Low energy scales of Kondo lattices: mean-field perspective

S. Burdin

Abstract A review of the low temperature properties of Kondo lattice systems is presented within the mean-field approximation, focusing on the different characteristic energy scales. The Kondo temperature, $T_K$, and the Fermi liquid coherence energy, $T_0$, are analyzed as functions of the electronic filling, the shape of the non-interacting density of states, and the concentration of magnetic moments. These two scales can vanish, corresponding to a breakdown of the Kondo effect when an external magnetic field is applied. The Kondo breakdown can also be reached by adding a superexchange term to the Kondo lattice model, which mimics the intersite magnetic correlations neglected at the mean-field level.

1 Introduction

Rare-earth and actinide based compounds exhibit extremely rich phase diagrams, with signatures of heavy fermion behavior, unconventional magnetism, or superconductivity [1,2]. At high temperature, the main physical properties of these systems are well reproduced by single impurity models, which describe the coupling between conduction electrons and one 4f or 5f ion. For dense systems, the single impurity models fail to describe the low temperature properties, which are characterized by the formation of a non local coherent state. In this regime, models with a periodic lattice of f ions are more appropriate.

Here, we consider more specifically dense compounds where the f orbital is occupied by one electron (Cerium) or one hole (Ytterbium). In the low temperature regime where the crystal field splitting lifts the degeneracy of the f orbital, these impurities are modeled by effective local spins $S_i = 1/2$. The system is thus de-
scribed by the Kondo lattice Hamiltonian,

\[ H = \sum_{k\sigma} (\xi_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + J_K \sum_i s_i S_i, \]  

(1)

where \( c_{k\sigma}^\dagger \) (\( c_{k\sigma} \)) describe creation (annihilation) operators of conduction electrons with spin \( \sigma = \uparrow, \downarrow \) and momentum \( k \). The Kondo interaction results from a local antiferromagnetic coupling \( J_K \) between the density of spin of conduction electrons at site \( i \), \( s_i \), and the Kondo impurities, \( S_i \). The chemical potential \( \mu \) fixes the electronic filling to \( n_c \) conduction electrons per site.

The Kondo model has been extensively studied throughout the last decades \cite{3}. At high temperature, the Kondo interaction can be considered a small perturbation: conduction electrons and Kondo ions are weakly coupled. The transport properties, which are determined by the conduction band, correspond to those of a normal metal. The magnetic susceptibility, governed by the Kondo free moments, has a Curie-Weiss form. The entropy is large, of the order of \( \ln 2 \) per site. A crossover occurs at the Kondo temperature, \( T_K \), below which the Kondo interaction cannot be treated by perturbative methods. Experimental signatures of this crossover include, for example, a logarithmic increase of the resistivity when the temperature decreases. Other signatures involve a saturation of the magnetic susceptibility, and a significant decrease of the entropy. At lower temperature, if we neglect magnetic or superconducting instabilities, the physical properties are characteristic of a universal heavy Fermi liquid: the specific heat vanishes linearly with the temperature.
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The local magnetic susceptibility, \( \chi(T) \), as well as the resistivity are constant at \( T = 0 \), with quadratic (i.e., \( T^2 \) like) variations at low \( T \). This low temperature regime is characterized by an energy scale, the coherence temperature, \( T_0 \), which can be equivalently determined from the specific heat Sommerfeld coefficient, \( T_0 \equiv 1/\gamma \), or the zero temperature magnetic susceptibility, \( T_0 \equiv 1/\chi(T = 0) \).

Figure 1 depicts the schematic phase diagram of the model, as a function of \( T_0/T_K \). The determination of \( T_0 \) and \( T_K \) from the entropy is illustrated by Fig. 2. The connection between \( T_0 \) and the thermal and electric transport properties have been analyzed by Zlatić et al. [5, 6].

Note that the authors of Ref. [7] discussed two energy scales: one of them corresponds to our definition of the Kondo lattice temperature, \( T_K \), from the temperature dependence of the entropy [see Fig. 2]. The second is the single impurity Kondo temperature, which, within the mean-field approach, is equal to the lattice Kondo temperature. The coherence temperature \( T_0 \) that we analyze here is not considered in Ref. [7].

![Fig. 2](Color online) Schematic plot of the electronic contribution to the entropy \( S_e \) as a function of the normalized temperature \( T/T_K \) for three cases: \( T_0 >> T_K \) (red dash dotted line), \( T_0 \approx T_K \) (blue solid line), and \( T_0 << T_K \) (green dashed line). The dotted lines indicate the linear Fermi liquid regime \( S_e(T) = T/T_0 \), with a rescaled slope \( T_K/T_0 \). For \( T > T_K \) the three curves are identical, reflecting the linear contribution from the conduction band \( S_e(T) = \ln 2 + T/D \). The black dot refers to a standard experimental determination of \( T_K \) from the electronic entropy: \( S_e(T_K) = p \ln 2 \). On this schematic plot, we used \( p = 1 \), which coincides with the vanishing of the effective hybridization, \( r = 0 \), defining \( T_K \) within the mean-field approach. Experimentally, where \( T_K \) is a crossover, one can choose, e.g., \( p = 1/2 \). Figure from Ref. [4].

