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Critical approach to the coherence transition in Kondo lattices

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We study the Kondo lattice from the point of view of the scaling theory of critical phenomena. The coherence temperature $\mathcal{T}_c$ is associated with a crossover from a paramagnetic state with local moments to a Fermi-liquid regime with strong magnetic correlations. We obtain an expression for $\mathcal{T}_c$ in terms of the Kondo-lattice parameters and a crossover exponent ϕ_t. The effect of a magnetic field is investigated and characterized by another critical exponent. These exponents obey scaling relations with a shifted dimensionality.

The Kondo lattice[1] provides a useful model to describe the physical behavior of heavy-fermion systems.[2] The energy scales in this problem are the intensity of the coupling between localized and conduction electrons J ($J>0$) and the bandwidth W of the conduction states ($W=1/\rho$ where ρ is the constant density of states). The existence of two competing effects in Kondo-lattice systems has been recognized,[1,3] both associated with the same renormalized coupling $J\rho$ between the localized and the itinerant electrons. The first is the Kondo effect that leads, as in the well studied impurity problem, to a compensation of the magnetic moments below a characteristic temperature. The second is an indirect coupling between the localized moments mediated by the conduction electrons. This coupling, of the Ruderman-Kittel-Kasuya-Yosida type, gives rise to a tendency for long-range magnetic order between the local moments. Recent studies of the two-impurity problem have led to new insights on the interplay between these competing effects.[4] Theoretical investigations[1] have shown the existence of a critical value of the coupling parameter $(J\rho)_c$ above which the Kondo effect dominates and a nonmagnetic, collective Kondo-type state is attained at zero temperature.[3] For $J\rho<(J\rho)_c$, long-range magnetic order, generally of the antiferromagnetic or ferromagnetic type, is established in the system at sufficiently low temperature.

An interesting phenomenon occurs in Kondo-lattice systems with $J\rho>(J\rho)_c$ when, with decreasing temperature, clusters of compensated spins start to behave "coherently" producing significant changes in the resistivity and Hall effect.[5] This transition, which is not a phase transition, occurs at temperatures below the single-impurity Kondo temperature $\mathcal{T}_K$ and marks the onset of a collective (dense) Kondo state. It is generally associated with a change in the behavior of the system from that of a paramagnet with partially compensated local moments to that of a Fermi liquid. The nature of this "coherence transition" is, however, elusive and it is not known yet how it relates to the relevant physical parameters. Nevertheless, this concept plays a central role in the study of heavy fermions and underlies explicitly or implicitly most of the recent literature on this subject.[2,5]

In this Rapid Communication we study the coherence transition in the Kondo lattice using the scaling theory of critical phenomena and phenomenological renormalization-group equations.[6] We assume that in the Kondo-lattice problem, at zero temperature, there is an unstable fixed point at $(J\rho)_c$ or $K_c=1/(J\rho)_c=(W/J)_c$, where $(J\rho)_c$ is the critical value of the parameter $J\rho$ that separates a phase with long-range magnetic order (ferromagnetic, antiferromagnetic, etc.) from a dense Kondo phase with Fermi-liquid behavior. This is in fact the picture that emerges from calculations using the renormalization group applied to the Kondo-lattice Hamiltonian.[3] Expanding the renormalization-group equations close to the zero-temperature fixed point at K_c we obtain

$$K_{n+1}=K_c+b^x(K_n-K_c)\,, \tag{1}$$

with $K=(1/J\rho)=W/J$ and for a change in the length scale of the system by a factor b. The quantity x is a positive number.

We would like to introduce now the effect of an increase in temperature in the system. In the renormalization-group approach one has to consider the question whether to treat this parameter as a relevant or an irrelevant "field." We shall treat it as relevant and the reason is that we expect, in general, the exponents governing the divergence of thermodynamic quantities in the paramagnetic to antiferromagnetic transition at finite temperatures to be different from those of the zero-temperature transition separating the Fermi liquid from the long-range magnetically ordered state. From the renormalization-group point of view this implies that the flow of the equations starting from a small but finite temperature is always away from the zero-temperature fixed point at K_c. In particular, at the critical line, in the $T\times J\rho$ plane, separating the paramagnetic from the antiferromagnetic phase, the flow is towards another fixed point that controls this finite-temperature transition.

