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Coherence scale of the Kondo lattice

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It is shown that the large- N approach yields two energy scales for the Kondo lattice model. The single-impurity Kondo temperature, T_K , signals the onset of local singlet formation, while Fermi liquid coherence sets in only below a lower scale, T^* . At low conduction electron density n_c (“exhaustion” limit), the ratio T^*/T_K is much smaller than unity, and is shown to depend only on n_c and not on the Kondo coupling. The physical meaning of these two scales is demonstrated by computing several quantities as a function of n_c and temperature.

How coherent quasi-particles form in the Kondo lattice has been a long-standing issue. For a single impurity, there is a single scale T_K below which the local moment is screened and a local Fermi liquid picture applies. T_K can be defined e.g. as the scale at which the effective Kondo coupling becomes large. All physical quantities (e.g. specific heat, susceptibility) obey scaling properties as a function of T/T_K in the limit where both T and T_K are smaller than the high-energy cutoff (bandwidth, denoted $2D$ in the following). In contrast, for a Kondo lattice, one may suspect that the physics is no longer governed by a single scale. Indeed, while magnetic moments can still be screened *locally* for temperatures lower than the single-impurity Kondo scale T_K , the formation of a Fermi-liquid regime (with coherent quasi-particles and a “large” Fermi surface encompassing both conduction electrons and the localized spins) is a global phenomenon requiring coherence over the whole lattice. If at all possible, it could be associated with a much lower coherence temperature T^* . The situation is reminiscent of strong-coupling superconductivity in which local pair formation may occur at a much higher scale than T_c , the scale at which long-range order sets in.

As was originally pointed out by Nozières [1], this issue becomes especially relevant when few conduction electrons are available to screen the local spins, i.e. in the limit of low concentration ($n_c \ll 1$). In this “exhaustion” regime, two possibilities arise: i) either magnetic ordering wins over Kondo screening or ii) a paramagnetic Fermi liquid state still manages to form, but with a much suppressed coherence scale $T^* \ll T_K$. Nozières has suggested in Ref. [2] that $T^* \sim n_c D$ for strong coupling $J_K/D \gg 1$ (where $T_K \sim J_K$), while $T^* \sim T_K^2/D$ for weak coupling $J_K \ll D$. Recently, several studies [3,4,5,6,7,8] have addressed this issue using dynamical mean-field theory (DMFT) [9]. The conclusion was that two scales are indeed present in the Kondo lattice, with the coherence scale with $T^* \ll T_K$ in the “exhaustion” regime. Because the DMFT equations require a numerical treatment, no detailed analytical insight into these

two scales was obtained, even though the validity of the estimate [2] $T^* \propto T_K^2/D$ was questioned [8].

In this letter, we solve this problem using the slave-boson approach, in the form of a controlled large- N solution of the $SU(N)$ Kondo lattice model. This approach has been extensively used in the past twenty years [10,11,12,13,14,15]. Surprisingly, the issue of the coherence scale and the temperature dependence of physical quantities has not been discussed in detail in the exhaustion limit $n_c \ll 1$ (See, however, Ref. [16]). We find that the large- N approach provides a remarkably simple and physically transparent realization of the two-scale scenario described above. Furthermore, because of its simplicity, it allows for an analytical calculation of the coherence scale, which is found to disagree (for weak coupling) with Nozières’ estimate in Ref. [2] (while it agrees with it at strong coupling). We also calculate the temperature dependence of several physical quantities and find remarkable agreement with the more sophisticated (and demanding) DMFT approach.

