# Non-Fermi-liquid behavior in Kondo lattices induced by peculiarities of magnetic ordering and spin dynamics

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A scaling consideration of the Kondo lattices is performed with account of singularities in the spin excitation spectral function. It is shown that a non-Fermi-liquid (NFL) behavior can be naturally connected with the regime which is marginal between the regions of strong coupling (Kondo lattice) and weak coupling ("usual" magnets). For complicated magnetic structures with several magnon branches, this regime occurs naturally between two critical values of the bare s-f coupling constant. Another kind of a NFL-like state (with different critical exponents) can occur for simple antiferromagnets with account of magnon damping, and for paramagnets, especially with two-dimensional character of spin fluctuations. The mechanisms proposed lead to some predictions about behavior of specific heat, resistivity, magnetic susceptibility, and anisotropy parameter, which can be verified experimentally. In particular, the Wilson ratio is predicted to weakly increase with lowering temperature.

#### I. INTRODUCTION

Recently, numerous experimental data have been obtained for anomalous *f* systems demonstrating so-called non-Fermiliquid (NFL) behavior.<sup>1,2</sup> Manifestations of the NFL behavior are unusual temperature dependences of magnetic susceptibility  $[\chi(T) \sim T^{-\zeta}, \zeta < 1]$ , electronic specific heat [C(T)/T]is proportional to  $T^{-\zeta}$  or  $-\ln T]$ , and resistivity  $[\rho(T) \sim T^{\mu}, 1 \le \mu < 2]$ , etc. Such a behavior is observed not only in alloys where disorder is present  $(U_x Y_{1-x} Pd_3, UPt_{3-x} Pd_x, CeCu_{6-x} Au_x, U_x Th_{1-x} Be_{13})$ , but also in some stoichiometric compounds, e.g.,  $Ce_7 Ni_3$ ,<sup>4</sup> CeCu\_2Si\_2, CeNi\_2Ge\_2,<sup>5</sup> UCu\_4Pd, UCu\_4Pt.<sup>6</sup> The latter situation is most interesting from the physical point of view.<sup>7</sup>

There are a number of theoretical mechanisms proposed to describe the NFL state: two-channel Kondo scattering,<sup>8–10</sup> "Griffiths singularities" in disordered magnets,<sup>11,6</sup> strong spin fluctuations near a quantum magnetic phase transition,<sup>12–15</sup> etc. Most of modern treatments of the NFL problem have a semiphenomenological character. The only microscopic model where formation of the NFL state is proven—the one-impurity two-channel Kondo model seems to be insufficient, since important role of intersite interactions is now a matter of common experience.<sup>1</sup>

In the present paper we start from the standard microscopic model of a periodical Kondo lattice. Main role in the physics of the Kondo lattices belongs to the interplay of the on-site Kondo screening and intersite exchange interactions. This interplay leads to the mutual renormalization of the characteristic energy scales: the Kondo temperature  $T_K$  and spin-fluctuation frequency  $\overline{\omega}$ . It was shown in our previous papers<sup>16–18</sup> that, depending on the model parameters, this may result in either entering strong-coupling region (the coupling constant diverges at a finite energy scale, i.e., effective Kondo temperature  $T_K^*$ ) or formation of magnetic state with partially suppressed moments. Here we consider the case of more complicated (but realistic) spin dynamics, presence of several singularities of spin spectral function being of crucial importance. In that case a marginal situation is demonstrated to occur, where the coupling constant does not diverge at a finite scale, but becomes infinite exactly at the Fermi surface. As a consequence, "soft" boson branches are formed during the renormalization process. Scattering of electrons by such soft collective excitations just leads to the formation of the NFL state (see Ref. 15).

In Sec. II the renormalization group (scaling) equations are presented. In Sec. III we consider the antiferromagnetic (AFM) state with account of the spin-wave damping and the paramagnetic state with simple spin-diffusive dynamics. It turns out that in these cases a NFL-like behavior (in a restricted temperature interval) is possible, especially in the case of quasi-two-dimensional (2D) spin fluctuations. In Sec. IV we consider the general problem of singularities of the scaling function. In Sec. V we show that the NFL behavior up to lowest temperatures can be naturally obtained provided that we take into account magnonlike excitations in the case of a complicated spin dynamics. The excitation picture required is characteristic for real f systems where several excitation branches exist. In Sec. VI we discuss various physical properties. Possible relation to experimental data is considered in Sec. VII.

#### **II. THE SCALING EQUATIONS**

To describe a Kondo lattice, we use the s-f exchange model

$$H = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} - I \sum_{i\alpha\beta} \mathbf{S}_{i} \boldsymbol{\sigma}_{\alpha\beta} c_{i\alpha}^{\dagger} c_{i\beta} + \sum_{\mathbf{q}} J_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \mathbf{S}_{\mathbf{q}} + H_{a},$$
(1)

where  $t_{\mathbf{k}}$  is the band energy,  $\mathbf{S}_i$  and  $\mathbf{S}_{\mathbf{q}}$  are spin-density operators, and their Fourier transforms, I is the *s*-*f* exchange parameter,  $J_{\mathbf{q}}$  are the intersite exchange parameters,  $\sigma$  are the Pauli matrices,  $H_a$  is the anisotropy Hamiltonian which results in occurrence of the gap  $\omega_0$  in the spin-wave spectrum. As well as in Refs. 16–18, we investigate the interplay

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of the Kondo effect and intersite interactions by the renormalization group approach. The latter starts from the secondorder perturbation theory with the use of the equation-ofmotion method (within the diagram technique in the pseudofermion representation for the spin operators, such an approximation corresponds to the one-loop scaling).

