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On the microscopic model of Fe and Ni: the possible breakdown of the ferromagnetic Fermi-liquid picture

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Abstract. A new model of strong itinerant ferromagnetism, taking into account the presence of a narrow density-of-states peak at E_F, which is due to merging of van Hove singularities, is proposed. The states of the peak (e_g-type states for Fe) are treated within the framework of the Hubbard model with strong correlations. The role of the non-quasi-particle states, which lie near E_F and are not described by the theory of the ferromagnetic Fermi liquid, is investigated. In particular, experimental data on the spin polarization of conduction electrons and T-dependence of resistivity are discussed.

1. Introduction

Despite the tremendous efforts made to construct the theory of transition-metal magnetism, a number of fundamental issues have not as yet been resolved. One of the most important of these is the problem of local magnetic moments (LMMs) which manifest themselves in the Curie–Weiss law for magnetic susceptibility and in the q- and T-dependences of the neutron magnetic scattering cross section in the paramagnetic phase. Spin fluctuation theories [1], based on the functional integral method for the Hubbard model, provide an interpolation description of strong ferromagnetism. Unfortunately, such approaches use essentially an uncontrolled static approximation that treats the translation-invariant many-particle system as a disordered alloy. This results in the violation of the Fermi-liquid picture: the 'spontaneous' spin splitting at $T > T_C$ contradicts the Landau postulate about the one-to-one correspondence of bare particles and quasi-particles, and the damping at E_F is large [2]. The question about the physical reality of this violation cannot be solved within the framework of spin fluctuation theories. Apparently, the dissipative character of spin dynamics is incompatible with the Fermi-liquid state (see, e.g., [3]), but this issue has not been investigated in detail.

Spontaneous spin splitting may be observed in optical [4] and photoemission [5,6] spectra and does exist in Fe, Co and Ni. Convincing evidence of its existence in Ni has been recently obtained by the positron annihilation technique [7]. Such a splitting is treated often as the correlation splitting between the Hubbard subbands. The picture including a large Hubbard splitting enables one to derive the Curie–Weiss law without using the functional integral formalism and the static approximation [8], the LMMs being treated as singly occupied states on a site which are stabilized by Hubbard correlations.

On the other hand, the applicability of the simple one-band Hubbard model for the description of ferromagnetic transition metals is questionable. A recent attempt of a consistent first-principles calculation of the Hubbard parameter for Fe [9] has yielded a

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large value $U \simeq 6$ eV. This value, if it were correct, would mean very strong correlation effects and the inadequacy of band theory (spin-density functional (SDF) approach) for Fe. However, the latter approach describes well such ground-state characteristics as saturation moment [10] and spin-wave stiffness [11]. At the same time, the elastic moduli and the phase diagram of Fe (stability of FCC and BCC phases) are not described satisfactorily by band theory [12]. The agreement between the theoretical and experimental cross sections of the Fermi surface for Fe is much worse than for non-magnetic transition metals [13]. In the paramagnetic phase, the SDF method does not yield the existence of LMMs in Ni and underestimates their value in Fe [14].

A number of physical properties are weakly sensitive to the model. First of all, this concerns the spin-wave (low-T) region where long-wave magnons play the dominant role and symmetry requirements result in identical T-dependences of electron and magnon spectra and of related quantities within the Fermi-liquid theory [15], the Hubbard model with strong correlations [16, 17] and even the s–d exchange model [18]. However, calculations within the microscopic models yield, unlike the phenomenological treatment [15], peculiar 'non-quasi-particle' contributions to the electron spectral density which correspond to branch cuts of the Green functions and yield appreciable contributions to thermodynamic and transport properties [16–18]. Their spectral weight is appreciable if the collective magnon mode is well defined in a large part of the q-space. The fulfilment of this condition is one of the criteria of the LMM existence [1]. Violations of the ferromagnetic Fermi-liquid picture are particularly important for the so-called 'half-metallic' ferromagnets (e.g. Heusler alloys [19]) where the Fermi level lies in the energy gap for one of the spin projections and the Stoner continuum is absent (see the model considerations in [16–18, 20]).

