Magnetic ordering and non-Fermi-liquid behavior in the multichannel Kondo-lattice model

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Abstract. Scaling equations for the Kondo lattice in the paramagnetic and magnetically ordered phases are derived to next-order leading with account of spin dynamics. The results are applied to describe various mechanisms of the non-Fermi-liquid (NFL) behavior in the multichannel Kondo-lattice model where a fixed point occurs in the weak-coupling region. The corresponding temperature dependences of electronic and magnetic properties are discussed. The model describes naturally formation of a magnetic state with soft boson mode and small moment value. An important role of Van Hove singularities in the magnon spectral function is demonstrated. The results are rather sensitive to the type of magnetic ordering and space dimensionality, the conditions for NFL behavior being more favorable in the antiferromagnetic and 2D cases.

PACS. 75.30.Mb Valence fluctuation, Kondo lattice, and heavy-fermion phenomena – 71.28.+d Narrow-band systems; intermediate-valence solids

1 Introduction

A number of 4f- and 5f-compounds, including so-called Kondo lattices and heavy-fermion systems, possess anomalous electronic properties, e.g., giant value of \( T \)-linear electronic specific heat \( C(T) \) and magnetic susceptibility \( \chi_m(T) \). Magnetism of such systems demonstrates also unusual features, including formation of an antiferro- or ferromagnetic state with small ordered moment value.

A common explanation of the heavy-fermion behavior is based on the Komdo effect. Unlike the one-impurity case \[7,8,9,10,11\]. Physically, this behavior is connected with overscreening of impurity spin by conduction electrons. The model permits a consistent description of the NFL behavior in the paramagnetic and magnetically ordered phases.

A great experimental material has been obtained for \( f \)-systems demonstrating so-called non-Fermi-liquid (NFL) behavior \[3\], which have unusual logarithmic or power-law temperature dependences of electron and magnetic properties, e.g., \( \chi_m(T) \sim T^{-\xi} \) (\( \xi < 1 \)), \( C(T)/T \) is proportional to \( T^{-\xi} \) or \(-\ln T\), for the resistivity \( R(T) \sim T^\mu \) (\( \mu < 2 \)), etc. The NFL behavior is observed in a number of rare-earth and actinide systems: not only in alloys like \( U_x Y_{1-x} Pd_3 \), \( UPt_{3-x} Pd_2 \), \( UCu_{5-x} Pd_x \), \( CeCu_{6-x}Au_x \), \( U_x Th_{1-x} Be_{13} \), but also in some stoichiometric compounds, e.g., \( Ce_{7}Ni_{13} \), \( CeCu_{2}Si_{2}CeNi_{2}Ge_{2} \). It can coexist with magnetic ordering and occur even in ferromagnets \[5\].

There are a number of theoretical mechanisms proposed to describe the NFL state, both single-site and intersite effects being discussed. In particular, proximity to magnetic quantum phase transitions \[6\] should be mentioned.

The NFL behavior in the \( M \)-channel Kondo model (especially in the large-\( M \) limit) was extensively investigated in the one-impurity case \[7\] \[8\] \[9\] \[10\] \[11\]. Physically, this behavior is connected with overscreening of impurity spin by conduction electrons. The model permits a consistent investigation since the fixed point is within the weak-coupling region (however, the marginal case \( M = 2 \) has some peculiarities). On the other hand, the lattice case is more difficult and only special approaches, in particular for one-dimensional models \[8\] \[12\] and infinite space dimension \[13\] were used. In the present paper we start from the standard microscopic model of a periodical Kondo lattice and treat the interplay of the on-site Kondo screening and intersite exchange interactions within a scaling approach. We will demonstrate that, besides the standard one-impurity NFL mechanism, "soft" boson branches can be formed during the renormalization process, the role of singularities in spin spectral function being important for the NFL behavior.
Earlier a similar consideration was performed in Refs. [2, 13] where the NFL behavior in $M = 1$ and large-$M$ Kondo lattices was treated within a simple approximation corresponding to one-loop scaling (in the pseudofermion representation). This approach yields NFL behavior in the formal limit $M \to \infty$ (where the coupling constant is unrenormalized, which is similar to occurrence of a fixed point), but for any realistic $M$ the NFL regime is achieved only in a very narrow interval of bare coupling constant (near the critical value for magnetic quantum phase transition). Thus this approximation is insufficient to describe consistently the NFL state. In the present work we perform the next-leading scaling analysis which changes radically the situation.

In Sect. 2 we write down the scaling equations in the one-impurity case and in the lattice situation (i.e. with account of spin dynamics). In Sect. 3, results of numerical calculations are presented. In Sect. 4 we discuss the physical consequences. Details of derivation of the scaling equations are presented in Appendices.

2 Scaling equations

To describe a Kondo lattice, we use the degenerate-band (multichannel) periodical $s - f$ exchange model

$$H = \sum_{km\sigma} t_k c_{km\sigma}^\dagger c_{km\sigma} - I \sum_{im\sigma\sigma'} S_i \sigma \sigma' c_{im\sigma}^\dagger c_{im\sigma'} + H_f \tag{1}$$

where $t_k$ is the band energy, $S_i$ are spin-1/2 operators, $I$ is the $s - f$ exchange parameter, $\sigma$ are the Pauli matrices, $m = 1...M$ is the channel index. For the sake of convenient constructing perturbation theory, we explicitly include the Heisenberg $f - f$ exchange interaction $H_f$ in the Hamiltonian, although in fact this interaction is usually the indirect RKKY coupling.

