Electron spectrum, thermodynamics and transport in antiferromagnetic metals at low temperatures

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Abstract

Electron spectrum of 2D and 3D antiferromagnetic metals is calculated with account of spin-fluctuation corrections within perturbation theory in the $s - f$ exchange model. Effects of the interaction of conduction electrons with spin waves in thermodynamic and transport properties are investigated. At lowest temperatures $T < T^* \sim (\Delta/E_F)T_N$ ($\Delta$ is the AFM splitting of the electron spectrum) a Fermi-liquid behavior takes place, and non-analytic $T^3\ln T$-contributions to specific heat are present for $D = 3$. At the same time, for $T > T^*$, in 2D and “nested” 3D systems the picture corresponds to a marginal Fermi liquid ($T\ln T$-contributions to specific heat and nearly $T$-linear dependence of resistivity). Frustrations in the spin system in the 3D case are demonstrated to lead to similar results. The Kondo contributions to electronic properties are analyzed and demonstrated to be strongly suppressed. The incoherent contributions to transport properties in the presence of impurity scattering are considered. In particular, in the 2D case $T$-linear terms in resistivity are present up to $T = 0$, and thermoelectric power demonstrates the anomalous $T\ln T$-dependence.

1 Introduction

The theory of electronic structure of highly correlated systems is up to now extensively developed. The interest in this problem has grown in connection with studying anomalous rare-earth and actinide compounds (e.g., heavy-fermion systems) and high-$T_c$ superconductors (HTSC). Last time, a possible formation of states, which differ from the usual Fermi liquid, is extensively discussed. The non-Fermi-liquid (NFL) behavior of the excitation spectrum up to lowest energies is now reliably established in the one-dimensional case (the “Luttinger liquid” [1]). However, Anderson [2] assumed occurrence of a similar situation in some two-dimensional (2D) and even three-dimensional (3D) systems with strong electron correlations, various mechanisms (resonating valence bond (RVB) state, scattering anomalies, Hubbard’s splitting etc.) being proposed. Recently, an attempt has been made [3] to revise the general formulation of the Luttinger theorem (conservation of the volume under the Fermi surface for arbitrary law of vanishing of electron damping at $E_F$) which is a basis of the Fermi liquid description.

Another approach to the problem of NFL behavior was proposed by Varma et al [4]. To describe unusual properties of HTSC (e.g., the $T$-linear dependence of resistivity), these
authors put forward a phenomenological “marginal Fermi liquid” (MFL) theory where electron damping is linear in energy $E$ (referred to the Fermi level), and the effective mass is logarithmically divergent at $E \to 0$. Such a behavior was supposed to result from the interaction with local Bose excitations which possess a peculiar (linear in their energy and weakly $q$-dependent) spectral density. Further the MFL theory was developed in a number of papers (see, e.g., \([5, 6, 7]\)). In a simplest way, the MFL electron spectrum can be reproduced in some crossover energy region for interacting electron systems under the requirement of almost perfect nesting in 2D case \([8, 9, 10, 11]\), which seems to be too strict for real systems. Similar results were obtained with account of antiferromagnetic (AFM) spin fluctuations in the vicinity of the AFM instability \([12]\). Almost $T$-linear behavior of the resistivity in paramagnetic 2D metals with strong AFM fluctuations was obtained by Moriya et al \([13]\) in a broad temperature region.

Besides HTSC, a NFL behavior in some temperature intervals was found experimentally in a number of uranium and cerium systems \((U_xY_{1-x}Pd_3 \ [14], UPt_{3-x}Pd_x \ [13], UCu_{5-x}Pd_x \ [16], CeCu_{6-x}Au_x \ [17], U_xTh_{1-x}Be_{13}, Th_{1-x}U_xRu_2Si_2, Ce_xLa_{1-x}Cu_2Si_2 \ [18, 19])\. In particular, $T \ln T$-term in electronic specific heat, $T$-linear corrections to resistivity (both positive and negative ones), unusual power-law or logarithmic $T$-dependences of magnetic susceptibility etc. were observed \([18]\). This behavior is as a rule interpreted within the two-channel Kondo scattering mechanism \([20]\), Griffith’s point mechanism \([21]\), etc. At the same time, in a number of systems \((UCu_{5-x}Pd_x, CeCu_{6-x}Au_x, U_xY_{1-x}Pd_3)\) the NFL behavior correlates apparently with the onset of antiferromagnetic (AFM) ordering \([17, 22]\).

An interesting behavior demonstrates the system is $Y_{1-x}Sc_xMn_2$ \([23, 24]\). YMn$_2$ is an itinerant AFM with a frustrated magnetic structure, and for $x = 0.03$ (or under pressure) the long-range magnetic order is suppressed and the linear specific heat is giant ($\gamma = 140$ mJ/mol K$^2$). This system demonstrates strong anomalies of transport properties (in particular, deviations from the quadratic $T$-dependence of resistivity). A hypothesis about formation of a spin-liquid state in this system was put forward in \([25]\). A detailed analysis of the neutron scattering in this compound seems to confirm this hypothesis \([26]\).

Most of systems under consideration possess peculiarities of band and spin-fluctuation spectra. The Fermi surfaces of the anomalous $f$-systems have complicated forms with several pieces \([27]\); we have to take into account that for some of these pieces the “nesting” condition can hold. It will be shown below that such cases need separate consideration (roughly speaking, in the nesting situation the effective dimensionality of the system diminishes by unity). Despite 3D picture of electron spectrum, spin fluctuations in such systems as $CeCu_{6-x}Au_x$, $CeRu_2Si_2$ demonstrate 2D-like behavior \([28, 29]\).