The choice of an adequate microscopic model of ferromagnetic transition metals, which takes into account all these circumstances, is not simple. The present paper is devoted to this problem. In section 2 we formulate such a model starting from the results of the band-structure calculations. In section 3 we investigate the character of electron states near the Fermi level within this model and demonstrate the important role of the non-quasi-particle contributions, described by branch cuts of the electron Green functions, in the thermodynamic and transport properties. In section 4 we discuss the general problem of the adequacy of the SDF approach and Fermi-liquid description for Fe and Ni. Preliminary results of the present paper were published as a short note [21].

2. The formulation of the model

The quantum Monte Carlo calculations [22] demonstrated that the occurrence of spin polarization in the homogeneous electron gas is energetically unfavourable at electron densities characteristic of d metals, and even for densities smaller by two orders of magnitude. Thus the existence of ferromagnetism in real metallic systems is intimately related to the inhomogeneity of the electron density. Considering the stability of the paramagnetic state of inhomogeneous electron gas within the SDF method, one obtains the 'Stoner' criterion of ferromagnetism

$$IN(E_F) > 1$$

(where $N(E)$ is the density of states (DOS)), the effective Stoner parameter I being approximately equal to that for the homogeneous electron gas with the same mean density.

Thus the occurrence of ferromagnetism is due to the large value of $N(E_F)$ which may exceed in real metals the free-electron values by one to two orders of magnitude. So, in the weak itinerant ferromagnets $ZrZn_2$ and $Ti_{1-x}Cu_xBe_2$ the fulfilment of the Stoner criterion is connected with the presence at E_F of sharp $N(E)$ peaks owing to the crystal structure of the C15 Laves compounds [23]. These peaks have a 'geometric' nature and result from the confluence of two square-root van Hove singularities, which yields a 'quasi-two-dimensional' singularity [24]

$$\delta N(E) \sim -\ln|E - E_F|$$

(at the same time, the crystal symmetry remains cubic). The situation for $ZrZn_2$ [23] is reminiscent of that for FCC Sr and Ca [24]. For the non-magnetic BCC Fe, the $N(E)$ peak at E_F, having a width $\Gamma \simeq 0.1$ eV [10] and responsible for ferromagnetism is due to the merging of van Hove singularities along the P–N line. When passing to the ferromagnetic phase, the peak becomes split but retains its form (spin splitting $\Delta \simeq 2\,\text{eV} \gg \Gamma$). A similar situation occurs for Ni. A detailed analysis of the corresponding merged van Hove singularities has been presented in [25].

An important difference between $ZrZn_2$ and α-Fe is that the peak capacity is small in the former case and is of the order of one electron per atom for Fe, the saturation moment being determined by this capacity. The formation of such a peak in Fe is connected with strong flattening of the spectrum in the directions perpendicular to the P–N line, i.e. with an appreciable localization of corresponding e_g-type 3d states in real space (unlike the 4d states in $ZrZn_2$). In the case of still stronger localization, the Stoner criterion is completely inadequate, Hubbard splitting occurs and ferromagnetism is possible even in the absence of $N(E)$ peaks. Such as situation was considered in [8] with application to the highly correlated system $Fe_{1-x}Co_xS_2$. However, in most metallic ferromagnets including Fe, Co and Ni, one can pick out a well defined group of states, which are connected with an $N(E)$ peak and responsible for magnetic instability. Up to now, this was underestimated when formulating models of itinerant magnetism.

