A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

OFFPRINT

Coexistence of ferromagnetism and Kondo effect in the underscreened Kondo lattice

N. B. Perkins, J. R. Iglesias, M. D. Núñez-Regueiro and B. Coqblin

EPL, **79** (2007) 57006

A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

September 2007

EPL, **79** (2007) 57006 www.epljournal.org
doi: 10.1209/0295-5075/79/57006

Coexistence of ferromagnetism and Kondo effect in the underscreened Kondo lattice

N. B. PERKINS[1,2], J. R. IGLESIAS[3], M. D. NÚÑEZ-REGUEIRO[4(a)] and B. COQBLIN[4]

[1] *Institute fur Theoretische Physik, TU Braunschweig - Mendelssohnstrasse 3, 38106 Braunschweig, Germany*
[2] *Bogoliubov Laboratory of Theoretical Physics, JINR - Dubna, Russia*
[3] *Instituto de Física, Universidade Federal do Rio Grande do Sul - 91501-970 Porto Alegre, Brazil*
[4] *Laboratoire de Physique des Solides, UMR 8502 CNRS, Université Paris-Sud - 91405 Orsay, France*

received 26 January 2007; accepted in final form 10 July 2007
published online 1 August 2007

PACS 71.27.+a – Strongly correlated electron systems; heavy fermions
PACS 75.30.Mb – Valence fluctuation, Kondo lattice, and heavy-fermion phenomena
PACS 75.20.Hr – Local moment in compounds and alloys; Kondo effect, valence fluctuations, heavy fermions

Abstract – The coexistence of ferromagnetic order and Kondo behavior, that has been experimentally observed in some uranium compounds, is studied in the framework of an underscreened Kondo lattice model within the mean-field approach. For small values of J_K compared to the bandwidth, a ferromagnetically ordered solution is obtained, while for larger values of J_K a Kondo regime occurs with a Kondo temperature larger than the Curie temperature, suggesting a scenario for the coexistence of Kondo effect and ferromagnetic order.

Historically, the KL model [1–4] has been proposed to account for properties of cerium compounds, where a competition between Kondo effect and magnetic order has been experimentally observed. In most of cerium-based compounds, cerium ions are in the $4f^1$ configuration. In this case, there exists one f-electron per site —giving a localized $S=1/2$ spin— which couples antiferromagnetically to a conduction electron spin density, via an on-site exchange interaction J_K. At very low temperatures the localized spin $S=1/2$ is completely screened by the conduction electrons, leading to the formation of coherent Kondo spin-singlet state. Besides, the local coupling between f-spins and conduction electrons may give rise to a magnetic order through the RKKY interaction. This interaction is usually added to the KL model as an additional inter-site interaction between f-spins [5,6].

The competition between the magnetic order and the Kondo effect was first considered by Doniach [7]. He proposed a phase diagram with a quantum phase transition between two distinct phases: a magnetically ordered one and a non-magnetic Kondo phase. The KL model has been proven to be an appropriate tool for describing these quantum transitions at different values of external parameters such as band filling, pressure, magnetic field or temperature [3].

In this paper, we are interested in the physical properties of another class of heavy-fermion systems, uranium compounds, whose behavior is quite different from cerium compounds, particularly due to the existence of several coexistence phenomena between magnetism, heavy-fermion behavior and superconductivity. Here, we would like to discuss one of them, namely, the coexistence between the ferromagnetic order and the Kondo behavior which has been observed experimentally in some uranium compounds.

The first experimental evidence of the coexistence between Kondo behavior and ferromagnetic order in the dense Kondo compound UTe has been obtained long ago [8,9]. More recently, this coexistence has been observed in $UCu_{0.9}Sb_2$ [10] and $UCo_{0.5}Sb_2$ [11]. Those systems undergo a ferromagnetic ordering at relatively high Curie temperatures of $T_C=102\,K$ (UTe), $T_C=113\,K$ ($UCu_{0.9}Sb_2$) and $T_C=64.5\,K$ ($UCo_{0.5}Sb_2$). Above the ordering temperatures, these materials exhibit a Kondo-like logarithmic decrease of the electrical resistivity, indicating a Kondo behavior. This logarithmic variation extends down to the ferromagnetic Curie temperature, T_C, suggesting that the Kondo behavior survives inside the ferromagnetic phase, implying that the ferromagnetic

(a) Our colleague and friend M. D. Núñez-Regueiro passed away on November 15, 2006 during the redaction of this article.

order and the Kondo behavior do coexist. We would like also to mention $UNiSi_2$ with a Curie temperature $T_C = 95\,K$ [12–14], $UCo_{0.6}Ni_{0.4}Si_2$ with $T_C = 62\,K$ [15] and $URu_{2-x}Re_xSi_2$ compounds where T_C increases rapidly with concentration x [16–18]. The same kind of coexistence has been recently observed in UAsSe with a $T_C = 109\,K$ [19] and in the neptunium compound $NpNiSi_2$, which becomes ferromagnetic at $T_C = 51.5\,K$ and presents a Kondo behavior [20].

