Ground state and electron-magnon interaction in an itinerant ferromagnet: half-metallic ferromagnets

1990 J. Phys.: Condens. Matter 2 7151

(http://iopscience.iop.org/0953-8984/2/34/009)

J. Phys.: Condens. Matter 2 (1990) 7151–7171. Printed in the UK

Ground state and electron–magnon interaction in an itinerant ferromagnet: half-metallic ferromagnets†

V Yu Irkhin and M I Katsnelson
Institute of Metal Physics, 620219 Sverdlovsk, USSR

Received 16 May 1989

Abstract. Electron and spin Green functions of a Hubbard ferromagnet are calculated, both starting from the Stoner ground state and for a ferromagnet with Hubbard subbands. The temperature dependences of the spin-wave stiffness and damping, the magnetisation, the local moment on a site and the thermodynamic properties are investigated. The role of non-quasiparticle contributions, described by branch cuts of electron Green functions, is discussed. The non-quasiparticle ('ferrospinon') correction to the linear term in the specific heat is obtained. Experimental data on 'half-metallic' ferromagnets (in particular, spin polarisation and longitudinal nuclear relaxation rate) are analysed.

1. Introduction

It is common practice to describe the properties of itinerant electron ferromagnets using the Hubbard [1] model. Considerable developments have been made in the last 15 years within the framework of the spin-fluctuation theory [2]. The latter treats the contribution of thermal spin fluctuations (mainly paramagnons) to thermodynamic and magnetic properties, and, as a rule, the ground state is assumed to be described by the Stoner theory. Such an approach, based on the Fermi-liquid theory, seems to be adequate for weak itinerant ferromagnets such as $ZrZn_2$ and Sc_3In. However, it is inapplicable for ferromagnets with strong electron correlations. In particular, the Mott–Hubbard splitting [1] may arise, which persists in the paramagnetic region, so that the Stoner picture is incorrect. For example, in the Hubbard-I approximation [1], the main effect of spin polarisation on the electron spectrum is the change in the widths of spin subbands rather than a constant spin splitting. Also, an explicit consideration of zero-point fluctuations is needed when determining the saturation magnetisation in a narrow-band Hubbard ferromagnet [3].

Another example of the influence of strong electron correlations is yielded by so-called 'half-metallic' ferromagnets (HFMs) where the Fermi level lies in the gap for one of the spin projections (in the non-degenerate Hubbard model these ferromagnets are described as saturated ferromagnets). Such a situation takes place, for example, in Heusler alloys MMnSb (M ≡ Ni, Co, Pt) [4]. This case is interesting from the theoretical point of view since it is opposite to the case of weak itinerant ferromagnets.

† Paper presented at the International Conference on Magnetism, Paris, July 1988.

Thus spin-fluctuation theories must be extended to include the case of strong electron correlations. The full realisation of this is a difficult problem. In the present paper we investigate in detail the effects of electron–magnon interaction on the magnetic and thermodynamic properties of itinerant ferromagnets, without restriction to the case of very weak ferromagnets. In particular, we demonstrate the important role of non-quasiparticle states which correspond to branch cuts of Green functions and are not taken into account in the Fermi liquid theory. In section 2 we calculate electron and spin Green functions both for the general case by using perturbation theory in the fluctuating part of the Coulomb interaction and, more accurately, for a HFM. In section 3 we consider the electron spectrum, damping, density of states and occupation numbers. In section 4 we investigate the magnon damping and the temperature dependence of the spin-wave stiffness (in particular, the non-analytic $T^2 \ln T$ contribution). In section 5 we find corrections to the magnetisation, and in section 6 to thermodynamic properties. In section 7 we derive the electron Green functions in the limit of strong electron correlations using the Hubbard many-electron representation [5]. In section 8 we demonstrate the occurrence of non-quasiparticle contributions to the electron specific heat, contradicting the Fermi-liquid theory. In section 9 we discuss available experimental data on HFMs.

2. Calculation of electron and spin Green functions

We proceed with the Hubbard Hamiltonian

$$H = \sum_{k\sigma} t_k c^+_{k\sigma} c_{k\sigma} + H_{\rm int}. \tag{2.1}$$

The intrasite Coulomb interaction $H_{\rm int}$ may be represented in various forms [2]

$$\begin{aligned} H_{\rm int} &= U \sum_i n_{i\uparrow} n_{i\downarrow} = U \sum_{kk'q} c^+_{k+q\uparrow} c_{k\uparrow} c^+_{k'\downarrow} c_{k'+q\downarrow} \\ &= \frac{U}{2} \sum_{k\sigma} c^+_{k\sigma} c_{k\sigma} - \frac{U}{2} \sum_q (S^-_{-q} S^+_q + S^+_q S^-_{-q}) \end{aligned} \tag{2.2}$$

$$S^\sigma_q = \sum_k c^+_{k\sigma} c_{k+q,-\sigma} \qquad \sigma = \uparrow, \downarrow (\pm). \tag{2.3}$$

Many of the results in the present paper hold also for the s–d(f) exchange model with the Hamiltonian

$$H = \sum_{k\sigma} t_k c^+_{k\sigma} c_{k\sigma} - I \sum_q \mathbf{S}_q \cdot \boldsymbol{\sigma}_{\alpha\beta} c^+_{k+q\alpha} c_{k\beta} + H_{\rm d} \tag{2.4}$$

with I the s–d exchange parameter, $\mathbf{S}_q$ the localised-spin operators, $\boldsymbol{\sigma}$ the Pauli matrices and $H_{\rm d}$ the Heisenberg Hamiltonian of the localised spin system.