To write the Hamiltonian of our model, we introduce the creation operators $d^+_{k\sigma}$ which describe the states forming the peak at E_F (e_g states for Fe) and responsible for ferromagnetism ('magnetic' states), and the operators $c^+_{k\sigma}$ which describe all the other (s, p, d) states (called for brevity hereafter 's electrons'). For simplicity, band indices will be omitted. We now consider the site representation, introducing the operators

$$D^+_{i\sigma} = \sum_{k \in K} d^+_{k\sigma} \exp(ik \cdot R_i) \tag{1}$$

where K is the region of quasi-momentum space filled by 'magnetic' electrons. Since the sum in (1) does not go over the whole Brillouin zone, the states created by the operators $D^+_{i\sigma}$ are not Wannier states; they are not orthogonal to each other and to the Wannier states of other bands. However, they may be mutually orthogonalized,

$$D^+_{i\sigma} \to d^+_{i\sigma}.$$

Because the DOS peak under consideration is narrow, it is natural to postulate strong localization of the orthogonalized functions in real space and to introduce a large Hubbard-type interaction. It is suitable to pass to the many-electron Hubbard representation which

diagonalizes the interaction term:

$$d_{i\sigma} = X_i^{0\sigma} + \sigma X_i^{-\sigma 2}$$
$$X_i^{\alpha\beta} = |i\alpha\rangle\langle i\beta| \tag{2}$$

$$H_{\rm int} = U\sum_i d_{i\uparrow}^+ d_{i\uparrow} d_{i\downarrow}^+ d_{i\downarrow} = U\sum_i X_i^{22} \tag{3}$$

where $|i\sigma\rangle$ are the singly occupied states with the spin projection σ, $|i2\rangle$ are the doubly occupied states (doubles) and $|i0\rangle$ are the empty states (holes). Since, according to the band calculations [10], the up-spin peak in Fe and Ni is completely filled, we assume that the concentration of 'magnetic' electrons is $n > 1$. Then, in the limit of the strong interaction $U \to \infty$, holes are absent and the number of doubles is minimal. (It should be noted that such a situation takes place also for strong non-contact interaction with positive Fourier transforms U_q [26].) Thus the Hamiltonian of magnetic electrons takes the form

$$H_{\rm d} = \sum_{ij} t_{ij} X_i^{2\sigma} X_j^{\sigma 2} = \sum_{k\sigma} \epsilon_k X_{-k}^{2\sigma} X_k^{\sigma 2} \tag{4}$$

where t_{ij} are the effective transfer integrals (renormalized after the orthogonalization), ϵ_k is the corresponding band spectrum and $X_k^{\alpha\beta}$ are the Fourier transforms of Hubbard operators.

It should be stressed that the width of the band ϵ_k, i.e. the peak width $\Gamma \simeq 0.1$ eV, is considerably smaller than the total d band width. The narrow band is submerged into a continuum of 's states'. In this sense, the situation is reminiscent of that in mixed-valence compounds where, however, the f peak width is still smaller and is determined by the s–f hybridization rather than by direct f–f overlap (with the possible exception of cerium [27]).

Similar to the derivation of the Anderson [28] model, the procedure considered results in the occurrence of a mixing term

$$H_{\rm sd} = \sum_{k\sigma} V_k (c_{k\sigma}^+ X_k^{-\sigma 2} + X_{-k}^{-\sigma 2} c_{k\sigma}). \tag{5}$$

In our case the overlap of the magnetic d states is more important than the hybridization V_k, so that to a zeroth-order approximation we may describe the magnetic electrons within the narrow-band Hubbard model (4). This enables one to explain naturally such LMM manifestations as the spontaneous spin splitting and the Curie–Weiss law, the Curie temperature being estimated as $\Gamma\phi(n)$ with $\phi(n) \sim 1$ being a function of magnetic electron concentration n (see, e.g., [8]). Thus the smallness of $T_C \simeq 10^3$ K in comparison with the 'Stoner' splitting Δ, which is a serious problem for strong itinerant ferromagnets, may be due to the small width of the 'magnetic' state band. It is worthwhile to note that the narrow $N(E)$ peak results in the Curie–Weiss behaviour of the paramagnetic susceptibility at $T > \Gamma$ even within the one-particle approach [29].