We consider the Kondo lattice model (KLM):

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \frac{J_K}{N} \sum_{i\sigma\sigma'} S_i^{\sigma\sigma'} c_{i\sigma'}^+ c_{i\sigma} \quad (1)$$

In this expression, the spin symmetry has been extended to $SU(N)$ ($\sigma = 1, \dots, N$) and the local spins will be considered in the fermionic representation: $S_i^{\sigma\sigma'} = f_{i\sigma}^+ f_{i\sigma'} - \delta_{\sigma\sigma'}/2$, with the constraint $\sum_{\sigma} f_{i\sigma}^+ f_{i\sigma} = N/2$. Standard methods [10] are used to solve this model at large N : a boson field $B_i(\tau)$ (conjugate to the amplitude $\sum_{\sigma} f_{i\sigma}^+ c_{i\sigma}$) is introduced in order to decouple the Kondo interaction, and the constraint is implemented through a Lagrange multiplier field $\lambda_i(\tau)$. For $N = \infty$, a saddle point is found at which the Bose field condenses $\langle B_i(\tau) \rangle = r$ and the Lagrange multiplier takes a uniform, static value $\langle i\lambda_i(\tau) \rangle = \lambda$. Two quasiparticle bands ω_k^{\pm} are formed, solutions of $(\omega + \lambda)(\omega + \mu - \epsilon_k) - r^2 = 0$. Changing variables to ω_k^{\pm} , the three saddle-point equations can be cast in the compact form:

$$\left\{ -\frac{1}{J_K}, \frac{1}{2}, \frac{n_c}{2} \right\} = \int_{-\infty}^{+\infty} d\omega n_F(\omega) \rho_0(\omega + \mu - \frac{r^2}{\omega + \lambda}) \times \left\{ \frac{1}{\omega + \lambda}, \frac{r^2}{(\omega + \lambda)^2}, 1 \right\}. \quad (2)$$

Here, n_F is the Fermi function, $n_c/2$ is the conduction electron density per spin colour, and $\rho_0(\epsilon) \equiv \sum_k \delta(\epsilon - \epsilon_k)$ is the non-interacting density of states.

In the large- N approach, the onset of Kondo screening is signaled by a phase transition at a critical temperature T_K , below which $r(T)$ becomes non-zero. The equation for T_K is $2/J_K = \int d\epsilon \rho_0(\epsilon) \tanh[(\epsilon - \mu_0)/2T_K]/(\epsilon - \mu_0)$, with μ_0 the non-interacting chemical potential (at $T = T_K$). This equation coincides with that for the single-impurity case: Kondo screening of individual local moments starts taking place in this approach *precisely at the single-impurity Kondo scale*. We have derived an explicit expression for T_K in the weak-coupling regime $J_K \ll D$:

$$T_K = D e^{-1/J_K \rho_0(\epsilon_F)} \sqrt{1 - (\epsilon_F/D)^2} F_K(n_c), \quad (3)$$

$$F_K(n_c) = \exp \left(\int_{-(D+\epsilon_F)}^{D-\epsilon_F} \frac{d\omega}{|\omega|} \frac{\rho_0(\epsilon_F + \omega) - \rho_0(\epsilon_F)}{2\rho_0(\epsilon_F)} \right), \quad (4)$$

where ϵ_F is the non-interacting Fermi level (given by $n_c/2 = \int_{-D}^{\epsilon_F} d\epsilon \rho_0(\epsilon)$). This expression is valid for an even d.o.s $\rho_0(-\epsilon) = \rho_0(\epsilon)$ which vanishes outside the interval $-D < \epsilon < +D$. The factor F_K , equal to unity for a constant density of states, varies smoothly with n_c (or ϵ_F). In contrast, the prefactor $[1 - (\epsilon_F/D)^2]^{1/2}$ vanishes in the low-density limit $n_c \rightarrow 0$, and suppresses T_K .

