Superconductivity from spoiling magnetism in the Kondo lattice model

Mohammad Zhih Asadzadeh, Michele Fabrizio, and Federico Becca

Democritos Simulation Center CNR-IOM Istituto Officina dei Materiali and International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy

We find evidence that superconductivity intrudes into the paramagnetic-to-magnetic transition of the Kondo lattice model if magnetic frustration is added. Specifically, we study by variational method the model on a square lattice in the presence of both nearest- (t) and next-nearest-neighbor (t’ ) hopping of the conduction electrons. We find that when t’/t is finite a d-wave superconducting dome emerges between the magnetic and paramagnetic metal phases and close to the compensated regime, i.e., the number of conduction electrons equal to the number of localized spin-1/2 moments. Superconductivity is further strengthened by a direct antiferromagnetic exchange between the localized moments, to such an extent that we even observe coexistence with magnetic order.

PACS numbers: 71.27.+a, 71.30.+h, 71.10.Fd

Introduction – The emergence of superconductivity in strongly-correlated electron systems has become quite a common phenomenon, observed by now in a wealth of different materials that include also so-called heavy-fermion compounds, where unconventional superconductivity was first reported in CeCu$_2$Si$_2$. \cite{1} The characteristic properties of heavy-fermions derive from the coexistence of itinerant electrons and localized moments residing on partly filled f-shells of rare earth or actinide ions. The pairing mechanism in heavy-fermions has been the subject of an intense debate, also in connection with high-temperature superconductors, \cite{2,3} with which heavy-fermions share unconventional pairing symmetry. For instance, recent scanning tunnelling spectroscopy on CeColn$_5$ unveiled the presence of nodal points in the superconducting gap compatible with a $d_{x^2−y^2}$ symmetry, \cite{4} just like in cuprates. The widely accepted picture is that pairing is mediated by spin fluctuations of a nearby antiferromagnetic phase, as suggested for CePd$_2$Si$_2$ and CeIn$_3$. \cite{5,6} This view is supported by the evidence that superconductivity in heavy-fermions almost ever appears in the vicinity of the quantum critical point that separates a paramagnetic metal phase from a magnetically-ordered one. \cite{7,8} Even more remarkably, some compounds show a coexistence of magnetism and superconductivity, as observed in CeRhSi$_2$, \cite{8} CeRhIn$_5$, \cite{9} and CeCo(In$_{1−x}$Cd$_x$)$_5$. \cite{10}

From the theoretical side, the Kondo lattice model (KLM), which has been introduced by Doniach in 1977, \cite{11} is believed to capture the basic properties of heavy fermions. While in one spatial dimension its physical behavior is well understood, \cite{12} the more relevant two- and three-dimensional cases are much less known, especially concerning (possible) superconducting properties. Most of the analytical understanding is based upon slave bosons and large-N approaches, \cite{13} which find that d-wave superconductivity can be indeed stabilized in two-dimension through the resonating-valence bond (RVB) mechanism, similarly to what has been suggested long ago by Anderson for high-temperature superconductors. \cite{14} As far as numerical calculations are concerned, unfortunately quantum Monte Carlo methods suffer from sign problems away from the compensated regime (where the number of itinerant electrons equals the number of localized spin-1/2 moments), while exact diagonalization and density-matrix renormalization group (DMRG) are limited to small clusters. Nonetheless, DMRG calculations suggest that the standard KLM does not support superconductivity. \cite{15} This is also the conclusion of variational Monte Carlo calculations, which show that d-wave pairing is indeed present in the paramagnetic sector of the KLM, but it is easily defeated by magnetism. \cite{16} Instead, recent dynamical mean-field theory (DMFT) results obtained some evidence for an unexpected s-wave superconductivity close to the compensated regime and relatively large Kondo coupling. \cite{17}