We apply the "poor man scaling" approach.<sup>19</sup> In this method one considers the dependence of effective (renormalized) model parameters on the flow cutoff parameter  $C \rightarrow$ -0 (here and hereafter the energy is referred to the Fermi energy  $E_F=0$ ) which occurs at picking out the Kondo singular terms. The relevant variables are the effective (renormalized) parameter of s-f coupling  $g_{ef}(C) = -2\rho I_{ef}(C)$  ( $\rho$ is the bare density of electron states at the Fermi level), characteristic "exchange" spin-fluctuation energy  $\bar{\omega}_{ex}(C)$ , gap in the spin-wave spectrum  $\omega_0(C)$ , and magnetic moment  $\overline{S}_{ef}(C)$ . The derivation of the scaling equations is described in detail in Ref. 17. In the magnetically ordered phase,  $\overline{\omega}_{ex}$  is the magnon frequency  $\omega_q$ , which is averaged over the wave vectors q=2k where k runs over the Fermi surface; in the case of dissipative spin dynamics (paramagnetic phase)  $\bar{\omega}_{ex}$ is determined by the second moment of the spin spectral density. Here we write down the set of scaling equations with account of the spin-wave damping  $\overline{\gamma}(C)$  which is determined from the imaginary part of the magnon polarization operator (see the next section). In this sense, the following equations generalize Eqs. (31)–(34) from Ref. 17:

$$\partial g_{ef}(C)/\partial C = \Lambda, \partial \ln \overline{S}_{ef}(C)/\partial C = -\Lambda/2,$$
 (2)

$$\partial \ln \bar{\omega}_{\text{ex}}(C) / \partial C = -a\Lambda/2, \partial \ln \omega_0(C) / \partial C = -b\Lambda/2, \quad (3)$$

$$\partial \ln \bar{\gamma}(C) / \partial C = -c \Lambda/2$$
 (4)

with

$$\Lambda = \Lambda [C, \overline{\omega}_{\text{ex}}(C), \omega_0(C)]$$
$$= \frac{g_{\text{ef}}^2(C)}{|C|} \eta \left( \frac{\overline{\omega}_{\text{ex}}(C)}{|C|}, \frac{\omega_0(C)}{|C|}, \frac{\overline{\gamma}(C)}{|C|} \right), \tag{5}$$

 $a=1-\alpha$  for the paramagnetic (PM) phase,  $a=1-\alpha', b=1$ for the antiferromagnetic (AFM) phase,  $a=2(1-\alpha''), b=2$ for the ferromagnetic (FM) phase;  $\alpha, \alpha', \alpha''$  are some averages over the Fermi surface (see Ref. 17); the quantity *c* is discussed below. The scaling function  $\eta$  is determined by

$$\eta = \operatorname{Re} \int_{-\infty}^{\infty} d\omega \langle \mathcal{J}_{\mathbf{k}-\mathbf{k}'}(\omega) \rangle_{t_{\mathbf{k}}=t_{\mathbf{k}'}=0} \frac{1}{1 - (\omega + i0)/C}, \quad (6)$$

where the electron spectrum  $t_{\mathbf{k}}$  is referred to the Fermi energy,  $\mathcal{J}_{\mathbf{q}}(\omega)$  is the normalized spectral density of the transverse spin susceptibility  $\chi^{+-}(\mathbf{q},\omega)$ , (for the AFM phase, in the local coordinate system). Equations that are similar to Eqs. (2)–(4) can be obtained for the Coqblin-Schrieffer model<sup>17</sup> and in the case of anisotropic *s*-*f* coupling.<sup>18</sup>

Further we shall need the expression for  $\alpha'$  in the case of the staggered AFM ordering for the 2D and 3D cubic lattices where

$$_{\mathbf{q}} = 2J_{1}\sum_{i=1}^{d} \cos q_{i} + 4J_{2}\sum_{i>j}^{d} \cos q_{i} \cos q_{j}$$

with  $J_1$  and  $J_2$  being the exchange integrals between nearest and next-nearest neighbors  $(|J_1| \ge |J_2|)$ . By averaging the Kondo correction to the magnon frequency (see Refs. 17,18) over the Fermi surface and using the expansion in small wave vectors q one can derive

$$\alpha' \simeq 2(d-1) \frac{J_2}{J_1} |\langle \exp(i\mathbf{k}\mathbf{R}_2) \rangle_{t_{\mathbf{k}}=0} |^2,$$
 (7)

where  $\mathbf{R}_2$  runs over the next-nearest neighbors.

