The Kondo-lattice state and non-Fermi-liquid behavior in the presence of Van Hove singularities

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Received 13 October 2010
Published 20 January 2011
Online at stacks.iop.org/JPhysCM/23/065602

Abstract

A scaling consideration of the Kondo lattices is performed with account of logarithmic Van Hove singularities (VHS) in the electron density of states. The scaling trajectories are presented for different magnetic phases. It is demonstrated that VHS lead to a considerable increase of the non-Fermi-liquid behavior region owing to softening of magnon branches during the renormalization process. Although the effective coupling constant remains moderate, the renormalized magnetic moment and spin-fluctuation frequency can decrease by several orders of magnitude. A possible application to f-systems and weak itinerant magnets is discussed.

1. Introduction

Anomalous rare-earth and actinide compounds have been studied extensively starting from the middle of the 1980s [1, 2]. They include the so-called Kondo lattices (with moderately enhanced electronic specific heat) and heavy-fermion systems demonstrating a huge linear specific heat. The main role in the physics of Kondo lattices [2–4] belongs to the interplay of the on-site Kondo screening and intersite exchange interactions. Following the Doniach criterion [5], it was believed in early works [2] that the total suppression of either magnetic moments or the Kondo anomalies takes place. However, later experimental data and theoretical investigations made it clear that the Kondo lattices as a rule demonstrate magnetic ordering or are close to this. This concept was consistently formulated and justified in a series of papers [6–9] treating the mutual renormalization of two characteristic energy scales: the Kondo temperature $T_K$ and the spin-fluctuation frequency $\bar{\omega}$. A simple scaling consideration of this renormalization process in the s–f exchange model [9, 10] yields, depending on the values of bare parameters, both the ‘usual’ states (a non-magnetic Kondo lattice or a magnetic state with weak Kondo corrections) and the peculiar magnetic Kondo-lattice state. In the latter regime, small variations of parameters result in strong changes of the ground-state moment. Thereby high sensitivity of the ground-state moment to external factors like pressure and doping by a small amount of impurities (a characteristic feature of heavy-fermion magnets) is naturally explained.

During the 1990s, a number of anomalous f-systems ($U_xY_{1-x}$Pd$_3$, $UPt_{3-x}$Pd$_x$, $UCu_{6-x}$Pd$_x$, $CeCu_{6-x}$Au$_x$, $U_xTh_{1-x}$Be$_{13}$, $CeCu_2Si_2$, $CeNi_2Ge_2$, $Ce_7Ni_3$, etc) demonstrating the non-Fermi-liquid (NFL) behavior became a subject of great interest (see, e.g., the reviews [11, 12]). These systems possess unusual logarithmic or power-law temperature dependences of their electronic and magnetic properties. Various mechanisms were proposed to describe the NFL behavior [13], including two-channel Kondo scattering [14, 15], ‘Griffiths singularities’ in disordered magnets [16], and strong spin fluctuations near a quantum magnetic phase transition [17, 18].

It is important that experimentally the NFL behavior (as well as the heavy-fermion behavior) is typical for systems lying on the boundary of magnetic ordering and demonstrating strong spin fluctuations [4, 11].

The NFL behavior close to the quantum phase transition was theoretically studied in a number of works [18–21]. In particular, renormalization group investigations near the quantum phase transitions connected with the topology of the Fermi surface were performed [20]. A scaling consideration of the Kondo lattices with account for singularities in the spin-excitation spectral function (which are due to Van Hove singularities in the magnon spectrum) yields the NFL behavior in an extremely narrow interval of bare parameters only [9]. As demonstrated in [22], when taking into account renormalization of spin-excitation damping, the region can become considerably broader.
The systems under consideration demonstrate both local moment and itinerant features. Moreover, large linear specific heat and NFL behavior is also observed in some d-systems including the layered ruthenates Sr₃RuO₄ [23] and Sr₂Ru₂O₇ [24].

It is well known that magnetism of itinerant systems is intimately related to the presence of Van Hove singularities (VHS) near the Fermi level. Therefore, it is instructive to treat the Kondo effect in systems with a singular electron spectrum. This is the aim of the present paper.

It is evident that the Kondo effect in such systems has a number of peculiar features. In particular, for the logarithmically divergent density of states

\[ \rho(E) = A \ln \frac{D}{B|E|} \]

(the energy is referred to the Fermi level, \( D \) is the half-bandwidth, the constants \( A \) and \( B \) are determined by the band spectrum) the Kondo singularities at \( E_F \) become double logarithmic. Perturbation expansion yields a non-standard expression for the one-center Kondo temperature,

\[ T_K \propto D \exp[-1/(AI)^{1/2}], \]

(1)

instead of the result for the smooth density of states, \( T_K \propto D \exp[1/2I\rho(0)] \), \( I \) being the s–f exchange parameter. The logarithmic divergence in \( \rho(E) \) is typical for the two-dimensional case (in particular, for the layered ruthenates). However, similar strong Van Hove singularities can occur also in some three-dimensional systems like Pd alloys and the weak itinerant ferromagnets ZrZn₂ and TiB₂ [25, 26].