From these examples we can see that Kondo-ferromagnetism coexistence, together with large Curie temperatures, is a rather common phenomenon in actinide compounds and it is clearly a novel feature compared to Ce-compounds, which cannot be explained by the standard KL ($S = 1/2$) model. It has been, to our knowledge, somewhat overlooked from a theoretical point of view. Nevertheless, we remark that a kind of coexistence of ferromagnetism and Kondo-like behavior has been observed in a few Ce-based dense Kondo systems, such as $CePt_xSi$ [21] and CeAg [22] compounds, but the Curie temperatures of these compounds are relatively small, typically of order 5 K. Therefore, these experimental findings can be considered rather as a sign of a strong competition rather than a real coexistence between the Kondo effect and ferromagnetic order. We also notice that the issue whether a disordered Kondo singlet state can coexist with an antiferromagnetically ordered state in KL model ($S = 1/2$) at half filling has been considered in ref. [23]. Using mean-field arguments, the authors have shown that such coexistence is possible for the half-filled anisotropic KL (AKL) model, although it remains very weak. They obtained a coexistence regime as a result of the balance between Kondo screening and magnetic interactions.

To account for the Kondo-ferromagnetism coexistence phenomena in uranium compounds, we propose the framework of the underscreened Kondo lattice (UKL) model, which consists of a periodic lattice of magnetic atoms with $S = 1$ interacting with a spin density of conduction electrons via an on-site antiferromagnetic Kondo coupling. In addition, the localized spins at neighboring sites interact ferromagnetically with each other. Because $S = 1$, the Kondo effect does not lead to a complete screening of the localized spins, and the ferromagnetic exchange between the (underscreened) spins may indeed lead to the formation of ferromagnetic order.

This model can be applied to uranium compounds if the majority of uranium ions are in $5f^2$ configuration, in which two f-electrons are bound into spin $S = 1$. We believe this is an appropriate description of electronic states for those compounds which have magnetic moments close to the free ion values [10,11,24]. However, we are aware that the choice of the $5f^2$ configuration with $S = 1$ is not free of controversy. Magnetism in uranium compounds comes from $5f$ electrons —this has been proven by many experimental observations, *e.g.*, by form-factor studies in neutron scattering. At the same time, $5f$ electrons states in uranium compounds are often in a crossover region between localized and itinerant behavior, and the strength of the localization depends strongly on a subtle balance between electronic correlations, crystal field, and spin-orbit coupling. It is often rather difficult to decide, on the basis of the experimental data, between Kondo behavior of well localized $5f^2$ configuration and mixed-valence behavior. Because of this dual nature of $5f$ states, the development of the adequate description of the electronic structure for uranium compounds has been a challenging problem [24–27]. However, it is reasonable to assume that $5f$ electrons are more localized in UTe, or in the previously described uranium compounds, than in other uranium monochalcogenides such as US or USe [24,28].

The UKL Hamiltonian can be written in the following form:

$$\begin{aligned} H \;=\; & \sum_{\vec{k},\sigma}(\epsilon_{\vec{k}}-\mu)\mathbf{n}^{c}_{\vec{k}\sigma} + \sum_{i\sigma\alpha} E_0 \mathbf{n}^{f\alpha}_{i\sigma} \\ & + J_K \sum_i \mathbf{S}_i \sigma_i + \frac{1}{2} J_H \sum_{ij} \mathbf{S}_i \mathbf{S}_j, \end{aligned} \tag{1}$$

where the first term represents the conduction band with dispersion ϵ_k, width $2D$ and constant density of states $1/2D$; μ is the chemical potential. Localized spins are represented by fermionic operators $\mathbf{f}^{\dagger}_{i\sigma\alpha}$ and $\mathbf{f}_{i\sigma\alpha}$ introduced in refs. [29,30], carrying spin, σ, and orbital, α, indexes. E_0 is a Lagrange multiplier which is fixed by a constraint for the total number of f-electrons per site, $n_f = \sum_\sigma (n^{f1}_\sigma + n^{f2}_\sigma) = 2$, and can be interpreted as a fictitious chemical potential for f-fermions. The third term is the on-site Kondo coupling, $J_K > 0$, between localized $\mathbf{S}_i = 1$ and conduction electron's $\sigma_i = 1/2$ spins, whose fermionic representation is done in the usual way. Finally, the last term is the ferromagnetic inter-site interaction, $J_H < 0$, between localized f-magnetic moments. It may result from two contributions: an effective RKKY interaction, which can be ferromagnetic for strong-coupling regime, large $|J_K|$, and for partial filling of the conduction band (as it has been shown by many authors for the usual KL model, see, for example, refs. [4,31]), and, possibly, a direct exchange.