Using Eqs. (2)-(4) we obtain the explicit expressions

$$\overline{\omega}_{ex}(C) = \overline{\omega}_{ex} \exp(-a[g_{ef}(C) - g]/2),$$

$$\omega_0(C) = \omega_0 \exp(-b[g_{ef}(C) - g]/2),$$

$$S_{ef}(C) = S \exp(-[g_{ef}(C) - g]/2),$$

$$\overline{\gamma}(C) = kg_{ef}^2(C)\overline{\omega} \exp[-c[g_{ef}(C) - g]/2].$$
(8)

In the last equation of Eq. (8), we have taken into account that the magnon damping is proportional to  $g^2$ ,  $\bar{\gamma} = kg^2\bar{\omega}$  (the factor *k* is determined by the bandstructure and magnetic ordering), and the scaling equations should contain only renormalized quantities.

One can see from Eqs. (8) that the behavior of all the relevant variables is determined by a single function  $g_{ef}(\xi)$ for the sake of convenience we introduce the variable  $\xi$  $\equiv \ln |D/C|$ , the scale D of order of the electron bandwidth being defined by  $g_{ef}(-D) = g$ ]. Generally speaking, depending on the bare model parameters, two simplest situations are possible: (i)  $g_{ef}(\xi)$  diverges at  $\xi = \xi^* = \ln(D/T_K^*)$ . Within our approach, that is based on perturbation theory, one cannot describe the scaling behavior of the system at  $\xi > \xi^*$ . By analogy with the exact results for the one-impurity Kondo problem, one can propose that the formation of a heavyfermion state takes place with a characteristic energy scale  $T_K^*$ . It should be noted that  $T_K^*$  can differ considerably from  $T_K$ , see Ref. 17. (ii)  $g_{ef}(\xi)$  remains finite at arbitrary  $\xi$ . This case corresponds to the usual magnet with local moments which are partially suppressed owing to the Kondo effect.

It is clear that a NFL behavior is in a sense intermediate between these cases. In particular, one has to expect for the magnetic susceptibility  $\chi(T) \propto 1/T_K^* = \text{const}(T)$  in the case (i), and  $\chi(T) \propto 1/T$  in the case (ii), whereas  $\chi(T) \propto T^{-\zeta}, 0$  $<\zeta < 1$  in the NFL state. Below we demonstrate that the NFL behavior can be associated with the marginal behavior of  $g_{ef}(\xi)$ , where  $g_{ef}(\xi) \rightarrow \infty$  at  $\xi \rightarrow \infty$ . Alternatively, the increase of  $g_{ef}(\xi)$  can take place in a wide  $\xi$  region. Of course, details of description of such situations in our approach (e.g., concrete exponents in the temperature dependences of physical characteristics) are not quite reliable, since higher-order corrections to the scaling function (beyond the one-loop approximation) may be important. However, it is natural to expect that the fact of existence of the marginal regime is reproduced correctly by the lowest-order scaling. Therefore we believe that our approach enables one, at least, to indicate physical factors which are favorable for the NFL state. In the next sections we consider concrete scenarios of the marginal behavior.

### III. THE SCALING BEHAVIOR IN THE PRESENCE OF DAMPING

As demonstrated in Ref. 17, the singularities of the scaling function  $\eta$  can result in occurrence of a NFL behavior in a restricted region due to fixing of the argument of the function  $\eta$  at the singularity during the scaling process, so that  $\overline{\omega}(C) \simeq |C|$ ,

$$g_{ef}(\xi) - g \simeq 2(\xi - \lambda)/a, \lambda \equiv \ln(D/\bar{\omega}).$$
(9)

This region becomes not too narrow only provided that the bare coupling constant  $g = -2I\rho$  is very close to the critical value  $g_c$  for the magnetic instability  $(|g - g_c|/g_c \sim 10^{-4} - 10^{-6})$ . Here we treat the scaling process with account of a not too small magnon damping  $\gamma_q$  (only very small damping was introduced in Ref. 17 to provide existence of the magnetic-nonmagnetic ground-state transition at  $g = g_c$ ).

Consider the scaling function  $\eta$  in the FM and AFM phases for simple magnetic structures. We use the expression for the spectral density, corresponding to the case of one magnon mode

$$\mathcal{J}_{\mathbf{q}}(\omega) = \frac{\gamma_{\mathbf{q}}}{\pi} \frac{1}{(\omega - \omega_{\mathbf{q}})^2 + \gamma_{\mathbf{q}}^2}.$$
 (10)

Substituting this into Eq. (6), we obtain

$$\eta(\bar{\omega}_{ex}/|C|,\bar{\gamma}/|C|) = \operatorname{Re}\langle (1 - (\omega_{\mathbf{k}-\mathbf{k}'} + i\gamma_{\mathbf{k}-\mathbf{k}'})^2/C^2)^{-1} \rangle_{t_k = t_{k'} = 0}$$
(11)

(for simplicity, magnetic anisotropy is neglected in this section). For an isotropic three-dimensional (3D) ferromagnet integration in Eq. (11) for  $\gamma_q = \text{const}$  and quadratic spin-wave spectrum yields

$$\eta(x,z) = \frac{1+z^2}{4x} \ln \frac{(1+x)^2 + z^2}{(1-x)^2 + z^2} + \frac{1+x}{z} \arctan \frac{z}{1+x} - \frac{1-x}{z} \arctan \frac{z}{1-x},$$
(12)

where  $x = \overline{\omega}_{ex}/|C|, z = \overline{\gamma}/|C|$ . Note that last two terms in Eq. (12) play a role similar to that of the "incoherent" contribution to the function  $\eta$ , which was treated in Ref. 17.