The physical properties of systems with a small concentration of magnetic ions are universal and characterized by a single energy scale, \( T_0 = T_K \). The identity relating the coherence and the Kondo temperatures is consistent with the exact solution of the single impurity model. The situation is different for dense systems for which more than one energy scale can be identified. As an example, the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, \( J_{RKKY} \), can compete with \( T_K \), and a magnetic instability can be obtained for a lattice system [8]. For a long time, it has
been believed that $T_0$ and $T_K$ remain equal to each other in the heavy Fermi liquid phase of a Kondo lattice model. In this context and in response to discrepancies between theory and photoemission spectroscopy on rare-earth-based compounds with respect to the scaling with $T_K$, alternative scenarios involving phonons have been proposed [9]. On this basis, whether the Kondo model is capable of predicting photoemission spectroscopy on YbAl$_3$ has been a subject of controversy [10, 11, 12].

The specificity of Kondo lattice systems, with $T_0$ different from $T_K$, has been confirmed by experiments including magnetic susceptibility, specific heat, Hall coefficient measurements and X-ray absorption spectroscopy in Cerium, Ce$_{1-x}$La$_x$Ir$_2$Ge$_2$, CeIr$_2$(-Rh,Pt)$_x$Ge$_2$, CeIr$_2$Ge$_2$(-Si,Sn), CeNiSi$_2$ [13], and Ytterbium compounds, YbXCu$_4$(X=Ag, Cd, In, Mg, Ti, Zn) [15], Yb$_{1-x}$Lu$_x$Al$_3$ [16].

The first suggestion that $T_0$ could be much smaller than $T_K$ was discussed by Nozières in the framework of the exhaustion problem [17, 18]. This prediction stimulated complementary theoretical works, including approximated methods based on a strong coupling approach [19] or mean-field calculations [20, 21, 22, 23], and numerical simulations [24, 25, 26, 27, 28] using dynamical mean-field theory (DMFT) [29, 30]. Even if the initial prediction of Nozières turned to be quantitatively wrong [21, 31], all the theoretical calculations converge to the same qualitative conclusion: in a Kondo lattice, $T_0$ can be different from $T_K$, and the ratio between these two energy scales can be tuned, for example, by varying the electronic filling of the system. Finally, these theoretical works shed some new light on the formerly controversial photoemission analysis.

The aim of this work is, first, to review how the two energy scales, $T_0$ and $T_K$ depend on physical parameters: electronic filling, shape of the density of states, concentration of magnetic ions. This is done within the simplest relevant approximation for the Kondo interaction: a mean-field decoupling. Then, we review how, within the mean-field approach, the Kondo phase can be destabilized by a magnetic field or by magnetic inter-ion interactions.

## 2 Mean-field formalism

The mean-field approximation for the Kondo lattice was first introduced by Lacroix and Cyrot [32]. It was reformulated by Coleman [33] and by Read, Newns and Doniach [34], as a large-$N$ approximation for the $N$-fold degenerate Coqblin-Schrieffer model [35]. It was shown that magnetic instabilities require expansions up to the order $1/N$, i.e. fluctuations around the mean-field. Nevertheless, the heavy Fermi liquid phase is well described in the limit $N = \infty$. The analysis of $T_0$ and $T_K$ can thus already be performed at the mean-field level. Here, we describe the main lines of the mean-field approximation for the Kondo lattice Hamiltonian [11].

The Kondo impurities are represented by local auxiliary fermions as follows: $S_i^z = \frac{1}{2}(f_i^\dagger \sigma_i f_i^\dagger \sigma_i)$, $S_i^+ = f_i^\dagger \sigma_i f_i^\dagger$, and $S_i^- = f_i^\dagger \sigma_i f_i^\dagger$. The Kondo interaction is thus rewritten as $J_K S_i^z S_j^z \mapsto \frac{J_K}{2} \sum_{\sigma\sigma'} \epsilon_{\sigma\sigma'} c_i^{\dagger \sigma\sigma'} c_j^{\dagger \sigma\sigma'} f_{\sigma\sigma'}^\dagger f_{\sigma\sigma'}$, which describes the spin-flip processes between conduction electrons and local moments. This mapping is exact as far
as the Hilbert space is restricted to the sector of one auxiliary fermion per site, $f_{i\uparrow}^\dagger f_{i\downarrow} + f_{i\downarrow}^\dagger f_{i\uparrow} = 1$. The mean-field solution is obtained within the two following approximations: (i) The local occupation of the auxiliary fermions is equal to one on average. This corresponds to describing the Kondo spins by an effective local $f-$level that is half full. This effective filling is controlled by introducing a second chemical potential, $\lambda$. (ii) The Kondo interaction is replaced by an effective one-body term, obtained from a mean-field decoupling of the $\uparrow$ and $\downarrow$ components. The mean-field approximation for the Kondo lattice Hamiltonian (1) yields

$$H = \sum_{k \sigma} (\varepsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + r \sum_{i \sigma} (c_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger c_{i\sigma}) - \lambda \sum_{i \sigma} f_{i\sigma}^\dagger f_{i\sigma},$$

where the effective hybridization is determined by the self-consistent relation

$$r = \frac{J_K}{2 \mathcal{N}} \sum_{i \sigma} \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle .$$