3. Non-quasi-particle states and their contributions to physical properties

Since in both Fe and Ni the spin-down subband of 'magnetic' electrons is filled, we have the saturated ('half-metallic') ferromagnetism situation, provided that s electrons are neglected. Calculation of the one-particle Green functions

$$G_k^\sigma(E) = \langle\langle X_k^{-\sigma 2} | X_{-k}^{2-\sigma} \rangle\rangle_E$$

at $T = 0$ in such a situation yields (cf [17, 20])

$$G_k^\downarrow(E) = (E - \epsilon_k)^{-1} \tag{6}$$

$$G_k^\uparrow(E) = \left[E - \epsilon_k + \left(\sum_q f_{k+q} G_{k+q}^\downarrow (E + \omega_q) \right)^{-1} \right]^{-1} \tag{7}$$

where $f_k = f(\epsilon_k)$ is the Fermi function and ω_q is the magnon spectrum. The expression (7) is reminiscent of the Hubbard-III result [30]. The latter does not contain the Fermi functions and may be represented for the paramagnetic phase at $U \to \infty$ in the form

$$G_k(E) = \left[E - \epsilon_k + \tfrac{1}{2} n \left(\sum_q G_q(E) \right)^{-1} \right]^{-1}. \tag{8}$$

This approximation yields a large damping at the Fermi level.

Provided that the concentration of the doubles (which play the role of current carriers), $n_2 = n - 1$, is not too large, $G_k^\uparrow(E)$ has no poles below E_F. At small n_2, (7) may be simplified to obtain [16]

$$G_k^\uparrow(E) = \sum_q \frac{f_{k+q}}{E - \epsilon_{k+q} + \omega_q}. \tag{9}$$

We see that there exists a 'non-quasi-particle' contribution to the density of states:

$$N_\uparrow(E) = -\frac{1}{\pi} \sum_k \mathrm{Im}[G_k^\uparrow(E)] \simeq \begin{cases} N_\downarrow(E) & E_F - E \gg \bar{\omega} \\ 0 & E > E_F \end{cases}$$

which is due to the branch cut. Contrary to the paramagnetic phase (see (8)), such contributions in ferromagnets vanish sharply (on the scale of the order of the characteristic magnon frequency $\bar{\omega}$) at $E \to E_F - 0$. Taking into account the behaviour $\omega_q = Dq_\delta^2$ at $q \to 0$, it is easy to derive [17, 18, 20]

$$N_\uparrow(E) \sim [(E_F - E)/\bar{\omega}]^{3/2} \qquad E_F - E \ll \bar{\omega}. \tag{10}$$

The non-quasi-particle states do not influence the characteristics of the Fermi surface at $T \ll \bar{\omega}$ and provide the correct value of the saturation moment

$$M_0 = \tfrac{1}{2}(n_\uparrow - n_\downarrow) = \tfrac{1}{2}(1 - n_2) = 1 - \tfrac{1}{2}n$$

($n_\sigma = \langle X_i^{\sigma\sigma} \rangle$ is the number of singly occupied sites with the spin projection σ), corresponding to the half-metallic state. Indeed, we obtain from the spectral representation for $G_k^\sigma(E)$

$$n_\sigma = \int \mathrm{d}E\, N_\sigma(E)[1 - f(E)] = (1 - n_2)\delta_{\sigma\uparrow} \tag{11}$$

and, for both σ, the sum rule holds:

$$\int \mathrm{d}E\, N_\sigma(E) f(E) = n_2. \tag{12}$$

However, they are important for the excitation spectrum near E_F and, consequently, for thermodynamic and transport properties.

As shown in [17], the branch cut terms contribute to the linear γT-term in the specific heat:

$$\delta C_\uparrow(T) = \sum_k \epsilon_k \int \mathrm{d}E\, f(E) \frac{\partial}{\partial T} \left(-\frac{1}{\pi} \operatorname{Im}[G_k^\uparrow(E)] \right) \tag{13}$$

owing to the temperature dependence of the Fermi functions which enter (7).