Since practically all the above-discussed highly-correlated systems are characterized by pronounced local moments and spin fluctuations, a detailed treatment of the electron-magnon mechanism seems to be important to describe their anomalous properties. In the present work we consider effects of interaction of conduction electrons with usual spin-wave excitations in metallic antiferromagnets with localized magnetic moments within the $s - d(f)$ exchange model. The latter condition results in that spin waves are well defined in a large region of the $q$-space. From the general point of view, presence of the localized-electron system is favorable for the violation of the Fermi-liquid picture. Indeed, we shall demonstrate that a number of physical properties of the AFM metals with 2$D$ electron spectrum (e.g.,
HTSC) exhibit a NFL behavior in some temperature interval, although the collective excitation spectrum is quite different from that in the theory [4]. A similar situation takes place for $D = 3$ provided that nesting features of the Fermi surface are present or spin-wave spectrum possesses reduced dimensionality (Ce- and U-based systems). We analyze also peculiar incoherent (“non-quasiparticle”) contributions to electronic density of states and thermodynamic and transport properties, which are not described by the standard Fermi-liquid theory.

In Sect.2 we calculate the electron Green’s function for a conducting antiferromagnet in the framework of the $s - d(f)$ exchange model. We investigate various contributions to the electron self-energy and density of states. In Sect.3 we calculate the electronic specific heat and transport relaxation rate owing to the electron-magnon interaction. We analyze also the incoherent contributions to transport properties, which are connected with impurity scattering. A consistent quasiclassical perturbation theory is discussed in Appendix A. A simple scaling consideration is performed in Appendix B. Some of preliminary results of the paper were briefly presented in Ref. [36].

2 Peculiarities of electron spectrum: perturbation theory

The peculiarities of spectrum and damping of quasiparticles near the Fermi level are due to the interaction with low-energy collective excitations, either well-defined or of dissipative nature (phonons, zero sound, paramagnons etc.). Migdal [31] proved for $D = 3$ in a general form that the corresponding non-analytic contributions to the self-energy $\Sigma(E)$ are of order of $E^3 \ln E$, which results in $T^3 \ln T$-terms in electronic specific heat [32]. The Fermi-liquid behavior might seem to take place for AFM metals since in the long-wavelength limit ($q \to 0$) the electron-magnon interaction is equivalent to the interaction with acoustical phonons (the spectrum of the Bose excitations is linear and the scattering amplitude is proportional to $q^{1/2}$). However, in the case of AFM spin waves there exists one more “dangerous” region $q \to Q$ ($Q$ is the wavevector of the AFM structure), where the magnon frequency $\omega_q$ tends to zero and the scattering amplitude diverges as $\omega_q^{-1/2}$. At very small $E$ such processes are forbidden because of the presence of the AFM splitting in the electron spectrum. At the same time, at not too small $E$ one may expect that these processes lead to stronger singularities. Thus the Fermi-liquid picture may become violated in this energy region.

To investigate effects of interaction of current carriers with local moments we use the Hamiltonian of the $s - d(f)$ exchange model

$$H = \sum_{k\sigma} t_k c_{k\sigma}^\dagger c_{k\sigma} - I \sum_{qk} \sum_{\alpha\beta} S_q c_{k\alpha}^\dagger \sigma_{\alpha\beta} c_{k\beta} - q - \alpha + \sum_q J_q S_q S_{-q}$$

(1)

where $c_{k\sigma}^\dagger$, $c_{k\sigma}$ and $S_q$ are operators for conduction electrons and localized spins in the quasimomentum representation, the electron spectrum $t_k$ is referred to the Fermi level, $I$ is the $s - d(f)$ exchange parameter, $\sigma$ are the Pauli matrices. We consider an antiferromagnet which has the spiral structure along the $x$-axis with the wavevector $Q$

$$\langle S^{z_i}_i \rangle = S \cos QR_i, \quad \langle S^{y_i}_i \rangle = S \sin QR_i, \quad \langle S^{x_i}_i \rangle = 0$$

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It is convenient to introduce the local coordinate system

\[
S_i^x = \hat{S}_i^x \cos QR_i - \hat{S}_i^y \sin QR_i, \\
S_i^y = \hat{S}_i^y \cos QR_i + \hat{S}_i^z \sin QR_i, \quad S_i^z = \hat{S}_i^z
\]

Further one can pass from spin operators \( \hat{S}_i \) to the spin deviation operators \( b_i^\dagger, b_i \), by the canonical transformation \( b_i^\dagger = u_i \beta_i^\dagger - v_i \beta_i \). to the magnon operators. Hereafter we consider for simplicity a two-sublattice AFM (2Q is equal to a reciprocal lattice vector, so that \( \cos^2 QR_i = 1, \sin^2 QR_i = 0 \)). Then the Bogoliubov transformation coefficients and the magnon frequency are given by

\[
u_q^2 = 1 + v_q^2 = \frac{1}{2}[1 + \overline{3} (J_{q+Q} + J_q - 2J_Q) / \omega_q] \\
\omega_q = 2 \overline{3} (J_{q-Q} - J_q)^{1/2} (J_q - J_Q)^{1/2}
\]

so that \( u_q \neq v_q \cong u_{q+Q} \pm v_{q+Q} \propto \omega_q^{\pm 1/2} \) at \( q \rightarrow 0 \).

Further we use at concrete calculations simple results of the usual perturbation theory in \( I \). Defining the self-energies by the perturbation expansion

\[
G_{k\sigma}(E) = \langle \langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E = [E - t_k - \sum_n \Sigma_k^{(n)} (E)]^{-1}
\]

we derive for the contributions which contain the Fermi distribution functions \( n_k = f(t_k) \)

\[
\Sigma_k^{(2)}(E) = I^3 \overline{3} \sum_q (u_q - v_q)^2 \left( \frac{1 - n_{k+q} + N_q}{E - t_{k+q} - \omega_q} + \frac{n_{k+q} + N_q}{E - t_{k+q} + \omega_q} \right) \\
\Sigma_k^{(3)}(E) = I^3 \overline{3} \sum_q \left( \frac{1 - n_{k+q} + N_q}{E - t_{k+q} - \omega_q} - \frac{n_{k+q} + N_q}{E - t_{k+q} + \omega_q} \right) \left( \frac{1}{E - t_{k-Q} - \omega_q} - \frac{1}{t_{k+q} - t_{k+q} - \omega_q} \right) \\
\Sigma_k^{(4)}(E) = I^3 \overline{3} \sum_q (u_q + v_q)^2 \left( \frac{1}{E - t_{k-Q}} - \frac{1}{E - t_{k+q} - Q} \right)^2 \left( \frac{1 - n_{k+q} + N_q}{E - t_{k+q} - \omega_q} + \frac{n_{k+q} + N_q}{E - t_{k+q} + \omega_q} \right)
\]

where \( N_q = N_B(\omega_q) \) is the Bose function.