For a 3D antiferromagnet integration in Eq. (11) for the linear spin-wave spectrum gives

$$\eta(x,z) = \frac{1}{2} \operatorname{Re}[(1+iz)\ln(1+x+iz) + (1-iz)\ln(1+x-iz)], \quad (13)$$

where we take into account the intersubband damping only,

$$\gamma_{\mathbf{q}} = \pi 2 I^2 \overline{S} (J_{\mathbf{q}} - J_{\mathbf{Q}}) \rho^2 \lambda_{\mathbf{q} + \mathbf{Q}}, \qquad (14)$$



FIG. 1. The scaling trajectories  $g_{ef}(\xi)$  in isotropic 2D antiferromagnets (solid lines,  $g=0.154 < g_c$ ,  $g=0.155 > g_c$ ) and 3D antiferromagnets (dashed lines,  $g=0.139 < g_c$ ,  $g=0.140 > g_c$ ) with k=0.5, a=c=1,  $\lambda = \ln(D/\bar{\omega}) = 5$ .

$$\lambda_{\mathbf{q}} = \rho^{-2} \sum_{\mathbf{k}} \delta(t_{\mathbf{k}}) \delta(t_{\mathbf{k}+\mathbf{q}}). \tag{15}$$

The damping (14) can be put nearly constant at not too large q (the threshold value determined by the AFM gap can be neglected due to formal smallness in I). In the 2D AFM case we obtain in the same approximation

$$\eta(x,z) = \frac{\nu^3(x,z)}{\nu^4(x,z) + z^2},$$
(16)  

$$\nu^2(x,z) = \frac{1}{2} [1 - x^2 + \sqrt{(1 - x^2)^2 + 4z^2}].$$

These expessions modify somewhat the cutoff procedure made in Ref. 17.

The function  $\lambda_q$  determines, in particular, the factor k in Eq. (8). For a parabolic electron spectrum we obtain

$$\lambda_{\mathbf{q}} = \frac{\theta(1-x)}{zx} \times \begin{cases} 1/6, & d=3, \\ (4\pi)^{-1}(1-x^2)^{-1/2}, & d=2, \end{cases}$$
(17)

where  $x = q/2k_F$ ,  $\theta(x)$  is the step function, z is the electron concentration (with both spin projections).

The main Kondo renormalization of the magnon damping comes from its proportionality to the factor of  $\overline{S}$ . Spin fluctuations can give correction to this factor, as well as for the magnon frequency.<sup>17</sup> For simplicity, we restrict ourselves in numerical calculations to the AFM case with  $\delta \gamma_q / \gamma_q$  $= \delta \omega_q / \omega_q = \delta \overline{S} / S$ , so that c = 1 in Eqs. (4), (8). The corresponding scaling trajectories are shown in Fig. 1. One can see that, unlike Ref. 17, the "linear" behavior, although being somewhat smeared, is pronounced in a considerable region of  $\xi$  for not too small  $|g - g_c|$ , especially in the 2D case. In the 3D case the linear region (9) is followed by a quasilinear behavior with

$$g_{ef}(\xi) \simeq A(\xi - \lambda), \overline{\omega}(C) \propto |C|^{aA/2}, \overline{S}_{ef}(C) \propto |C|^{A/2}, \quad (18)$$

where A < 2/a.

To investigate the latter behavior in more details, it is instructive to consider also the case of a paramagnet with pure dissipative dynamics. In the case of spin-diffusion behavior we have (see Ref. 17)



FIG. 2. The scaling trajectories  $g_{ef}(\xi)$  in 2D (solid lines) and 3D (dashed lines) paramagnets with  $a=1/2,\lambda=5$ . The bare coupling parameters are g=0.135 and g=0.145, higher curves corresponding to larger g. The values of  $g_c$  in 2D and 3D cases are 0.148 and 0.152.

$$\eta^{PM}\left(\frac{\bar{\omega}}{C}\right) = \sum_{\mathbf{q}} \lambda_{\mathbf{q}} [1 + (\mathcal{D}q^2/C)^2]^{-1}, \bar{\omega} = 4\mathcal{D}k_F^2, \quad (19)$$

where  $\mathcal{D}$  is the spin diffusion constant. As demonstrate numerical calculations (see Fig. 2), for  $g \leq g_c$  the one-impurity behavior  $1/g_{ef}(\xi) = 1/g - \xi$  is changed at  $\xi \simeq \lambda$  by the behavior (18) with

$$A \simeq [g_{ef}(\lambda)]^2 \Psi(0), g_{ef}(\lambda) \simeq g/(1 - \lambda g), \Psi(0) = \eta(1) \sim 0.5.$$
(20)

In the 3D case where  $\eta^{PM}(x) = \arctan x/x$  the quasi-linear NFL-like behavior  $g_{ef}(\xi)$  takes place in a rather narrow region. However, in the 2D case we obtain

$$\eta^{PM}(x) = \left[\frac{1 + (1 + x^2)^{1/2}}{2(1 + x^2)}\right]^{1/2}$$
(21)

and the NFL-like region becomes more wide due to a more slow decrease of  $\eta^{PM}(x)$  at  $x \to \infty$ . Note that such regions are not observed for  $g > g_c$ .