Consider the anticommutator retarded one-electron Green function [6]

$$G^\sigma_k(E) = \langle\langle c_{k\sigma} | c^+_{k\sigma} \rangle\rangle_E = [E - t_k - \Sigma^\sigma_k(E)]^{-1}. \tag{2.5}$$

The equation of motion for it has the form

$$\begin{aligned} (E - t_{k\sigma}) G^\sigma_k(E) &= 1 - U \sum_q F^\sigma_{kq}(E) \\ F^\sigma_{kq}(E) &= \delta \langle\langle S^{-\sigma}_{-q} c_{k+q,-\sigma} | c^+_{k\sigma} \rangle\rangle_E. \end{aligned} \tag{2.6}$$

The symbol δ means that the Hartree–Fock decouplings must be excluded when treating the corresponding Green function

$$t_{k\sigma} = t_k + Un_{-\sigma} = t_k + U(n/2 - \sigma\langle S^z\rangle) \qquad n_\sigma = \sum_k \langle c^+_{k\sigma} c_{k\sigma}\rangle$$

$$n_\uparrow + n_\downarrow = n \qquad n_\uparrow - n_\downarrow = 2\langle S^z\rangle.$$

In the Hartree–Fock approximation,

$$\langle c^+_{k\sigma} c_{k\sigma}\rangle = f(t_{k\sigma}) \equiv n_{k\sigma} \tag{2.7}$$

with $f(E)$ the Fermi function. The next equation of motion reads

$$\begin{aligned}(E - t_{k+q,-\sigma} + \sigma\omega_q)F^\sigma_{kq}(E) &= -U\sum_p \langle\langle S^{-\sigma}_{-q} S^\sigma_p c_{k+q-p,\sigma} - 2\sigma S^z_{p-q} S^{-\sigma}_{-p} c_{k+q,-\sigma} | c^+_{k\sigma}\rangle\rangle_E \\ &\simeq -U(\langle S^{-\sigma}_{-q} S^\sigma_q\rangle + 2\sigma\langle S^z\rangle n_{k+q,-\sigma})G^\sigma_k(E).\end{aligned} \tag{2.8}$$

Here we have carried out the simplest decouplings. The magnon frequency ω_q arises owing to spin dynamics. The simplest way to derive this term is to add to the Hamiltonian (2.1) an effective Heisenberg interaction H_d. Spin dynamics may be taken into account more strictly if one uses the diagram technique [7, 8] or passes to the representation of exact eigenfunctions of H_d [9]. Then we get

$$\Sigma^\sigma_k(E) = Un_{-\sigma} - U^2 \sum_q \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \operatorname{Im}\langle\langle S^\sigma_q | S^{-\sigma}_{-q}\rangle\rangle_\omega \frac{N_B(\omega) + n_{k+q,-\sigma}}{E - t_{k+q,-\sigma} + \omega} \tag{2.9}$$

with $N_B(\omega)$ the Bose function. Retaining only the spin-wave (magnon pole) contribution to the spectral density,

$$-(1/\pi)\operatorname{Im}\langle\langle S^\sigma_q | S^{-\sigma}_q\rangle\rangle_\omega = 2\sigma\langle S^z\rangle\delta(\omega - \sigma\omega_q) \tag{2.10}$$

$$\langle S^-_{-q} S^+_q\rangle = 2\langle S^z\rangle N_B(\omega_p) \equiv 2\langle S^z\rangle N_p \tag{2.11}$$

i.e. neglecting the Stoner excitations, we obtain both from (2.8) and from (2.9)

$$\Sigma^\uparrow_k(E) = Un_\downarrow + U\Delta\sum_q \frac{N_q + n_{k+q\downarrow}}{E - t_{k+q\downarrow} + \omega_q} \tag{2.12}$$

$$\Sigma^\downarrow_k(E) = Un_\uparrow + U\Delta\sum_q \frac{1 + N_q - n_{k-q\uparrow}}{E - t_{k-q\uparrow} - \omega_q} \tag{2.13}$$

where $\Delta = 2U\langle S^z\rangle$ is the spin splitting. Equations (2.12) and (2.13) are valid for the s–d model ($U \to I$) to first order in the small parameter $1/2S$ [10].