Non-analytic contributions to the self-energies at \( E \rightarrow 0, T = 0 \) originate from spin waves with small \( q \) and \( |q - Q| \). Because of \( q \)-dependence of interaction matrix elements \( (u_q \neq v_q)^2 \propto q, (u_q \pm v_q)^2 \propto q^{-1} \) at \( q \rightarrow 0 \) and \( q \rightarrow Q \) respectively, the intersubband contributions \( (q \rightarrow Q) \) are, generally speaking, more singular than intrasubband ones ( \( q \rightarrow 0 \)). However, owing to quasimomentum and energy conservation laws, the intersubband transitions are possible at \( |q - Q| > q_0 \sim \Delta / v_F \) (\( \Delta = 2I\overline{3} \) is the antiferromagnetic splitting, \( \overline{S} \) is the sublattice magnetization, \( v_F \) is the electron velocity at the Fermi level). Therefore, when using simple perturbation expressions, one has to bear in mind that the singular intersubband transition contributions should be cut at \( |E|, T \sim T^* \) where

\[
T^* = c q_0 \sim T_N \Delta / v_F
\]

with \( c \) being the magnon velocity. A more general perturbation theory is considered in Appendix A.
It should be noted that, despite absence of long-range order at finite temperatures, the results (3)-(6) are valid also in the 2D case up to $T \sim J$, $S$ being replaced by square root of the Ornstein-Cernike peak intensity in the pair correlation function \[33\]. We have also to replace $T_N \rightarrow JS^2$ in (7). A similar situation occurs for frustrated magnetic systems with suppressed long-range order. In particular, one can think that the consideration of electron-spin interactions, that is based on the spin-wave picture, is qualitatively applicable to $Y_{1-x}Sc_xMn_2$, despite this is not an antiferromagnet, but a spin liquid with strong short-range AFM order.

The correction to the density of states owing to $s - d(f)$ interaction reads

$$\delta N(E) = -\sum_{k\sigma} \{ \frac{1}{\pi} \text{Im} \Sigma^{(i)}_{k}(E)/(E - t_k)^2 + \text{Re} \Sigma^{(i)}_{k}(E) \delta'(E - t_k) \}$$

(8)

The first term in (8) corresponds to incoherent (non-quasiparticle) contribution, and the second one describes the renormalization of quasiparticle spectrum.

The third-order contribution (4) describes the Kondo effect in the AFM state \[38, 39\]. It should be noted that an account of spin dynamics is important at treating this contribution, and its neglect leads to incorrect results: the transition to the usual Kondo behavior $\text{Im} \Sigma(E) \propto \ln |E|$ discussed in Ref.[37] takes place in fact only at

$$|E| \gg \omega(2k_F) \simeq 2ck_F.$$

Unlike $\Sigma^{(2)}_k(E)$, $\Sigma^{(4)}_k(E)$ does not contain “dangerous” divergences since the factor $(u_q + u_q)^2$ is singular at $q \to 0$ (rather than at $|q - Q| \to 0$) and the next factor is proportional to $q^2$. Thus this term results in unimportant renormalizations of $\Sigma^{(2)}_k(E)$. Summation of higher-order correction within a scaling approach is presented in Appendix B.

Averaging $\Sigma^{(2)}_k(E)$ over the Fermi surface $t_k = 0$, we obtain for the intrasubband contribution at $T \ll |E|$ in the 3D case

$$\left\{ \begin{array}{c} \text{Re} \\ \text{Im} \end{array} \right\} \Sigma^{(2)}(E) = \frac{2I^2\rho}{3\omega^2(J_0 - J_Q)E^3}E^3 \times \left\{ \begin{array}{c} \ln |E/\omega| \\ -\left(\pi/2\right)\text{sgn} E \end{array} \right\}$$

(9)

Thus, after analytical continuation, the contributions to $\text{Im} \Sigma(E)$, proportional to $E^2|E|$, result in corrections of the form $\delta \text{Re} \Sigma(E) \propto E^3\ln|E|$, which is in agreement with the microscopic Fermi-liquid theory \[31\]. Then the second term in (8) yields the contributions of the form $\delta N(E) \propto E^2\ln|E|$. For $D = 2$, $\text{Im} \Sigma^{(2)}(E)$ is proportional to $E^2$ and does not result in occurrence of non-analytic terms in $\text{Re} \Sigma(E)$ and $N(E)$. Note that in a 2D paramagnet electron-electron scattering results in the contributions $\text{Im} \Sigma(E) \propto E^2 \ln |E|$, and in $T^2 \ln T$-terms in resistivity \[12\].

As for the “Kondo” (third-order) term (5), picking out the most singular contribution yields

$$\delta \Sigma^{(3)}_k(E) = -\frac{2I^2S^2}{E - t_{k-Q}} \frac{1}{t_{k-Q}} \sum_{k'} \frac{n_{k'}(E - t_{k'})^2}{(E - t_{k'})^2 - \omega_{k-k'}^2}$$

(10)

Thus the singularity in this term is by a factor of $|E|$ weaker in comparison with the intrasubband contribution to $\Sigma^{(2)}(E)$ (note that the corresponding results of Ref.[35, 36] are not correct since not all $q$-dependent factors were taken into account).
Now we investigate the intersubband contributions. Averaging (1) in $k$ over the Fermi surface $t_k = E_F = 0$ we obtain

$$\text{Im}\Sigma(E) = -2\rho^{-1} \sum_{q \geq Q, T^* \leq \omega_q < |E|} \frac{\lambda_q}{\omega_q}$$

with $\rho = \sum_k \delta(t_k)$ the bare density of states at the Fermi level,

$$\lambda_q = 2\pi I^2 S^2 (J_0 - J_Q) \sum_k \delta(t_k) \delta(t_{k+q})$$

In the general 3D case we have $\text{Im}\Sigma(E) \propto E^2$. For $D = 2$ we derive