Here $\mathcal{N}$ is the number of lattice sites. The chemical potentials for $c-$electrons, $\mu$, and $f-$fermions, $\lambda$, are determined by the constraints $n_c = \sum_{\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$ and $1 = \frac{1}{\mathcal{N}} \sum_{i \sigma} \langle f_{i\sigma}^\dagger f_{i\sigma} \rangle$. The mean-field Hamiltonian (2) describes an effective system of conduction electrons hybridized with local $f$ levels. The correlation effects are renormalized into the self-consistent hybridization $r$. This approximation captures two important features of the Kondo lattice: at high temperature, we find $r = 0$, and the system is described as a paramagnetic light metal ($c$ electrons) decoupled from local free moments ($f-$fermions). This picture is oversimplified but it succeeds in describing qualitatively the experimental situation, in which, above the Kondo temperature, conduction electrons are weakly coupled to the local moments. Within the mean-field approach, the Kondo temperature $T_K$ is thus defined as the temperature for which a hybridization $r \neq 0$ occurs. At very low temperature, the physical properties correspond to a Fermi liquid and the excitations of the system correspond to the creation of non-interacting, heavy, fermionic quasiparticles. The latter are a linear combination of the light $c-$electrons and the heavy $f-$fermions. The Fermi-liquid regime is characterized by an energy scale, $T_0$, which can be defined identically from different physical properties of the ground state: the quasiparticle density of states, $\rho = 1/T_0$, the Sommerfeld coefficient, $\Gamma = \lim_{T \to 0} C_V(T)/T = 1/T_0$, or the local impurity spin susceptibility, $\chi_{\text{loc}}(T = 0) = 1/T_0$. We have obtained explicit expressions for $T_K$ and $T_0$ in the limit of small $J_K$ [4,21]:

$$T_K = F_K [n_c, \rho_0] \varepsilon^{-1/2} \rho_0^{1/2} \rho_0^{1/2},$$

and

$$T_0 = F_0 [n_c, \rho_0] \varepsilon^{-1/2} \rho_0^{1/2} \rho_0^{1/2},$$

which depend on the Kondo coupling $J_K$ only within the non-analytic exponential factor $e^{-1/2 \rho_0^{1/2} \rho_0^{1/2}}$. The prefactors $F_K$ and $F_0$ are functions of the electronic filling, $n_c$, and the non-interacting density of states (DOS), $\rho_0(\omega) \equiv \sum_k \delta(\omega - \varepsilon_k)$. Here,
$\mu_0$ is the non-interacting chemical potential, corresponding to an electronic filling $n_c = \int_{-D}^{D} \rho_0(\omega) d\omega$. For the sake of clarity, we do not write the explicit expressions of $F_K$ and $F_0$ here, as they are given in Refs. [4, 21]. The exponential factor in both $T_0$ and $T_K$, results in a very sensitive dependence of these energy scales with respect to small changes in the system (e.g., pressure or doping). Since the ratio $T_0/T_K$ does not depend on $J_K$, it is more likely to be analyzed experimentally as a universal function. The mean-field solution yields [4]

$$\frac{T_0}{T_K} = \left( \frac{D + \mu_0}{D - \mu_0} \right)^{1/2} \frac{F_{\text{shape}}}{\alpha \rho_0(\mu_L) \Delta \mu}.$$  

(6)

Here, $D$ is the half-bandwidth of the non-interacting DOS. The interacting chemical potential, $\mu_L$, corresponds to a filling $n_c + 1$, and the energy $\Delta \mu = \mu_L - \mu_0$ is related to the enlargement of the Fermi surface. $\alpha = 1.13$ is a number. $F_{\text{shape}}$ is an explicit function depending on the shape of $\rho_0$ as follows:

$$F_{\text{shape}} \equiv \exp \left[ \left( \int_{-(D+\mu_0)}^{D-\mu_0} - \frac{1}{2} \int_{-(D+\mu_0)}^{D-\mu_0} \frac{\rho_0(\mu_0 + \omega) - \rho_0(\mu_0)}{\omega |\rho_0(\mu_0)|} d\omega \right) \right].$$  

(7)

3 Tuning $T_0$ and $T_K$

### 3.1 Variation of electronic filling

The effect of electronic filling on the temperature scales of the Kondo lattice has been discussed by Nozières who suggested a possible exhaustion problem [17, 18]. Considering $N_S$ Kondo spins coupled to $N_c \leq N_S$ conduction electrons, Nozières started with the following remark: the magnetic entropy which can be released at the temperature $T \approx T_K$ by the formation of incoherent Kondo singlets (i.e., by the single impurity Kondo effect) is $\Delta S = N_c \ln 2$. However, the formation of a coherent Fermi liquid ground state is characterized by a vanishing entropy, $S(T) \approx T / T_0$. The freezing of the remaining entropy, $S(T_K) \approx (N_S - N_c) \ln 2$, thus requires a collective mechanism and can lead to $T_0 \ll T_K$ when $N_c \ll N_S$.