In the present work we consider the Kondo problem and the NFL behavior with the singular electron density of states for the lattice of d(f)-spins where a competition with spin excitation damping is considered. In section 4 we treat the scaling behavior for the magnetic phases with account of spin-excitation damping.

In section 2 the renormalization group equations in the presence of Van Hove singularities (VHS) near the Fermi level. Therefore, it is instructive to treat the Kondo effect in systems with a singular electron spectrum. This is the aim of the present paper.

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The density of states corresponding to the spectrum \( n_k \) is supposed to contain a Van Hove singularity near the Fermi level. In particular, for the square lattice with the spectrum

\[ n_k = 2t (\cos k_x + \cos k_y) + 4t' (\cos k_x \cos k_y + 1) \]

we have the density of states

\[ \rho(E) = \frac{1}{2\pi^2 \sqrt{t^2 + Et' - 4t'^2}} K\left(\frac{\sqrt{t^2 - (E - 8t')^2/16}}{t^2 + Et' - 4t'^2}\right) \]

\[ \simeq \frac{1}{2\pi^2 \sqrt{t^2 - 4t'^2}} \ln \frac{16\sqrt{t^2 - 4t'^2}}{|E|} \]

(3)

where \( K(E) \) is the complete elliptic integral of the first kind; the bandwidth is determined by \( |E - 8t'| < 4|t'| \). For \( t' = 0 \) we derive

\[ \rho(E) = \frac{2}{\pi^2 D} K\left(\sqrt{1 - \frac{E^2}{D^2}}\right) \approx \frac{2}{\pi^2 D} \ln \frac{4D}{|E|}, \]

(4)

so that, according to (1),

\[ T_K \propto D \exp\left[-\left(\frac{\pi^2 D}{2I}\right)^{1/2}\right]. \]

(5)

Note that the expression for the Kondo temperature in the parquet approximation has a different form [27]:

\[ T_K \propto D \exp\left[-\frac{1}{2I}\right] = D \exp\left[-\left(\frac{\pi^2 D}{4I}\right)^{1/2}\right]. \]

(6)

However, the expression (5) agrees with the numerical Wilson renormalization group calculation for the square lattice [28], unlike the result (6); the corresponding problems of the parquet approximation in the Hubbard model are discussed in the works [29].

In [9, 10, 22], the interplay of the Kondo effect and intersite interactions was investigated by the renormalization group method. This starts from the second-order perturbation theory with the use of the equation-of-motion method (within the diagram technique for pseudofermions such an approximation corresponds to the one-loop scaling).

We apply the ‘poor man scaling’ approach [30]. This considers the dependence of effective (renormalized) model parameters on the cutoff parameter \( C \) which occurs on picking out the singular contributions from the Kondo corrections to the effective coupling and spin-fluctuation frequencies. Using the results of [9, 22] we can write down the system of scaling equations in the case of the Kondo lattice for various magnetic phases.

In the calculations below we use the density of states for a square lattice with \( t' = 0 \) in both the two-dimensional (2D) and three-dimensional (3D) cases as a phenomenological one, so that

\[ \varphi(E) = \varphi(-D) F(E), \varphi(-D) = \frac{2 \ln 4}{\pi^2 D}, \]

(7)

\[ F(E) = \ln \frac{D}{|E|} + 1. \]

We adopt the definition of the effective (renormalized) and bare s–f coupling constant

\[ g_{sf}(C) = -2g_{sf}(C), \quad g = -2I\varphi, \quad \rho = \varphi(-D) \]

(8)
where $C \to -0$ is a flow cutoff parameter. Other relevant variables are the characteristic spin-fluctuation energy $\tilde{\omega}_q(C)$ and magnetic moment $\tilde{S}_{\text{eff}}(C)$.

To find the equation for $I_{\text{ef}}(C)$ we have to treat the electron self-energy. For a ferromagnet (the case of an antiferromagnet is considered in a similar way, see [9]) the second-order Kondo contribution reads
\[
\Sigma_{k\bar{k}}^{(2)}(E) = \pm 2I^2S \sum_q \frac{n_{k-q}}{E - k_{-q} \pm \omega_q}
\]  
where $n_k = f(t_k)$ is the Fermi function. Then we have
\[
\delta I_{\text{ef}} = [\Sigma_{k\bar{k}}^{(2)}(E) - \Sigma_{k\bar{k}}^{(2)}(E)]/(2S). 
\]
Picking out in the sums the contribution of intermediate electron states near the Fermi level with $C - k_{\pm q} < C + \delta C$ we obtain
\[
\delta I_{\text{ef}}(C) = 2\rho F(C)I^2\eta\left(-\frac{\tilde{\omega}}{C}\right)[\delta C/C] 
\]  
where $\eta(x)$ is a scaling function which satisfies the condition $\eta(0) = 1$ which guarantees the correct one-impurity limit. In the magnetically ordered phase, $\tilde{\omega}$ is the magnon frequency $\omega_q$, which is averaged over the wavevectors $q = 2k$ where $k$ runs over the Fermi surface (for simplicity we use a spherical Fermi surface). In the paramagnetic phase (the problem of localized moment screening) $\tilde{\omega}$ is determined from the second moment of the spin spectral density.