We now consider the low-temperature limit $T \ll T_K$, in which the large- N approach leads to an extremely simple Fermi liquid picture [10]. It is somewhat oversimplified in that the conduction electron self-energy $\Sigma_c(k, \omega) = r^2/(\omega + \lambda)$ is purely real (finite lifetime effects are absent at $N = \infty$) and momentum independent. Even so, it captures some of the most important features of the problem. The zero-frequency shift $\Sigma_c(\omega = 0, T = 0) = r(T = 0)^2/\lambda(T = 0)$ is precisely such that the Fermi surface has a *large volume* containing both conduction electrons and local spins. Indeed, adding the last two saddle point equations in (2), one obtains: $\mu - \Sigma_c(\omega = 0, T = 0) = \epsilon_F^>$ where $\epsilon_F^>$ is the non-interacting value of the Fermi-level corresponding to $(n_c + 1)/2$ fermions per spin color. As detailed below, all physical quantities at $T = 0$ are directly related to a single energy scale, proportional to the boson condensation amplitude $T^* = r^2(T = 0)/D$. It is possible to derive an analytical expression for T^* in the weak coupling limit, which is valid for a general (bounded) density of states and arbitrary density n_c . This expression, which has apparently not been reported before, reads:

$$T^* = D e^{-1/J_K \rho_0(\epsilon_F)} (1 + \epsilon_F/D) \frac{\Delta \epsilon_F}{D} F^*(n_c), \quad (5)$$

$$F^*(n_c) = \exp \left(\int_{-(D+\epsilon_F)}^{\Delta \epsilon_F} \frac{d\omega}{|\omega|} \frac{\rho_0(\epsilon_F + \omega) - \rho_0(\epsilon_F)}{\rho_0(\epsilon_F)} \right), \quad (6)$$

where $\Delta \epsilon_F = \epsilon_F^> - \epsilon_F$. As F_K , F^* varies smoothly with n_c [17]. The total density of states at the Fermi level $\rho(\omega = 0) = \rho_{cc}(0) + \rho_{ff}(0)$ is given by: $\rho(0) = \rho_0(\epsilon_F^>)/Z_c$, with Z_c the conduction electron quasiparticle residue $1/Z_c \equiv 1 - \partial \Sigma_c(\omega)/\partial \omega|_{\omega=0} = 1 + (\epsilon_F^> - \epsilon_F)^2/r_0^2$. In the weak coupling limit, all physical quantities at $T = 0$ are directly related to $\rho(0) \simeq \rho_0(\epsilon_F^>)(\Delta \epsilon_F)^2/(T^*D)$, and are thus renormalized by the ratio T^*/D . For instance, the f -electron susceptibility and the specific heat coefficient (per spin color), are given by $\chi_f \propto \rho(0)$ and $\gamma = \pi^2 \rho(0)/3$. The Drude weight may also be computed with the result $D_R \propto T^*D \rho_0(\epsilon_F^>)/(\Delta \epsilon_F)^2$.

The physical content of these expressions and of Eqs.(3-6) is that *two different energy scales* are relevant for the Kondo lattice model: one (T_K) is associated with the onset of local Kondo screening; the other (T^*) with Fermi liquid coherence and the behaviour of physical quantities at $T = 0$. These two scales have *the same* exponential dependence on J_K/D at weak coupling, but very different dependence on the conduction electron density in the ‘‘exhaustion’’ limit $n_c \ll 1$, in which $T^* \ll T_K$. This is in qualitative agreement with Nozières proposal in [2], but not with his estimate $T^*/T_K \propto T_K/D$ (which would thus depend on the coupling). We find that the ratio T^*/T_K depends only on n_c in this limit, in a manner which reflects the behavior of the bare d.o.s $\rho_0(\epsilon)$ at the bottom of the band. For a d.o.s vanishing as $(\epsilon + D)^\alpha$, Eqs.(3-6) yield $T^*/T_K \propto n_c^{1/[2(1+\alpha)]}$.