In the more general $SU(N) \otimes SU(M)$ model we have $\sigma = 1...N$ and the Hamiltonian can be written as [10]

$$H = \sum_{km\sigma} t_k c_{km\sigma}^\dagger c_{km\sigma} - I \sum_{im\sigma\sigma'} |\sigma\rangle \langle i\sigma| c_{im\sigma}^\dagger c_{im\sigma'} + H_f \tag{2}$$

A somewhat more realistic model including angular momenta is discussed in Ref. [2]; generalization to arbitrary spin is also possible (see, e.g., Ref. [15]).

Similar to Ref. [2], we use the “poor man scaling” approach [16]. In this method one considers the dependence of effective (renormalized) model parameters on the cutoff parameter $C < 0$ which occurs at picking out the Kondo singular terms and approaching the Fermi level.

To describe the renormalization process we introduce the dimensionless coupling constants

$$g_{ef}(C) = - N \rho I_f(C), \quad g = - N \rho I \tag{3}$$

where $\rho$ is the bare electron density of states per channel at the Fermi level. In the one-impurity case the scaling behaviour is governed by the beta function

$$\beta(g) = - g^2 + (M/N) g^2 + ... \tag{4}$$

At $M > N$ the fixed point $g^* = N/M$ (zero of $\beta(g)$) lies in a weak coupling region which makes possible successful application of perturbation and renormalization group approaches.

The scaling equation reads

$$\int_0^{g_{ef}(C)} \frac{dg}{\sqrt{\beta(g)}} = \int_0^C \frac{dC}{C} = \ln \left| \frac{C}{D} \right| \tag{5}$$

where the cutoff energy $D$ is defined by $g_{ef}(-D) = g$. Solving this equation yields

$$\frac{g^* - g_{ef}(C)}{g^* - g} = g^* \left( \frac{C}{T_K} \right)^\Delta \exp \left( - \frac{g^*}{g_{ef}(C)} \right) \tag{6}$$

with $\Delta = N/M$ and the Kondo temperature

$$T_K = D g^{M/N} \exp(-1/g). \tag{7}$$

It should be noted that we have no divergence of $g_{ef}(\xi)$, and the power-law critical behavior in [6] takes place in a wide region, including $|C| > T_K$ [9].

Generally, the critical exponents are defined by the slope $\Delta = \beta'(g)$. Taking into account higher orders in $1/M$ one has

$$\Delta = \frac{N}{M} \left( 1 - \frac{N}{M} \right) \approx \frac{N}{M + N}, \tag{8}$$

the latter value being in agreement with the exact results of Bethe ansatz and conformal field theory (see Ref. [10]). The corresponding value of $g^*$ for $N = 2$ reads [9]

$$g^* = \frac{2}{M} \left( 1 - \frac{2 \ln 2}{M} \right) \tag{9}$$

which differs weakly from $\Delta$.

Using the results of Appendices A, B we can write down the system of scaling equations for paramagnetic (PM), ferromagnetic (FM) and antiferromagnetic (AFM) phases in the lattice case. Similar to Ref. [2], but taking into account next-leading contributions, we find the equation for $I_{ef}$ by picking up in the sums in the corresponding self-energies the contribution of intermediate electron states near the Fermi level with $C < t_k < C + \delta C$. We derive

$$\delta I_{ef}(C) = \rho I^2 N(1 + M \rho I) \eta(\frac{C}{C}) \delta C/C \tag{10}$$

where $\eta$ is a characteristic spin-fluctuation energy, $\eta(x)$ is the scaling function satisfying the condition $\eta(0) = 1$, which guarantees the correct one-impurity limit, see Appendix C. The third-order term, proportional to $M$, comes from corrections which contain summation over the orbital index $m$ (in the diagram approach, they correspond to diagrams containing a closed electron loop).

The leading renormalization of spin-fluctuation frequencies is already of order of $M$:

$$\delta \omega_{ef}(C)/\omega = a \delta S_{ef}(C)/S = a M N \rho^2 \eta(\frac{C}{C}) \delta C/C \tag{11}$$
where the parameters $a$ for a concrete lattice and magnetic structure are expressed in terms of averages over the Fermi surface (see Refs. [2][11] and Appendices A, B). It turns out that, owing to the structure of perturbation theory for magnetic characteristics, the $M^2$ corrections do not occur in the third order in $I$, so that Eq. 11 is sufficient.

