Localized spin ordering in Kondo lattice models

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(January 2, 2022)

Using a non-Abelian density matrix renormalization group method we determine the phase diagram of the Kondo lattice model in one dimension, by directly measuring the magnetization of the ground-state. This allowed us to discover a second ferromagnetic phase missed in previous approaches. The phase transitions are found to be continuous. The spin-spin correlation function is studied in detail, and we determine in which regions the large and small Fermi surfaces dominate. The importance of double-exchange ordering and its competition with Kondo singlet formation is emphasized in understanding the complexity of the model.

The Kondo lattice model (KLM) describes the interaction between a conduction electron (CE) band and a half-filled narrow impurity, e.g. \( f \) electron, band and is thought to capture the essential physics of the rare earth compounds. Although intensively studied for two decades, the KLM is still far from being completely understood. Recently, after the discovery of Kondo insulators and the non-Fermi liquid behavior, interest in this field has been greatly renewed, especially due to the non-Fermi liquid behavior discovered in most of the heavy fermion compounds, which resembles a Griffiths phase.\textsuperscript{\textcopyright}

In order to understand the role of the impurity spin in determining the properties of KLM we must develop a better understanding of the magnetic correlations. The Griffiths phase in the one dimensional KLM occurs naturally; it is, therefore, the prototypical model for heavy fermion compounds. Hence, this is an ideal system to study since we have the bosonized solution\textsuperscript{\textcopyright} and we know the behavior of the CEs in both the paramagnetic (PM) and ferromagnetic (FM) phases. However, less attention has been given to understand the correlations between the impurity spins. This is the focus of our study.

The Hamiltonian for the KLM is

\[
H = -t \sum_{j=1}^{L} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.}) + J \sum_{j=1}^{L} S_j^z S_j^z, \quad (1)
\]

where \( t > 0 \) is the CE hopping parameter, \( S_j \) are spin \( 1/2 \) operators for the localized spins, e.g. \( f \), and \( S_j^z = \frac{1}{2} \sum_{\sigma, \sigma'} c_{j,\sigma}^\dagger \sigma_{\sigma, \sigma'} c_{j,\sigma'} \) with \( \sigma \) the Pauli spin matrices and \( c_{j,\sigma}, c_{j,\sigma}^\dagger \) the electron annihilation and creation site operators. The Kondo coupling \( J \) is measured in units of the hopping \( t \) and partial conduction band filling, \( n = N/L < 1 \), is assumed throughout.

The method that we use is density matrix renormalization group (DMRG) which, however, is extended to explicitly preserve \( SU(2) \) spin and pseudospin symmetry. Hence we can measure the magnetization directly and determine rigorously the PM - FM phase boundary. The obtained result is in excellent agreement with a recent bosonized solution\textsuperscript{\textcopyright} and contradicts common view that this phase boundary goes to infinite Kondo coupling \( J \) as the CE density approaches half-filling.\textsuperscript{\textcopyright} We also determine the regions of the phase diagram where large and small Fermi surfaces are dominant, which has been a central issue for much of the research in this area for some years.

In addition, we have discovered a second FM region not seen before. For most dopings, this region of FM separates the regions of large and small Fermi surface. This most likely resolves the question as to the applicability of the Luttinger theorem to the KLM, shown by Yamanaka \textit{et al.}\textsuperscript{\textcopyright} since the Fermi points are not expected to remain constant across a phase transition.