We first introduce the relevant bosonic fields. To describe Kondo effect, we introduce the operator $\widehat{\lambda}_{i\sigma} = \sum_\alpha \mathbf{c}^{+}_{i\sigma}\mathbf{f}^{\alpha}_{i\sigma}$ which couples electrons and auxiliary fermions at the same site. To describe magnetic properties of the system, we introduce the operators of magnetization for both f- and c-subsystems: $M_i = S^z_i = \frac{1}{2}(n^f_{i\uparrow} - n^f_{i\downarrow})$ and $m_i = \sigma^z_i = \frac{1}{2}(n^c_{i\uparrow} - n^c_{i\downarrow})$, respectively. We restrict our consideration to self-consistent analysis (equivalent to slave boson mean-field description), and evaluate all physical quantities in terms of these bosonic fields. We then introduce four real order parameters $\lambda_\sigma = \langle\widehat{\lambda}_{i\sigma}\rangle$, $M = \langle \mathbf{M}_i\rangle$ and $m = \langle \mathbf{m}_i\rangle$, and decouple the Hamiltonian (1) to obtain self-consistent equations on λ_σ, M and m. The non-zero values of M and m correspond to the magnetically ordered phase, while a non-zero values of λ_σ describes the Kondo effect and the formation of the heavy-fermion state.

Our computational procedure is basically equivalent to other mean field (MF) approaches developed for studying normal KL, such as the path-integral calculation restricted to a saddle point solution performed by Coleman and Andrei [5], or large-N formulation performed by Burdin *et al.* [32], where the saddle point solution yields a mean-boson-field approximation. However, all these approximate schemes have some caveats. The MF approximation neglects magnetic fluctuations, and the system may possess spurious charge fluctuations such that the exact constraint $f^\dagger_\uparrow f_\uparrow + f^\dagger_\downarrow f_\downarrow = 2$ is actually satisfied only on average. However, despite all these caveats, mean-field approximation captures essentially the correct low-temperature physics of Kondo systems. It also yields a right Kondo temperature, for example in the study of the Kondo impurity problem [33]. Finally the validity of MF and slave-boson approaches for the KL model has been extensively discussed in ref. [32].

Within this MF approximation, the Hamiltonian (1) is given by

$$\begin{aligned} H_{MF} = {} & \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}\sigma} n^c_{\vec{k}\sigma} + \sum_{i\alpha\sigma} E_{0\sigma} n_{i\alpha\sigma} - \frac{1}{2} J_K \sum_{i\alpha\sigma} (\lambda_{\bar\sigma} \widehat{\lambda}^\alpha_{i\sigma} + \text{h.c.}) \\ & + 2J_K N \sum_\sigma \lambda_{\bar\sigma}\lambda_\sigma - J_K N m M - \frac{1}{2} J_H N z M^2, \end{aligned} \quad (2)$$

where, remembering that $J_K > 0$ and $J_H < 0$, energies read

$$\begin{aligned} \varepsilon_{\vec{k}\sigma} &= \varepsilon_{\vec{k}} + J_K \sigma M - \mu, \quad \text{with } \sigma = \pm 1/2, \\ E_{0\sigma} &= E_0 + J_K \sigma m - \frac{1}{2} J_K \lambda_\sigma \lambda_{\bar\sigma} + J_H z \sigma M. \end{aligned} \quad (3)$$

The diagonalization of the MF Hamiltonian (2) gives two non-hybridized f-levels (one for each spin) at energies $E_{0\sigma}$ and two quasiparticle bands $E^\sigma_\pm(\vec{k})$ with energies

$$E^\sigma_\pm(\vec{k}) = \frac{1}{2}\left[E_{0\sigma} + \varepsilon_{\vec{k}\sigma} \pm \sqrt{(E_{0\sigma} - \varepsilon_{\vec{k}\sigma})^2 + 8\alpha^2_{\bar\sigma}}\right], \quad (4)$$

where $\alpha_{\bar\sigma} = -\frac{1}{2} J_K \lambda_{\bar\sigma}$. The $\pm$ sign refers to the upper (lower) hybridized band. Let us point out here one of the main differences between the mean-field treatment of the standard KL and UKL models: in the underscreened case one f-localized level remains non-hybridized and for the other level the resulting c-f effective hybridization is twice that of the normal case.