Now we treat the singular correction to $\tilde{\omega}_{\text{ef}}$ and the effective magnetic moment $\tilde{S}_{\text{ef}}$. We have within the spin-wave picture
\[
\delta \tilde{S} = -\sum_q \delta\langle b^+_q b_q \rangle. 
\]
The singular contribution to magnon occupation numbers occurs owing to the electron–magnon interaction. Calculation for a ferromagnet from the corresponding magnon Green’s function yields [9]
\[
\delta\langle b^+_q b_q \rangle = I^2S \sum_k \frac{n_{k}(1-n_{k-q})}{(k_{-q} - k_{-q} - \omega_q)^2}.
\]
We see that, when considering the characteristics of the localized spin subsystem, the lowest-order Kondo corrections originate from double integrals over both electron and hole states. Then we have to introduce two cutoff parameters $C_c$ and $C_h$ with $C_c + C_h = C$ ($C$ is the cutoff parameter for the electron–hole excitations), $\delta C_c = -\delta C_h$ to obtain
\[
\delta \tilde{S}_{\text{ef}}(C)/S = 2\rho^2I^2F(C/2)F(-C/2)\eta\left(-\frac{\tilde{\omega}}{C}\right)[\delta C/C]. 
\]
The renormalization of the spin-wave frequency owing to magnon–magnon scattering is given by
\[
\delta \omega_q/\omega_q = -a\tilde{\omega}/\tilde{S}_{\text{ef}}(C)/S. 
\]
Now we pass to the magnon frequency averaged over the Fermi surface. Then we have ($a_q \to a$)
\[
\delta \tilde{\omega}_{\text{ef}}(C)/\tilde{\omega} = a\delta \tilde{S}_{\text{ef}}(C)/S
= 2a\rho^2I^2F(C/2)F(-C/2)\eta\left(-\frac{\tilde{\omega}}{C}\right)[\delta C/C]. 
\]
The latter result holds for all magnetic phases with $a = 1 - \alpha$ for the paramagnetic (PM) phase, $a = 1 - \alpha'$ for the antiferromagnetic (AFM) phase, $a = 2(1 - \alpha'')$ for the ferromagnetic (FM) phase. Here $\alpha, \alpha', \alpha''$ are some averages over the Fermi surface (see [9]), $\alpha' = 0$ in the nearest-neighbor approximation. This approximation enables us to use a single renormalization parameter, rather than the whole function of $q$. For simplicity, we put in the numerical calculations below $a = 1$ (although the deviation $1 - a$ just determines critical exponents for physical properties, see [22] and conclusions).

The scaling picture (which determines the NFL behavior) is influenced by not only the real, but also the imaginary part of the spin-fluctuation energy. The latter is even dominating in the paramagnetic phase (e.g., in the Heisenberg model a spin-diffusion picture can be adopted at high temperatures). In the magnetically ordered phases, the damping comes from paramagnon-like excitations. They can be taken into account starting from the magnon picture of the localized spin-excitation spectrum. In the s-f exchange model the damping is proportional to $I^2$ and to the magnon frequency (for the details, see [22]). The dependence of the damping on the magnetic moment $S$ (which is strongly renormalized) is crucial for the size of the NFL region. The calculation of the damping in the second order in $I$ yields the contributions of the order of both $I^2S$ and $I^2$ [31, 32] (formally, they correspond to the first and second orders in the quasiclassical parameter $1/2S$). The corresponding problems from a semiphemenological point of view are discussed in [33]. Similarly to [22], here we do not introduce the additional factor of $S$ to obtain in terms of renormalized quantities
\[
\tilde{\gamma}_{\text{ef}}(C) = kF(C/2)F(-C/2)\tilde{g}_{\text{ef}}(C)\tilde{\omega}_{\text{ef}}(C),
\]
the factor $k$ being determined by the bandstructure and magnetic ordering. In the numerical calculations we take $k = 0.5$.