The exhaustion problem remained for several years an open issue, and its first solution was obtained within a mean-field approach [21, 31], which provides a quantitative description of the electronic filling effect. First, from the analytical expressions [4, 5], $T_K$ and $T_0$ have the same $J_K$ dependence, $e^{-1/J_K \rho_0(\mu)}$ factor, and the ratio $T_K/T_0$ does not depend on the Kondo coupling. This is in contradiction with the result of Nozières, who predicted a ratio $T_0/T_K \approx T_K/D \approx e^{-1/J_K \rho_0(\mu)}$ [17, 18]. The mean-field result, $T_0/T_K$ independent of $J_K$, was later confirmed by DMFT calculations [50], and finally accepted by Nozières [31]. Nevertheless, $T_0$ and $T_K$ define two energy scales with different dependencies with respect to the electronic filling, as depicted by Fig. 3 where $T_0 \ll T_K$ in the limit $n_c \to 0$. The mean-field result obtained here is remarkably similar to the one obtained within DMFT combined
with Quantum Monte Carlo simulation [see Fig. 1 in Ref. [26]]. The filling effects can also be analyzed from the expression (6). Neglecting the band shape effects [discussed in section 3.2], we find $T_0 / T_K \approx \left( \frac{n_c + \mu_0}{n_c - \mu_0} \right)^{1/2}$, which vanishes when $\mu_0$ approaches the band edge $-D$, i.e., when $n_c \to 0$.

![Fig. 3](image)

Fig. 3 (Color online) $T_K / D$ (black solid line) and $T_0 / D$ (red dashed line) versus electronic filling, for the Kondo lattice. Numerical result obtained within the mean-field approximation, for a semi-elliptic non-interacting DOS and $J_K / D = 0.75$ [21].

![Fig. 4](image)

Fig. 4 (Color online) Electronic occupation $n_c(\epsilon_k)$ for $T / T_K = 1.0$ (black dashed line), $T / T_K = 0.5$ (black dotted line), and $T / T_K = 0.005$ (red solid line). Numerical result obtained within the mean-field approximation for a semi-elliptic non-interacting DOS, $n_c = 0.15$, and $J_K / D = 0.75$. $\mu_0$ and $\mu_L$ indicate the chemical potential corresponding to a small and a large Fermi surface, respectively. Inset: focus around $\mu_L$. Figure from Ref. [21].
The analysis of the electronic occupation, \( n_c(\epsilon_k) \equiv \langle c_k^\dagger c_k \rangle \), provides an important insight for understanding the physical mechanism leading to two different energy scales. For \( T \approx T_K \), the mean-field result, depicted by Fig. 4, looks like a Fermi distribution with a thermal window around the non-interacting chemical potential, \( \mu_0 \), corresponding to \( n_c \) electrons (small Fermi surface). For \( T \ll T_K \), in the Fermi liquid regime, the distribution is spread and forms a step around \( \mu_L \) (large Fermi surface). Figure 4 only describes the occupation of the \( c^- \)electrons, which is fixed to \( n_c \). At \( T = 0 \), there are states of given momentum \( k \) which are not fully occupied by \( c^- \)electrons. The Fermi liquid picture is recovered because the quasiparticles are not pure \( c^- \)states, but a linear combination of \( c^- \)and \( f^- \)states. The quasiparticle occupation is complete, i.e., equal to one, for states with an energy \( \epsilon_k < \mu_L \), and it vanishes for states with higher energy. This behavior is consistent with the Luttinger theorem which predicts that, at \( T = 0 \), the Fermi surface contains both \( c^- \)electrons and \( f^- \)fermions. It is not surprising that the Kondo lattice satisfies the Luttinger theorem within the mean-field approximation. The reason is that the effective mean-field model (2) does not contain an explicit many body interaction term. We expect this result to survive beyond the mean-field in the Fermi liquid phase. The enlargement of the Fermi surface might be a key point in the origin of the difference between \( T_0 \) and \( T_K \): the Kondo temperature is associated with the incoherent scattering of the conduction electrons which are in the Fermi window of width \( T_K \) around \( \mu_0 \) [see Fig. 5]. The coherence temperature, \( T_0 \), results from the Kondo effect, but, unlike \( T_K \), characterizes a Fermi liquid with a large Fermi surface.

3.2 Shape of the non-interacting density of states

![Fig. 5](Color online) Schematic plot of the non-interacting DOS. (a) For a regular DOS and far from the electronic half-filling \( T_0 \ll T_K \). Close to the half-filling, the shape of the DOS around \( \mu \) is crucial for determining \( T_0/T_K \); (b) \( \rho_0(\omega) \) is nearly constant around \( \omega = \mu \) and \( T_0 \sim T_K \). (c) \( \mu \) is close to a minimum of \( \rho_0 \) and \( T_0 \gg T_K \). Here, \( \mu_0 \approx \mu \) indicates the chemical potential corresponding to \( n_c \) non-interacting \( c^- \)-electrons (small Fermi surface), and \( \mu_L \) is the chemical potential corresponding to \( n_c + 1 \) non-interacting \( c^- \)-electrons (large Fermi surface). Figure from Ref. [4].