The expansion of the renormalization-group equations for the Kondo lattice, close to the zero-temperature fixed point, can be generalized for finite temperature and is given by

$$K_{n+1}=K_c+b^x(K_n-K_c)-T_n\,,\qquad T_{n+1}=b^yT_n\,. \tag{2}$$

where $T=\mathcal{T}/W$ (or $\mathcal{T}/J$ since W and J scale with the same exponent at K_c) and y is a positive number since temperature is included as a relevant field in the problem. Notice that Eq. (2) implies $J_{n+1}=b^{-y}J_n$ close to K_c. The coupling between temperature and the exchange energy was taken to lowest order in the equations above which can be iterated to yield

$$K_l=l^x(K-K_c-aT)+K_c+al^yT\,, \tag{3}$$

where $l=b^n$, $a=(b^x-b^y)^{-1}$, $K=W/J$, and K_c is the zero-temperature fixed point governing the magnetic to Fermi-liquid transition. At $T=0$ we can define a correlation length $\xi=(K-K_c)^{-1/x}$ which for $K<K_c$ or $(J\rho)>(J\rho)_c$ gives the typical size of magnetically correlated regions. In analogy with a temperature-induced phase transition, we introduce the exponent $\nu=1/x$ characterizing the divergence of the correlation length at the critical value of the parameter $(J\rho)$. At finite temperatures we obtain the following relation for the correlation length:

$$\xi=(K-K_c)^{-\nu}f[T/(K-K_c)^{\phi_t}]\,, \tag{4}$$

where $f[x]$ is a scaling function and we introduced a crossover exponent ϕ_t defined by $\phi_t=y/x=\nu y$. We neglected a regular, linear temperature-dependent term which does not affect our results as long as $\phi_t\gtrsim 1$. If this is not the case it should be taken into account.

Although we derived above explicit results only for the scaling expression of the correlation length, scaling theory implies that for any other thermodynamic quantity like specific heat, susceptibility, etc., temperature will appear in the same combination as in Eq. (4). It also implies[7] that the equation for the critical line, separating the antiferromagnetic phase from the disordered paramagnetic state, is given by $T_N=A\,|K-K_c|^{\phi_t}$. If $\phi_t<1$ we write $T_N=A\,|K-K_c-aT|^{\phi_t}\equiv A\,|K-K_c(T)|^{\phi_t}$ or alternatively, $J_c(T)=J_c(T=0)-cT-gT^{1/\phi_t}$, where J_c is the critical value of J and c and g are constants. The regular linear term can be identified with the result found by Doniach[1] and it is dominant at low temperatures if $\phi_t<1$. The critical line $T_N(J)$ is shown in Fig. 1 together with the crossover line which has the equation $T_c=B\,|K-K_c(T)|^{\phi_t}$. This line in the noncritical region of the $T\times J\rho$ plane, i.e., $J\rho>(J\rho)_c$, is characterized by the same exponent ϕ_t of the critical line.[7] It describes the change of behavior of the correlation length, or any other thermodynamic quantity, from a temperature-dominated region with local moments to a collective, Kondo-type regime with $(K-K_c)^{\phi_t}\gg T$. This occurs because the scaling functions for the thermodynamic quantities, that we represent quite generally by $g(x)$ where $x=T/(K-K_c)^{\phi_t}$, have different asymptotic behavior for $x\gg 1$ or $x\ll 1$. Consequently the line $T_c=B\,|K-K_c(T)|^{\phi_t}$ defines the crossover between two different physical regimes; one dominated by thermal fluctuations that we identify with a paramagnetic state with local moments and the other with $x\ll 1$ where the Kondo effect dominates. Furthermore, the scaling approach predicts that all anomalies in the thermodynamic quantities in the noncritical regime and for $T\ll T_K$ ($T_K=\mathcal{T}_K/W$ where $\mathcal{T}_K$ is the Kondo temperature) should occur along the crossover line $T_c\propto|K-K_c|^{\phi_t}$. We can alternatively express these results writing the scaling functions in the form $g(x)=g(T/T_c)$ for $T\ll T_K$.