$$\left\{ \begin{array}{ll}
\text{Re} & \Sigma^{(2)}(E) = \frac{2}{\pi^2 \rho c^2} \lambda_Q E \times \left\{ \begin{array}{c}
\ln |E/\omega| \\
-(\pi/2)\text{sgn}E
\end{array} \right. \\
\text{Im} & \end{array} \right.$$

so that $\text{Im}\Sigma(E)$ is linear in $|E|$. The residue of the electron Green’s function

$$Z = \left( 1 - \frac{\partial \text{Re}\Sigma(E)}{\partial E} \bigg|_{E=E_F} \right)^{-1}$$

yields the renormalization of the effective mass

$$m^*/m = 1/Z \sim \ln (\omega/\omega^*) .$$

The second term of (8) yields at $|E| > T^*$

$$\delta N(E) = - \frac{4}{\pi^2 c^2} \lambda_Q \ln |E|$$

Consider the peculiar 3D case where the electron spectrum satisfies approximately the “nesting” condition $t_k = -t_{k+Q}$ in a significant part of the Brillouin zone (however, the system is still metallic since the gap does not cover the whole Fermi surface). Such a situation is typical for itinerant-electron AFM systems since onset of AFM ordering is connected with the nesting. Besides that, for localized-moment metallic magnets, that are described by the $s-f$ model, the value of $Q$ is also often determined by the nesting condition [38]. As discussed in the Introduction, such a situation can be also assumed for some anomalous $f$-systems.

In the case under consideration the electron spectrum near the Fermi surface is strongly influenced by the AFM gap, so that we have to use the “exact” spectrum (19) and replace in (12)

$$\delta(t_k) \delta(t_{k+q}) \rightarrow \delta(E_{k1}) \delta(E_{k+q2})$$

Then we have in some $q$-region (which is determined not only by $I$ but also by characteristics of the Fermi surface) $\lambda_q \propto 1/|q - Q|$. Thus the effective dimensionality in the integrals is reduced by unity, and the energy and temperature dependences become similar to those in the 2D case.
For the 2D “nested” antiferromagnet, the perturbation theory damping is very large,

\[ \text{Im}\Sigma(E) \propto \ln |E|. \]  

(17)

Replacing the denominator in (4) by the exact electron Green’s function and making the ansatz \( \text{Im}\Sigma(E) \propto |E|^\alpha \) we can estimate the damping in the second-order self-consistent approximation as

\[ \text{Im}\Sigma(E) \propto |E|^{1/2}. \]  

(18)

Thus one has to expect in this case a strongly non-Fermi-liquid behavior at not too small \( |E| \). Note that the situation is different from the power-law non-analyticity in the Anderson model at very small \( |E| \), which is an artifact of the NCA approximation [39].

The damping (13) becomes stronger also in the case of frustrations in the localized spin subsystems where the \( \mathbf{q} \)-dependence of magnon frequency

\[ \omega_q^2 = c_x^2 q_x^2 + c_y^2 q_y^2 + c_z^2 q_z^2 + \Phi^{(4)}(\mathbf{q}) + \ldots \]  

(19)

(\( \Phi^{(4)}(\mathbf{q}) \)) is a quartic form of \( q_x, q_y, q_z \) becomes anomalous. As discussed above, such a situation is typical for systems demonstrating NFL behavior. Instabilities of magnetic structures with competing exchange interactions are often accompanied by softening of magnon spectrum. Usually this takes place in one direction, i.e. \( c_z \ll c_x, c_y \) near the instability point. In some peculiar models, the softening can occur in two or even three directions. In all the cases, the energy dependences of \( \Sigma \) are changed. We have

\[ \text{Im}\Sigma(E) \simeq -2\rho^{-1} \lambda_{\mathbf{Q}} \int_{T^*} |E| \frac{d\omega}{\omega} g(\omega) \propto |E|^\alpha \]  

(20)

where

\[ g(\omega) = \sum_{\mathbf{q} = \mathbf{Q}} \delta(\omega - \omega_\mathbf{q}) \propto \omega^\alpha, \omega \to 0 \]  

(21)

Provided that \( c_z \ll c_x, c_y \), one has to take into account quartic terms, and we obtain after passing to cylindrical coordinates \( \alpha = 3/2 \). In the opposite case \( c_z \gg c_x, c_y \) we get in a similar way \( \alpha = 1 \). For \( c_x, c_y, c_z \to 0 \) we derive \( \alpha = 1/2 \). In the 2D case we have \( \alpha = 1/2 \) at \( c_x \ll c_y \) and \( \alpha = 0 \) (\( \text{Im}\Sigma(E) \propto \ln |E/T^*| \)) at \( c_x, c_y \to 0 \). Thus we can explain violations of the Fermi-liquid picture by peculiarities of not only electron, but also magnon spectrum. The frustration problem for an itinerant AFM was considered in Ref. [40].

Now we treat the incoherent contribution to \( N(E) \) (first term in (8)). We have at \( T = 0 \)

\[ \delta N_{\text{incoh}}(E) \simeq I^2 S \sum_{\mathbf{q}, \sigma} (u_\mathbf{q} - v_\mathbf{q})^2 \sum_k \frac{P}{(E - t_k)^2} \times [(1 - n_{k+\mathbf{q}})\delta(E - t_{k+\mathbf{q}} - \omega_\mathbf{q}) + n_{k+\mathbf{q}}\delta(E - t_{k+\mathbf{q}} + \omega_\mathbf{q})], \]  

(22)

where \( P \) stands for the principal value of the integral. After a little manipulation we obtain

\[ \delta N_{\text{incoh}}(E) \simeq I^2 S \sum_{\mathbf{q}, \omega \sigma < |E|} (u_\mathbf{q} - v_\mathbf{q})^2 P \sum_{k\sigma} \frac{\delta(|E| - t_{k+\mathbf{q}} - \omega_\mathbf{q})}{(E - t_k)^2}. \]  