Here we consider the effects due to the shape variation of the non-interacting DOS, \( \rho_0(\omega) \) [4]. In order to separate this effect from the electronic filling effects, we assume that \( n_c \) is close to 1, but not exactly half full, so that the system is metallic.
Eqs (6) and (7) are thus simplified to

$$\frac{T_0}{T_K} \approx F_{shape} \approx \exp \left[ \int_{-(D+\mu_0)}^{D-\mu_0} \frac{\rho_0(\mu + \omega) - \rho_0(\mu_0)}{2|\omega|\rho_0(\mu_0)} d\omega \right].$$

A constant $\rho_0$ gives $T_0 \sim T_K$, which explains the $T/T_K$ scaling observed in some compounds. If $\mu_0$ is close to a local maximum of $\rho_0(\omega)$, the integrand in Eq. (5) is negative in the main part of the integration range, and $T_0 \ll T_K$. In the opposite situation, when $\mu_0$ is close to a local minimum [see Fig. 5(c)], we find $T_0 \gg T_K$, which can be understood by the following argument. The incoherent Kondo screening which begins at $T \approx T_K$ involves a small number of conduction electrons which are in the Fermi thermal window of width $T_K$, around $\mu_0$. At lower temperature, $T < T_K$, the Fermi surface is enlarged, due to the contribution of the $f-$electrons [see Fig. 4]. This results from a non-zero hybridization, $r \neq 0$, in the Kondo phase. The formation of a coherent Fermi liquid ground state thus involves all the states of the large Fermi surface. In the situation described by Fig. 5(c), where $\mu_0$ is close to a local minimum of the DOS, the further we are from $\mu_0$, the more states are available for the formation of the coherent Fermi liquid. In this case, there is a kind of self-amplification resulting in $T_0 \gg T_K$. With this picture, the magnetic screening of the Kondo impurities involves not only the $c-$conduction electrons but also, in a dynamical way, ”growing” quasiparticles which contain some $f-$components.

### 3.3 Substitution of magnetic ions

Here, our analysis focuses on the concentration of Kondo impurities, $x$. In rare-earth based Kondo systems, the latter can be varied, e.g., by Ce-La or Yb-Lu substitution. For this purpose, we have introduced a Kondo alloy model, which is a generalization of the Hamiltonian (1) where each site of the lattice can randomly either contain a Kondo impurity, with a probability $x$, or not [37, 38]. The Kondo interaction is then treated within the mean-field approximation, and the different configurations of impurity distributions are averaged using a generalization of the coherent potential approximation [39]. Results described here remain valid beyond the coherent potential approximation [38].

Figure 6 illustrates the evolution of $T_0/T_K$ as a function of the impurity concentration, $x$, for different values of electronic filling, $n_c$. The dilute limit of the model, $x \ll 1$, reproduces the universal behavior of the single impurity model, with $T_0 = T_K$. The crossover to the dense Kondo-lattice regime, with $T_0 \neq T_K$ occurs for $x \approx n_c$.

The data presented in Fig. 7 are identical to those in Fig. 6 with a rescaled axis, $x \rightarrow n_c/x$. From this rescaling, an exhaustion regime is identified, for $n_c < x$, where $T_0/T_K$ is a universal function of $n_c/x$. Note that this numerical result has been obtained here for a non-interacting semi-elliptic DOS which mimics, at low $n_c$, the band edge of a three-dimensional system. We expect the universal exhaustion regime to depend on the dimension via the exponent characterizing the vanishing of the
Fig. 6 (Color online) $T_0/T_K$ as a function of the impurity concentration. From top to bottom, $n_c = 1; 0.8; 0.6; 0.4; 0.2$. The solid lines are included as a guide for the eye. The curves have been computed for a semi-elliptic non-interacting DOS and $J_K/D = 0.75$. From Ref. [37].

Fig. 7 (Color online) Same data as Figure 6 with a rescaled horizontal axis which represents $n_c/x$ here. Each curve corresponds to a given electronic filling, $n_c$, as indicated by the legend. The parameter $n_c/x$ has been tuned by varying $x$, and the curves are cut-off by the finite physical minimal value $n_c/x = n_c$.

DOS at the band edge. Apart from the possibility of magnetic ordering, which is not considered here, the exhaustion regime might be difficult to access experimentally for the following reason: the maximal concentration of Kondo impurities is $x = 1$. The only way to reach $n_c \ll x$ thus involves decreasing the electronic filling. Yet, in rare-earth compounds, conduction electrons usually involve more than one band. With a single band description, the exhaustion regime would be observable.
by increasing the concentration of magnetic ions, \( x \). A multi-band system, however, allows for another scenario to materialize as \( x \) increases: instead of exhausting one conduction band, the system might energetically prefer transferring electrons from other bands, preventing the filling from accessing the exhaustion regime, \( n_c \ll x \). In this case, a single band Kondo lattice model would not be appropriate anymore. Nevertheless, we expect that other Kondo systems can be realized experimentally, in which the universal regime \( n_c \ll x \) could be observed. For most of dense compounds, \( x \approx 1 \), the electronic filling is \( n_c \approx x \). This is a non-universal regime, where all the lattice structure becomes relevant.

