_1 S_2 \rangle < 0$. We notice several features in Fig. 3: (a) Increasing the Coulomb interaction $U$ leads to smaller values of $\langle S_1 S_2 \rangle$. (b) The magnetic correlations $\langle S_1 S_2 \rangle$ fall off with increasing distance due to the decreasing RKKY coupling $\mathcal{K}$. (c) As shown in the inset, all data points can be scaled onto a universal curve by using the lengthscale $\xi$ shown in Fig. 3. The overall behavior of $\xi$ is quite similar to the Kondo screening length $v_F/T_K$, which, roughly speaking, determines the extent of the electronic screening cloud around the

\begin{equation}
\langle S_1 S_2 \rangle = \frac{3}{4} \left( 1 - \exp(\mathcal{K}/k_B T) \right) - \frac{3}{4} \exp(\mathcal{K}/k_B T). 
\end{equation}
impurity. Since \( T_K \) increases with correlations, the observed decrease of \( \xi \) with increasing \( U \) is in accordance with the results of Ref. [1]. In that sense, electronic correlations imply a smaller screening cloud.

As depicted in Fig. 4, DMRG results for the \( J \)-dependence of \( \langle S_1 S_2 \rangle \) at the fixed distance \( R = 5 \) explicitly demonstrate the competition between RKKY and Kondo-dominated behavior. Since almost the same curves were found for \( N = 30 \), finite-size effects seem to play only a very minor role here. For small \( J \), the (here antiferromagnetic) RKKY interaction leads to a singlet, \( \langle S_1 S_2 \rangle \to -\frac{3}{4} \), while the Kondo effect destroys magnetic order for large \( J \) such that \( \langle S_1 S_2 \rangle \to 0 \). The qualitative influence of Coulomb correlations can be read off from Figs. 2 and 3. The magnetic correlations \( |\langle S_1 S_2 \rangle| \) are significantly reduced by switching on and increasing the Coulomb interaction \( U \). Regarding the impurity spins, RKKY-related magnetic order is suppressed by electronic correlations. The same qualitative finding was obtained for quarter-filling and other values of \( U \) or \( R \) under consideration.

This behavior can be simply rationalized as follows. Switching on the Hubbard-\( U \) implies an increase in the Kondo temperature and enhances the importance of Kondo screening. Since the correlated RKKY law [4] does not change appreciably with increasing \( U \) for the values of \( R \) studied in the DMRG simulations, the increase in \( T_K \) is decisive here and leads to the observed partial destruction of magnetic order.

Next we study the distance dependence of \( \langle S_1 S_2 \rangle \) in the bulk limit \( R \ll N/2 \), for which DMRG results are shown in Fig. 3. For the quarter-filled case and the configurations considered here (odd \( R \)), the impurity correlations \( \langle S_1 S_2 \rangle \) exhibit an oscillatory behavior. We plot here only the negative values; similar conclusions are reached for the positive ones. For small enough \( J \), the RKKY interaction locks the impurity spins in a singlet state irrespective of the distance \( R \). Increasing \( J \) causes two effects: (a) The Kondo effect leads to smaller values of \( |\langle S_1 S_2 \rangle| \). (b) There is an (approximate) power-law decrease in the distance dependence

\[
\langle S_1 S_2 \rangle \sim \cos(2k_F R)/R^\alpha .
\]

The exponent \( \alpha \) is shown in Fig. 3 for the data of Fig. 3. Clearly, \( \alpha = 0 \) for very small \( J \), and then \( \alpha \) continuously increases with \( J \). For large \( J \), the limiting value \( \alpha = 2 \) is approached for arbitrary \( U \) and filling factor.

Since the RKKY coupling \( K \to 0 \) as \( R \to \infty \), the large-distance behavior should effectively be determined by the large-\( J \) behavior. Therefore, from our DMRG results we expect the asymptotics

\[
\langle S_1 S_2 \rangle \sim \cos(2k_F R)/R^2
\]
for any value of $J$. For $J \to \infty$, Eq. (4) holds on all lengthscales. Furthermore, additional DMRG results not shown here reveal that the asymptotic law (9) is approached faster in the case of strong electronic correlations.

The large-$J$ value $\alpha = 2$ can be understood analytically. For $J = \infty$, each impurity spin forms a strongly coupled singlet with the conduction electron spin at that site (see Fig. 1). This singlet cannot be broken up, and therefore the Hubbard chain is effectively cut at the impurity sites. The leading $1/J$ contribution to $\langle S_1 S_2 \rangle$ can then be computed by open boundary bosonization. To proceed, we write

$$\langle S_1 S_2 \rangle = (2\pi/k_F)^2 \langle s(x_1) s(x_2) \rangle,$$  

(5)

since $s(x_i)$ is antiparallel to $S_i$ in $1/J$ accuracy. We then compute $\langle s(x) s(y) \rangle$ under open boundaries at the impurity locations (we take $x_1 = 0$ and $x_2 = R$),

$$\langle s(x) s(y) \rangle = \frac{3k_F^2}{4\pi^2} \cos[2k_F(x-y) - f(2x) + f(2y)]$$

$$\times \left[ P(2x) P(2y) \right]^{1+g/2} \left( \frac{P(x-y)}{P(x+y)} \right)^{1+g} - 1$$

$$+ (y \to -y),$$

with the functions (we consider $k_F R \gg 1$)

$$P(x) = \left\{ 1 + \left[ \frac{2k_F R}{\pi} \sin \left( \frac{\pi x}{2R} \right) \right]^2 \right\}^{-1/2}$$

$$f(x) = \arctan \left( \frac{\sin(\pi x/R)}{\exp(\pi/k_F R) - \cos(\pi x/R)} \right).$$

Evaluating this result for $x$ near $x_1$ and $y$ near $x_2$ reproduces the numerically observed behavior (9). Of course, the prefactor in Eq. (9) depends on the interaction strength parameter $g$.

To conclude, we have employed DMRG simulations to study the two-impurity Kondo problem for interacting 1D electrons. On-site Coulomb interactions were shown to partially destroy magnetic ordering between the impurities. The main reason for this effect is the increase of the Kondo temperature for correlated electrons. For the impurity spin-spin correlations, we obtain a $\cos(2k_F R)/R^2$ behavior at large distances.

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17. Taking directly $x = x_1$ and $y = x_2$, the spin density correlations would vanish due to the open boundary conditions.