Replacing in the right-hand parts of (10) and (11) $g \rightarrow g_{ef}(C)$, $\omega \rightarrow \omega_{ef}(C)$ we obtain the system of scaling equations

\[
[1 - \gamma g_{ef}(C)]^{-1} \partial g_{ef}(C)/\partial C = -A
\]

\[
a \partial \ln \omega_{ef}(C)/\partial C = \partial \ln \omega_{ef}(C)/\partial C = a \gamma A
\]

with $\gamma = M/N$,

\[
A = A(C, \omega_{ef}(C)) = [g_{ef}^2(C)/C] \eta(-\omega_{ef}(C)/C).
\]

Writing down the first integral of the system (12), (13) we have

\[
\ln [1 - \gamma g_{ef}(C)] - (1/a) \ln \omega_{ef}(C) = \text{const}
\]

\[
\frac{\omega_{ef}(C)}{S} = \left( \frac{\omega_{ef}(C)}{\omega} \right)^{1/a} = \frac{1 - \gamma g_{ef}(C)}{1 - \gamma g} = \frac{g^* - g_{ef}(C)}{g^* - g},
\]

\[
(M/N)g_{ef}(C) = 1 - [1 - (M/N)g] \left( \frac{\omega_{ef}(C)}{\omega} \right)^{1/a}
\]

Thus we have a soft-mode situation at approaching the fixed point.

Provided that $\omega_{ef}(C)$ is weakly renormalized (e.g., $a \ll 1$ at small $k_F$) we obtain

\[
g^* - g_{ef}(C) = g^* \exp \left( - \frac{g^*}{g_{ef}(C)} \right) \left| \frac{D \exp[G(C)]}{T_K} \right|^{1/\Delta}
\]

\[
G(C) = - \int_{-D}^{C} \frac{C'}{C'} \eta \left( - \frac{C}{C'} \right),
\]

cf. the treatment of the large-$N$ limit [2]. In particular, in the paramagnetic state

\[
G^{PM}(C) = \frac{1}{2} \ln((C^2 + \omega^2)/D^2) + \frac{C}{\omega} \arctan(\frac{\omega}{C}) - 1
\]

so that $C \rightarrow \sqrt{C^2 + \omega^2}$ in the Kondo divergences in comparison with (6), cf. discussion in Refs. [17][18].

However, in the general case the scaling behavior is much more rich and interesting. Introducing the function

\[
\chi(\xi) = \ln \frac{\omega}{\omega_{ef}(C)} = a \ln \frac{\omega_{ef}(C)}{S}
\]

the scaling equation takes the form

\[
\frac{\partial \chi}{\partial \xi} = a \frac{1}{\gamma} [1 - (1 - \gamma g) \exp(-\chi/a)]^2 \Psi(\lambda + \chi - \xi)
\]

where

\[
\Psi(\xi) = \eta(e^{-\xi}), \quad \xi = \ln |D/C|, \quad \lambda = \ln(D/\omega) \gg 1
\]

In Ref. [2], an approximation was proposed for magnetically ordered cases, which takes into account not only the magnon pole, but also incoherent contribution, namely

\[
A = [g_{ef}^2(C)/C] \times [Z \eta_{coh}(-\omega_{ef}(C)/C) + (1 - Z) \eta_{incoh}(-\omega_{ef}(C)/C)]
\]

(21)

where $\eta_{coh}$ corresponds to the magnetic phase, and the function $\eta_{incoh}$ is unknown; for estimations we may put $\eta_{incoh} = \eta^{PM}$. The quantity $Z = Z(-\omega_{ef}(C)/C)$ is the residue at the magnon pole, which is given by

\[
\frac{1}{Z(\xi)} = 1 + \ln \frac{S}{S(\xi)}
\]

Then we have instead of (20)

\[
\frac{\partial \chi}{\partial \xi} = a \frac{1}{\gamma} [1 - (1 - \gamma g) \exp(-\chi/a)]^2 \Psi(\lambda + \chi - \xi)
\]

(23)

with $Z = 1/(1 + \chi/a)$.

\section{3 Scaling behavior}

Our scaling equations are written in terms of $\gamma$ rather than $M$ and $N$ separately. Therefore, to establish properly the correspondence with the one-impurity case [5], we may put $\gamma = M/N + 1 = 1/\Delta$. This yields, at least for $M > 2$, correct critical exponents for magnetic susceptibility, specific heat and resistivity.

The important case $M = 2$ is more difficult from the theoretical point of view, see [10][8][11]. However, a fixed point is still present for $M = 2$, the resistivity being satisfactorily described by simple scaling approach [10].

In numerical calculations, we put $M = 3$, which may be relevant for Ce$^{3+}$ ion [10]. Then for $M = 3$, $N = 2$ we have $\gamma = 5/2$.

Since $\Psi(\xi > 1) \simeq 1$, in the PM phase $\chi(\xi)$ increases according to (19), (16). Provided that $g$ is not too small, at large $\xi$ we can put for rough estimations $g_{ef}(\xi) \simeq g^* = 1/\gamma$ to obtain

\[
\chi(\xi) \simeq a \gamma g_{ef}(\xi) \xi - a/\gamma g \simeq (a/\gamma)(\xi - 1/g).
\]

(24)

Thus a power-law behavior occurs

\[
\omega_{ef}(C) \simeq (C/T_K)^{\beta}, \quad \beta = a/\gamma = a \Delta
\]

\[
\omega_{ef}(C) \simeq (C/T_K)^{\Delta},
\]

(25)

which corresponds to the standard one-impurity NFL behavior (see below the discussion of physical properties).
Note that the scale of $T_K$ occurs here, unlike the lowest-order scaling in the large-$M$ limit [2]. The dependence [24] takes place up to the point

$$
\xi_1 \simeq (\lambda - \beta/g)/(1 - \beta).
$$

(26)

For $\xi > \xi_1$, $\chi(\xi) \simeq \chi(\xi_1) \simeq \lambda \beta/(1 - \beta)$ is practically constant since $\Psi(\lambda + \chi - \xi)$ becomes small, and $g_{ef}(\xi)$ increases slowly tending at $\xi \to \infty$ to an asymptotic value which is, however, smaller than the one-impurity $g^{*}$ since $\chi(\xi)$ remains finite.