The energy spectra $E^\sigma_\pm(k)$ depend on a set of external parameters such as band filling, n_c, Kondo coupling, J_K, and exchange interaction, J_H, and a set of internal parameters, M, m, λ_σ, μ and E_0, which should be calculated in a self-consistent way. To this end, we construct a close self-consistent scheme, and evaluate bosonic fields $\lambda_\uparrow$, $\lambda_\downarrow$, M and m together with the chemical potential μ and the Lagrange multiplier E_0 self-consistently. The first self-consistent equation can be obtained from the constraint on the total number of f-electrons:

$$n_f = n^\uparrow_f + n^\downarrow_f = 2. \quad (5)$$

The second self-consistent equation is obtained by setting the average number of conduction electrons to be equal to the filling value n_c:

$$n_c = n^\uparrow_c + n^\downarrow_c. \quad (6)$$

The expressions of n^σ_f and n^σ_c can be evaluated by straightforward calculation from the Green functions of the system:

$$\begin{aligned} n^\sigma_f = {} & \frac{1}{2D}\int_{-D+\Delta_\sigma}^{D+\Delta_\sigma} \mathrm{d}\varepsilon_\sigma \bigg[n_F(E_{0\sigma}) - n_F(E_{+\sigma}) \frac{\varepsilon_\sigma - E_{+\sigma}}{W_\sigma(\varepsilon_\sigma)} \\ & + n_F(E_{-\sigma}) \frac{\varepsilon_\sigma - E_{-\sigma}}{W_\sigma(\varepsilon_\sigma)} \bigg], \\ n^\sigma_c = {} & \frac{1}{2D}\int_{-D+\Delta_\sigma}^{D+\Delta_\sigma} \mathrm{d}\varepsilon_\sigma \bigg[-n_F(E_{+\sigma}) \frac{E_{0\sigma} - E_{+\sigma}}{W_\sigma(\varepsilon_\sigma)} \\ & + n_F(E_{-\sigma}) \frac{E_{0\sigma} - E_{-\sigma}}{W_\sigma(\varepsilon_\sigma)} \bigg], \end{aligned} \quad (7)$$

where $n_F(\omega) = \frac{1}{e^{\frac{\omega-\mu}{T}} + 1}$ is the Fermi distribution function, $\Delta_\sigma = J_K \sigma M$ and $W_\sigma(\varepsilon) = \sqrt{(E_{0\sigma} - \varepsilon)^2 + 8\alpha^2_{\bar\sigma}}$. In the mean-field approximation, as we discussed above, we substitute the strong constraint, $n_{if} = 2$ in each site, by a softer one for its average, and set the band filling by the averaged number of c-electrons, n_c, which we consider in the usual range of partial filling, *i.e.* $0 < n_c \leqslant 1$.

The third and the forth self-consistent equations are obtained from the Luttinger theorem, and from the condition that the total magnetization M_{tot} is the sum of the average magnetization of f -and c-electrons. This gives

$$n_f + n_c = 3 + \frac{\mu_\uparrow + \mu_\downarrow}{2D} \quad (8)$$

and

$$M + m = 1 + \frac{\mu_\uparrow - \mu_\downarrow}{4D}. \quad (9)$$

We use here $M = \frac{1}{2}(n^\uparrow_f - n^\downarrow_f)$ and $m = \frac{1}{2}(n^\uparrow_c - n^\downarrow_c)$, respectively. We remark that the Fermi surface encloses both conduction electrons and partially localized f-levels. The quantities $\mu_\uparrow$ and $\mu_\downarrow$ in eqs. (8) and (9) correspond to the limits of integration over $\epsilon_\uparrow$ and $\epsilon_\downarrow$, respectively, and are related to the Fermi level μ through the equalities: $E^\uparrow_+(\mu_\uparrow) = E^\downarrow_-(\mu_\downarrow) = \mu$.

The last two equations are self-consistent relations for the bosonic fields $\lambda_\uparrow, \lambda_\downarrow$:

$$\lambda_\sigma = \frac{1}{D}\int_{-D+\Delta_\sigma}^{D+\Delta_\sigma} \mathrm{d}\varepsilon_\sigma [n_F(E_{+\sigma}) - n_F(E_{-\sigma})] \frac{\alpha_{\bar\sigma}}{W_\sigma(\varepsilon_\sigma)}. \quad (10)$$

Equations (5)–(10) constitute the full set of self-consistent equations for six variables: $\lambda_\uparrow$, $\lambda_\downarrow$, M, m, μ and E_0. We solved this equations numerically by iterations.

We first discuss the properties of the model at $T = 0$. In order to establish the region of coexistence of Kondo effect and ferromagnetic ordering (Kondo-ferromagnetism coexistence) in the phase space set by the parameters of the model, we study the parameter-dependent behavior of λ_σ and the magnetization M and m.