Fig. 1 displays the n_c -dependence of T_K and of the inverse of the f -electron susceptibility, obtained by solving the large- N equations, both for a single-impurity and for the lattice. It is seen that T_K and $1/\chi_f(T = 0)$ are identical energy scales for the single impurity case, but have very different density dependence for the lattice model ($T^*/T_K \propto n_c^{1/3}$ at low density for the semi-circular d.o.s used here). Near $n_c = 1$, T_K falls below $1/\chi$ reflecting the vanishing χ for the Kondo insulator. These curves are remarkably similar to those obtained by Tahvildar-Zadeh *et al.* in their Quantum Monte Carlo studies of the periodic Anderson model in infinite dimensions [5] (see also [5]- [8]). In the inset of Fig. 1, we plot the dimensionless number $T_K \chi_f(0)$ as a function of $\ln T_K/D$. This number goes to a universal value at weak coupling in the single-impurity case, while it has intrinsic density dependence for the lattice. This shows that T_K is not the appropriate low-temperature scale, especially for $n_c \rightarrow 0$. The inset in Fig. 2 shows the effective mass ratio m/m^* (computed from the specific heat) and the Drude weight, as a function of n_c . This vanishes in the limits $n_c \rightarrow 0$ and $n_c \rightarrow 1$. The effective mass m^* is proportional to $e^{+1/J_K \rho_0(\epsilon_F)}$, with a density dependent prefactor which diverges as $n_c \rightarrow 0$ and vanishes at half filling.

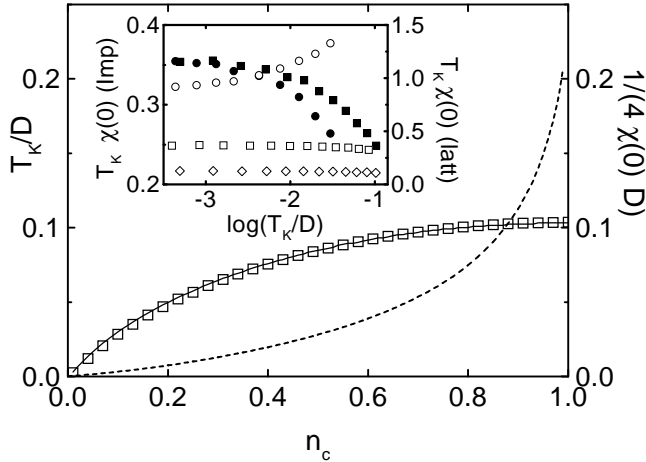


FIG. 1. Solid line: density-dependence of T_K (defined as the slave boson condensation temperature). Squares: $1/4\chi_f(T=0)$ for a single impurity. Dashed line: $1/4\chi_f(T=0)$ for the lattice. $J_K/D=0.75$. Inset: $T_K\chi_f(0)$ for the impurity (left scale, solid symbols) and the lattice (right scale, open symbols) for $n_c=0.1, 1.0$ (impurity) and $n_c=0.1, 0.5, 0.9$ (lattice) from top to bottom. All plots are for a semi-circular d.o.s.

We have also studied the behavior of several physical quantities as a function of temperature, by solving numerically Eqs.(2). Fig.2 shows the product $T_K\chi(T)$ for the Kondo lattice, for several values of n_c , as a function of T/T_K . All the curves merge at $T/T_K = 1$, where the boson decondenses and χ_f reaches the free spin value ($\chi_f(T) = 1/4T$ for $T > T_K$). No universal scaling function of T/T_K describes the temperature dependence in Fig.2, in contrast to the single-impurity case. Plotting $\chi(T)/\chi(T=0)$ does not restore scaling, since qualitative differences in the T-dependence are seen for different densities. Fig.3(a) shows the T-dependence of the entropy. A linear behavior $S(T) = \gamma T$ is found at low temperature for all densities $n_c \neq 1$. The slope $\gamma \propto \rho(0)$ decreases with increasing density as does the temperature scale T_F^* up to which $S(T)$ is linear. T_F^* is of the order of T^* ($\ll T_K$) at low n_c , while it can be estimated by comparing γT to $e^{-T_K/T}$ as $T_F^* \simeq T_K/|\ln(1-n_c)| \ll T_K \simeq T^*$ for $n_c \rightarrow 1$. For $n_c \simeq 1$, T_F^* is a better estimate of the coherence scale than T^* itself.