To accelerate the computation, we make use of several operators that commute with the Hamiltonian, \( S^+, S^-, S^z, I^+, I^-, I^z \), respectively the generators of the spin \( SU(2) \) and pseudospin \( SU(2) \) algebras.\textsuperscript{\textcopyright} Combined, the generators form the algebra \( SO(4) \). All of the states in our DMRG calculation transform as irreducible representations of this algebra. Since \( SO(4) \) is non-Abelian these representations have, in general, degree \( > 1 \), which implies that a single basis state in the \( SO(4) \) representation is equivalent to multiple states of the purely Abelian representation of most previous DMRG calculations. This is the origin of the dramatic performance improvements of the non-Abelian DMRG. The states are labeled by the eigenvalues of the Casimir operators of \( SO(4) \), which are \( S^2 = s(s+1) \) and \( I^2 = i(i+1) \). Hence we can label all irreducible representations by \( [s, i] \), which has degree \( (2s+1)(2i+1) \). In this construction, a chemical potential would appear as a term in the Hamiltonian proportional to \( I^z \), acting in an identical way a magnetic field coupled to \( S^z \). Although the basis states in the calculation are eigenstates of \( S^2 \) and \( I^2 \), rather than \( S^z \) and \( I^z \), all these operators mutually commute so it is possible to simply replace \( S^2 \) and \( I^2 \) by the chosen eigenvalues in this case. A single site of the Kondo lattice contains just three such states. The simplest is the
Kondo singlet state, transforming as the $[0,0]$ representation of degree 1. The Kondo triplet state transforms as the $[1,0]$ representation of degree 3, and encapsulates the three projections $|\uparrow\uparrow\rangle$, $\sqrt{1/2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, $|\downarrow\downarrow\rangle$ in a single state. Here, $\uparrow$ denotes localized $f$, and $\downarrow$ the conduction electron spins, respectively. Finally, the holon state (actually; the tensor product of a holon and an $f$ spin) transforms as the $[1/2,1/2]$ representation of degree 4 and has the projections $|\uparrow 0\rangle$, $|\downarrow 0\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$. The single-site operators are $3 \times 3$ matrices over this basis. The matrix elements can be determined by the Wigner-Eckart theorem, which specifies the relationship between the 3 dimensional reduced basis and the full 8 dimensional basis. For a comprehensive description of the new algorithm, see Ref. 3.

At half filling (where the ground state is a pseudospin singlet) 400 block states are equivalent to around 2500 states of a calculation using $N$ and $S^z$ quantum numbers, although the relative advantage of $SO(4)$ decreases as the system is doped away from half filling. We used the new DMRG algorithm to obtain the ground state energy, magnetization and different correlation functions, i.e., the momentum distribution, density-density, conduction electron spin-spin and the $f$ spin structure factor, $S(k)$. The obtained results can be summarized with the phase diagram presented in Fig. 1, which will be analyzed in detail hereafter. The main properties of the phase diagram have been confirmed on chains of 120 or more sites. Results for the magnetization were calculated on smaller chains, 40 - 60 sites, where the energies can be calculated more accurately. We found no finite size effects that would affect the properties of Fig. 1. In all cases, we extrapolate to zero truncation error based on well-converged sweeps of between 200 and 500 $SO(4)$ states kept.

As it can be seen from Fig. 1, the main feature dominating the KLM is $f$ spin FM ordering. The FM ordering is due to the double-exchange (DE) interaction which appears as a consequence of an excess of localized spins over CEs, each CE has to screen more than one localized spin, and since hopping is energetically most favorable for CEs which preserve their spin, this tends to align the localized spins. This element was missing in the early approaches, which concentrated on the competition between Kondo singlet formation at large $J$ and the RKKY interaction in the weak coupling limit. This picture is borrowed from the single impurity Kondo model and is inadequate for the lattice case.

Starting the analysis of the phase diagram for large $J$, we see that all CEs form singlets with the localized $f$ spins which become inert. The uncoupled $f$ spins order FM in a mechanism similar to the $J < 0$ case. Here, there is no competition between Kondo singlet formation and DE. The fully polarized state with $S = (L - N)/2$ appears for any value of $n < 1/2$, contrary to the suggestion of Refs. 4, 6 that close to half filling the PM phase extends to $J \rightarrow \infty$. As $J$ is lowered, KLM can be rigorously mapped into a random transverse field Ising model, hence the phase transition (the solid curve in Fig. 1) is identical to the quantum order - disorder transition. It should be emphasized that this is also true for the second FM phase, as will be shown later on.

FIG. 1. The obtained phase diagram of KLM. The two shaded areas are the FM phases. The open circles and triangles correspond to points at which the FM energy level crosses the $S = 0$ level. The dashed curves are the derived phase transition lines (the solid curve was already obtained in Ref. 2).

The phase transition obtained via DMRG fits exceptionally well this picture, confirming the bosonization result of Ref. 2. The open circles correspond to points at which the energy of the FM state crosses the energy of the singlet state. Since the phase transition is second order, this is only an upper bound on the true transition line. However the partially polarized region is very small, of the order of $J/t \sim 0.01$, which is why this phase transition has not previously been observed to be continuous. A typical example of the energy versus the magnetization ($M$) is presented in Fig. 2. This shows that in the transition regime, $\partial^2E/\partial M^2$ is positive. We have accounted...
for all known random errors, these are errors arising from
the tolerance of the matrix diagonalization, variations in
the energy across the DMRG sweep, and error arising
from the extrapolation to zero truncation error. These
errors are of the order of the symbol size in this figure.