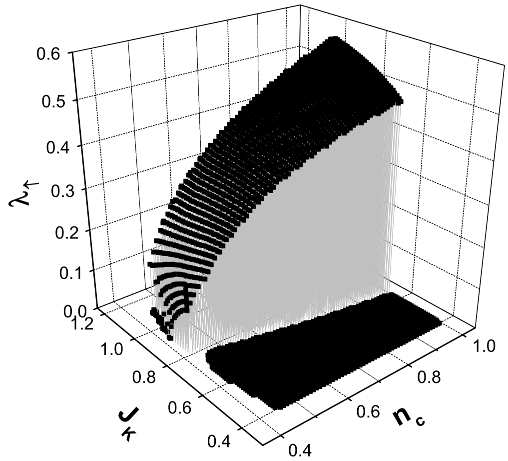

Fig. 1: Plot of the parameter $\lambda_\uparrow$ as a function of J_K and n_c for $T = 0$. The ferromagnetic interaction between localized f moments is $J_H = -0.01$. There is a discontinuous transition as a function of J_K and a behavior in $\sqrt{n_c}$ for constant values of J_K, as explained in the text.

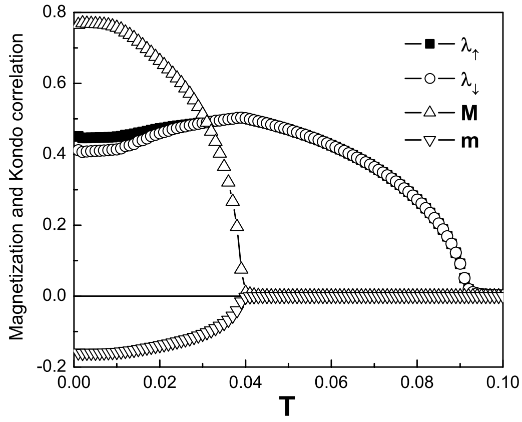

Fig. 2: Plot of $\lambda_\uparrow$, $\lambda_\downarrow$, M and m as a function of temperature. Self-consistent solutions are obtained for the following parameters: $J_K = 0.8$, $J_H = -0.01$ and $n_c = 0.8$ (in units of the half-bandwidth D).

In fig. 1 we present a summary of the results for $T = 0$. The region of the parameters J_K and n_c that provide finite values of $\lambda_\uparrow$ corresponds to a coexistence between the heavy-fermion behavior and ferromagnetic order. The values of $\lambda_\downarrow$ are close to $\lambda_\uparrow$, so the former is not shown in the fig. 1, to keep the figure transparent. In this and all other figures all energies and temperatures are given in units of half-bandwidth D. It is possible to see in fig. 1 that $\lambda_\uparrow$ decreases smoothly as a function of n_c, following an approximate square root behavior [3], while it undergoes a sharp transition as a function of J_K. When $\lambda_\uparrow$ goes to zero the ground state is magnetically ordered with no Kondo effect and the hybridization gap $\Gamma_\sigma = 8\alpha_\sigma^2$ vanishes simultaneously, signaling a quantum phase transition. Moreover, even if the magnetization goes through a discontinuity for this critical value of J_K, it is always different from zero. So, one observes a quantum phase transition from a pure magnetically ordered state for small values of J_K to a coexistence of magnetic order and Kondo effect for high values of J_K. It is worth to notice that both the Kondo and magnetic behaviors extend up to the case of half-band filling, *i.e.* it is not an effect of the low density of conduction electrons, but a true consequence of the underscreened $S = 1$ spin, that is only partially screened by the sea of conduction electrons.

We now present the results obtained at finite temperatures which allows us to determine the Curie temperature and the Kondo temperature. Figure 2 shows the behavior of the f and c magnetization, M and m, respectively, and λ_σ, as a function of the temperature. The parameters here and in following figures are chosen to be $J_K = 0.8$, $J_H = -0.01$ and $n_c = 0.8$. The two magnetization curves clearly show the existence of a continuous phase transition at T_C from a ferromagnetic to a non-magnetic state. At zero and low temperatures we observe the coexistence of magnetic order and heavy-fermion behavior, but as both spin systems are strongly polarized the Kondo effect is smaller. When the magnetization decreases, λ_σ grows up to a maximum at the Curie temperature. Due to the breakdown of the spin symmetry $\lambda_\downarrow$ and $\lambda_\uparrow$ are slightly different in the magnetic region but they coincide when the magnetization vanishes for $T = T_C$, *i.e.* when the spin symmetry is restored. For $T > T_C$ the system exhibits only Kondo behavior ($\lambda_\sigma \neq 0$, $M = 0$ and $m = 0$). Finally, above a characteristic temperature, the Kondo temperature, T_K, both λ_σ are zero and the two electron systems are decoupled. The result that λ vanishes at a particular temperature is a well-known artifact of the mean-field approximation. Actually, T_K is a crossover temperature, associated with the onset of local Kondo screening. We notice that T_K increases when the Kondo coupling value J_K also increases.