#### **IV. SINGULARITIES OF THE SCALING FUNCTION**

To get further insight into the NFL-behavior problem, we perform a general analysis of singularities of the scaling function  $\eta$ . In the absence of damping, after averaging over the Fermi surface we can rewrite Eq. (11) as

$$\eta(\overline{\omega}_{ex}/|C|,\omega_0/|C|) = \sum_{\mathbf{q}} \lambda_{\mathbf{q}}(1-\omega_{\mathbf{q}}^2/C^2)^{-1}.$$
 (22)

The singularities of  $\eta$  correspond to the Van Hove singularities in the magnon spectrum and to the boundary points q = 0 and  $q = 2k_F$ .

For  $q \rightarrow 2k_F$  the magnon spectrum has the Kohn anomaly

$$\delta\omega_{\mathbf{q}} \propto \begin{cases} (q-2\dot{k}_F)\ln|q-2k_F|, & d=3, \\ \sqrt{q^2-4k_F^2}\theta(q-2k_F), & d=2. \end{cases}$$
(23)

Taking into account the dependences (17), which hold qualitatively in a general situation, we obtain for  $v = C^2 - \bar{\omega}^2 \rightarrow 0$ 

$$\eta(v) \propto \begin{cases} \ln \ln |v|, & d=3, \\ \theta(v)v^{-1/2}, & d=2. \end{cases}$$
(24)

Note that the singularity of the form  $\ln v$  obtained for the 3D case in Ref. 17 (see also previous section), is a consequence of a simplified "Debye" model of the magnon spectrum. In fact, such a dependence corresponds qualitatively to an intermediate asymptotics at approaching the singularity. In any case, a small damping of spin excitations should be introduced to cut the singularity. In the calculations below we put the damping parameter  $\delta = 1/100$  (see Ref. 17). In fact, pronounced extrema of  $\eta$ , but not singularities themselves turn out to be important for the scaling behavior discussed below.

For  $q \to 0$  we have  $\lambda_q \propto q^{-1}$ . Near the points of minimum (maximum) in the magnon spectrum we have  $\omega_q^2 - \omega_m^2 \propto \pm q^2$ , and for  $v = C^2 - \omega_m^2 \to 0$  we obtain

$$\eta(v) \propto \begin{cases} \pm \ln|v|, & d=3, \\ \mp \theta(\mp v)|v|^{-1/2}, & d=2 \end{cases}$$
(25)

so that  $\eta \rightarrow -\infty$  near the band bottom and  $\eta \rightarrow +\infty$  near the band top. The Van Hove singularities in the magnon band at  $\omega = \omega_c$  for  $q \neq 0$  yield weaker singularities in  $\eta(v)$  ( $|v|^{1/2}$  for d=3 and a finite jump for d=2) and will not be treated below.

#### V. THE SCALING PICTURE AND NFL BEHAVIOR IN MANY-SUBLATTICE MAGNETS

Using the results of the previous section we can propose a rather realistic and universal mechanism of the NFL behavior. Suppose that the spin excitation spectrum contains several branches which make additive contributions to the function  $\eta$ .

As a simple model example we can consider a twosublattice ferrimagnet with the localized-system Hamiltonian

$$H_{f} = \sum_{i \in A, j \in A} J_{ij} \mathbf{S}_{i} \mathbf{S}_{j} + \sum_{i \in B, j \in B} J'_{ij} \mathbf{S}_{i} \mathbf{S}_{j} + \sum_{i \in A, j \in B} \widetilde{J}_{ij} \mathbf{S}_{i} \mathbf{S}_{j}$$
$$= \sum_{\mathbf{q}} (J_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \mathbf{S}_{\mathbf{q}} + J'_{\mathbf{q}} \mathbf{S}'_{-\mathbf{q}} \mathbf{S}'_{\mathbf{q}} + \widetilde{J}_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \mathbf{S}'_{\mathbf{q}}), \qquad (26)$$

the *s*-*f* exchange interaction being taken into account only at one sublattice A (spins without primes). Similar to Eq. (22) we obtain

$$\eta = \sum_{\mathbf{q},i=1,2} \lambda_{\mathbf{q}} \frac{\omega_{\mathbf{q}i}}{B_{\mathbf{q}}} \left( 1 - \frac{\omega_{\mathbf{q}i}^2}{C^2} \right)^{-1}, \tag{27}$$

where

$$B_{\mathbf{q}} = \{ [S(J_{\mathbf{q}} - J_{0}) + S'(J'_{\mathbf{q}} - J'_{0}) - (S + S')\tilde{J}_{0}]^{2} - 4SS'\tilde{J}_{\mathbf{q}}^{2} \}^{1/2},$$

$$(28)$$

$$\omega_{\mathbf{q}1,2} = B_{\mathbf{q}} \mp |S(J_{\mathbf{q}} - J_{0}) - S'(J'_{\mathbf{q}} - J'_{0}) + (S - S')\tilde{J}_{0}|$$

are the acoustical and optical modes.