When taking into account the spin-wave damping $\tilde{\gamma}$ we have
\[
\eta\left(\frac{\tilde{\omega}_{\text{ef}}(C)}{|C|}\right) \to \eta\left(\frac{\tilde{\omega}_{\text{ef}}(C)}{|C|}, \frac{\tilde{\gamma}_{\text{ef}}(C)}{|C|}\right). 
\]
Replacing in the Kondo corrections $g \to g_{\text{ef}}(C)$, $\tilde{\omega} \to \tilde{\omega}_{\text{ef}}(C)$ we derive the set of scaling equations with account of the energy dependence of the electron density of states:
\[
\partial g_{\text{ef}}(C)/\partial C = F(C)\Lambda,
\]
\[
\partial \ln \tilde{\omega}_{\text{ef}}(C)/\partial C = -aF(C/2)F(-C/2)\Lambda/2,
\]
\[
\partial \ln \tilde{S}_{\text{ef}}(C)/\partial C = -F(C/2)F(-C/2)\Lambda/2 
\]
with
\[
\Lambda = \Lambda(C, \tilde{\omega}_{\text{ef}}(C), \tilde{\gamma}_{\text{ef}}(C)) = \tilde{g}_{\text{ef}}(C)\eta\left(\frac{\tilde{\omega}_{\text{ef}}(C)}{|C|}, \frac{\tilde{\gamma}_{\text{ef}}(C)}{|C|}\right). 
\]
Similar equations can be obtained for the general $SU(N)$ Coqblin–Schrieffer model [9] where $a/2 \to a/N$ (there are some peculiarities for the FM case owing to the asymmetry of the spin-up and spin-down states).

One can see that the renormalizations of the spin-fluctuation energy $\tilde{\omega}_{\text{ef}}(C)$ and the damping are stronger than...
that of $g_{ef}(C)$ owing to the factors of $F(\pm C/2)$. We obtain from (19), (20)

$$\frac{S_{\text{ef}}(C)}{S} = \left(\frac{\tilde{\omega}_{\text{ef}}(C)}{\tilde{\omega}}\right)^{1/\nu}. \quad (21)$$

However, the simple expression for $\rho = \text{const}$,

$$\tilde{\omega}_{\text{ef}}(C) = \tilde{\omega} \exp(-a[g_{\text{ef}}(C) - g]/2), \quad (22)$$

does not hold for the logarithmic density of states; no simple relation with the quantity $\tilde{g}_{\text{ef}}(C) = F(C)g_{\text{ef}}(C)$ is obtained either. Expanding in $1/\ln |D/C|$, we derive

$$\tilde{\omega}_{\text{ef}}(C) \approx \tilde{\omega} \exp\left[-a \ln \frac{\tilde{g}_{\text{ef}}(C) - g}{2}\right]. \quad (23)$$

Now we treat the scaling functions $\eta$. In the paramagnetic case we use the spin-diffusion approximation (dissipative spin dynamics) to obtain (cf [9])

$$\eta^\text{PM}(\frac{\tilde{\omega}}{C}) = \left(\frac{1}{1 + D(k-k)^2/C^2}\right)_{k_{F} = 0}, \quad \tilde{\omega} = 4Dk_{F}^2 \quad (24)$$

where $D$ is the spin-diffusion constant, the averages go over the Fermi surface. Integration yields

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

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

$$\eta(\tilde{\omega}_{\text{ef}}/|C|, \tilde{\gamma}_{\text{ef}}/|C|) = \text{Re}((1 -(\alpha k-k + iyk-k)^2/C^2)^{-1})_{k_{F} = 0}. \quad (25)$$

For an isotropic 3D ferromagnet integration in (25) for $\gamma =$ const and quadratic spin-wave spectrum $\omega_q \propto q^2$ yields

$$\eta^\text{FM}(x, z) = \frac{1}{4x} \ln \frac{(1 + x^2)^{2} + z^2}{(1 - x^2)^{2} + z^2}, \quad (26)$$

where $x = \tilde{\omega}_{\text{ef}}/|C|$, $z = \tilde{\gamma}_{\text{ef}}/|C|$. Although the details of the spin-wave spectrum are not reproduced in such an approach, the renormalization of the spin-wave frequency (which is a cutoff for the Kondo divergences) is adequately reproduced.

In the 2D case we obtain in the same approximation

$$\eta^\text{PM}(x, z) = \frac{1}{2} \text{Re}[[1 + iz](1 + iz - x)]^{-1/2}$$
$$\quad + [(1 - iz)(1 - iz + x)]^{-1/2}. \quad (27)$$

For an antiferromagnet integration in (25) with the linear spin-wave spectrum $\omega_q \propto cq$ gives

$$\eta^\text{AFM}(x, z) = \begin{cases} -\frac{1}{2x^2} \ln[(1 + z^2 + x^2)^2 - 4x^2] & d = 3 \\ -2 \ln(1 + z^2) & d = 2 \\ 2 \ln(x^2 - 1 - 2iz + z^2)^{-1/2} & d = 2. \end{cases} \quad (28)$$

which somewhat modifies the results of [9].