This behavior can be further clarified by the plot of the densities of states at different temperatures. As the c densities of states are almost constant (except in the hybridization gap region) we present the results only for the f densities of states, which are calculated numerically from the imaginary part of the f-f Green functions. In fig. 3 we plot $\rho_{f\sigma}(\epsilon - \mu)$ for four different temperatures.

At zero and low temperatures, $T < T_C$, the bands for the two spin polarizations are shifted, as expected for the magnetically ordered state. The hybridization gap due to Kondo effect is present for both directions of the spin, and the non-hybridized f-level stays inside this gap. This localized f-level is occupied for spin-up states and it is empty for spin-down states. This implies a semi-metal behavior in the magnetic phase. When $T > T_C$, the Fermi level is inside the gap for both up and down spin directions and coincides with the energy of the f-level, E_0, (see fig. 3c and d). Finally, when λ_σ goes to zero, the hybridization gap closes and the system becomes metallic.

At last, from the quasiparticle spectrum, eq. (4), one can estimate the mass enhancement [34], which is

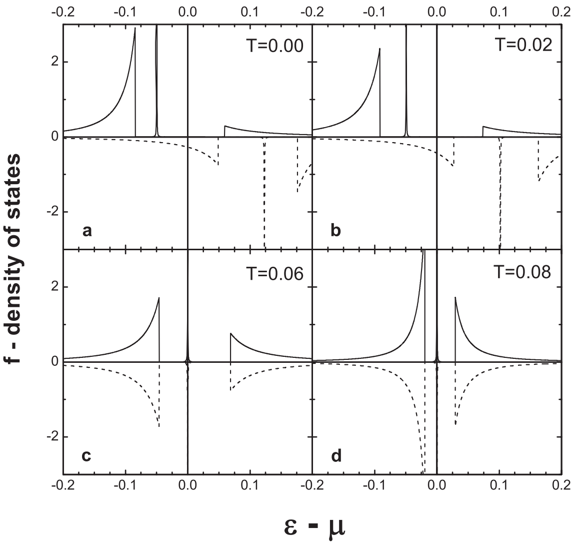

Fig. 3: Temperature variation of the up- (solid line) and down- (dashed line) f-density of states, $\rho_{f\sigma}(\epsilon-\mu)$. Panel (a) corresponds to $T=0$, (b) $T=0.02$, (c) $T=0.06$ and (d) $T=0.08$. The parameters are the same as in fig. 2.

spin-dependent in this case:

$$\frac{m^*_\sigma}{m}=1+\frac{2\alpha^2_{\bar\sigma}}{(E_{0\sigma}-\mu-\Delta_\sigma)^2}. \tag{11}$$

We plot the temperature variation of the mass enhancement in fig. 4.

For both spin directions two peaks are clearly seen: one corresponds to the Curie temperature, and the second (at a higher temperature) to the onset of Kondo effect. In the region of coexistence, the effective mass increases as a function of temperature following the position of the Fermi level inside the $E^{\downarrow}_{-}(k)$ band. The mass enhancement becomes very large in the pure Kondo regime. In fact, in this regime the denominator of eq. (11) goes to zero and the effective mass formally diverges. A finite width of the f-level eliminates the divergence, but still yields a very large mass.

Although this result for the effective mass probably overestimates the strength of the enhancement, it still provides a qualitatively good explanation of the heavy-fermion behavior.

In fig. 5, we plot the Curie temperature T_C and the Kondo temperature T_K *vs.* J_K for fixed values of J_H and n_c. It is possible to see that the Kondo temperature T_K becomes finite only at the critical value $J^c_K\simeq 0.65$ (for $J_H=-0.01$ and $n_c=0.8$), then rapidly increases for larger values of J_K. On the other hand, the Curie temperature, T_C, is finite for all studied values of J_K. The two curves $T_K(J_K)$ and $T_C(J_K)$ cross slightly above J^c_K and for larger values of J_K the Kondo temperature, T_K, is always larger than T_C. Indeed, the ferromagnetic order persists for all values of the ratio J_K/J_H, while the Kondo-ferromagnetism coexistence exists only for sufficiently large values of this ratio. In the purely magnetic region

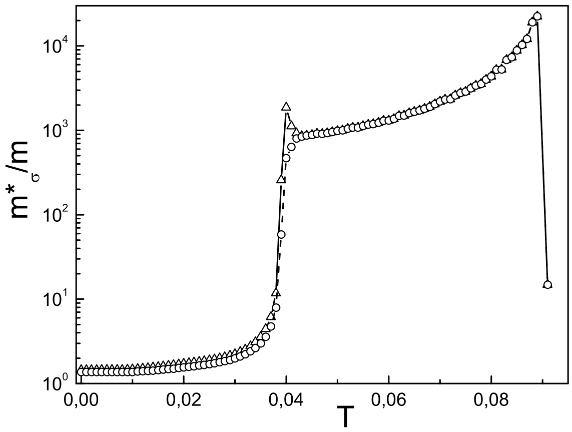

Fig. 4: Temperature dependence of the effective mass enhancement. The parameter set is the same as in fig. 2.