Note that lowest-order (one-loop) scaling for finite $M$ yields the NFL behavior in a very narrow interval of bare coupling constant $g$ only, since with increasing $g$ we come rapidly to strong-coupling regime where $g_{ef}(\xi > \lambda) \to \infty$. Unlike the lowest-order scaling, such a critical $g$ value does not occur in the present calculation for the paramagnetic case: $g_{ef}(\xi)$ remains finite for any $g$.

The dependence $g_{ef}(\xi)$ and $\chi(\xi)$ in the paramagnetic phase are shown in Fig.1 for the 3D case (the results for the 2D case differ here very weakly). The behavior $g_{ef}(\xi)$ between $\xi_1$ and $\xi_2$ may be described as nearly linear, but is somewhat smeared since $\Psi(\xi)$ differs considerably from the asymptotic values 0 and 1 in a rather large interval of $\xi$. Remember that Fig.1a demonstrates also the behavior of magnetic moment according to Eq.(15).

In magnetically ordered phases, the behavior for for $\xi < \xi_1$ is similar, but the situation for $\xi > \xi_1$ changes since the Van Hove singularity of $\Psi_{coh}(\xi)$ at $\xi = 0$ plays an important role. Instead of decreasing, $\Psi(\lambda + \chi - \xi)$ starts to increase at approaching $\xi_1$. At sufficiently large $g$, provided that

$$
a g_{ef}^2(\xi \simeq \xi_1)\Psi_{coh}^{\max} \simeq a g^{*^2}\Psi_{coh}^{\max} > 1,
$$

(27)

at $\xi > \xi_1$ the argument of the function $\Psi_{coh}$ in (20) becomes almost constant (fixed), and we obtain

$$
\chi(\xi) \simeq \xi - \lambda, \quad \Psi_{ef}(C) \simeq |C|.
$$

(28)

Thus, instead of divergence of $\chi(\xi)$ in the one-channel model [2], we have a linear NFL behavior since $g_{ef}(\xi)$ remains finite. Such a behavior has a critical nature and corresponds to $g = g_c$ in the one-channel Kondo model.

Unlike the PM case, a sharp crossover occurs here with changing $g$ since we do not reach the regime [28] at small $g < g_c$. The value of $g_c$ is determined by the value of $\delta$, i.e. the magnon damping, see (24). One can see that the influence of the singularity is considerably stronger and conditions of the NFL behavior are more favorable in the 2D rather than 3D case, and in the AFM rather than FM case. Above the critical value $g_c$, the picture of scaling trajectories (in particular, the size of NFL behavior region ) does not practically depend on $g$.

In the case of equation (20), the linear behavior takes place up to $\xi = \infty$. On the other hand, when taking into account the incoherent contribution the increase of $\chi$ stops at $a g^{*^2}\Psi_{coh}^{\max} = 1/Z = 1 + \chi/a$, i.e., at

$$
\xi_2 = \lambda + \chi_{\max} = \lambda + a(a g^{*^2}\Psi_{coh}^{\max} - 1).
$$

(29)

The dependences $\chi(\xi)$ for a 3D and 2D antiferromagnet are shown in Figs.2-3. In the presence of the incoherent contribution, the region, where the linear dependence [28] holds, is sensitive to the value of $\delta$ and is not wide, especially in the 3D case; the width does not increase with further increasing $g$. However, a more exact consideration of spin dynamics may change considerably the results. Probably, using the spin diffusion approximation underestimates the coherence and the picture should be somewhat intermediate between solid and dashed lines.

4 The non-Fermi-liquid behavior in physical properties

Now we discuss the NFL behavior of physical properties for the most important case $N = 2$. The temperature dependences of magnetic moment and magnetic susceptibility in the PM case are obtained directly from the above results by the replacement $|C| \to T$,

$$
S_{ef}(T) \propto (T/T_K)^{2 \Delta}, \quad \chi_m \propto S_{ef}^2(T)/T \propto (T/T_K)^{2 \Delta}/T.
$$

(30)

However, unlike the one-impurity case, such dependences are somewhat smeared and take place only up to temperatures determined by (28). A similar dependence is obtained for specific heat [9].
As discussed above, the logarithmic factor in $\chi_m$ for $M=2$ ($\Delta=1/2$) is not described by our approach; an accurate treatment is obtained by more sophisticated methods, e.g., Bethe ansatz and conformal field theory.