The plot of the functions $\eta(x) = \eta(x, 0)$ for different magnetic phases is shown in figure 1. Note that for a 2D antiferromagnet $\eta(x)$ vanishes discontinuously at $x > 1$. However, a smooth non-zero contribution can occur for more realistic models of the magnon spectrum.

3. The scaling behavior in the paramagnetic and magnetic phases

We start the discussion of scaling behavior from the simple case of the Coqblin–Schrieffer model in the limit $N \to \infty$. Then the renormalization of the magnon frequency is absent and the scaling behavior can be investigated analytically, similar to [9]. We have

$$1/g_{\text{ef}}(C) - 1/g = G(C) = -\int_{-D}^{C} \frac{dc'}{C'} F(C')\eta\left(-\frac{\tilde{\omega}}{C}\right). \quad (29)$$

Equation (29) can be used even for $N = 2$ provided that $g$ is considerably smaller than the critical value $g_c$. The effective coupling $g_{\text{ef}}(C)$ begins to deviate strongly from its one-impurity behavior

$$1/g_{\text{ef}}(C) = 1/g - \frac{1}{2} \ln^2 |D/C| \quad (30)$$

at $|C| \sim \tilde{\omega}$. The boundary of the strong coupling region (the renormalized Kondo temperature) is determined by $G(C) = -T_{K}^{\text{ren}} = -1/g$. Of course, $T_{K}^{\text{ren}}$ means here only some characteristic energy scale extrapolated from high temperatures, and the detailed description of the ground state requires a more detailed consideration. In the PM, FM and 2D
AFM phases spin dynamics suppresses $T_{K}^{*}$. To leading order in $\ln(D/\bar{\omega})$ we have

$$T_{K}^{*} \simeq (T_{K}^{2} - \bar{\omega}^{2})^{1/2}$$

with $T_K$ given by (5). (However, owing to the minimum of the scaling function (28) (figure 1(b)), in the 3D AFM case spin dynamics at small $\bar{\omega}$ results in an increase of $T_{K}^{*}$.)

Provided that the strong coupling regime does not occur, i.e. $g$ is smaller than the critical value $g_{c}$, $g_{c}(C \to 0)$ tends to a finite value $g^{*}$. To leading order in $\ln(D/\bar{\omega})$ we have

$$1/g_{c} = \frac{1}{2} \ln \frac{D}{\bar{\omega}} = \frac{1}{2} \lambda^{2}$$

(31) (which yields also a rough estimate of $g_{c}$ for $N = 2$). An account of next-order terms results in an appreciable dependence on the type of magnetic ordering and space dimensionality. For the PM, FM and 2D AFM phases the critical value $g_{c}$ is given by $1/g_{c} = -G(0)$, and in the 3D AFM case $g_{c}$ is determined by the minimum of the function $G(C)$.

Numerical calculations for $N = 2$ were performed for $\lambda = \ln(D/\bar{\omega}) = 5$. The plots are presented in figures 2–5 for both smooth and singular bare densities of states. We compare these cases in the same relative interval of the coupling constant $|g - g_{c}|/g_{c}$. The scaling process for finite $N$ in the former case is described in [9]. It turns out that the qualitative picture near the critical value of the coupling constant is rather
universal for the same interval $|g - g_c|/g_c$ depending mainly on the scaling function and the damping, but not on the details of the bare electron density of states (even on its singularities). The shift of the Van Hove singularity below the Fermi level does not strongly influence the results either, although we cross the singularity during the scaling process (the singularity is in fact integrable).

An important quantitative difference in the presence of VHS is that the renormalized coupling constant is considerably smaller. Moreover, the relative renormalization of the coupling constant is also smaller (figures 2–4). This makes using smaller. Moreover, the relative renormalization of the coupling constant is considerably fact integrable).

The shift of the Van Hove singularity below the Fermi level of the bare electron density of states (even on its singularities).

on the scaling function and the damping, but not on the details $\xi \rightarrow \xi \sim |D/(D/C)| = 1/\xi \rightarrow -\xi \approx (a/2A)\xi$ (32) with $A < 2/\alpha$. Such a behavior takes place both for $g < g_c$ and $g > g_c$ in a wide region of $\xi$, i.e. up to rather low temperatures (figure 2(b); for a discussion of physical properties see conclusions).

For magnetic phases, the singularities of the scaling function $\eta(x \rightarrow 1)$ play the crucial role. A rather distinct NFL behavior takes place in a narrower region where the argument of the function $\eta$ is fixed at the singularity during the scaling process, so that

$$\tilde{\omega}_{\text{eff}}(C) \approx |C|, \quad \ln[\tilde{\omega}/\tilde{\omega}_{\text{eff}}(\xi)] \approx \xi. \quad (33)$$

Then for a smooth density of states we obtain from (22)

$$g_{\text{eff}}(\xi) - g \approx 2(\xi - \lambda)/\alpha. \quad (34)$$

However, in the presence of VHS the relation (23) between $\tilde{\omega}_{\text{eff}}(C)$ and $g_{\text{eff}}(C)$ is more complicated.