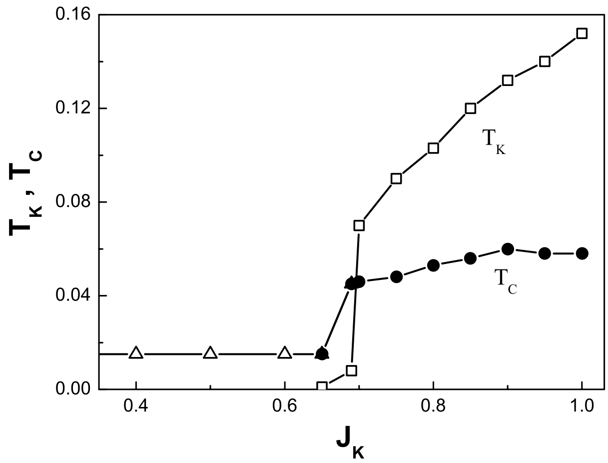

Fig. 5: The ferromagnetic Doniach diagram: plot of the Curie temperature T_C (the triangles are analytical values, the circles numerical ones) and the Kondo temperature T_K (squares) *vs.* J_K with $J_H=-0.01$ and $n_c=0.8$.

the Curie temperature can be easily evaluated, and it is equal to $T_C=\frac{z|J_H|}{4}$.

The diagram presented in fig. 5 can be called the "ferromagnetic Doniach diagram" for the UKL model. It is qualitatively very different from the well-known Doniach diagram derived for the Kondo lattice with $S=1/2$ [3,6], where the ordering temperature tends to zero at a finite J_K and the magnetic order and the Kondo effect compete rather than co-exist.

In conclusion, in this work we introduced and studied the underscreened Kondo lattice model with localized spins $S=1$. The main result is that this model naturally exhibits coexistence of ferromagnetic order and heavy-fermion behavior. We analyzed this behavior by deriving and solving self-consistent equations for the relevant bosonic fields.

Within this treatment, we obtained a region in the phase space where the order parameters, λ_σ, M, and m are all different from zero, characterizing a coexistence between the heavy fermion (Kondo) properties and ferromagnetic order. As temperature increases, the magnetic order disappears first at the temperature T_C. At this temperature λ_σ is still different from zero, indicating a Kondo or NFL regime. This is in agreement with the experiments for uranium compounds in which the Kondo behavior is observed above the Curie temperature. The phase transition at T_C is then the transition from the ferromagnetic Kondo phase at low temperature to the non-magnetic Kondo phase at higher temperature. Another transition is obtained at $T=0$ by varying J_K. This transition is discontinuous and leads to a non-Kondo magnetically ordered state, as seen in fig. 1.

We emphasize that the coexistence between ferromagnetism and Kondo effect is due to the presence of one non-hybridized and one hybridized f-level (see fig. 3). The coexistence arises from the fact that localized f-spins are only partially screened. The presence of the localized f-level is the key difference between our model and a conventional $S=1/2$ Kondo lattice model, for which it is well known that magnetism and Kondo effect just compete. In this way, our UKL model explains the behavior of some uranium compounds, and even one neptunium compound, where a ferromagnetically ordered state has been observed to coexist with a heavy fermion Kondo state.

Finally, we stress that besides its applicability to the physics of ferromagnetic uranium compounds, the UKL model is an interesting problem on its own, but yet it has attracted a little attention. The UKL model in the form we use here was first proposed in ref. [29]. It is one of the theoretical models which can capture the physics of the lattice of underscreened magnetic moments in a metal. A more extended analysis of the UKL model, including the study by numerical simulations, is under way and will be published elsewhere.

***

The authors acknowledge stimulating discussions with S. Burdin, P. Fulde, R. Ramazashvili and J. Schoenes and the financial support of Brazilian agencies CNPq and FAPERGS. JRI thanks the kind hospitality and financial support from MPI for Complex Systems, Dresden and MPI for Dynamics and Self-Organization, Göttingen, Germany, during the realization of this work. BC thanks the European COST P16 for financial support.