Below the solid curve, Fig. 1, the Kondo singlets are
not inert anymore and they greatly contribute to the
properties of KLM. Excluding the Kondo triplet states,
the CE wave function in the continuum limit satisfies a
nonlinear Schrödinger equation which has finitely delo-
calized solitonic solutions. This corresponds to a dress-
ing of the CE by a cloud of antiparallel local spins, i.e.,
spin polarons are formed. The polaronic length scale
competes with the length scale set by the free CE mean
free path and introduces competing time scales: slow mo-
tion of the polarons with low energy dynamics and fast
motion of the free CEs with high energies. This sce-
nario resembles a two-fluid picture with intrinsic inhomo-
genieties which involves spin fluctuations and short-range
spin correlations, which we call a polaronic liquid.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig3.pdf}
\caption{Typical $J$ dependence of the spin structure factor,
$S(k)$, and the momentum distribution, $n(k)$ ($n = 0.6$).}
\end{figure}

Finite temperature DMRG confirmed the presence of
short-range $f$ spin correlations in the van-Hove singulari-
ties. Consequently the structure factor peaks at $2k_F - \pi$, where
$k_F$ is the Fermi point determined by the filling of the
CE band. This means that the localized $f$ spins, even
though they are completely immobile, contribute to the
volume of the Fermi sea. This conventionally is called a
large Fermi surface, the effect of which is also seen in the
momentum distribution function, see Fig. 3. As the po-
larons are formed the peak of $S(k)$ shifts from the small
$J/t$ value of $2k_F$: the slow motion of the spin polarons
will dominate the low energy dynamics of the quasiparti-
cles. This proves that the appearance of the large Fermi
surface is a dynamical effect since it involves local inho-
genieties, impurity spin fluctuation, and short-range
correlations of the $f$ spins. This phase is related to a
Griffiths phase, suggesting that the small - large Fermi
surface crossover is a Griffiths singularity.

The large Fermi surface is conventionally explained
by reference to the periodic Anderson model (PAM) ancestry.
Our results imply that even for PAM, this simple picture is inadequate. In particular, we see no rea-
son why a small - large Fermi surface crossover, marked
by a FM phase, should not also appear in PAM. How-
ever, the behavior of the Fermi surface crossover close to
quarter filling is numerically difficult to determine (dot-
ted line in Fig. 1), hence we are not yet able to rule out the possibility that the large and small Fermi surface
regions are adiabatically connected. Even prior to the
current calculation, the nature of the Fermi surface in
the weak-coupling regime was not clear, with the sug-
 gestion from Ref. 7 that the Fermi surface vanishes at a point
in proximity to where we find the ferromagnetic phase.
For $n < 0.5$ the width of the polarons is over several lat-
tice spacings (diverging for $n \rightarrow 0$) hence the energy
needed to excite these polarons is too large for this effect
to happen. The polarons will not contribute to the low
energy dynamics and the system behaves as an RKKY
liquid, as we explain below.