In the case of a constant magnon damping considered in [9], the region (33) is not too narrow only provided that the bare coupling constant $g$ is very close to the critical value $g_c$ for the magnetic instability ($|g - g_c|/g_c \sim 10^{-4}$). However, when taking into account the magnon damping renormalization, this region is considerably wider, although being smeared [22], and the influence of the energy dependence $\rho(E)$ becomes stronger.

One can see that VHS lead to a considerable increase of the effective moment $S^* = \tilde{S}(\xi \rightarrow \infty)$. For the chosen deviation $|g - g_c|/g_c \sim 1\%$ the moment renormalization $S/S^*$ can make up one to two orders of magnitude; even for $|g - g_c|/g_c \sim 10-20\%$, the moment can decrease by several times.

Since in a 2D antiferromagnet $\eta(x \rightarrow 1) = 0$, a sharp transition to the saturation plateau occurs, unlike the FM case (cf figures 3 and 4). The situation in 3D systems with a logarithmic density of states can be considered in a similar way. Surprisingly, for 3D ferromagnets the scaling trajectories (except for a narrow critical region near $g_c$) and the critical values $g_c$ turn out to be very close to the 2D case (for both smooth density of states and with VHS). Therefore we do not show the corresponding plot. On the other hand, for 3D antiferromagnets VHS do not lead to suppression of magnon frequencies (figure 5). This is due to the influence of the minimum in the scaling function (figure 1(b)).

4. The scaling behavior with account of incoherent contributions

The magnon approximation used in section 3 is not quite valid since this underestimates the role of the damping. In fact, the spin spectral function should have an intermediate form between large damping and spin-wave pictures, containing both coherent (magnon-like) and incoherent contributions. A simple attempt to construct the corresponding scaling function as a linear combination was performed in [9]. In particular, in the case of a ferromagnet we have near the magnon pole

$$\langle \langle S_{q}^{+} | S_{-q}^{-} \rangle \rangle_{\omega} = \frac{2}{\omega} \frac{Z_{q}}{\omega - \omega_{q}^{*}} + \langle \langle S_{q}^{+} | S_{-q}^{-} \rangle \rangle_{\omega}^{\text{inc}} \quad (35)$$
where the inverse residue at the pole is determined by
\[
\frac{1}{Z_q} = 1 - \left( \frac{\partial \Pi_q(\omega)}{\partial \omega} \right)_{\omega = \omega_q},
\]

\(\Pi_q(\omega)\) being the polarization operator of the magnon Green’s function. Besides that, there exists the singular contribution which comes from the incoherent (non-pole) part of the spin spectral density. Then we get
\[
\partial g_{ef}(C)/\partial C = F(C)\Lambda, \tag{37}
\]

\[
\partial \ln S_{ef}(C)/\partial C = -a F(C/2) F(-C/2)\Lambda/2, \tag{38}
\]

\[
\partial (1/Z)/\partial C = \partial \ln S_{ef}(C)/\partial C = -F(C/2) F(-C/2)\Lambda/2 \tag{39}
\]

where
\[
\Lambda = \frac{[g_{ef}^2(C)/|C|][Z \eta_{coh}(\omega_{ef}(C)/|C|)]}{(1 - Z)\eta_{incoh}(\omega_{ef}(C)/|C|)} \tag{40}
\]

with \(\eta_{coh} = \eta_{PM}\). The choice of \(\eta_{incoh}\) is a more difficult problem; here we put simply \(\eta_{incoh} = \eta_{PM}\).

According to (39) we have
\[
\frac{1}{Z(\xi)} = 1 + \ln \frac{S}{S_0(\xi)} \tag{41}
\]

Consequently, the increase of magnetic moment owing to the Kondo screening leads to a considerable logarithmic suppression of the magnon contributions to the spectral density.

The role of the incoherent contribution becomes important only provided that \(S/S_0(\xi)\) and \(Z\) deviate appreciably from unity. However, such a momentum suppression just occurs when passing the region of singularity in \(\eta_{coh}(\xi = 1)\), the further scaling process being determined by the incoherent contribution.

The corresponding scaling trajectories are shown in figure 6. Now we have a two-stage renormalization. One can see that the well-linear ‘coherent’ behavior region (which is rather narrow in figure 6) is changed to a PM-like ‘quasi-linear’ behavior (32) with increasing \(\xi\). This crossover occurs when the function \(\eta_{coh}\) reaches its maximum value at the singularity (cf [9]).