4 Destabilizing the Kondo phase

Microscopically, the Kondo effect is characterized by the formation of local singlets. The Kondo phase can be destabilized by an external magnetic field, or by the fluctuations of the internal Weiss field induced by RKKY interactions. Here, these two situations are analyzed from the mean-field approximation: the breakdown of the Kondo effect is identified to a continuous vanishing of the \( f-c \) effective hybridization, \( r \), which occurs at \( T = 0 \).

4.1 Effect of a magnetic field

We consider an external magnetic field, \( h \), applied to the Kondo spins in the longitudinal direction \( z \). This mimics a situation where the Landé factor of the magnetic ions is much larger than the one of \( c \)-electrons. A supplementary contribution is thus added to the Hamiltonian \( H \rightarrow H - h \sum \vec{S} \). The mean-field approximation described in Sec. 2 is generalized \[4\], resulting in an effective Hamiltonian formally similar to Eq. (2), with spin-dependent \( f-c \) fermion potentials, \( \lambda \rightarrow \lambda + \sigma h \). The effective hybridization, \( r \), remains spin-independent.

For a sufficiently small magnetic field, a low temperature solution with \( r \neq 0 \) is obtained. This situation, depicted by Fig. 8, characterizes a phase where the Kondo effect coexists with a partial polarization of both Kondo spins and \( c \)-electrons. A finite critical field \( h_c(T) \) is obtained, above which \( c \)-electrons decouple from fully polarized local moments. At \( T = 0 \), in the weak coupling limit, \( J_K \ll D \), the mean-field approximation yields the universal relation \( h_c^0 \equiv h_c(T = 0) = T_K / \alpha \). Since \( \alpha = 1.13 \), we have \( h_c^0 \approx T_K \). This result is not surprising if we consider the Kondo temperature as the energy scale characterizing the local singlet formation: the Kondo effect is destroyed when the Zeeman energy becomes larger than \( T_K \). At finite temperature, assuming a constant \( c \)-DOS yields the critical line \( [h_c(T)/h_c^0]^2 + [T/T_K]^2 = 1 \).

The \( T = 0 \) magnetization \( m_z(h) \equiv \frac{1}{N} \sum_i \left( \langle f_i^\dagger \sigma_i \rangle - \langle f_i^\dagger \sigma_i \rangle \right) \) obtained from the mean-field solution is plotted in Fig. 8 as a function of the reduced magnetic field.
Fig. 8 (Color online) Left: Schematic phase diagram of the Kondo lattice as a function of a magnetic field \( h \). The red solid line indicates \( h_c(T) \) which separates the Kondo phase (\( r \neq 0 \)) from the decoupled phase (\( r = 0 \)). Right: Schematic plot of the magnetization \( m_z(h/T_K) \). For \( T_0 \gg T_K \) (red dash dotted line), \( T_0 \approx T_K \) (blue solid line), and \( T_0 \ll T_K \) (green dashed line). The dotted line indicates the initial slope in the linear response regime, where \( m_z(h) = h/T_0 \). The black dot refers to the complete polarization of the local Kondo spins, \( m_z = 1/2 \), which occurs at the critical field \( h_0^c = T_K \). Figures from ref. [4].

\( h/T_K \). The low field regime is given by the linear response, \( m_z(h) = h\chi_{\text{loc}}(T = 0) \), which, by definition, yields \( m_z(h) = h/T_0 \). Since the critical field characterizing a full polarization of the local moments is of the order of the Kondo temperature, \( h_0^c \approx T_K \), we distinguish three typical cases. \( T_0 \approx T_K \) is a standard situation, where \( m_z \) increases linearly with \( h \), until saturation. For \( T_0 \gg T_K \), the linear regime allows only a small magnetization when \( h < h_0^c \). Thus, at about \( h \approx h_0^c \), such systems exhibit a meta-magnetic transition from an unpolarized Fermi-liquid to the polarized spin lattice. In the opposite case, \( T_0 \ll T_K \), the linear regime saturates around \( h \approx T_0 \ll h_0^c \). The intermediate regime \( T_0 < h < T_K \) is expected to be non-universal. Eventually, a magnetization plateau can occur, at \( m_z \approx (1 - n_c)/2 \), similar to the one obtained for the entropy [see Fig. 2].

It is well known that the transition \( r = 0 \), defining \( T_K \) within the mean-field approximation, becomes a crossover when more accurate methods are used. There are several examples of systems where a finite temperature crossover ends up to a quantum critical point, i.e. a transition at zero temperature. Whether the transition at the critical field \( h_0^c \) would survive beyond the mean-field is an open issue.

### 4.2 Extra-RKKY interaction

The possibility of destabilizing a Kondo phase in favor of a magnetically ordered ground state was first discussed by Doniach [8], by comparison of the Kondo temperature, \( T_K \sim De^{-1/J_{\text{RKKY}}(\mu_0)} \), with the RKKY energy, \( J_{\text{RKKY}} \sim \rho_0(\mu_0)T_K^2 \).