At low densities, after a steep initial rise, $S(T)$ remains close to $\ln 2$ up to T_K . This can be interpreted in terms of the strong-coupling picture discussed below. At higher densities, most of the variation takes place in the range $T_F^* < T < T_K$. The specific heat $C(T)$, shown in Fig.3(b), has a two-peak structure [18]: the peak at T_K signals the onset of Kondo screening and appears in this mean-field description as a discontinuity of $C(T)$. The second peak, at T_F^* , signals the Fermi liquid heavy-fermion regime. As n_c increases, weight is gradually transferred to the high-temperature peak until the low temperature peak disappears completely in the

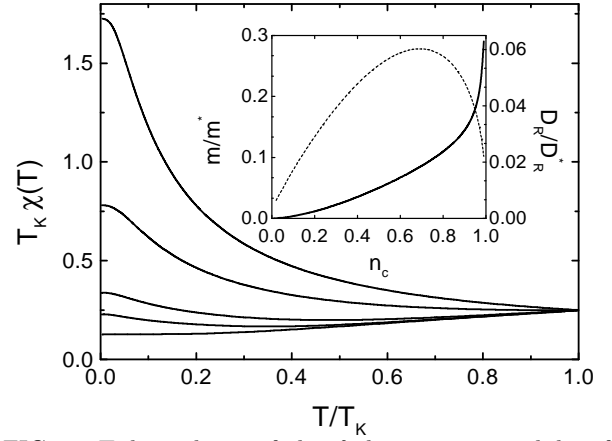


FIG. 2. T -dependence of the f -electron susceptibility for the lattice for $n_c=0.01, 0.2, 0.5, 0.8$ and 0.9 , from top to bottom. Inset: Inverse effective-mass(left scale, full line) and Drude factor (right scale, dashed line) as functions of density. In all plots, $J_K/D = 0.75$

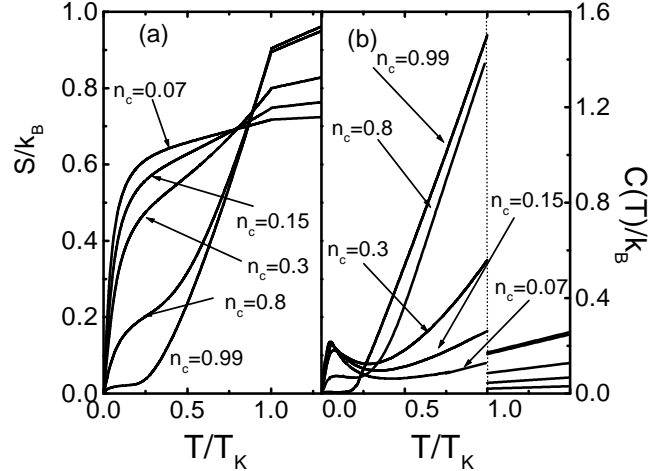


FIG. 3. Entropy (a) and specific heat (b) for the lattice model for several values of the density. $J_K/D=0.75$.

Kondo insulator limit.

In the strong coupling limit $J_K/D \gg 1$, the large- N results support the physical picture proposed by Lacroix [19] and further discussed in [2]. In this picture, the conduction electrons bind to n_c spins, forming singlets below $T \sim J_K \sim T_K$, the binding energy of a singlet. The remaining $1 - n_c$ “bachelor spins” behave as itinerant fermions subject to a constraint of no double occupancy. The hopping integral of the resulting effective infinite- U Hubbard model is $t_{\text{eff}} = -t/2$. The (hole-like) sign of this matrix element implies that these $1 - n_c$ fermions have a Fermi surface volume corresponding precisely to $n_c + 1$ particles. In the exhaustion limit $n_c \ll 1$, one has effectively a weakly doped $U = \infty$ Hubbard model. Solving Eqs.(2) at strong-coupling yields a quasiparticle residue $Z_c \propto n_c$, and hence a coherence scale $T^* \sim n_c D$ corresponding to a Brinkman-Rice estimate for this doped Mott insulator [2]. Notice, however, that at finite N