To avoid misunderstanding, it should be stressed that this fact means inapplicability of the Fermi-liquid description in terms of dynamical quasi-particles only, which are determined by the poles of the Green functions. It may be shown rigorously that the entropy of interacting Fermi systems at low T is expressed in terms of Landau quasi-particles with the energies determined as variational derivatives of the total energy with respect to occupation numbers [31]. Thus, even in the presence of non-pole contributions to the Green functions, the description of thermodynamics in terms of statistical quasi-particles [31] holds. (However, the quasi-particle description is insufficient for spectral characteristics, e.g. optical and emission data.) The anomalous γT-term is determined by the difference between the spectra of statistical and dynamical quasi-particles. Within the perturbation theory in U, such terms arise in order U^2 for the ferromagnetic phase [17] and in order U^3 for the paramagnetic phase (cf [31]). In the case of the strong correlations (large U) under consideration the anomalous specific heat may be large [15].

The spin fluctuation enhancement of γ does exist [32] in the Heusler alloys X_2MnY which possess the half-metallic electron structure [33], so that the usual paramagnon enhancement is absent and the mechanism considered should be relevant. As for ferromagnetic transition metals, experimental data demonstrating the difference between the γ-values for Ni at $T < T_C$ (7.0 mJ mol^{-1} K^{-2} [34]) and at $T > T_C$ (5.8 mJ mol^{-1} K^{-2} [35]) are of interest. From the viewpoint of simple band theory, $\gamma(T < T_C)$ should be

smaller than $\gamma(T > T_C)$ since the spin splitting results in a shift in the $N(E)$ peak from E_F.

Within the picture including the non-quasi-particle states, the behaviour of the spin polarization $P(E)$ of emitted electrons turns out to be non-trivial. According to the band theory, $N_\downarrow(E_F) \gg N_\uparrow(E_F)$ and P must be negative and large in absolute value because of the large peak for spin-down states at E_F [10]. In our model, P should be small after averaging over the energy interval $|\Delta E| \gg \tilde{\omega}$ since $N_\uparrow(E < E_F) \simeq N_\downarrow(E)$. At not too small n_2 and finite Hubbard parameter U, this equality is violated, but in any case we may expect strong deviations from the predictions of the band theory. This conclusion should be reliable irrespective of the details of the spin-polarization measurement.

Experimental data for Ni yield small values of $P \simeq -5$ to $+10\%$ [36]. The data for Fe [36] are contradictory because of the difficulty of surface preparation. As follows from our model, P should be small for well prepared Fe samples.

An old problem of the metallic ferromagnetism theory is the temperature dependence of resistivity at $T \ll T_C$ [37]. Experimental data are usually fitted as

$$\rho(T) = aT + bT^2$$

or

$$\rho(T) \sim T^{3/2}.$$

The factor a exceeds by two to three orders of magnitude the value corresponding to relativistic interactions, and the T^2-term is present at temperatures much lower than those predicted by the theory considering the one-magnon scattering processes (which have the threshold energy determined by the boundary of the Stoner continuum).

In our model, the $T^{3/2}$-dependence may be explained by impurity scattering $\bar{V}$ with account of the non-quasi-particle contribution to the DOS (cf [38]). As follows from (10),

$$\delta\rho(T) \sim \bar{V}^2 \int dE \left(\frac{-\partial f(E)}{\partial E}\right) N_\uparrow(E) \sim T^{3/2}. \tag{14}$$

Spin-polaron contributions of another nature (see, e.g., [39]) may also play a role. In high-purity samples the $T^{3/2}$-contribution should vanish.

As to the T^2-contribution, this may be due to scattering of 's electrons' by 'magnetic electrons' via the Mott s–d hybridization mechanism [40]. Unlike the usual s–d exchange model, there is no threshold energy for such processes; so they should be effective at low T.

4. Adequacy of the spin-density functional description

Now we treat an important problem: to what extent does the statement about the crucial role of correlation effects in Fe and Ni agree with the standard microscopic theory of these metals, based on the Fermi-liquid picture and SDF approach? As discussed in the introduction, the successes of band-structure calculations in the description of transition-metal properties should not be overestimated. The difficulties available (in particular, for the elastic moduli and crystal structure of Fe [12]) are apparently connected with the local approximation for

the SDF. The Kohn–Hohenberg theorem guarantees the existence of a (generally speaking, non-local) SDF which yields exact results for the ground-state energy and the distribution of the spin and charge densities. This functional should enable one to calculate to any accuracy such quantities as the elastic moduli (expressed as differences between the ground-state energies) and some magnetic characteristics: saturation magnetization (connected with the spin density), spin-wave stiffness and exchange parameters (expressed in terms of the energies of the corresponding magnetic configurations). An improvement in the local-density approximation for itinerant magnets was discussed in [41].