REFERENCES

[1] Fazekas P. and Muller-Hartmann E., *Z. Phys. B*, **85** (1991) 282.
[2] Coqblin B., Núñez-Regueiro M. D., Alba Theumann, Iglesias J. R. and Magalhaes S. G., *Philos. Mag.*, **86** (2006) 2567 and references therein.
[3] Coqblin B., Lacroix C., Gusmao M. S. and Iglesias J. R., *Phys. Rev. B*, **67** (2003) 064417.
[4] Tsunetsugu H., Sigrist M. and Ueda K., *Rev. Mod. Phys.*, **69** (1997) 809.
[5] Coleman P. and Andrei N., *J. Phys.: Condens. Matter*, **1** (1989) 4057.
[6] Iglesias J. R., Lacroix C. and Coqblin B., *Phys. Rev. B*, **56** (1997) 11820 .
[7] Doniach S., *Proceedings of the International Conference on Valence Instabilities and Related Narrow-band Phenomena*, edited by ParksR. D. (Plenum Press) 1976, p. 168.
[8] Schoenes J., *J. Less-Common Met.*, **121** (1986) 87.
[9] Schoenes J., Frick B. and Vogt O., *Phys. Rev. B*, **30** (1984) 6578.
[10] Bukowski Z., Troc R., Stepien-Damm J., Sulkowski C. and Tran V. H., *J. Alloys Compd.*, **403** (2005) 65.
[11] Tran V. H., Troc R., Bukowski Z., Badurski D. and Sulkowski C., *Phys. Rev. B*, **71** (2005) 094428.
[12] Kaczorowski D., *Solid State Commun.*, **99** (1998) 949.
[13] Das A., Paranjpe S. K., Raj P., Satyamoorthy A., Shashikala K. and Malik S. K., *Solid State Commun.*, **114** (2000) 87.
[14] Taniguchi T., Morimoto H., Miyako Y. and Ramakrishnan S., *J. Magn. & Magn. Mater.*, **177-181** (1998) 55.
[15] Kaczorowski D., *37èmes Journées des Actinides, Sesimbra, Portugal*, March 2007 (private communications).
[16] Dalichaouch Y., Maple M. B., Torikachvili M. S. and Giorgi A. L., *Phys. Rev. B*, **39** (1989) 2423.
[17] Torikachvili M. S., Rebelsky L., Motoya K., Shapiro S. M., Dalichaouch Y. and Maple M. B., *Phys. Rev. B*, **45** (1992) 2262.
[18] Bauer E. D., Zapf V. S., Ho P. C., Butch N. P., Freeman E. J., Sirvent C. and Maple M. B., *Phys. Rev. Lett.*, **94** (2005) 046401.
[19] Schoenes J., Withers R. L. and Hulliger F., *J. Magn. & Magn. Mater.*, **310** (2007) 1778.
[20] Colineau E., Wastin F., Sanchez J. P. and Rebizant J., *37èmes Journées des Actinides, Sesimbra, Portugal*, March 2007 (private communications).
[21] Lee W. H., Ku H. C. and Shelton R. N., *Phys. Rev. B*, **38** (1988) 11562.
[22] Eiling A. and Schilling J. S., *Phys. Rev. Lett.*, **46** (1981) 364.
[23] Zhang G.-M. and Yu Lu, *Phys. Rev. B*, **62** (2000) 76.
[24] Schoenes J., Vogt O., Lohle J., Hulliger F. and Mattenberger K., *Phys. Rev. B*, **53** (1996) 14987.
[25] Durakiewicz T., Batista C. D. and Thompson J. D. *et al.*, *Phys. Rev. Lett.*, **93** (2004) 267205.
[26] Zwicknagl G., Yaresko A. N. and Fulde P., *Phys. Rev. B*, **65** (2002) 081103(R); **68** (2003) 052508.
[27] Pourovskii L. V., Katsnelson M. I. and Lichtenstein A. I., *Phys. Rev. B*, **72** (2005) 115106.
[28] Sheng Q. G. and Bernard R. Cooper, *J. Magn. & Magn. Mater.*, **164** (1996) 335.
[29] Perkins N. B., Núñez-Regueiro M. D., Iglesias J. R. and Coqblin B., *Physica B*, **378-380** (2006) 698.
[30] Di Matteo S., Perkins N. B. and Natoli C. R., *Phys. Rev. B*, **65** (2002) 054413.
[31] Honner G. and Gulacsi M., *Z. Phys. B*, **104** (1997) 733.
[32] Burdin S., Georges A. and Grempel D. R., *Phys. Rev. Lett.*, **85** (2000) 1048.
[33] Lacroix C. and Cyrot M., *Phys. Rev. B*, **20** (1979) 1969.
[34] Barzykin V., *Phys. Rev. B*, **73** (2006) 094455.