In general, the weakness of superconductivity seems the consequence of the strength of magnetism, reinforced in the model calculation by the bipartite square lattice and by the unfrustrated hopping. Since lack of magnetic frustration is rather exceptional in real materials, it is worth and legitimate to investigate how frustration modifies the phase diagram of the KLM. \cite{18} Frustration in real heavy-fermion materials may take various forms. In certain cases, it can appear as a direct geometric frustration, as in the pyrochlore material Pr$_2$Ir$_2$O$_7$ \cite{19} and in the Shastry-Sutherland lattice compound Yb$_2$Pt$_2$Pb, \cite{20} in others by competing interactions of various kinds. The role of frustration in the KLM has been investigated in different works, especially focusing on magnetic properties. \cite{21,24}

There is another ingredient worth to be included to better reproduce the phase diagram of heavy fermions. Realistically, one expects that f-electrons are mutually coupled mostly through the conduction electrons, i.e., via the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange. However, most of the approximate methods used to study the KLM are unable to account for the RKKY interaction, unless long-range magnetic order is explicitly assumed. This inserts a bias in the calculations, since mag-
netic solutions can profit of RKKY, while non-magnetic ones cannot even exploit short-range magnetic correlations, e.g., to stabilize superconductivity. A way to mitigate this flaw is to add a direct $f-f$ exchange $J_H$ mimicking the actual RKKY interaction. The role of $J_H$ for reproducing the magnetic properties of heavy fermions has been highlighted several times. \[16\] Moreover, there are also suggestions that $J_H$ may be important to understand superconductivity in UP$_2$Al$_3$. \[31\]

In this letter, we thus explore the phase diagram of an extended KLM on a square lattice described by the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_i^\dagger c_j + h.c.) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (c_i^\dagger c_j + h.c.) + J \sum_i \mathbf{S}_i \cdot \mathbf{s}_i + J_H \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{s}_j,$$

(1)

where $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ imply that $i$ and $j$ are, respectively, nearest neighbors and next-nearest neighbors, $\mathbf{s}_i$ is the spin $1/2$-operator of the local moment at site $i$, and $\mathbf{S}_i$ that of the conduction electrons. Hereafter, we shall refer to the frustrated Kondo lattice model (FKLM) when $t' \neq 0$ but $J_H = 0$, and to the Kondo-Heisenberg lattice model (KHLM) in the opposite case of $t' = 0$ but $J_H \neq 0$. We take $t = 1$ as the energy unit, and study the phase diagram in the uncompensated regime, where the density of $c$-electrons $n_c < 1$, by varying the frustrating hopping $t'$ (both positive and negative), the Kondo coupling $J$, and the super-exchange $J_H$.

Method – We study the ground state of Eq. (1) by variational Monte Carlo technique. The variational wave function is defined by:

$$|\Psi_v\rangle = \mathcal{P}_f |\Phi_{MF}\rangle,$$

(2)

where $\mathcal{P}_f$ is the Gutzwiller projector that enforces single occupancy of $f$ electrons on each site, while $|\Phi_{MF}\rangle$ is an uncorrelated wave function defined as the ground state of a non-interacting variational Hamiltonian, $\mathcal{H}_{MF}$, that in general contains as variational parameters $c-c$, $c-f$ and $f-f$ hybridization terms, an energy shift of the $f$-orbitals, staggered magnetic fields acting on $c$- and $f$-electrons, as well as BCS coupling terms. Depending on $\mathcal{H}_{MF}$ we can access different uncorrelated states: 1) a paramagnetic metal when the staggered fields and the BCS terms are not allowed, which we denote by PM; 2) a superconductor when the BCS coupling is allowed, denoted by PM+BCS; and finally 3) an antiferromagnetic metal, where all Hamiltonian parameters in $\mathcal{H}_{MF}$ are allowed. We remind that when antiferromagnetism is considered, two possible states can be variationally obtained that differ by the topology of their Fermi surface, \[32\] either electron- or hole-like, which we refer to as AFe and AFh, respectively. Should antiferromagnetism coexist with superconductivity, we would use as labels AFh+BSC or AFe+BSC. The variational parameters are fixed by minimizing the total energy by quantum Monte Carlo simulations. \[33\] Calculations have been performed on clusters with 64, 100, 144 and 196 sites.