An interesting phenomenon appears as we further lower $J$. The residual weight attached to the Kondo sin-
glets vanishes, hence all CEs which participated in the
formation of these singlets, become delocalized. The dis-
tance between these CEs is much larger than the lattice
spacing, and below $J \leq 2\sqrt{n}\sin(\pi n)$ their continuum
limit takes the regular quantum sine-Gordon form. In
the bosonization language of Ref. 2 this means that the
spin Bose fields, $\Phi_\sigma$ cannot be approximated by their
noninteracting expectation values, rather by their expect-
ation value corresponding to a sine-Gordon (sG) model,
$\Phi_\sigma \approx \langle \Phi_\sigma \rangle_{\text{sG}}$. However, the charge degrees of freedom
not being affected by the sine-Gordon spin gap, their
Corresponding Bose fields, $\Phi_\sigma$ may be still approximated
by their noninteracting values. Extending the bosonized
results of Ref. 2 to a finite $\langle \Phi_\sigma \rangle_{\text{sG}}$, we obtain the crit-
cal Hamiltonian governing the PM - FM phase tran-
sition at intermediate $J$ values in the form: $H_{\text{crit}} =
- J^2 A / (2\pi^2 v_F) \sum_j S^a_j S^a_{j+1} + 2JB \sum_j \{ (\langle \Phi^a_\sigma \rangle_{\text{sG}}^2 / 2) [1 + J/(2\pi v_F)]^2 + \cos(2k_{Fj}) \} S^a_j$, where $A$ and $B$ are func-
tions which depend only on the cutoffs introduced by
the bosonization scheme. Following closely previous
bosonization approaches we can prove that the critical
behavior of the FM transition for the intermediate $J$
below is of a random transverse-field Ising model type,
where the transverse field $h = 2JB \{ 1 - (\langle \Phi_\sigma \rangle_{\text{sG}}^2 / 2)[1 + J/(2\pi v_F)]^2 + \cos(2k_{Fj}) \}$ is driven by a displaced co-
sine distribution of the form: $\rho(h) = [1/(2\pi J B)] \{ 1 - [h/(2JB)] + (\langle \Phi_\sigma \rangle_{\text{sG}}^2 / 2)[1 + J/(2\pi v_F)]^2 - [1/2] - [1/2] \}$. Ac-
cordingly, the FM transitions emerging at intermediate
values of $J$ are of a quantum order - disorder type.
These transitions are driven by spin polarons, contrary
to the FM phase emerging at high $J$ values, which is
given by the uncoupled $f$ spins (in a mechanism simi-
lar to the $J < 0$ case). The new critical line is $J_c =
\alpha(A, B) \sin(\pi n/2) / [1 - \beta(A, B)] - \gamma(A, B, \langle \Phi_\sigma \rangle_{\text{sG}}^2)$. The
bosonization (conformal field-theory) arguments does not
determine the magnitude of $\alpha$, $\beta$ and $\gamma$, accordingly these constants are used as fitting parameters to the numerically obtained points. The best fits are the dashed curves in Fig. 1.

This is the second FM phase in Fig. 1, which has proven difficult to detect with conventional (Abelian) DMRG. Previous DMRG calculations did show a weak FM signal at $n = 0.8$ and $J = 1.6$ and $1.8$ but the results were discarded in later papers by the same authors. Likewise an exact diagonalization of a very small system gave FM for $n = 0.75$ and $J = 1.5$. Using the non-Abelian DMRG algorithm we could also check the energy of each total spin state, shown in Fig. 4, which clearly shows a second ferromagnetic region although we have not yet confirmed numerically the order of the phase boundaries. For the FM Kondo lattice model, $J < 0$, a phase separated regime was observed in numerical approaches. However for $J > 0$ we found no change in sign of the inverse charge compressibility. Thus, this phase is a true FM rather than a phase separated region.

![FIG. 4. The gap, $\Delta E$, from the fully polarized ferromagnetic state to every other spin state vs. $J$, for $n = 0.8$, and 60 site lattice, measured along intervals of $J = \pm 0.05$. For most data points the error bars are of order $\sigma_{\Delta E} \sim 10^{-4}$ or less, except for the $S = 0$ curve for very low and very high $J$, where the errors are of order $\sigma_{\Delta E} \sim 5 \times 10^{-5}$. The inset shows the second ferromagnetic region.](image)

Below the second FM region the KLM reduces to a system of free localized spins in fields determined by CE scattering: dominant $2k_F$ modulations are manifest, see Fig. 3, superimposed on an incoherent background. This reflects the momentum transferred from the CE band to the spin chain in backscattering interactions, together with incoherent forward scattering. This case is referred to as an RKKY liquid as the scattering processes give an RKKY-like correlation for the $f$ spins, even though the RKKY interaction strictly diverges in one dimension.

In conclusion, using a non-Abelian DMRG method a most comprehensive analysis of the short- and long-range ordering of the localized moments in KLM is presented. We show that DE ordering and its competition with Kondo singlet formation is the dominant feature of the phase diagram. The non-Abelian DMRG method allowed us to discover that FM does not only appear at large $J$ but also at intermediate values. This second FM phase was missed in previous approaches. We also show that at large $J$ FM is due to ordering of uncoupled $f$ spins, while for intermediate $J$, i.e., the second FM region, FM is due to ordering of the spin polarons. The inhomogeneous polaronic state between these two FM phases is analogous to a two-fluid system and it exhibits a large Fermi surface.

Work in Australia was supported by the Australian Research Council. In Sweden by the Swedish Natural Science Research Council.

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