Phase diagram of the 1D Kondo lattice model

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We determine the boundary of the fully polarized ferromagnetic ground state
in the one dimensional Kondo lattice model at partial conduction electron
band filling by using a newly developed infinite size DMRG method which
conserves the total spin quantum number. The obtained paramagnetic to
ferromagnetic phase boundary is below \( J \approx 3.5 \) for the whole range of band
filling. By this we solve the controversy in the phase diagram over the extent
of the ferromagnetic region close to half filling.

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The central problem posed by heavy fermion materials is to understand
the interaction between an array of localized moments (generally f-electrons
in lanthanide or actinide ions) and conduction electrons (generally p- or d-
band). The magnetic properties of the localized moments and conduction
electron interplay is well described by the Kondo lattice model:

\[
H = -t \sum_{\langle i,j \rangle, \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} + J \sum_j S_{cj} S_j ,
\]

where \( t > 0 \) is the conduction electron (or simply electron) hopping, \( \langle i,j \rangle \)
denotes nearest neighbors, \( S_j \) are spin 1/2 operators for the localized spins,
and where \( S_{cj} = \frac{1}{2} \sum_{\alpha, \alpha'} c_{j,\alpha}^\dagger \sigma_{\alpha, \alpha'} c_{j,\alpha'} \) with \( \sigma \) the Pauli spin matrices and
c_{j,\alpha}, c_{j,\alpha}^\dagger the electron site operators.
In the following, we concentrate on the region of the disordered paramagnetic - ferromagnetic phase boundary which appears at partial conduction band filling \( n = \frac{N_c}{L} < 1 \), where \( N_c \) is the number of electrons, and \( L \) the number of localized spins, of the one dimensional case. The transition has been identified both analytically and in numerical simulations by a variety of methods. We focus on the \( J > 0 \) case, relevant to heavy-fermion systems, in which the localized spins model \( f \)-electrons in lanthanide or actinide ions.

The bulk of the numerical simulations are based on the DMRG approach and are devoted to values of filling factor less than quarter filling. Accordingly, our first focus is to extend the region of the numerically available results up to very close to half filling. However, our main focus is to determine as accurately as possible the paramagnetic - ferromagnetic phase boundary. For this we developed a DMRG code which keeps track of the total spin. In this way we can exactly determine the phase boundary where the one dimensional Kondo lattice model becomes ferromagnetic. These results will clarify the controversy over the paramagnetic - ferromagnetic phase boundary close to half filling which has been a central issue for much of the research in this area for some years.

The density-matrix renormalization group (DMRG) method has become a widespread method for the investigation of (mostly) one dimensional strongly correlated electron systems. Even though a lot of new additions were made to the original method, the problem of keeping track of the total spin of the analysed model was still a challenge. The problem emerges as a consequence of the fact that the density matrix is not block diagonal with respect to the total spin, except in the special case of \( S = 0 \).

In order to properly keep track of the ferromagnetic phase appearing in the one dimensional Kondo lattice model, we developed an infinite DMRG method which conserves the total spin. This is the first DMRG method that we are aware of to do this task. In the following we give a brief description of the method, while a detailed analysis will be published elsewhere.

Suppose the basis is partitioned into states of total spin, with the basis vectors written as

\[
|S, i\rangle, \quad i = 1, 2, \ldots, n_S,
\]

(2)

where \( n_S \) is the number of basis states having total spin \( S \).

Let the density matrix eigenstates be \( |\rho_k\rangle \), with corresponding eigenvalues \( \rho_k \). The density matrix in the original basis is

\[
\rho_{S_1, i; S_2, j} = \sum_k \rho_k \langle S_1, i | \rho_k \rangle \langle \rho_k | S_2, j \rangle.
\]

(3)
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Fig. 1. The truncation error as a function of the length of the chain for \( n = 0.9 \) and \( J = 3.1 \).

The problem is to find the optimum basis state

\[
|b\rangle = \sum_{i=1}^{ns} b_i |S, i\rangle,
\]

which is an eigenstate of total spin \( S \). After the best basis state is found, the density matrix can be reduced in dimension and the procedure applied iteratively until the best \( m \) basis states are found.

The measure of how good a basis state is, is given by the probability,

\[
\mathcal{P}(|b\rangle) = \rho_k |\langle \rho_k | b\rangle|^2.
\]

Maximizing \( \mathcal{P}(|b\rangle) \), subject to the condition that \( |b\rangle \) is normalized, gives one unique state, given by the highest weight eigenvector of the density matrix with off-diagonal (with respect to total spin) elements removed.

Neglecting the off diagonal elements results in a tendency for the spread of eigenvalues of the quasi-density matrix to be increased, so it is necessary to keep more block states at each step. However in every case we have tried, this still leads to a significant overall reduction in the number of states in the super block. To exemplify, we present in Fig. 1 the truncation error. As it can be seen it fluctuates to accommodate all the states corresponding...
to a given total spin value, since it is necessary to keep all members of a spin multiplet to be able to keep the Clebsch-Gordan transformation exact. The corresponding number of kept states, \( m \) is given in Fig. 2.

We calculated the total spin of the system for \( n = 0.5, 0.6, 0.7, 0.8, 0.9 \) and 0.95 fillings. As the phase transition is crossed, the total spin of the system changes from 0 to \( (L - N_c)/2 \). The fully polarized configuration is \( N_c \) Kondo singlets, and \( L - N_c \) unscreened localized spins coupled ferromagnetically. This type of configuration, seen to exist in the bosonization approach also, signals the presence of spin polarons.

We have not yet determined from the numerical data the order of the phase transition. In Fig. 3 we present the case of \( n = 0.8 \). As it can be seen, the system is paramagnetic up to \( J = 2.8 \). The oscillations in the total spin are of finite size origin. It may be that immediately above the phase transition there is a region where the total spin is not fully polarized. This would imply that the paramagnetic - ferromagnetic phase transition in the one dimensional Kondo lattice model is not of first order type, rather second order, or a quantum ordered-disordered phase transition with variable exponents. However, close to the critical line, the total spin states become numerically degenerate so the results in this intermediate region are not reliable. Indeed, we have not yet seen any fractionally polarized states where the total spin can be determined unambiguously.
In Fig. 4 we present the phase diagram of the 1D Kondo lattice model. We plotted only those cases which represent fully polarized localized spins. Accordingly, these points (denoted by stars in Fig. 4) represent an upper bound on the true thermodynamic phase transition. As a comparison we also plotted the previous numerical results (square is DMRG data, the diamond is the quantum Monte Carlo data, the open circles are the exact numerical diagonalization data, and the filled circles are the infinite size DMRG results) and the phase transition curve obtained via bosonization.

The most significant contribution of the present work is to establish the existence of a ferromagnetic regime extending up to half filling, see Fig. 4 for $n = 0.9$ and $n = 0.95$ filling factors. For $n = 0.95$ the impurity spins are already fully polarized above $J \approx 3.5$. This suggests that, contrary to the ferromagnetic Kondo lattice model, in the present case ferromagnetism will exist for any band filling. For $J < 0$ the ferromagnetic phase only asymptotically approaches half filling. The reason for this is that a phase separated regime appears between ferromagnetism and the insulating phase at exactly half filling. Such a phase separated regime cannot appear for the $J > 0$ Kondo lattice model and, as such, the present DMRG results clearly confirms the predictions of the bosonization approach.
Fig. 4. The phase diagram of the 1D Kondo lattice model. The stars are the results of the present work, they represent the first fully polarized impurity spin states. For details, see text.

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