The dependence

$$\Psi(\xi) = \sum_{i} z_{i} \eta_{i} [(\bar{\omega}_{ex,i}/D) e^{\xi}, (\omega_{0,i}/D) e^{\xi}]$$
(29)



FIG. 3. The scaling functions  $\Psi(\xi)$  defined by Eq. (29) in the case of a 3D antiferromagnet with two excitation modes. The parameters are  $z_1 = 0.4$ ,  $z_2 = 0.6$ ,  $\ln(D/\bar{\omega}_2) = 4$ ,  $\bar{\omega}_2/\bar{\omega}_1 = 3$ ,  $\omega_{0,1}/\bar{\omega}_{ex,1} = 0.2$ ,  $\omega_{0,2}/\bar{\omega}_{ex,2} = 0.6$  ( $\bar{\omega}_i^2 = \bar{\omega}_{ex,i}^2 + \omega_{0,i}^2$ ).

is shown in Fig. 3 for the case of two excitation modes in a 3D antiferromagnet (the expressions for the function  $\eta_i$  in the case of one mode with inclusion of anisotropy are given in Ref. 18). The only property of the function  $\Psi$ , which will be important below, is the occurrence of the *second* zero with decreasing |C| (or increasing  $\xi$ ). This property follows immediately from existence of the 'positive' singularity in  $\Psi$  near the maximum frequency of the lower branch and of the 'negative' singularity near the minimum frequency of the upper branch [e.g., for  $\omega_1(q=2k_F) < \omega_2(q=0)$ ]. One can expect that this is a general property of many-sublattice magnets. The singularities can be also connected with the crystal-field excitations.<sup>3</sup>

As demonstrate both numerical calculations and analytical treatment, in some interval of the bare coupling parameter,  $g_{c1} < g < g_{c2}$ , the argument of the function  $\Psi$  becomes fixed at the second zero,  $C = C_0$ , during the scaling process which is described by Eq. (2). This can be illustrated for the simple case where a = b for all the modes (e.g., for an antiferromagnet in the nearest-neighbor approximation we have a = b = 1). On substituting Eq. (8) into Eq. (2) we obtain

$$\partial (1/g_{ef})/\partial \xi = -\Psi(\xi - a[g_{ef} - g]/2).$$
 (30)

Then we derive

$$g_{ef}(\xi \to \infty) \simeq (2/a)(\xi - \xi_0) - 1/[\Psi'(\xi_0)\xi^2],$$
 (31)

where  $\xi_0 \sim \ln(D/\bar{\omega})$  is the second zero of the function  $\Psi(\xi)$ . Note that the first zero does not work since the unrestricted increase of  $g_{ef}$  corresponds to a decrease of the argument of the function  $\Psi$  in Eq. (30), so that  $\Psi \rightarrow +0$ . According to Eq. (8) we obtain

$$\overline{\omega}_{\text{ex}}(C), \omega_0(C) \propto |C|, \overline{S}_{ef}(C) \propto |C|^{1/a}.$$
(32)

Within the approach used, the behavior (31), (32) takes place up to  $C=0(\xi=\infty)$ . As discussed in Sec. II, the one-loop scaling equations themselves may become invalid with increasing  $g_{ef}$ , but the tendency to the formation of the "soft" magnon mode seems to be physically correct. The scaling picture for three possible cases is shown in Fig. 4. One can see that the interval  $[g_{c1}, g_{c2}]$  where the NFL behavior occurs is not too small, unlike Ref. 17.

In a more general case, where  $a \neq b$  and the exponents in Eq. (3) differ for different frequencies, the linear *C* depen-



FIG. 4. The scaling trajectories  $g_{ef}(\xi)$  in a 3D antiferromagnet with the parameters of Fig. 3 and  $a_i = b_i = 1$ . The bare coupling parameters are  $g = 0.158 \approx g_{c2}$  (upper solid line with the asymptotics),  $g = 0.154 \approx g_{c1}$  (lower solid line), and  $g_{c1} < g = 0.156 < g_{c2}$  (dashed line).

dence takes place only for the total characteristic frequency  $\bar{\omega}$  (e.g., for an anisotropic antiferromagnet with one mode we have  $\bar{\omega}^2 = \omega_0^2 + \bar{\omega}_{ex}^2$ ), and the behavior  $g_{ef}(\xi)$  and  $\bar{S}_{ef}(\xi)$  is more complicated. As follows from Eq. (7), for the AFM state with small next-nearest exchange interactions the case of small |a-1| and b=1 is realized.