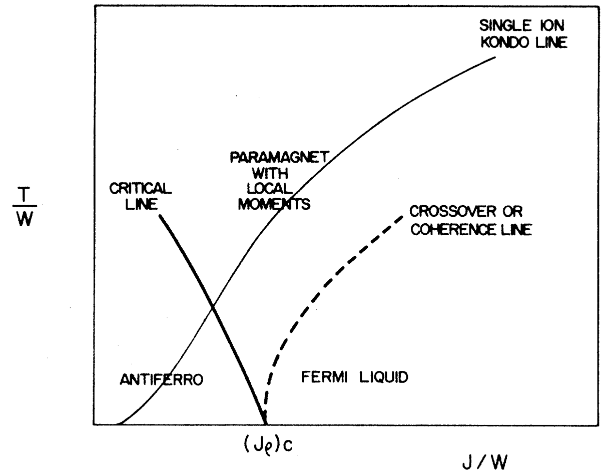

FIG. 1. Finite-temperature phase diagram for the Kondo lattice (schematic plot for $\phi_t=\frac{2}{3}$). Below the single-ion Kondo line, the local moments are partially compensated both in the critical $[J\rho<(J\rho)_c]$ and in the noncritical region.

The analysis above shows that the crossover line provides the relevant characteristic energy scale for the Kondo lattice in the noncritical region at very low temperatures ($T\ll T_K$). It leads to the main result of this Rapid Communication: *We identify the crossover line with the so-called "coherence transition" observed in heavy fermions and which marks the onset of the dense Kondo regime with decreasing temperature.*

In order to complete the phase diagram shown in Fig. 1, we must include the one-impurity Kondo line $T_K=\exp(-1/J\rho)$. This is important since single-ion Kondo effects may be relevant both in the critical and in the noncritical region of the diagram. In the critical region, i.e., for $J\rho<(J\rho)_c$, the system crosses with decreasing temperature both the single-ion Kondo line and the critical frontier. This is the reason for the existence of reduced moments in long-range-ordered magnetic Kondo-lattice systems.[8] The same phenomenon occurs in the noncritical region where single-ion Kondo effect becomes effective before the coherence transition.

The scaling function $f[x]$, characterizing the correlation length, is such that $f[0]=\text{const}$ implying that at $T=0$, $\xi \propto (K-K_c)^{-\nu}$ for $J\rho > (J\rho)_c$. The existence of a finite correlation length, which gives the typical size of magnetically correlated regions at zero temperature, is a direct consequence of the scaling approach. We point out that a finite ξ has been observed in recent inelastic neutron scattering experiments[9] in $CeCu_6$ at very low temperatures. The correlation length ξ diverges only in the critical region $J\rho \leq (J\rho)_c$ and for $T=T_N$. Also because we took temperature as a relevant field, the exponent ν does not describe the divergence of the correlation length at T_N which is given by a different exponent $\dot{\nu}$, such that $\xi \propto (T-T_N)^{-\dot{\nu}}$. The specific heat can also be obtained in the scaling theory. We write the singular part of the free energy as

$$F \propto (K-K_c)^{2-\alpha} q[T/|K-K_c|^{\phi_t}] , \tag{5}$$

where $q[x]$ is a scaling function, with $q[0]=\text{const}$, and α is a critical exponent. For the specific heat we obtain to first order in temperature, $C \propto (K-K_c)^{2-\alpha-2\phi_t}T$. Because we are dealing with a zero-temperature fixed point,[10] the scaling relations which involve the dimension d are modified according to the rule $d \rightarrow d+y$ [y is defined in Eq. (2)] so that we get an increase in the effective dimensionality of the system. The hyperscaling relation, for example, is now given by $2-\alpha=(d+y)\nu$. Using standard scaling relations but with d substituted by $d+y$ we can write $C \propto (K-K_c)^{\nu(d-y)}T$ for $y<1$. If $y \geq 1$ and $d=3$, the exponents associated with the zero-temperature fixed point attain, due to the dimensionality shift, their classical (mean field) values and $C/T \propto (K-K_c)^{2-y}$. The enhancement of the specific heat at low temperatures for $y>2$ can be related to the proximity of a magnetic instability and the presence of strong magnetic correlations.