The ‘quasi-linear’ behavior, although being somewhat smeared, is pronounced in a considerable region of \(\xi\) even for larger \(|g - g_c|\) values. The difference with the PM case is that \(g_{ef}(\xi)\) increases considerably at the first stage of renormalization owing to the singularity of the function \(\eta_{coh}\).

A similar consideration can be performed for the antiferromagnetic phase (cf [9]). The account of the incoherent contribution results in a smearing of the non-monotonic behavior of \(g_{ef}(\xi)\) in the 3D AFM case, so that at small \(|g - g_c|\) the maximum in the dependences \(g_{ef}(\xi)\) and \(\ln[\omega/\omega_{ef}(\xi)]\) vanishes completely.

5. Discussion and conclusions

In the general problem of metallic magnetism, the peaks in the bare density of states (which are usually connected with VHS) near the Fermi level play a crucial role. Here we have investigated their influence starting from the Kondo-lattice \((s - d(f)\) exchange) model.

For \(g \rightarrow g_c\) we obtain the magnetic state with small effective moment \(S^*\) and a NFL-type behavior. The corresponding dependences \(S(T) = S_{ef}(C) \rightarrow T\) describe an analog of the ‘temperature-induced magnetism’ [34]. Such a picture is based on the many-electron renormalization (compensation) of localized magnetic moments and differs outwardly from the ordinary mechanism for weak itinerant ferromagnets with small \(S\), which are assumed to correspond to the immediate vicinity of the Stoner instability.

However, the physical difference is not radical. In fact, a continuous transition exists between the highly correlated Kondo lattices and the ‘usual’ itinerant-electron systems. In particular, one may view Pauli paramagnets as systems with high \(T_K\) of the order of the Fermi energy; for enhanced Pauli paramagnets like Pd, Pt and UAl\(_2\), where the Curie–Weiss law holds at high temperatures, one introduces instead of the Kondo temperature the so-called spin-fluctuation temperature. A combined description of the Kondo-lattice state and weak itinerant magnetism has been considered recently by Okahiva [35]. Remember that the Kondo systems with VHS near the Fermi level under consideration just possess high values of \(T_K\) (see section 1).

In this context, it would be instructive to describe weak itinerant magnets not from the ‘band’ point of view, but from the perspective of local magnetic moments which are nearly compensated. Since a number of cerium NFL
systems demonstrate itinerant-electron behavior [13] and it is customary now to treat UPt3, CeSi2 and CeRh2B2 as weak itinerant magnets, the second approach appears already to be far less natural than the first (see [7, 37]). From the formal point of view, perturbation calculations in the Hubbard model, which describes itinerant-electron systems, are similar to those in the s–d(f) model, provided that one postulates the existence of local moments. Besides that, for two-dimensional itinerant systems with strong spin fluctuations the semiphenomenological spin-fermion model can be used which separates electron and spin degrees of freedom and is somewhat similar to the s–d exchange model [36, 38].

Further on, the question arises about the role which many-electron effects play in the ‘classical’ weak itinerant 3D magnets like ZrZn2 and TiBe2. Indeed, one can hardly believe that the extreme smallness of $\tilde{S}$ in these systems is due to accidental bare values of $N(E_F)$ and the Stoner parameter. Moreover, the Stoner criterion is not valid even qualitatively (in particular, due to spin fluctuations the critical coupling $U_c$ in the Hubbard model is finite when the Fermi level tends to VHS [38]). Thus a scaling consideration in the presence of VHS would be of interest, especially with account of chemical potential renormalizations (cf [25]). In particular, owing to VHS the chemical potential can depend weakly on the electron concentration (the pinning phenomenon [39]). In the Kondo systems such a treatment may lead to a renormalization of the scale $|g - g_c|$ itself.

Now we discuss some real layered systems. The specific heat is considerably enhanced in ruthenates, Sr2RuO4. A gradual enhancement of the electronic specific heat and a more drastic increase of the static magnetic susceptibility were observed in Sr2–xLa2RuO4 with increasing y. Furthermore, the quasi-2D Fermi-liquid behavior observed in pure Sr2RuO4 breaks down near the critical value $y = 0.2$. The enhancement of the density of states can be ascended to the elevation of the Fermi energy toward a Van Hove singularity of the thermodynamically dominant Fermi-surface sheet. The NFL behavior is attributed to two-dimensional FM fluctuations with short-range correlations at VHS [23].

The bilayered ruthenate system Sr3Ru2O7 in the ground state is a paramagnetic Fermi liquid with strongly enhanced quasiparticle masses. The Fermi-liquid region of the phase diagram extends up to 10–15 K in zero field and is continuously suppressed towards zero temperature upon approaching the critical field of $B = 8$ T. In the vicinity of the putative quantum critical end point, NFL behavior has been observed in various macroscopic quantities including specific heat, resistivity and thermal expansion and has been described on the basis of phenomenological models [24].