In the spin-wave region for an AFM structure with the wavevector $Q$, we write down in terms of a retarded Green’s function

$$\chi_m = \lim_{q \to 0} \langle \langle S^z_q | S^z_q \rangle \rangle_{\omega \to 0} \propto \bar{S}/\bar{\sigma}. \quad (31)$$

On replacing $\bar{\sigma} \to \bar{\sigma}(C)$, $\bar{S} \to \bar{S}_{ef}(C)$ with $|C| \sim T$ in spirit of scaling arguments we obtain

$$\chi_m(T) \propto T^{-\zeta}, \quad \zeta = \left\{ \begin{array}{ll} (a - 1)/a, & \text{if } \delta R_m(T) \propto -T/T_K^2 \text{ is observed } \delta R_m(T) \propto g_{ef}(T) - g^* \propto -T/T_K^2 \text{ is observed } \end{array} \right. \quad (32)$$

for the regimes corresponding to (25) and (28), respectively. Note that the spin-wave description of the magnon-magnon interaction can be adequate not only in the AFM phase, but also for systems with a strong short-range magnetic order, including 2D and frustrated 3D systems at finite temperatures.

According to (67), the non-universal exponent $\zeta$ is determined by details of magnetic structure and can be both positive and negative. For a qualitative discussion, we can use Figs.2-3 and treat the difference $\delta = 2.10^{-4}$ as a perturbation.

Following to Ref. 14, the temperature dependence of the electronic specific heat in magnetic phases can be estimated from the spin-wave perturbation theory, $C_{el}(T)/T \propto 1/\Delta(T)$, where $\Delta(T)$ is the residue of the electron Green’s function at the distance $T$ from the Fermi level (cf. Ref. 17). Then we have in the AFM case

$$C_{el}(T)/T \propto g_{ef}^2(T)\bar{S}_{ef}(T)/\bar{\sigma}_{ef}(T) \propto \chi_m(T). \quad (33)$$

The dependence $C_{el}(T)/T \propto \chi_m(T)$ was obtained experimentally for a number of NFL systems 7,10. In the paramagnetic case the temperature correction to magnetic resistivity can be calculated from (13) as 9

$$\delta R_m(T) \propto g_{ef}(T) - g^* \propto -T/T_K^2 \text{ for } T \ll T_K. \quad (34)$$

The $T^{1/2}$ dependence (which corresponds to $M=2$) is indeed observed in a number of $f$-systems 10.

In the regime (28), the contribution to resistivity owing to scattering by spin fluctuations in AFM phase is given by

$$\delta R(T) \propto T^2 g_{ef}^2(T)\bar{S}_{ef}(T)/\bar{\sigma}_{ef}(T) \propto T^2 C_{el}(T)/T \propto T^{2-\zeta}. \quad (35)$$

For electron-electron scattering one has another temperature dependence.
5 Conclusions

To conclude, we have treated various mechanisms of the NFL behavior in the multichannel Kondo lattice. In comparison with one-impurity model, the lattice version provides a more rich picture. The NFL phenomenon seems to have a complicated nature being influenced by both single-site Kondo effect and spin dynamics. The corresponding dependences of physical properties can be different in different temperature intervals. Moreover, various scattering mechanisms can give different temperature dependences.

The most important result is occurrence of an intermediate coupling fixed point, which makes formation of reduced magnetic moment or even its vanishing in the NFL regime, the dependence on the bare coupling parameter being different. Scaling behavior of physical properties can be different in comparison with one-impurity model, the lattice version provides a more rich picture. The NFL phenomenon seems to be close to one-impurity model, the lattice version provides a more rich picture. The NFL phenomenon seems to be a consequence of the corresponding dependences of physical properties can be different in different temperature intervals. Moreover, various scattering mechanisms can give different temperature dependences.

The model used describes naturally formation of an intermediate phase with small moment value. Besides that, the model provides an example of essential renormalization of the effective coupling constant according to (15). This may be of interest for the general theory of metallic magnetism (in particular, for weak itinerant ferro- and antiferromagnets): the magnetic state is determined by the renormalization process rather than by bare Stoner-like criterion (cf. discussion in Ref. [18]).

An important problem is stability of the fixed point: lifting of the degeneracy of electron subbands with different $m$ in the Hamiltonian (1) should result in a change of scaling behavior, so that anomalous temperature dependences may take place in a restricted region.

Possible applications of the two-channel model to rare-earth and actinide systems, including corresponding difficulties of interpretation, are discussed in Ref. [19]. For uranium systems, application of this model is possible due to time-reversal symmetry of subbands.

The model used describes naturally formation of a magnetic state with small moment value. Besides that, the model provides an example of essential renormalization of the effective coupling constant according to (15). This may be of interest for the general theory of metallic magnetism (in particular, for weak itinerant ferro- and antiferromagnets): the magnetic state is determined by the renormalization process rather than by bare Stoner-like criterion (cf. discussion in Ref. [18]).

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Appendix A. Renormalization in the paramagnetic phase

The Kondo-lattice problem in the paramagnetic state describes the process of screening of localized magnetic moments. The correction to the effective magnetic moment is obtained from the static magnetic susceptibility [17,2]

\[
\chi_{\text{m}} = \frac{\text{S}_{\text{eff}}^2}{3T}, \quad \text{S}_{\text{eff}}^2 = S(S + 1)[1 - L] \quad (37)
\]

\[
L = 4MN/2 \int_{-\infty}^{\infty} d\omega \sum_{kq} \frac{n_{k\uparrow}(1 - n_{k\downarrow})}{(E - t_{k\uparrow} - \omega)^2}
\]

\[
\delta R(T) \propto T^2 [C_\text{eff}(T)/T]^2 \propto T^{2-2\eta}\quad (36)
\]

with $\mathcal{J}_q(\omega)$ the spectral density of the spin Green’s function for the Hamiltonian $H_I$, which is normalized to unity. We use the simple spin diffusion approximation

\[
\mathcal{J}_q(\omega) = \frac{1}{\pi} \frac{Dq^2}{\omega^2 + (Dq^2)^2} \quad (38)
\]

($D$ is the spin diffusion constant), which corresponds to dissipative spin dynamics.