(23)
In the sum over \( k \) we can neglect \( |E| \) and \( \omega_q \) in comparison with \( v_F q \). Main contribution comes from the intersubband transitions,

\[
\delta N_{\text{incoh}}(E) \simeq I^2 S \sum_{\omega_q \ll |E|} \frac{2S(J_0 - J_Q)}{\omega_q} \sum_{k} \frac{\delta(t_k)}{(t_k + q - t_k)^2} \propto \int_{-E}^E d\omega g(\omega) \propto |E|^\alpha
\]  

(24)

This contribution can have any sign depending on the dispersion law \( t_k \). For the general electron and magnon spectra we have \( \delta N_{\text{incoh}}(E) \propto E^2 \) for \( D = 3 \) and \( \delta N_{\text{incoh}}(E) \propto |E| \) for \( D = 2 \). Unlike the quasiparticle contribution (16), the incoherent one is not cut at \( |E| \approx T^* \) since the conservation laws do not work for virtual magnons. In the case of “frustrated” magnon spectrum the values of \( \alpha \) are given above. In the nesting situation the additional divergent factor \( 1/|q - Q| \) occurs which is, however, cut at \( q = q_0 \). This leads to that, at \( |E| > T^* \), \( \delta N_{\text{incoh}}(E) \propto |E| \) for \( D = 3 \) and \( \delta N_{\text{incoh}}(E) \propto -\ln |E| \) for \( D = 2 \). Due to the factor \( (u_q - v_q)^2 \), the contribution from the region of small \( q \) in (23) contains higher powers of \( E \), despite the singularity in the denominator. The third-order “Kondo” contribution to \( \delta N_{\text{incoh}}(E) \) is small owing to cancellation of intra- and intersubband transitions in (3). The “incoherent” contributions may be in principle observed in tunneling experiments.

Now we treat for comparison the case of a metallic ferromagnets with the parabolic dispersion law of magnons \((Q = 0)\). We have for a given spin projection

\[
\Sigma_{\sigma}(E) = 2I^2 S \sum_q \frac{f(\pm t_k + q + IS) + N_q}{E - t_k + q \mp IS \pm \omega_q}
\]  

(25)

This yields for \( D = 3 \) the one-sided singular contributions

\[
\text{Im} \Sigma_{\sigma}(E) \propto \theta(\sigma E)|E|^{3/2}, \quad |E| > T^* \sim (\Delta/v_F)^2 T_C,
\]  

(26)

the crossover energy scale being considerably smaller than in the AFM case (see \cite{51, 50}; these papers treat also the quasiparticle damping at small \( |E| \) due to electron-magnon scattering, which occurs in the second order in \( 1/2S \) and turns out to be small). Then we obtain \( \delta N_{\sigma}(E) \propto -\ln |E| \) for \( |E| > T^* \). At the same time, the incoherent contribution, which survives up to \( E = 0 \), has the form \( \delta N_{\sigma}(E) \propto \theta(\sigma E)|E|^{3/2} \) and can be picked up in the half-metallic case \cite{52, 51}.

The situation in a 2D ferromagnet is similar to that in the above-discussed “nested” 2D antiferromagnet: the damping in the perturbation theory is large, \( \text{Im} \Sigma(E) \propto |E|^{1/2} \), this result being valid in the self-consistent approximation too.

### 3 Thermodynamic and transport properties

To calculate the electronic specific heat \( C(T) \) we use the thermodynamic identity

\[
\left( \frac{\partial n}{\partial T} \right)_\mu = \left( \frac{\partial S}{\partial \mu} \right)_T
\]  

(27)

with \( n \) the number of particles, \( S \) the entropy, \( \mu \) the chemical potential. Taking into account the expression

\[
n = \int_{-\infty}^{\infty} dE f(E) N(E)
\]  

(28)
and integrating by part, we obtain from the second term of (8)

$$\delta n = \frac{\partial}{\partial \mu} \Phi, \delta C(T) = \delta S(T) = \frac{\partial}{\partial T} \Phi$$

where, to lowest order in $I$

$$\Phi = -2I^2S \sum_{k,q}(u_q - v_q)^2 \frac{\omega_q n_k(1 - n_{k+q})}{(t_k - t_{k+q})^2 - \omega_q^2}. \quad (29)$$

It should be noted that the same result for $C(T)$ can be derived by calculating the transverse-fluctuation contribution to the interaction Hamiltonian

$$\delta \langle H_{sd} \rangle = -I(2S)^{1/2}\langle b_q^\dagger c_{k+q} \downarrow c_{k-q}^\dagger \rangle = -2\Phi \quad (30)$$

(the last equality in (30) is obtained from the spectral representation for the corresponding Green’s function, cf. Ref. [42]) and using the Hellman-Feynman theorem for the free energy, $\partial F/\partial I = \langle \partial H/\partial I \rangle$.

Using the identity

$$\frac{\partial}{\partial T} \int \int dE dE' f(E)[1 - f(E')] F(E - E') = \frac{1}{T} \int \int dE dE' \frac{\partial f(E)}{\partial E} \frac{\partial f(E')}{\partial E'} \int_{E - E'}^{E + E'} dx F(x) \quad (31)$$

we obtain for the intrasubband ($q \to 0$) contribution to (29) at $D = 3$

$$\delta_{\text{intra}}(T) = \frac{74}{135}(J_0 - J_Q)\frac{\omega^2}{\pi T^3} \ln \frac{\bar{\omega}}{T} \quad (32)$$

The term, proportional to $T^3 \ln(T/T_{sf})$ ($T_{sf}$ is a characteristic spin-fluctuation energy, in our case $T_{sf} \sim |J|$) was derived earlier within the Fermi-liquid theory [32]. Note that the $T^3 \ln T$-corrections were not obtained in the spin-fluctuation theory by Moriya et al [43] since only fluctuations with $q \simeq Q$ were taken into account.

The intersubband contribution to specific heat is transformed as

$$\delta_{\text{inter}}(T) = \frac{8}{3} \pi T \sum_{q \simeq Q, T \leq \omega_q} \lambda_q / \omega_q^2 \quad (33)$$

In the 2D or “nesting” 3D situation the integral is logarithmically divergent at $q \to Q$, and the divergence is cut at $\omega_q \simeq \max(T, T^*)$, so that we obtain the $T \ln T$-dependence of specific heat. For $D = 2$ we have

$$\delta_{\text{inter}}(T) = \frac{4\Omega_0}{3c^2} \lambda_Q T \ln \frac{\bar{\omega}}{\max(T, T^*)} \quad (34)$$

Since the integral in (33) is determined by the magnon spectrum only, the result (34) holds also in the case the frustrated (2D-like) magnon spectrum. This contribution may explain the anomalous dependences $C(T)$ in a number of rare-earth and actinide systems (see the
Introduction), which are observed in some restricted temperature intervals. At $T < T^*$ we have an appreciable logarithmic enhancement of the electronic specific heat.