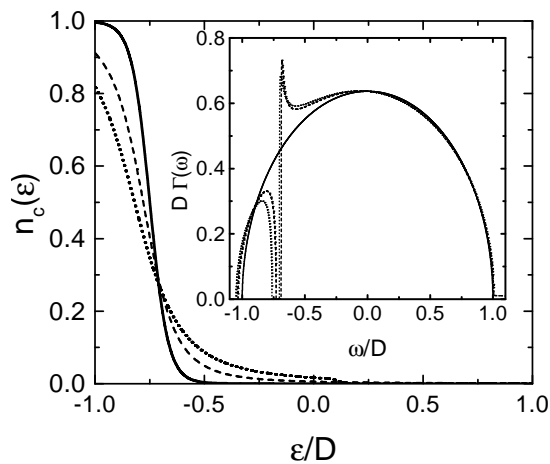


FIG. 4. $n_c(\epsilon)$ for $T/T_K=1.0$ (solid line), 0.5 (dashed line), 0.005 (dotted line). $n_c=0.15$. Inset: Spectral density $\Gamma(\omega)$ for $T/T_K=1$ (solid line), 0.5 (dashed line) and 0.25 (dotted line). For $T < T_K$ there is a δ -function peak in the gap not shown for clarity. $n_c=0.2$. In all plots $J_K/D=0.75$.

this uniform solution may become unstable to magnetism or phase separation of localized singlets and unscreened spins. This picture sheds some light on the T -dependence of the entropy and specific heat in the exhaustion limit reported above. As the system goes through T_K , it loses the magnetic entropy ($\sim n_c \ln 2$) of the n_c bound spins. The remaining entropy ($\sim (1 - n_c) \ln 2$), is lost below T^* . The two peaks of unequal weight in the specific heat reflect these processes [20].

We display in Fig. 4 the distribution function of the conduction electrons $n_c(\epsilon_k) \equiv \langle c_k^\dagger c_k \rangle$. Very close to T_K , $n_c(\epsilon_k)$ has the shape of a Fermi function centered around the *non-interacting* Fermi level ϵ_F , with a small thermal broadening of order T_K ($\ll D$ in weak coupling). As T is reduced below T_K , weight is transferred to scales of order $\epsilon_F^>$, the *interacting* Fermi level associated with the large Fermi surface. The feature at ϵ_F *broadens* as T is decreased. When Fermi liquid coherence establishes at $T \simeq T_F^*$, a discontinuity (of amplitude Z_c) develops at $\epsilon = \epsilon_F^>$. Finally we note that, in the large- N approach, the Kondo lattice model can be exactly mapped onto an effective single-impurity model coupled to a self-consistent bath of electrons. This mapping holds more generally for any approach in which the conduction electron self-energy depends only on frequency, such as dynamical mean-field theory [9]. For a semi-circular d.o.s, the Green's function of the self-consistent bath is $\mathcal{G}_0(i\omega_n) = [i\omega_n + \mu - D^2 G_c(i\omega_n)/4]^{-1}$. The inset of Fig. 4 displays the continuous evolution of the spectral density $\Gamma(\omega) = -\text{Im}\mathcal{G}_0(\omega + i0^+)/\pi$ as T is reduced below T_K . Above T_K , it coincides with the non-interacting d.o.s ρ_0 , while the bath is split into two bands below T_K . The width of the lower band depends on n_c and is small for $n_c \ll 1$, leading to the low coherence scale. The existence of a sharp gap separating the two bands is an artifact of

the large- N limit (except at $n_c = 1$). In more realistic treatments it is replaced by a pseudo-gap [5,7,8].

In conclusion, we have reconsidered the time-honored large- N approach to the Kondo lattice model, with special emphasis on the “exhaustion” limit of low electron density. We showed that two energy scales appear for which we have obtained explicit analytic expressions: the Kondo scale associated with the onset of local Kondo screening and a much lower scale associated with Fermi liquid coherence. Physical quantities reflect the crucial role played by these two scales. In this approach, magnetic ordering is suppressed by quantum fluctuations: more elaborate treatments such as DMFT must be used to assess whether the coherence scale can actually be reached or magnetic ordering sets in at a higher temperature.

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