The spin-fluctuation frequency in the paramagnetic phase is determined from the second moment of the spin Green’s function with the result [17,2]

\[
\delta \omega_q^2/\omega_q^2 = (1 - \alpha_q)\delta S_{\text{eff}}^2/S_{\text{eff}}^2 = -(1 - \alpha_q)L \quad (39)
\]

where $\alpha_q$ is expressed in terms of exchange integrals

\[
\alpha_q = \sum_{R} J_R^{\uparrow} \left( \sin \frac{k_F R}{R} \right)^2 \left[ 1 - \cos \frac{q R}{R} \right] / \sum_{R} J_R^{\uparrow} \left[ 1 - \cos \frac{q R}{R} \right] \quad (40)
\]

In the approximation of nearest neighbors at the distance $d$, $\alpha_q = \alpha = (e^{ikQ})_{g=0} = \left( \sin \frac{k_F d}{R} \right)^2$, so that we may use a single renormalization parameter. It should be stressed that we do not need here to search for higher order corrections to magnetic properties (leading corrections are already proportional to $M$).

To construct a self-consistent theory of Kondo lattices we have to find the renormalization of the effective $s - f$ exchange parameter. To this end, we calculate the Kondo correction to the electron self-energy with account of spin dynamics. We use the method of irreducible Green’s functions (see Ref. [20] and the review paper [21]) which enables one to construct a consistent perturbation expansion in a small parameter. We write down

\[
\Sigma_k(E) = \langle \langle \hat{c}_{k\sigma}, H_{\text{int}} \rangle \rangle \langle H_{\text{int}}, \hat{c}_{k\sigma}^\dagger \rangle \rangle_{\text{eff}} \quad (42)
\]

where $H_{\text{int}}$ is the $s - f$ interaction term. In the second order in $I$ we have

\[
\Sigma_k^{(2)}(E) = I^2 PR(E), \quad R(E) = \sum_q \frac{1}{E - t_{k\uparrow - q}} \quad (43)
\]

The next-order singular contributions read

\[
\Sigma_k^{(3)}(E) = -I^3 PN \int_{-\infty}^{\infty} d\omega \sum_{q,p} \mathcal{J}_q(\omega) \frac{n_{k\uparrow - q}}{(E - t_{k\uparrow - q} - \omega)^2} \times \left( \frac{1}{E - t_{k\uparrow - p}} - \frac{1}{t_{k\uparrow - q} - t_{k\uparrow - p}} \right) \quad (44)
\]

\[
\Sigma_k^{(4)}(E) = -I^4 P M N \sum_{q,p} \int_{-\infty}^{\infty} d\omega d\omega' \mathcal{J}_q(\omega) \mathcal{J}_{q' - p}(\omega') \times \left( \frac{1}{E - t_{k\uparrow - q} - \omega} \right)^2 \frac{n_{k\uparrow}(1 - n_{k\downarrow})}{(E - t_{k\uparrow - q} + t_{k\uparrow} - t_{k\downarrow} - \omega)(E - t_{k\uparrow - q} - \omega)} \quad (45)
\]
where \( P = 1 - 1/N^2 \), \( n_k = n(t_k) \) is the Fermi function. When neglecting spin dynamics Eqs. (13-15) agree with the one-impurity results [9]. The Kondo renormalization of the \( s-f \) parameter \( I \rightarrow I_f = I + \delta I_f \) is determined by “incorporating” \( \text{Im} \Sigma^{(3)}_k(E) \) into \( \text{Im} \Sigma^{(2)}_k(E) \). The imaginary parts required are simplified:

\[
- \text{Im} \Sigma^{(2)}_k(E) = \pi^2 P \rho \times \left( 1 - N \int_{-\infty}^{\infty} d\omega \sum_{q,\sigma} J_q(\omega / E - t_{k-q} - \omega) \right)
\]

\[
- MN^2 \int_{-\infty}^{\infty} d\omega d\omega' \sum_{q,\nu} J_q(\omega / E - t_{k-q} - \omega) \times \left( \frac{n_k(1 - n_k)}{(t_k - t_{k'}, - \omega + \omega')^2} \right) . \quad (46)
\]

Note that the structure of \( \text{Im} \Sigma^{(4)}_k(E) \) is similar to that for magnetic susceptibility and magnetic moment [37]. Averaging over \( t_k = t_k' = t_k = E_F = 0 \) we obtain to leading accuracy the result [10].

**Appendix B. Renormalization in magnetically ordered phases**

Now we investigate the renormalization of the \( s-f \) interaction in FM and AFM phases. For simplicity we treat only the \( s-f \) model with \( N = 2 \) (a more general case is discussed in Ref. [2]).