For $T > T^*$ the $T \ln T$-term is present also in specific heat of a ferromagnet, both for the case of weak itinerant-electron ferromagnetism [16] and in the regime of local moments [33, 50]. However, we shall see below that the ferromagnets do not exhibit an important property of the MFL state - the $T$-linear resistivity.

In the model accepted, the non-analytic contributions to magnetic susceptibility should mutually cancel, as well as for electron-phonon interaction [41]. However, such contributions may occur in the presence of relativistic interactions (e.g., for heavy actinide atoms). This effects may be responsible for anomalous $T$-dependences of $\chi$ in the 4$f$- and 5$f$-systems [18].

The first term in (8) (i.e. the branch cut of the self-energy) yields the incoherent (non-quasiparticle) $T$-linear contribution to specific heat (cf. the consideration for a ferromagnet in Ref. [50]), which is owing to the temperature dependence of $N(E)$ and is not described by the Fermi liquid theory. After substituting this term into (28) we obtain

$$\frac{\partial}{\partial T} \delta n_{\text{incoh}} = \frac{2I^2S}{3} \sum_{k,q,\alpha=\pm} \left( u_q - v_q \right)^2 \frac{f(t_{k+q} - \alpha \omega_q)}{(t_{k+q} - t_k - \alpha \omega_q)^2} \frac{\partial}{\partial T} n_{k+q}$$

(35)

At low temperatures we have

$$f(t_{k+q} + \omega_q) \rightarrow 0, \quad f(t_{k+q} - \omega_q) \rightarrow 1$$

and we derive

$$\delta C_{\text{incoh}}(T) = \frac{2}{3} \pi I^2 S \rho T \sum_q \left\langle \left( \frac{u_q - v_q}{t_{k+q} - t_k} \right)^2 \right\rangle_{t_k=0}$$

(36)

Note that the contribution (36) can be also obtained by direct differentiating in temperature the total electronic energy

$$\mathcal{E} = \int_{-\infty}^{\infty} dEE f(E) N(E)$$

(37)

Now we discuss transport properties. To second order in $I$, using the Kubo formula [44] we obtain for the inverse transport relaxation time

$$\frac{1}{\tau} = \pi I^2 S \sum_{k,q} (u_q - v_q)^2 (v_{k+q} - v_k)^2 \delta(t_{k+q} - t_k - \omega_q) \delta(t_k) / \sum_k v_k^2 \delta(t_k)$$

(38)

with $v_k = \partial t_k / \partial k$. Picking out the intersubband contribution ($q \approx Q$) we obtain after standard transformations

$$\frac{1}{\tau} = \frac{\left\langle (v_{k+Q} - v_k)^2 \right\rangle_{t_k=0}}{v_F^2 \rho} \sum_q \lambda_q \left( -\frac{\partial N_q}{\partial \omega_q} \right)$$

(39)

For $D = 3$ we have the quadratic temperature dependence of spin-wave resistivity,

$$R(T) \propto (T/T_N)^2.$$  

(40)

This dependence was obtained earlier within an itinerant model [19]. Note that this contribution dominates at not too low temperatures over the intrasubband contribution (the latter is analogous to the electron-phonon scattering one and is proportional to $T^5$ [18]).
For the 2D magnon spectrum (or “nested” 3D) situation one obtains
\[ R(T) \propto T \ln(1 - \exp(-T^*/T)) \simeq T \ln(T/T^*) \] (41)

Thus in our model, unlike [4], the linear dependence of \( \text{Im}\Sigma(E) \) results in \( T \ln T \) rather than \( T \)-linear behavior of the resistivity because of the lower-limit divergence of the integral with the Bose function. However, the deviation from the linear law is hardly important from the experimental point of view. As for concrete experimental data, the systems CePd\(_2\)Si\(_2\) and CeNi\(_2\)Ge\(_2\) [53] demonstrate under pressure anomalous temperature dependence \( \rho(T) \sim T^\mu, \mu = 1.2 \div 1.5 \). The data of Ref. [54] on CeNi\(_2\)Ge\(_2\) yield for the resistivity exponent \( \mu = 3/2 \).

For a ferromagnet, the spin-wave resistivity at \( T > T^\ast \) is proportional to \( T^2 \) for \( D = 3 \) (and \( T^3/2 \) for \( D = 2 \)) because of the factor \( (\mathbf{v}_k - \mathbf{v}_{k+q})^2 \) in (38). (However, extra powers of \( q \) are absent for the scattering between spin subbands, which yields the \( T \ln T \)-term in resistivity of ferromagnetic alloys [55].) A similar situation takes place in the case of “flat” regions of the Fermi surface in AFM. This may explain absence of \( T \)-linear resistivity in some above-discussed rare-earth and actinide systems which demonstrate \( T \ln T \)-corrections to specific heat.