Results – We start by discussing the results for the FKLM of Eq. (1) with $J_H = 0$. First, we focus on the paramagnetic sector, namely on PM and PM+BCS states. The best superconducting wave function has $d_{x^2-y^2}$ symmetry. We report in Fig. 1 the condensation energy, computed as the energy difference between the best superconducting solution and the best normal one, for $n_c = 0.93$ and different values of $t'$. The presence of a positive next-nearest-neighbor $t'$ is found to considerably enhance the condensation energy, while negative values slightly suppresses it. The enlargement of the stability region of superconductivity for $t' > 0$ is also remarkable: while for $t' = 0$ the condensation energy vanishes for $J \simeq 1.5$, for $t' = 0.4$ superconductivity survives up to $J \simeq 2.3$.

Let us now consider magnetic states. We recall that, in the absence of frustration, the magnetic solution has always lower energy than the superconducting one, when the latter is stable, hence the actual phase diagram does not include superconductivity at all. \[16\] \[32\] This situation changes when frustration is added. In Fig. 2 we report the optimized energy of PM+BCS, AFh, and AFe...
states relative to the PM one, for $t' = \pm 0.4$ and $n_c = 0.93$ (we do not find any appreciable gain by allowing both magnetism and superconductivity). The first finding is that the AFh state is strongly hindered by $t'$ (both positive and negative). This is also true for the AFe state when $t' < 0$, while $t' > 0$ actually lowers AFe energy. The most important feature is the superconducting state now taking over the AFh phase, for both signs of the frustrating hopping (even though for $t' < 0$ the condensation energy is rather small). Therefore, the final outcome is the existence of a true superconducting phase in the vicinity of the magnetic transition (especially for large values of $J$ and $t'$). Finally, further away from compensated regime (i.e., for $n_c \lesssim 0.8$) the superconducting phase is defeated by the AFe state, and eventually disappears.

We now turn to the KHLM, with $t' = 0$ but $J_H > 0$ in Eq. (1). We observe that a variational wave function could in principle account for the RKKY exchange, hence not require any $J_H$, through spin-spin Jastrow factors. However, in practice this is unfeasible unless spin SU(2) symmetry is explicitly broken. Therefore, even though our variational approach is more accurate than Hartree-Fock, we still need to include a direct $f-f$ exchange to add magnetic short-range correlations provided in reality by the RKKY interaction.

As before, we start by the paramagnetic sector. Also in this case the superconducting state has $d_{x^2-y^2}$ symmetry. In Fig. 3 we show the condensation energy for different values of $J_H$ at $n_c = 0.93$. The case of $J_H = 0$ has been also reported for comparison. The maximum gain remains peaked around $J = 0.5$ but increases monotonically with $J_H$. Remarkably, even tiny values of $J_H$ substantially enhance the condensation energy. The inclusion of $J_H$ not only enlarges the condensation energy but also the stability region of superconductivity. While at $J_H = 0$ the transition to a normal metal occurs at $J \simeq 1.5$, for $J_H = 0.1$ the superconducting state remains stable up to $J \simeq 2.2$. To better highlight the enhancement of pairing due to $J_H$, in Fig. 4 we plot the pair-pair correlations for different values of $J_H$ at $J = 1.1$ and $n_c = 0.86$ (similar results are obtained for $n_c = 0.93$). Correlations remain pretty constant at large distances, indicating the existence of a true off-diagonal long-range order. To assess whether superconductivity does exist in the phase diagram, we now examine also magnetic states.

Obviously, a direct antiferromagnetic interaction $J_H$ enhances the tendency towards Néel order, hence enlarges the stability region of antiferromagnetism. In Fig. 4 we show the energy of magnetic and superconducting states relative to the paramagnetic state, for different values of $J_H$ and $n_c = 0.93$. The case $J_H = 0$ has been also included for comparison. Interestingly, upon increasing $J_H$ the superconducting phase finally gets energetically more favorable than AFh. Therefore, a superconducting region in the vicinity of the magnetic quantum critical point emerges as before, this time thanks to a finite $J_H$.