The possibility of calculation of the whole excitation spectrum within the SDF method may not be justified and is doubtful even in principle. There exist a number of attempts to describe the quasi-particle structure of d metals by combining band and model approaches (see, e.g., [42]). The practice of band calculations for heavy-fermion systems [43], where correlation effects are important, demonstrates that the shape of the Fermi surface is described with high accuracy, but the discrepancy with experimental results, say, for the electron effective mass can be up to one to two orders of magnitude. The characteristics of the Fermi surface at $T = 0$ K, measured by photoemission or the de Haas–van Alphen effect, are determined by the electron self-energy $\Sigma(k, 0)$ at $E = E_F$ and are fixed to some extent by the Luttinger theorem and the crystal structure. Therefore we can assume that these ground-state characteristics of 3d metals are described by band calculations too. However, temperature variations in the Fermi surface are strongly influenced by the existence of local magnetic moments, as can be seen from recent data on the spin splitting of Ni [7]. Similar to the case of heavy-fermion systems, the linear γT-term in the specific heat is not given correctly by the calculated $N(E_F)$, as we have demonstrated in section 2.

The question about the adequacy of the SDF description for the states far from E_F is still more complicated, since the many-particle theory yields no corresponding rigorous results. These states may be investigated by optical and thermionic emission experiments. In this connection, recent thermoemission data for Fe and Ni [44] are of interest. The emission intensity for caesiated Fe (with a work function of 1.4 eV) is determined by the group of states in the region of the spin-down $N(E)$ peak [10], so that one may expect strong spin polarization of thermoelectrons. However, null polarization has been observed both for Fe and for Ni. It is shown in [45] that the situation in Ni may be explained even within the band approach, but for Fe the discrepancy is connected with strong correlations. Thus the results [44, 45] yield direct evidence of incomplete adequacy of the band theory for Fe.

From the viewpoint of our model, for providing a basis for considering correlation effects, band calculations in only the ground state should be used. The spin dependence of the spectrum in the narrow-band Hubbard model, even in the ground state, differs drastically from that in the band theory (e.g. the narrowing of the band in the simplest Hubbard-I approximation [46] instead of the spin splitting).

5. Conclusions

Our model, which separates d electrons into two subsystems, revives to some extent the idea about the different natures of e_g and t_{2g} states suggested by Goodenough [47] who considered e_g states in Fe as localized and t_{2g} states as itinerant. Two-band models of transition metals with localized and itinerant d electrons were used also in [48, 49], where magnetism was assumed to arise owing to the RKKY interaction.

In our treatment, the e_g states which form the DOS peak are assumed to be localized, and other states are itinerant. This assumption leads to some consequences which may be

useful for first-principles electronic structure calculations. So, when calculating the Hubbard parameter U (e.g. in the approach in [9]), it is natural to consider e_g electrons as 'Hubbard' electrons, and t_{2g} electrons, together with s and p electrons, as taking part in the screening of the Coulomb interaction (since only states near E_F contribute to the screening, the incorrect treatment of the e_g states, which are far from E_F, is not important). This may result in a considerable decrease in U. When applying the s–d model to Fe, only e_g ('magnetic') states should be treated as 'd states'. As for finite-T calculations in the SDF approach, the ratio T_C/Γ (with Γ being the effective band width) is not small; so using the alloy analogy, i.e. adiabatic approximation for spin degrees of freedom, in spin fluctuation theories [1] and band calculations [14] needs verification.

A consistent qualitative treatment of magnetic and transport properties as well as electron emission data within our model seems to be of interest.

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