The mean-field approximation for the Kondo lattice Hamiltonian [1] can hardly provide a correct description of a transition from a Kondo ground state to a phase with magnetic ordering. This results from the two following reasons:
(i) **Difficulty in driving the system to a second order magnetic transition:** this would require a mechanism leading to a continuous vanishing of the zero temperature effective hybridization, \( r(T=0) \). However, from the Kondo lattice Hamiltonian (1), the only possibility of vanishing \( r(T=0) \) involves the non-interacting DOS, \( \rho_0(\mu) \) vanishing. This does not correspond to the physical situation of a magnetic transition induced by the RKKY interaction.

(ii) **Difficulty in describing the criticality of transport properties:** Within the mean-field approach, the system is either in a strong coupling regime, with \( r \neq 0 \) and a heavy Fermi liquid ground state, or in a fully decoupled regime, with \( r = 0 \). Since the transport properties are governed by the conduction electrons, no universal non-Fermi-liquid behavior can be predicted at the mean-field level.

These two difficulties can be understood from the large-\( N \) formulation of the mean-field approximation: Coleman \[33\], and Read, Newns and Doniach \[34\] have shown that magnetic ordering involves at least processes of order \( 1/N \), i.e., fluctuations around the mean-field. Describing the criticality obtained from calculations taking into account the fluctuations and the emerging compact gauge field theory is beyond the scope of this presentation. We simply refer to the works of Senthil, Sachdev, and Vojta \[40, 41\], who analysed the possibility of a quantum phase transition between a Fermi liquid phase with a large Fermi surface, and a (partially) fractionalized Fermi liquid phase. A Kondo breakdown quantum critical point has also been identified by Pepin \[42, 43\], who obtained, for example, a specific exponent diverging logarithmically in temperature, as observed in a number of heavy fermion metals.

Whilst **Difficulty (ii)** can not be easily cured without the fluctuations, we describe here how **Difficulty (i)** can be fixed at the mean-field level. The Kondo lattice Hamiltonian (1) is generalized to a so-called Kondo-Heisenberg lattice, by adding a supplementary superexchange term, as follows: \( H \rightarrow H + \sum_{ij} J_{ij} S_i S_j \). This general model has been introduced first by Sengupta and Georges \[44\], and studied later within various methods. In terms of auxiliary fermions, introduced in Section 2, the superexchange term is rewritten as \( J_{ij} S_i S_j = \frac{J_{ij}}{2} \sum_{\sigma\sigma'} f_{i\sigma}^\dagger f_{j\sigma'} f_{j\sigma'}^\dagger f_{i\sigma} \), which describes the spin-flip processes between two Kondo impurities, on sites \( i \) and \( j \). Up to now, this description is very general and holds for any magnetic coupling \( J_{ij} \), which can be periodic (ferro or antiferromagnetic), or randomly distributed (disorder case). We will now describe two complementary mean-field approaches for the superexchange.

The first one was introduced by Coqblin et al. \[45\] in the case of an antiferromagnetic nearest neighbor exchange \( J_{ij} = J_{AF} < 0 \). In the paramagnetic Kondo phase, the intersite exchange is approximated within a Resonant Valence Bound decoupling: \( J_{ij} S_i S_j \rightarrow \Gamma_{ij} \sum_{\sigma} f_{i\sigma}^\dagger f_{j\sigma} f_{j\sigma}^\dagger f_{i\sigma} \), with \( \Gamma_{ij} = \frac{J_{AF}^2}{4} \sum_{\sigma} \langle f_{i\sigma} f_{j\sigma}^\dagger \rangle \). The magnetic, Heisenberg-like, interaction generates an effective self-consistent dispersion for the \( f \)-fermions. Using this method, Coqblin et al. show that the Kondo effect disappears abruptly for low band filling and/or strong intersite coupling \[22, 23\].