In order to calculate the zero-temperature susceptibility, for the ferromagnetic case, one has to consider the effect of a magnetic field in the system. Defining an exponent σ through the recursion relations for the magnetic field close to the zero-temperature fixed point at K_c, $h_{n+1}=b^\sigma h_n$, we derive the generalized scaling form for the ground-state energy,

$$E \propto (K-K_c)^{\nu(d+y)} v[(h/J)/|K-K_c|^{\nu(\sigma+y)}] , \tag{6}$$

where $v[z]$ is a scaling function and $\nu(d+y)=2-\alpha$. The susceptibility $\chi=-(\partial^2E/\partial^2h)_{h=0}$ at $T=0$ and we get $\chi \propto (K-K_c)^{-\gamma}$ where $\gamma=\nu(2\sigma+y-d)$. It is also enhanced due to the proximity of the magnetic instability at K_c. When $y<1$ and $d=3$, we find for the Wilson ratio $\chi/\gamma_0 \propto (K-K_c)^{-2\nu\sigma}$ which turns out to be nonuniversal. For $y \geq 1$ and $d=3$, $\chi/\gamma_0 \propto (K-K_c)^{y-3}$ which is universal for $y=3$. γ_0 is the coefficient of the linear term of the specific heat.

More interesting, the shift in the coherence temperature (defined, for example, by some particular anomaly in a thermodynamic quantity for $T \ll T_K$) due to the magnetic field follows the relation $\Delta T_c \propto h^{1/\phi_h}$, where $\phi_h=\nu\sigma$. For antiferromagnetic interactions, it is the staggered susceptibility that diverges at K_c but we expect enhancement of the uniform susceptibility and $\Delta T_c \propto h^{2/\phi_h}$. The scaling theory predicts that the same exponent yields the shift in the critical (Néel) temperature due to an external field, i.e., $\Delta T_N \propto h^{2/\phi_h}$. Finally defining the critical exponent δ through the field dependence of the magnetization m for $K=K_c$, $m \propto h^{1/\delta}$, also $\phi \equiv \phi_t+\phi_h$ and β through $m \propto (K-K_c)^\beta$ for $T=0$, we obtain the scaling relations $\alpha+2\beta+\gamma=2$ and $\delta=\phi/\beta$ for the exponents associated with the zero-temperature fixed point.

The exponent y in Eq. (2) can be identified[11] with the dynamic exponent z. Since at $T=0$ there are only quantum fluctuations in the system, we have $\Delta J \propto (\Delta t)^{-1}$ and consequently time scales as the inverse of energy and $z=y$. The dynamic exponent z reflects the nature of the low-frequency excitations[11] but the character of these excitations in the dense Kondo state[12] and in particular their wave-vector dependence are not yet known. We recall that for $y=z=3$, we found the susceptibility and effective mass to diverge with the same exponent close to J_c. This value of z is associated with paramagnon type of excitations.[11] Most probably y or z is close to three ($\phi_t \cong \frac{3}{2}$) in heavy fermions since the Wilson ratio does not vary very much from one system to another.[11]

It has been shown using renormalization-group calculations[2] that in one dimension the Kondo-lattice problem has $(J\rho)_c=0$ so that any coupling between localized moments and the conduction electrons leads to Fermi-liquid behavior. This situation can be described by scaling theory and corresponds to the case $x=0$ showing that in one dimension the fixed point at $(J\rho)_c=0$ is marginal. In this case of course there is no critical line since the system does not order magnetically. The crossover line can, however, still be obtained and we find $T_c \propto \exp(-y/J\rho)$. Then in one dimension, the expression for the coherence or crossover line depends exponentially on the coupling parameter as the single-ion Kondo temperature.

In conclusion, our scaling theory accounts in a simple and unambiguous way for the coherence transition in heavy fermions. It characterizes this transition in terms of the Kondo-lattice parameters and critical exponents. It is a one exponent theory since given $y(d+y \geq 4)$ all other exponents can be found. We show that universality concepts may be useful in the study of heavy fermions.

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