Furthermore, $J_H$ also stabilizes coexistence of pairing and magnetism, both close to the quantum critical point and well inside the AFe phase for small Kondo coupling. Indeed, we find a large energy gain when adding superconducting parameters on top of the AFh state. In other words, upon reducing the Kondo coupling, the paramagnetic metal first becomes superconducting through a second-order transition and then acquires magnetic order, still displaying a sizable electron pairing, see Fig. 4. By further reducing the Kondo exchange, a first-order transition to an AFe state occurs. Its energy can be even lowered by allowing for a BCS coupling, although the

FIG. 3: (Color on-line) Left panel: superconducting condensation energy versus the Kondo exchange $J$ for different values of $J_H$ and $n_c = 0.93$. The same quantity for fixed value of $J$ versus $J_H$ is also reported in the inset. Right panel: pair-pair correlations as a function of distance for $n_c = 0.86$, $J = 1.1$, and different values of $J_H$. The correlations for free electrons are also reported for comparison.

FIG. 4: (Color on-line) Energy difference of magnetic and superconducting phases with respect to paramagnetic state as a function of the Kondo exchange $J$, for different values of $J_H$ and $n_c = 0.93$. The cases with $J_H = 0$ (bottom left), $J_H = 0.01$ (bottom right), $J_H = 0.05$ (top left), and $J_H = 0.1$ (top right) are reported.
energy gain is tiny, see Fig. 4.

For lower electron densities, namely for $n_c \lesssim 0.8$ the AFh state cannot be stabilized anymore, similarly to the $J_H = 0$ case. In addition, the pure superconducting phase PM+BCS is now defeated by the AFh state, although the latter may still allow for a coexisting superconductivity.

In summary, we have shown that the inclusion of magnetic frustration in the Kondo lattice model through a next-nearest-neighbor hopping has the important role of suppressing magnetic order hence uncovering superconductivity, which we find intrudes between the paramagnetic and antiferromagnetic metal phases, see Fig. 5. Superconductivity is further stabilized by short-range magnetic correlations, which in reality are yielded by the RKKY exchange but which we had to enforce in our variational calculation through a direct antiferromagnetic exchange $J_H$ between the localized moments. Even for quite small $J_H$, a superconducting dome appears between the antiferromagnet and the paramagnetic metals, for $n_c \gtrsim 0.8$, see Fig. 5. We also have indications for a coexistence of magnetism and superconductivity when the Kondo exchange is small.

Therefore, both the occurrence of a superconducting dome right in the vicinity of the quantum critical point separating the magnetic metal from the paramagnetic one, the typical example being CePd$_2$Si$_2$, and the coexistence of antiferromagnetism and superconductivity, observed in CeRhSi$_2$, CeRhIn$_5$, and, more recently, CeCo(In$_{1-x}$Cd$_x$)$_5$, are reproduced by an enriched Kondo lattice model.

This work was partially supported by PRIN 2010-11.