### VI. NFL BEHAVIOR OF PHYSICAL PROPERTIES

Consider the temperature dependence of the magnetic susceptibility. In the spin-wave region we have for an AFM structure with the wave vector  $\mathbf{Q}$ 

$$\chi = \lim_{q \to 0} \langle \langle S_{\mathbf{q}}^{x} | S_{-\mathbf{q}}^{x} \rangle \rangle_{\omega=0} = (J_{0} - J_{\mathbf{Q}})^{-1} \propto \overline{S} / \overline{\omega}.$$
(33)

One can assume that the spin-wave description of the electron-magnon interaction is adequate not only in the AFM phase, but also for systems with a strong short-range AFM order (e.g., for 2D and frustrated 3D systems at finite temperatures). Using the scaling arguments we can replace  $\bar{\omega} \rightarrow \bar{\omega}(C), \bar{S} \rightarrow \bar{S}_{ef}(C)$  with  $|C| \sim T$ , which yields

$$\chi(T) \propto T^{-\zeta}, \zeta = (a-1)/a. \tag{34}$$

According to Eq. (7), the nonuniversal exponent  $\lambda$  is determined by details of magnetic structure and can be both positive and negative. For a qualitative discussion, we can still use Fig. 4 and treat the difference a-1 as a perturbation. The increase of  $\chi(T \rightarrow 0)$  (which is usually called NFL behavior) takes place for a > 1 and, as follows from Eq. (8), corresponds to an increase of magnetic anisotropy parameter with lowering T (see Ref. 18). Such a correlation may be verified experimentally. The negative  $\zeta$  values correspond to an anomalous power-law temperature dependence  $\chi(T)$ . It should be noted that corrections to  $\chi(T)$  and  $C_{el}(T)/T$  that are proportional to  $T^{1/2}$ , are discussed sometimes for some f-systems, e.g.,  $U_x Y_{1-x} P d_3$ ,<sup>1</sup> but picking out them is not unambiguous (see the fittings of experimental data in Refs. 1 and 6).

The temperature dependence of electronic specific heat can be estimated from the second-order perturbation theory,

TABLE I. Scenarios of the NFL behavior (the values of the exponent  $\zeta$ ) in various magnetic phases.

	3D AFM (two regions)	2D AFM	РМ	AFM, several branches
a-1 $\zeta$	both signs $(a-1)/a$ , $(a-1)A/2$	both signs $(a-1)/a$	<0 ( <i>a</i> -1) <i>A</i> /2<0	both signs $(a-1)/a$

 $C_{\rm el}(T)/T \propto 1/Z(T)$  where Z(T) is the residue of the electron Green's function at the distance *T* from the Fermi level (see Ref. 20). Then we have

$$C_{\rm el}(T)/T \propto g_{ef}^2(T)\overline{S}_{ef}(T)/\overline{\omega}_{\rm ex}(T) \propto \chi(T) \ln^2(T/T^*),$$
(35)

where  $T^*$  is a characteristic energy scale (crossover temperature in the scaling process). With decreasing temperature, the Wilson ratio

$$W(T) = T\chi(T)/C_{\rm el}(T) \propto \ln^{-2}(T/T^*)$$
 (36)

should decrease with lowering  $T(T \le T^*)$ .

Generally, the temperature behavior of magnetic characteristics ( $\overline{S}$  and  $\overline{\omega}$ ), which depend exponentially on the coupling constant, is decisive for our NFL mechanisms. The transport relaxation rate determining the temperature dependence of the resistivity owing to scattering by spin fluctuations in AFM phase is given by<sup>22</sup>

$$\frac{1}{\tau} = \frac{2\pi}{v_F^2} I^2 \overline{S}^2 (J_0 - J_{\mathbf{Q}}) \rho \langle (\mathbf{v}_{\mathbf{k}+\mathbf{Q}} - \mathbf{v}_{\mathbf{k}})^2 \rangle_{t_{\mathbf{k}}=0} \sum_{\mathbf{q} \approx \mathbf{Q}} \lambda_{\mathbf{q}} \left( -\frac{\partial N_{\mathbf{q}}}{\partial \omega_{\mathbf{q}}} \right).$$
(37)

Then we obtain

$$\frac{1}{\tau} \propto g_{ef}^2(T) \overline{S}_{ef}(T) / \overline{\omega}_{ex}(T) T^2 \propto T^2 C_{el}(T) / T \propto T^{2-\zeta}.$$
 (38)

Considering electron-electron scattering as the main scattering mechanism one can expect another temperature dependence, namely,

$$\frac{1}{\tau} \propto [\rho/Z(T)]^2 T^2 \propto T^2 [C_{\rm el}(T)/T]^2 \propto T^{2-2\zeta}.$$
 (39)

One can expect that the dependence close to Eq. (38) should hold in localized-moment systems, and that close to Eq. (39) in itinerant-electron compounds.

As for paramagnets with purely dissipative spin dynamics, the value of  $\zeta$  is always negative since a < 1. Thus, to produce NFL behavior with positive  $\zeta$ , spin dynamics should include strong spin fluctuations (short-range order, sufficiently well defined spin waves). The temperature dependences of specific heat, magnetic susceptibility and resistivity in the case of a NFL-like behavior considered in Sec. III differ from those discussed above by the value of  $\zeta = (a - 1)A/2$  (for the second "linear" region).

The results for the exponent  $\zeta$  in various magnetic phases are summarized in Table I. Remember once more that the corresponding behavior takes place in a restricted region, except for the AFM case with several excitation branches.