We have developed another mean-field method \[46\], based on the DMFT, which we first applied to a disordered system where \( J_{ij} \) are given by a Gaussian distribution with an average \( \langle J_{ij} \rangle = 0 \), and a variance \( \langle J_{ij}^2 \rangle \equiv J_d^2 \). In this case, the superexchange
term generates a local energy-dependent self-energy for the $f-$fermions, which is determined by self-consistent relations similar to the ones obtained by Sachdev and Ye for a pure spin disordered system \[47\]. We have also applied this method to a model with constant nearest-neighbor antiferromagnetic exchange \[48\], where the self-consistent equation for the $f-$fermions self-energy depends on the lattice structure. In both cases, disordered or periodic model, we obtained a quantum critical point corresponding to the breakdown of Kondo effect, characterized by a vanishing of the effective hybridization, $r(T=0) = 0$. Figure 9 depicts the phase diagram that we obtained for the disordered Kondo-Heisenberg model \[46\]. We also have obtained a similar phase diagram for the periodic, i.e., non-disordered, case \[48\]. Here, one relevant point is that the quantum critical point emerging from our mean-field approach does not necessarily correspond to the onset of magnetic ordering. This suggests an interpretation in terms of topological transition, without breaking of symmetry, but with a violation of Luttinger theorem, as discussed in Refs. \[40\] \[41\]. Furthermore, $1/N$ corrections can reveal a magnetic instability at a value of the coupling, $J_d$ which is smaller than $J_d^c = T_K$. In this latter case, a symmetry breaking is expected. Whereas criticality in heavy fermions is governed by a Kondo breakdown critical point or by a magnetic transition, what is the nature of the non-Kondo phase, and whereas the Kondo breakdown coincides or not with magnetic ordering are still open questions. The answers probably depend on the system.
The quantum critical transition obtained here results from the competition between the Kondo effect and the fluctuations of the \( f \)-fermions. These fluctuations are precisely the microscopical mechanism which is required to fix Difficulty (i), i.e., the difficulty in driving the system to a second order magnetic transition within the mean-field approximation. In the approach introduced by Coqblin et al., the \( f \)-fermion fluctuations are generated by an effective dispersion, which is connected to the Resonant Valence Bound decoupling. In our approach, the fluctuations are included within a self-consistent local self-energy. In both approaches, fluctuations are characterized by an energy, \( J_{RKKY} = J_{AF} \) or \( J_d \), and the Kondo effect disappears above the critical value \( J_{RKKY} \approx T_K \).

5 Conclusions

Important properties of Kondo systems can be obtained from the mean-field approximation. Some of them have not been presented here, like, for example, the effect of a pseudo-gap [49, 50]. Also, for the sake of clarity, the description was restricted to the ‘standard’ Kondo model. Of course, the mean-field approximation has been generalized and applied to more realistic models, with, for example, a momentum-dependent hybridization between conduction electrons and \( f \) ions [51].

Here we have focused on the low energy scales: the Kondo temperature, \( T_K \), characterizing the temperature crossover below which conduction electrons and local moments are strongly coupled; the coherence energy, \( T_0 \), characterizing the Fermi liquid ground state; and \( J_{RKKY} \), the intersite magnetic correlation energy. At the mean-field level, \( J_{RKKY} \) is negligible or neglected, and any study of magnetic criticality requires the inclusion of fluctuations around the mean-field. Nevertheless, the Kondo effect can break down at the mean-field level if the RKKY interaction is added ‘by hand’, generalizing the Kondo lattice to a Kondo-Heisenberg model.

For the ‘pure’ Kondo lattice, the mean-field approximation provides explicit expressions for \( T_0 \) and \( T_K \). Both quantities depend on the Kondo coupling with the same exponential factor, \( e^{-1/J_K \rho_0/\mu_0} \). This explains the strong sensitivity of these energy scales with respect to changes in the system (e.g. doping, or pressure). The ratio \( T_0/T_K \), which does not depend on \( J_K \), appears to be a promising quantity for analyzing universal behaviors of heavy fermion compounds. Whilst it is equal to one in dilute systems, \( T_0/T_K \) depends in fact on the electronic filling, \( n_e \), the band shape, and the impurity concentration, \( x \). A universal regime with \( T_0 \ll T_K \) is expected in the exhaustion limit, \( n_e \ll x \), which might be difficult to access experimentally. More typical situations correspond either to the universal dilute regime, \( n_e \gg x \), or to the non-universal dense regime \( x \sim n_e \). In the latter case, the shape of the non-interacting DOS becomes relevant, and can lead to \( T_0 \ll T_K \) if the chemical potential, \( \mu_0 \), is close to a local maximum of the DOS, or to \( T_0 \gg T_K \) if \( \mu_0 \) is close to a local minimum.

The experimental determination of \( T_0 \) and \( T_K \) is straightforward for systems which are ‘deeply’ in a Fermi liquid phase: for example, one can determine \( T_0 \) from
the specific heat Sommerfeld coefficient, and $T_K$ from the temperature dependence of the magnetic part of the entropy. The determination of $T_K$ might become more tricky in the vicinity of a magnetic transition, where the freezing of the entropy is no longer due to Kondo singlet formation, but to magnetic intersite correlations instead. In this case, one should find another physical observable which would enable an unambiguous determination of $T_K$. In this case, a systematic experimental analysis of the ratio $T_0/T_K$ might reveal interesting universal behavior.

Some of the results obtained at the mean-field level have been confirmed by exact numerical methods. For example, DMFT calculations have shown that $T_0/T_K$ does not depend on the Kondo coupling. One limitation of the mean-field is also well known: its weakness in describing criticality, where fluctuations become important. Nevertheless, some predictions of the mean-field have not been checked yet with more accurate methods (DMFT or $1/N$ corrections). This is, for example, the case of the band shape effect.

Acknowledgements I thank the organizers of the NATO Advanced Research Workshop on Properties and Applications of Thermoelectric Materials. I acknowledge my collaborators on the works presented here: P. Fulde, A. Georges, M. Grilli, and V. Zlatic. I am also grateful to A. Rosch, M. Vojta, A. Klopper, H. Weber and N.B. Perkins for useful discussions regarding this manuscript, and to P. Nozières, B. Coqblin, and C. Lacroix for fruitful advise.

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