Now we treat the impurity contributions to transport properties in the presence of potential scattering (in the case of a ferromagnet they were considered in [15]). To second order in impurity potential \( V \) we derive

\[ \langle \langle c_{k\sigma}^\dagger | c_{k'\sigma} \rangle \rangle_E = \delta_{kk'} G_{k\sigma}(E) + VG_{k\sigma}(E)G_{k'\sigma}(E) [1 + V \sum_p G_{p\sigma}(E)] \] (42)

Neglecting vortex corrections and averaging over impurities we obtain for the transport relaxation time

\[ \delta\tau^{-1}_{imp}(E) = -2V^2 \text{Im} \sum_p G_{p\sigma}(E) \] (43)

Thus the contributions under consideration are determined by the energy dependence of \( N(E) \) near the Fermi level. The correction to resistivity reads

\[ \delta R_{imp}(T)/R^2 = -\delta \sigma_{imp}(T) \propto -V^2 \int dE (-\partial f(E)/\partial E) \delta N(E) \] (44)

Note that the quasiparticle renormalization effects owing to \( 1 - d\text{Re}\Sigma(E)/dE = 1/Z \) do not contribute impurity scattering since \( \tau \to \tau/Z \) and \( v_F \to v_F Z \), so that the mean free path is unrenormalized [1]. At the same time, incoherent terms in \( N(E) \) yield \( \delta R_{imp}(T) \propto T^2 \) in the 3D case and \( \delta R_{imp}(T) \propto T \) in the 2D case up to lowest temperatures (in the “nested” 3D case, the \( T \)-linear term has lower cutoff, as well as the “coherent” contribution [14]). In the “frustrated” 3D case with \( \alpha = 1/2 \) we have \( \delta R_{imp}(T) \propto T^{3/2} \).

The impurity contributions are important in “dirty” nearly AFM metals where anomalous contributions to the temperature dependence of resistivity can be both positive and negative. In particular, for the system \( U_x Y_{1-x}Pd_3 \) the experimental data [18] demonstrate the negative contribution to resistivity, \( \delta \rho(T) \sim -T^\mu, \mu = 1.1 \div 1.4 \). In such cases the explanation of these terms by the spin-wave renormalization of impurity scattering seems to be reasonable.

The correction to thermoelectric power, which is similar to (44), reads (cf. [43]):

\[ \delta Q(T) \propto \frac{1}{T} \int dE (-\partial f(E)/\partial E) E \delta N(E) \] (45)
Besides that, an account of higher orders in impurity scattering leads to the replacement of the impurity potential \( V \) by the \( T \)-matrix. For the point-like scattering the latter quantity is given by

\[
T(E) = \frac{V}{1 - V \mathcal{R}(E)}, \quad \mathcal{R}(E) = \mathcal{P} \sum_k G_{k\sigma}(E).
\] 

(46)

Expanding (46) yields also the term

\[
\delta Q(T) \propto \frac{1}{T} \int dE (-\partial f(E)/\partial E) E \delta \mathcal{R}(E)
\]

(47)

with \( \delta \mathcal{R}(E) \) being obtained by analytical continuation from \( \delta N(E) \). Unlike the case of a ferromagnet where \( \delta Q(T) \propto T^{3/2} \) for \( D = 3 \), the \( I^2 \)-contribution to \( \delta N_{\text{coh}}(E) \) in the AFM case is even in \( E \) and does not contribute \([47]\). At the same time, in the 2D case, where \( \delta \mathcal{R}(E) \propto E \ln |E| \), Eq.(47) yields

\[
\delta Q(T) \propto T \ln(T/\Omega)
\]

(48)

For the “nested” 3D case such contributions are present at \( T > T^* \) only. In this connection, experimental data on the systems \( Y(\text{Mn}_{1-x}\text{Al}_x)_2 \), \( \text{Y}_{1-x}\text{Sc}_x\text{Mn}_2 \) \([30]\) are of interest which demonstrate anomalous behavior of \( Q(T) \).

4 Conclusions

We have investigated peculiarities of electron spectrum and corresponding anomalies of thermodynamic and transport properties in metallic antiferromagnets with well-localized magnetic moments. The use of perturbation theory in the electron-magnon interaction within the \( s-d(f) \) exchange model seems to be a reasonable phenomenological approach for highly-correlated electron systems, which takes into account the SU(2) symmetry of exchange interactions. It is often used, e.g., in the theoretical description of high-\( T_c \) copper-oxide superconductors (see, e.g., Ref.[58]). The electron spectrum \( t_k \) and parameter \( I \) may be considered as effective ones (including many-electron renormalizations). Note that similar results for the electron-magnon interaction effects may be obtained in the Hubbard model \((I \to U, \text{cf.}[50, 42])\).

We have demonstrated that, owing to intersubband scattering processes, electronic properties of 2D and “nested” 3D metallic antiferromagnets are close to those in the MFL picture \([4]\) in a rather wide interval \( T^* < T < J \), the value of the crossover temperature being determined by the \( s-f \) exchange parameter and characteristics of electron spectrum. In contrast to \([4]\), no special assumptions about the spectrum of the Bose excitations are used: in our model they are just spin waves with the linear dispersion law. Unlike Refs.[12, 13], we need not to consider the special case of the vicinity to AFM instability. Thus AFM ordering itself, together with rather natural assumptions about a peculiar form of the electron or magnon spectrum, may explain violations of the Fermi-liquid picture which are observed in some rare-earth and actinide systems.

At \( T < T^* \) the MFL behavior is changed by the usual Fermi-liquid one, although some non-quasiparticle contributions are present, which are connected with the presence of local
magnetic moments. These incoherent contributions, which are beyond the Fermi liquid theory, play the crucial role for half-metallic ferromagnets [57]. In AFM metals they are not so important and are hardly observable for perfect crystals. Nevertheless, such contributions may be important for the temperature dependences of transport properties in the “dirty” case (metals with impurities).

We have also analyzed the Kondo contributions to electronic properties in the AFM state. In the case under consideration, they turn out to be strongly suppressed by spin dynamics. Thus main role belongs to the second-order corrections, and higher orders in $I$ are not important. Formally it is a consequence of the divergence of the factors $(u_q - v_q)^2$ at $q \to Q$; the Kondo terms do not contain this divergence [35, 47]. The situation should change with increasing $|I|$ when renormalization of magnon frequencies becomes important and summation of the higher orders is needed. Within a simple scaling approach, such a problem was considered in Ref. [47]. Thus, the transition from “usual” magnets with well-defined local moments, which are weakly coupled to conduction electrons, to the anomalous Kondo magnets is accompanied by a reconstruction of the structure of perturbation theory (different diagram sequences dominate in these two regimes). Therefore the problem of the formulation of an unified picture of metallic magnetism appears to be very complicated not only for itinerant $d$-electron magnets [43, 57], but also for $f$-electron ones.