---

[1] F. Steglich, J. Aarts, C.D. Bredl, W. Lieke, D. Meschede, W. Franz, and H. Schafer, Phys. Rev. Lett. 43, 1892 (1979).
[2] M.R. Norman, Science 332, 196 (2011).
[3] D.J. Scalapino, Rev. Mod. Phys. 84, 1383 (2012).
[4] M.P. Allan, F. Massee, D.K. Morr, J. Van Dyke, A.W. Rost, A.P. Mackenzie, C. Petrovic, and J.C. Davis, Nat. Phys. 9, 468 (2013).
[5] N.D. Mathur, F.M. Grosche, S.R. Julian, I.R. Walker, D.M. Freye, R.K.W. Haselwimmer, and G.G. Lonzarich, Nature (London) 394, 39 (1998).
[6] F.M. Grosche, I.R. Walker, S.R. Julian, N.D. Mathur, D.M. Freye, M.J. Steiner, and G.G. Lonzarich, J. Phys.: Condens. Matter 13, 2845 (2001).
[7] Q. Si and F. Steglich, Science 329, 1161 (2010).
[8] R. Movshovich, T. Graf, D. Mandrus, J.D. Thompson, J.L. Smith, and Z. Fisk, Phys. Rev. B 53, 8241 (1996).
[9] M. Yashima, S. Kawasaki, H. Mukuda, Y. Kitaoaka, H. Shishido, R. Settai, and Y. Onuki, Phys. Rev. B 76, 020509 (2007).
[10] S. Nair, O. Stockert, U. Witte, M. Nicklas, R. Schedler, K. Kiefer, J.D. Thompson, A.D. Bianchi, Z. Fisk, S. Wirth, and F. Steglich, PNAS 107, 9537 (2010).
[11] S. Doniach, Physica B & C 91, 231 (1977).
[12] H. Tsumetugu, M. Sigrist, and K. Ueda, Rev. Mod. Phys. 69, 809 (1997).
[13] P. Coleman, in Handbook of Magnetism and Advanced Magnetic Material, Volume 1: Fundamentals and Theory, pag. 95 (eds H. Kronmuller and S. Parkin) (Wiley, 2007).
[14] P.W. Anderson, Science 235, 1196 (1987).
[15] J.C. Xavier, Phys. Rev. B 68, 134422 (2003).
[16] M.Z. Asadzadeh, F. Becca, and M. Fabrizio, Phys. Rev. B 87, 205144 (2013).
[17] O. Bodensiek, R. Zitko, M. Vojta, M. Jarrell, and T. Pruschke, Phys. Rev. Lett. 110, 146406 (2013).
[18] P. Coleman and A.H. Nevidomskyy, J. of Low Temp. Phys. 161, 182 (2010).
[19] S. Nakatsuji, Y. Machida, Y. Maeno, T. Tayama, T. Sakakibara, J. van Duijn, L. Balicas, J.N. Millican, R.T. Macaluso, and J.Y. Chan, Phys. Rev. Lett. 96, 087204 (2006).
[20] M.S. Kim, M.C. Bennett, and M.C. Aronson, Phys. Rev. B 77, 144425 (2008).
[21] Y. Motome, K. Nakamikawa, Y. Yamaji, and M. Udagawa, Phys. Rev. Lett. 105, 036403 (2010).
[22] B.H. Bernhard, B. Coqblin, and C. Lacroix, Phys. Rev. B 83, 214427 (2011).
[23] R. Peters, N. Kawakami, and T. Pruschke, J. Phys.: Conf. Ser. 320, 012057 (2011).
[24] J.G. Rau and H.-Y. Kee, Phys. Rev. B 89, 075128 (2014).
[25] P. Coleman and N. Andrei, J. Phys.: Condens. Matter 1, 4057 (1989).
[26] J.R. Iglesias, C. Lacroix, and B. Coqblin, Phys. Rev. B 56, 11820 (1997); B. Coqblin, C. Lacroix, M.A. Gusmao, and J.R. Iglesias, Phys. Rev. B 67, 064417 (2003).
[27] M.D. Kim, C.K. Kim, and J. Hong, Phys. Rev. B 68, 174424 (2003).
[28] J.C. Xavier and E. Dagotto, Phys. Rev. Lett. 100, 146403 (2008).
[29] Y. Liu, H. Li, G.-M. Zhang, and L. Yu, Phys. Rev. B 86, 024526 (2012).
[30] L. Isakov and I. Vekhter, Phys. Rev. Lett. 110, 026403 (2013).
[31] N.K. Sato, N. Aso, K. Miyake, R. Shiina, P. Thalmeier, G. Varelogiannis, C. Geibel, F. Steglich, P. Fulde, and T. Komatsubara, Nature (London) 410, 340 (2001).
[32] H. Watanabe and M. Ogata, Phys. Rev. Lett. 99, 136401 (2007).
[33] S. Sorella, Phys. Rev. B 71, 241103 (2005).