For a ferromagnet the electron spectrum possesses the spin splitting, \( E_{k\sigma} = t_k - \sigma M \bar{S} \). The second-order correction to \( I_f \) is determined by the corresponding electron self-energies:

\[
\delta I_f = [\Sigma^{FM}_k(E) - \Sigma^{FM}_k(E)]/(2\bar{S})
\]

which are defined by

\[
\sum_{m,n} \langle \psi_{k\sigma} | c_{k-m\sigma}^\dagger c_{k-n}\sigma \rangle_E = M/(E - t_k - \sigma \bar{S} - \Sigma_{k\sigma}(E))
\]

As described in Ref. [20], using equation-of-motion method, we write down the self-energy in terms of the irreducible Green’s function

\[
\Sigma_{k\sigma}(E) = I^2 \sum_{m,n} \langle S_q^{-}\sigma c_{k-q-m\sigma} + \sigma \delta S_q^{\dagger} c_{k-q+m\sigma} \rangle c_{k+p\sigma}^\dagger S_p \quad (48)
\]

with \( \delta \Lambda = \Lambda - \langle \Lambda \rangle \). Writing down the equations of motion for the Green’s function [18] we derive with account of singular terms

\[
\Sigma_{k\uparrow}(E) = 2I^2 \bar{S} \sum_{q} \frac{n_{k-q}}{E - t_{k-q} - \omega_q}
\]

\[
\Sigma_{k\downarrow}(E) = 2I^2 \bar{S} \sum_{q} \frac{1 - n_{k-q}}{E - t_{k-q} - \omega_q} \quad (49)
\]

The next-leading singular contribution, similarly to (43) (second term in the brackets), come from static correlators and are formally reduced to renormalization of occupation numbers:

\[
\tilde{n}_{k\uparrow} = n_{k\uparrow} - \frac{1}{S} \sum_{m\sigma} \langle c_{k+q\sigma}^\dagger c_{k}\sigma \rangle S_q^+ \quad (50)
\]

\[
\tilde{n}_{k\downarrow} = n_{k\downarrow} + \frac{1}{S} \sum_{m\sigma} \langle c_{k+q\sigma}^\dagger c_{k}\sigma \rangle S_q^- \quad (51)
\]

Calculating the corresponding Green’s function yields

\[
\langle \psi_{k\uparrow}^\dagger c_{k+q\uparrow} c_{k}\sigma \rangle \langle \psi_{k\uparrow} c_{k-q\uparrow}^\dagger c_{k}\sigma \rangle E = - \frac{2I^2}{\bar{S}} \frac{n_{k\uparrow} - n_{k+q\uparrow}}{\omega_q + \omega_{q'} + t_k - t_{k+q}} \quad (52)
\]

Using the spectral representation for the retarded Green’s function we obtain

\[
\langle \psi_{k\uparrow}^\dagger c_{k+q\uparrow} c_{k}\sigma \rangle \langle \psi_{k\uparrow} c_{k-q\uparrow}^\dagger c_{k}\sigma \rangle E = \int_{-\pi}^{0} d\omega d\omega' \left( \partial_{n_{k\uparrow}} \right) \frac{2I^2}{\bar{S}} \delta(\omega + t_k - t_{k+q}) \quad (53)
\]

the coefficient at the \( \delta \)-function being just the contribution of the layer \( f_{k+q} - f_k = \bar{C} \). Note that the correction to magnon frequency and magnetization can be obtained in the same manner via magnon damping (cf. Ref. [17]).

This just gives the singular correction to \( \Sigma^{(3)}_k(E) \). Note that this does not survive in the limit of large \( N \). At the same time, corrections to \( \Sigma^{(3)}_k(C) \) are absent since \( C = t_{k+q} \neq t_{k} \). The coefficient at \( \bar{C} \bar{S} \) is also present since \( \bar{C} \bar{S} \) is the Fermi function.

The correction to the magnon frequency is the same as in the one-loop consideration [2]

\[
\bar{\omega}_q/\omega_q = 2(1 - \bar{\alpha}_q) \bar{S}/S \quad (56)
\]

\[
\bar{\alpha}_q = \int_{R} \left| \psi_{kR}^R \right|^2 - \left| \psi_{kR}^{L} \right|^2 \left[ 1 - \cos qR \right] / \sum_{R} \int_{Q} \left[ 1 - \cos qR \right]
\]

For an antiferromagnetic structure with the wavevector \( Q \) the electron spectrum contains the AFM gap \( \bar{S} \)

\[
E_k = \frac{1}{2} (t_k + t_{k+Q}) \pm \frac{1}{4} (t_k - t_{k+Q})^2 + \bar{S}^2/2 \quad (58)
\]
The calculation of the off-diagonal self-energy gives (we consider for simplicity a two-sublattice system with \( \omega = \omega_q \pm q \))

\[
\Sigma^{AFM}_{k,k+q}(E) = \frac{1}{4} M^2 \sum_{m,q} \left( (S^+_{q} - S^-_{q}) c_{k-q,m \uparrow} \right)
\]

so that

\[
\delta E_{\text{loc}} = -\Sigma^{AFM}_{k,k+q}(E)/\mathcal{S}.
\]

The calculation of the off-diagonal self-energy gives (we consider for simplicity a two-sublattice system with \( \omega = \omega_q \pm q \))

\[
\Sigma^{AFM}_{k,k+q}(E) = \frac{1}{4} M^2 \sum_{m,q} \left( (S^+_{q} + S^-_{q}) c_{k-q,m \uparrow} + (S^+_{q} - S^-_{q}) c_{k-q,m \downarrow} \right)
\]

\[
-2\delta S^z_{k+q,m \downarrow} \langle q \rangle.
\]