## VII. DISCUSSION OF EXPERIMENTAL DATA AND CONCLUSIONS

Now we discuss relevant experimental data on the anomalous *f* systems. They demonstrate indeed pronounced spin fluctuations. These can have quasi-2D nature, see, e.g., data of Refs. 15,21,23 for the systems  $\text{CeCu}_{6-x}\text{Au}_x$  and  $\text{CePd}_2\text{Si}_2$ . Note that for other compositions the first system demonstrates complicated magnetic ordering.<sup>24</sup> According to Ref. 25, for x=0.45 the system  $U_xY_{1-x}\text{Pd}_3$  has antiferromagnetic ordering with  $T_N \approx 20$  K and the saturation moment about  $1 \mu_B$ . The inelastic neutron scattering demonstrates existence of several branches in spin excitation spectrum, which is probably connected with crystal field effects.

The systems CePd<sub>2</sub>Si<sub>2</sub> and CeNi<sub>2</sub>Ge<sub>2</sub> (Ref. 12) possess complicated magnetic structure with several magnetic atoms per unit cell (and, consequently, spin-wave branches). Under pressure, these systems demonstrate anomalous temperature dependence  $\rho(T) \sim T^{\mu}$ ,  $\mu = 1.2-1.5$ . Unfortunately, data on specific heat and magnetic susceptibility for these systems are not presented. The data of Ref. 5 on CeNi<sub>2</sub>Ge<sub>2</sub> yield for the resistivity exponent  $\mu = 3/2$ , and the dependence  $C_{\rm el}(T)/T$  is described by a logarithmic law with square-root corrections. Provided that electron-electron scattering dominates, we obtain from Eq. (39) the dependence  $C_{\rm el}(T)/T$  $\propto T^{-0.25}$ , which cannot be easily distinguished from the logarithmic one [see different fittings of the dependences  $C_{\rm el}(T)$ in Refs. 6 and 1 for the same systems]. Thus the question needs further investigations.

The dependence  $C_{el}(T)/T \propto \chi(T)$  has been recently obtained experimentally for a wide class of NFL systems, e.g.,  $U_x Y_{1-x} Pd_3$ , UCu<sub>4</sub>Pd, UCu<sub>4</sub>Pt, the value of  $\zeta$  being about 0.2-0.3.<sup>6</sup> Such a correlation itself is in agreement with a number of theoretical microscopic mechanisms, including the Griffiths point one, and cannot provide any definite arguments. At the same time, the Griffiths point mechanism predicts nearly temperature independent Wilson ratio, but our mechanism yields the dependence (36). One can expect that usually the accuracy of the experimental data is insufficient to pick out the factor of  $\ln^2(T/T^*)$ . However, the data of Ref. 24 for the system CeCu<sub>6-x</sub>Au<sub>x</sub> definitely demonstrate a considerable dependence W(T), which is in a qualitative agreement with Eq. (36) (unfortunately, no quantitative fitting is presented in Ref. 24).

Therefore obtaining data on resistivity for the same samples is of crucial importance (as demonstrated in Ref. 1, the resistivity for  $U_{1-x}Th_xPd_2Al_3$  is described by different power-law temperature dependences at varying x in the interval 0.6<x<0.95). It should be noted that our approach does yield nonuniversal exponents in the temperature dependences, which depend on characteristics of the Fermi surface. For the systems such as  $U_xY_{1-x}Pd_3$  the experimental data<sup>1</sup> demonstrate the negative contribution to resistivity,  $\delta\rho(T)$  $\sim -T^{\mu}, \mu = 1.1-1.4$ . However, the negative temperature coefficient probably indicates importance of disorder effects.

In the whole, despite existence of plentiful data on the NFL behavior, it is difficult to choose unambiguously a theoretical mechanism because of the problem of fitting experimental data and absence of the complete set of physical characteristics [temperature dependences of  $C_{\rm el}(T), \chi(T), \rho(T)$ , and spin dynamics] for the same sample compositions. One of more features of our mechanism is correlation of electronic properties with magnetic anisotropy parameter. The existing data seem to not exclude the NFL mechanism proposed, at least for the systems with pronounced magnetic ordering. To get further insight, detailed measurements for stoichiometric systems such as CeNi<sub>2</sub>Ge<sub>2</sub> would be useful.

To conclude, phenomenon of the NFL behavior seems to have a complicated nature (both magnetic fluctuations and the on-site Kondo effect are important). The mechanisms considered above are not based on disorder effects, but describe naturally the NFL state in ideal crystals. At the same time, the damping makes the quasi-NFL behavior considered in Sec. III more pronounced and in a sense plays the role of disorder.

The damping is not important for the NFL behavior mechanism considered in Sec. V. This NFL picture is "true" (i.e., holds up to lowest temperatures) within the lowest-

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order scaling approach; treatment of higher-order corrections to the scaling equations would provide additional information. Unlike previous phenomenological works, existence of peculiar long-range critical fluctuations near the quantum phase transition is not needed for this mechanism, but local reconstruction of electronic states owing to the Kondo effect is essential, the concrete form of spin spectral function being of crucial importance. More detailed investigations of the NFL behavior for complicated spectral functions, in particular with account of crystal-field effects and incoherent contributions, would be also of interest.

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