We can mention also some layered f-systems. The layered Kondo lattice model was proposed for quantum critical beta-YbAlB4 where the two-dimensional boron layers are Kondo coupled via interlayer Yb moments [40]. CeRuPO seems to be one of the rare examples of a ferromagnetic Kondo lattice where LSDA + $U$ calculations evidence a quasi-2D electronic band structure, reflecting a strong covalent bonding within the CeO and RuP layers and a weak ionic-like bonding between the layers [41].

To describe layered antiferromagnetic cuprates, the 2D $t$–$t'$ Hubbard model is often used which also describes the Fermi-liquid and NFL regimes. Despite the density-of-states logarithmic singularity, the staggered spin susceptibility in this model does not diverge within the Fermi-liquid approach, the reason being the appearance of the logarithmic singularity in the quasiparticle mass [42]. The effective mass renormalization is beyond our lowest-order (one-loop) scaling consideration, but may play a role in an accurate treatment. The two-loop considerations of the flat-Fermi-surface and $t$–$t'$ Hubbard models [43, 44] yield a (generally speaking, anisotropic) suppression of the quasiparticle weight (inverse effective mass) along the Fermi surface, the staggered spin susceptibility remaining divergent, although the divergence is considerably weakened.

Note that the pictures in the Hubbard model and s–d(f) model (where ‘direct’ exchange interaction is present) can be considerably different. Recently, the $\epsilon$-expansion has been used for a scaling consideration of the 2D antiferromagnetic Kondo lattice with the use of a non-linear sigma model [45].

In the case of a smooth electron density of states, various physical properties of NFL systems are discussed within our approach in [22]. The temperature behavior of the magnetic characteristics $\tilde{S}$ and $\tilde{\omega}$, which depend exponentially on the coupling constant, is decisive for the NFL picture under consideration. At the same time, the presence of VHS near the Fermi level influences strongly all the electronic, magnetic and transport properties in the scaling approach, as well as in the one-electron theory. The replacement $\rho^2 g_{el}^2(T) \to \rho^2(T)g_{el}^2(T)$ with $\rho(T)$ being considerably temperature dependent owing to VHS possibly modifying somewhat the behavior of the observable quantities.

Consider the temperature dependence of the magnetic susceptibility $\chi \propto \tilde{S}/\tilde{\omega}$. Using scaling arguments we can replace $\tilde{\omega} \to \tilde{\omega}_{el}(C)$, $\tilde{S} \to \tilde{S}_{el}(C)$ where $|C| \sim T$, which yields $\chi(T) \propto T^{-\xi}$. The non-universal exponent $\xi$ is determined by the details of the magnetic structure (the difference $a - 1$ can be used as a perturbation, see [22]). Besides that, a number of crossovers are characteristic for the NFL behavior under consideration. In the coherent ‘magnon’ regime we have $\xi = (a - 1)/a$, and in the ‘quasi-linear’ (incoherent) region $\xi = (a - 1)/2$.

The temperature dependence of the electronic specific heat can be estimated from the second-order perturbation theory, $C_{el}(T)/T \propto 1/Z(T)$, where $Z(T)$ is the residue of the one-electron Green’s function at the distance $T$ from the Fermi level. Then we have

$$C_{el}(T)/T \propto \rho^2(T)g_{el}^2(T)\tilde{S}_{el}(T)/\tilde{\omega}_{el}(T) \propto \rho^2(T)g_{el}^2(T)\chi(T)$$

(42)

which results in a non-trivial behavior of the Wilson ratio.

Following [22], a simple estimation of the transport relaxation rate (which determines the temperature dependence of the resistivity owing to scattering by spin fluctuations in the AFM phase) yields

$$\frac{1}{\tau} \propto T^2 \rho^2(T)g_{el}^2(T)\tilde{S}_{el}(T)/\tilde{\omega}_{el}(T) \propto T^2 C_{el}(T)/T.$$  (43)
However, a more refined treatment in the spirit of [42] would be useful in some cases.

In [22], a mechanism of NFL behavior owing to the peculiar behavior of the spin spectral function was proposed. Here we treated a similar, but somewhat simpler and more natural mechanism which is connected with the singularities in the bare electron spectrum. Of course, a more accurate treatment of the magnetic fluctuations near the quantum phase transition is required. Therefore detailed investigations of the NFL behavior for a realistic Fermi surface and spin spectral function are of interest. An accurate investigation of the situation where the VHS is shifted from $E_F$, or two peaks are present below and above $E_F$ [25], would also be instructive.

Acknowledgments

The research described was supported in part by the Program ‘Quantum Physics of Condensed Matter’ from the Presidium of the Russian Academy of Sciences. The author is grateful to M I Katsnelson and A A Katanin for discussions of the problem.

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