The Green’s function needed is calculated as

\[
-\sum_{m,q} \left( (S^+_{q} + S^-_{q}) c_{k+q+m \uparrow} c_{k-m \downarrow} \right) / \omega
\]

\[
= \sum_{m,q} \left( (S^+_{q} - S^-_{q}) c_{k+q+m \uparrow} c_{k-m \downarrow} \right) / \omega
\]

\[
= 2M^2 \sum_{m,q} \left( \frac{\omega}{\omega^2 - \omega^2_{q} - \omega_{k+q} + \omega_k} \right)
\]

so that we obtain

\[
\delta(E^{(2)}_{\text{AFM}}(C))/\delta C = 2M^2 \sum_{k,k'} \delta(t_k) \delta(t_{k'}) \frac{C}{C^2 - \omega_{k-k'}}
\]

\[
\delta(E^{(3)}_{\text{AFM}}(C))/\delta C = -2M^3 \sum_{k,k',k''} \delta(t_k) \delta(t_{k'}) \delta(t_{k''}) \frac{C^3}{C^2 - \omega_{k-k'})(C^2 - \omega_{k'-k''})}
\]

in agreement with [10].

For the staggered AFM ordering in a cubic lattice with the dimensionality \( d \) one has [11]

\[\delta \omega/\omega = (1 - \alpha') \delta \omega/\omega,\]

\[\alpha' \approx 2(d - 1)/J^2 \frac{1}{J^2} \left| \exp(ikR_2) \right|_{t_k=0}^1 \]

where \( J_1 \) and \( J_2 \) are the exchange integrals between nearest and next-nearest neighbors (\(|J_1| \gg |J_2|\)). \( R_2 \) runs over the next-nearest neighbors.

**Appendix C. Scaling functions**

For the paramagnetic phase we have

\[\eta^{PM}(\overline{\omega}/C) = \text{Re} \int_{-\infty}^{\infty} d\omega \langle \mathcal{J}_{k-k'}(\omega) \rangle_{t_k=t_{k'}=E_F} \frac{1}{1 - (\omega + i0)/C}
\]

In the spin-diffusion approximation [38] we obtain

\[\eta^{PM}(\overline{\omega}/C) = \left( \frac{1}{1 + D(k-k')^2/C^2} \right)_{t_k=t_{k'}=0}
\]

where \( \overline{\omega} = 4Dk^2_F \), the averages go over the Fermi surface. Integration yields

\[\eta^{PM}(x) = \left\{ \begin{array}{ll}
\arctan x/x & d = 3 \\
\left\{ \frac{1}{2} \ln \left[ 1 + \left( 1 + x^2 \right) \right] \right\} & d = 2
\end{array} \right.
\]

In the FM and AFM phases for simple magnetic structures we have

\[\eta(\overline{\omega}_f/C, \delta) = \text{Re} \left( \frac{1 - (\omega - \omega_k - i\delta)^2/C^2}{(C^2 - \omega_k)} \right)_{t_k=t_{k'}=0}
\]

where \( \delta \) is a cutoff owing to damping. (Note that in the FM case with \( N > 2 \) this expression should be generalized since spin-up and spin-down contributions are asymmetric [2].) For an isotropic 3D ferromagnet integration in [71] for quadratic spin-wave spectrum \( \omega_k \propto q^2 \) yields

\[\eta^{FM}(x) = \left\{ \begin{array}{ll}
\frac{1}{4\pi} \ln \left[ \left( 1 + x^2 \right) + 2 \right] & d = 3 \\
\frac{1}{4\pi} \ln \left[ \left( 1 + i(x + \delta) \right)^2 \right] & d = 2
\end{array} \right.
\]

where \( x = \overline{\omega}_f/C, \omega = \omega_k F \).

For an antiferromagnet integration with the linear spin-wave spectrum \( \omega_k \propto q \) gives

\[\eta^{AFM}(x, z) = \left\{ \begin{array}{ll}
-(2x^2)^{-1} \ln \left[ (1 - x^2)^2 + 4\delta^2 \right] & d = 3 \\
\ln \left[ x^2 + (1 + i\delta)^2 \right]^{1/2} & d = 2
\end{array} \right.
\]

Thus \( \Psi \) becomes bounded from above:

\[\Psi_{\text{max}} = \eta_{\text{max}} \approx \eta(1) \approx \left\{ \begin{array}{ll}
\frac{1}{4\pi} \ln \delta & 3D \text{ FM} \\
\ln \delta & 3D \text{ AFM}
\end{array} \right.
\]

One can see that the scaling functions for the ordered phases contain Van Hove singularities at \( x = 1 \). Presence
of such singularities is a general property which does not depend on the spectrum model. The function \( \eta_{AFM}(x) \) \((d = 3)\) changes its sign at \( x = \sqrt{2} \). For \( d = 2 \), \( \eta_{AFM}(x) \) vanishes discontinuously at \( x > 1 \), but a smooth contribution occurs for more realistic models of magnon spectrum.

A more detailed analysis of the scaling function singularities is presented in Ref. [14].

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