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### A Self-energies in the $1/S$-expansion

The electron spectrum in the AFM phase contains two split subbands. In the mean-field approximation we have

$$E_{k1,2} = \theta_k \pm E_k, E_k = (\tau_k^2 + I^2 S^2)^{1/2},$$

$$\theta_k = \frac{1}{2}(t_k + t_{k+q}), \tau_k = \frac{1}{2}(t_k - t_{k+q})$$  \hspace{1cm} (50)

To calculate the fluctuation corrections in a consistent way, we have to separate effects of transition within and between the AFM subbands by including the AFM splitting in the zero-order approximation. Introducing spinor operators $\Psi_k^\dagger = (c_k^{\uparrow}, c_{k+q}^{\downarrow})$ and passing to the magnon representation for spin operators, we calculate the matrix electron Green’s function $\hat{G}(k, E)$ to second order in the electron-magnon interaction (this approximation corresponds to first order in the quasiclassical small parameter $1/2S$, see [12]).

We do not write down the whole cumbersome expression for the matrix $\hat{G}(k, E)$, but present the correction to the density of states

$$\delta N(E) = -\sum_{jk}[\frac{1}{\pi} \text{Im} \Sigma_j(k, E)/(E - E_{kj})^2 + \text{Re} \Sigma_j(k, E)\delta'(E - E_{kj})]$$  \hspace{1cm} (51)

The self-energies are given by

$$\Sigma_i(k, E) = \frac{1}{2} I^2 S \sum_q \sum_{j,l=1,2} \{L_{qk}([-1]^{i+j+1} + (-1)^{i+l} M_{qk}([-1]^{i+j+1})] \frac{f((-1)^l E_{k+q}) + N_q}{E - E_{k+q} + (-1)^l \omega_q}$$

\hspace{1cm} (52)
where
\[
L_{kq}(\pm) = (u_q^2 + v_q^2)(1 \pm \frac{I^2 q^2}{E_k E_{k+q}}) \pm 2u_q v_q \tau_k \tau_{k+q}/E_k E_{k+q}
\]
\[
M_{kq}(\pm) = \frac{I^2}{S_k} (1/E_k \pm 1/E_{k+q})
\]
(53)

(54)

The intra- and intersubband contributions correspond to \(i = j\) and \(i \neq j\).

The calculations in the narrow-band limit can be performed by using the many-electron Hubbard operator \([58, 33]\) or slave boson representations \([59]\). The contribution of intersubband processes turns out to have a different structure and does not lead to occurrence of the singular factors \((u_q - v_q)^2\). In particular, the factors of \((u_q t_k - v_q t_k)^2\) occur which tend to zero both at \(q \to 0\) and \(q \to Q\) (cf. Refs.\([33, 59]\)). The problem of interpolation between perturbation regime and narrow-band case, which is important for HTSC, needs further investigations.

For example, averaging \(\Sigma_i(k, E)\) over the Fermi surface \(E_{ki} = 0\), we obtain instead of (9) for the intrasubband contribution at \(T \ll |E|\):
\[
\text{Im} \Sigma_i^{(a)}(E) = -\frac{I^2 S_k}{6\pi c^3} F_i^{(a)}(E) \times \left\{ \begin{array}{lcr} |E|(E^2 + \pi^2 T^2) & D = 3 \\ E^2 c & D = 2 \end{array} \right.
\]
(55)

with
\[
F_i^{(a)}(E) = \langle [L_{kq}(-) - (-1)^i \text{sgn} E M_{kq}(-)]/\omega_q \rangle_{E_{ki} = E_{k+q}, \omega_q = 0} [\omega_q (\delta(E_{k+q}))]_{E_{k} = 0} q = 0.
\]
(56)

B  
A simple scaling consideration

The singularities of matrix elements at \(q \simeq Q\) could lead to the formation of marginal Fermi liquid if they would not cut at \(E \simeq \omega^*\); when taking into account the cutoff they are formally safe. Let us consider the summation of the divergences from the dangerous region \(q \simeq Q\) using the “poor-man scaling” approach \([10]\).

We neglect here the Kondo renormalizations of the effective coupling constant and magnon frequency, which are considered in Ref.\([47]\), since they do not contain the factors of the type \((u_q - v_q)^2\) and can be treated separately.

During the scaling process, the cutoff frequency is renormalized itself owing to the renormalization of the electron spectrum, \(t_k \to Z t_k\), so that \(q_0 \to q_0/Z, \omega^* \to \omega^*/Z\).

In the simplest scaling theory we have to pass to \(E = 0\) (effective mass at the Fermi surface exactly). Supposing that there is no cutoff of the dangerous electron-magnon scattering processes, we can consider the effective mass as a function of \(C\) which is the flow cutoff parameter (see, e.g., Ref.\([47]\)). Usually one has to treat the limit \(C \to 0\). Here we have to remember that \(\omega_{\text{max}} > C > \omega^*\) and to stop scaling at the boundary of this region \(\omega^*\).

The electron damping owing to \(s - d(f)\) interaction is determined by the imaginary part of the polarization operator which is obtained as the convolution of the one-electron Green’s functions,
\[
\Pi_q(\omega) = Z^2 \sum_k \frac{f(Z t_k) - f(Z t_{k+q})}{Z t_{k+q} - Z t_k - \omega}
\]
(57)
Thus the quantity $\lambda Q$ in (11), which is proportional to the spin-wave damping, turns out to be unrenormalized.

The correction to effective electron mass in the 2D case according to (14) reads

$$\delta Z^{-1}(C) = \frac{2}{\pi^2 \rho c^2} \lambda Q \ln (\frac{\omega}{C})$$

(58)

Equation for the renormalization factor $Z = Z(C \rightarrow 0)$ has the form

$$1/Z = 1 + \frac{2}{\pi^2 \rho c^2} \lambda Q \ln (\frac{Z \omega}{\omega^*})$$

(59)

This possesses the only solution with $0 < Z < 1$ which can be estimated as $Z \sim \ln^{-1} (\frac{\omega}{\omega^*})$. Thus, despite an appreciable renormalization of the effective mass, formation of the true MFL state does not take place because of the presence of the cutoff.

Note that the effective mass enhancement for 3D ferromagnets [35, 50] can be treated in a similar way.

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