For the saturated HFM at $T = 0$ (where $n_\downarrow = 0$, $\Sigma_k^\uparrow(E) \equiv 0$), $G_k^\downarrow(E)$ may be calculated more accurately. Reducing the operator products to the 'normal' form where the $c_\downarrow^+$ stay before the $c_\uparrow^+$ and neglecting terms proportional to $n_\downarrow$, we have

$$[\delta(S_q^+ c_{k-q\uparrow}), H_{\text{int}}] \simeq (1 - n_{k-q\uparrow}) \sum_{k_1 k_2} c_{k_1\uparrow}^+ c_{k_2\uparrow} c_{k+k_1-k_2\downarrow}$$

$$= (1 - n_{k-q\uparrow}) \left(n_\uparrow c_{k\downarrow} - \sum_p \delta(S_p^+ c_{k-p\uparrow}) \right).$$

Then we obtain the integral equation

$$(E - t_{k+q} - \omega_q) F_{kq}^\downarrow(E) = U(1 - n_{k+q\uparrow}) \left(n_\downarrow G_k^\downarrow(E) - \sum_p F_{kp}^\uparrow(E) \right). \tag{2.14}$$

Solving this we find that

$$\Sigma_k^\downarrow(E) = \Delta \left(1 - U \sum_q \frac{1 - n_{k-q\uparrow}}{E - t_{k-q} - \omega_q} \right)^{-1}. \tag{2.15}$$

The result (2.15) (the 'parquet' approximation) is similar to the corresponding result for the s–d model [11–13], which is exact in the limit of zero conduction electron concentration. For the Hubbard model it was derived by Edwards and Hertz [8]. (Note that the results of the Ward-identity approach [8] and of the parquet approximation are different for a non-saturated state.)

Consider the commutator spin Green function

$$G_q(\omega) = \langle\langle S_q^+ | S_{-q}^- \rangle\rangle_\omega \qquad \operatorname{Im} \omega > 0. \tag{2.16}$$

We obtain the following equations of motion:

$$\omega G_q(\omega) = 2\langle S^z \rangle + \sum_k (t_{k+q} - t_k) M_{kq}(\omega) \tag{2.17}$$

$$M_{kq}(\omega) = \langle\langle c_{k\uparrow}^+ c_{k+q\downarrow} | S_{-q}^- \rangle\rangle_\omega \tag{2.18}$$

$$(\omega - t_{k+q} + t_k - \Delta) M_{kq}(\omega) = (n_{k\uparrow} - n_{k+q\downarrow})[1 - UG_q(\omega)] - U \sum_p L_{kqp}(\omega) \tag{2.19}$$

where we have introduced the 'irreducible' Green function

$$L_{kqp}(\omega) = \delta \langle\langle X_{kqp} | S_{-q}^- \rangle\rangle_\omega \tag{2.20}$$

$$X_{kqp} = c_{k\uparrow}^+ S_p^+ c_{k+q-p\uparrow} - c_{k+p\downarrow}^+ S_p^+ c_{k+q\downarrow} - \delta_{pq}(n_{k\uparrow} - n_{k+q\downarrow}) S_q^+. \tag{2.21}$$

Then we have

$$G_q(\omega) = [2\langle S^z \rangle - \Omega_q(\omega)/U]/[\omega - \Omega_q(\omega) - \Pi_q(\omega)] \tag{2.22}$$

$$\Omega_q(\omega) = U \sum_k \frac{t_{k+q} - t_k}{t_{k+q} - t_k + \Delta - \omega} (n_{k\uparrow} - n_{k+q\downarrow}). \tag{2.23}$$

When neglecting Π (i.e. the function L), equations (2.22) and (2.23) provide an alternative form of the random-phase approximation (RPA). Unlike the standard RPA expression, equations (2.22) and (2.23) yield the magnon pole $\omega_q \simeq \Omega_q(0)$ explicitly. To calculate Π, we differentiate the function (2.20) with respect to the time on the right and obtain the contribution

$$\Pi_q(\omega) = \sum_{kpk'p'} \frac{t_{k+q} - t_k}{t_{k+q} - t_k + \Delta - \omega} \frac{t_{k'+q} - t_{k'}}{t_{k'+q} - t_{k'} + \Delta - \omega} \times \delta[U\langle\langle X_{kqp}|X^{+}_{k'q'p'}\rangle\rangle_\omega + \delta_{kk'}\langle c^{+}_{k+q\downarrow} S^{+}_p c_{k+q-p\uparrow} + c^{+}_{k+p\downarrow} S^{+}_p c_{k\uparrow}\rangle]. \tag{2.24}$$

In the s–d model, such a contribution corresponds to the second order in $1/2S$ [14]. Using the spectral representation we get

$$\begin{aligned}\langle\delta(c^{+}_{k+p\downarrow} S^{+}_p)c_{k\uparrow}\rangle &= -\frac{1}{\pi}\int \mathrm{d}E f(E)\, \mathrm{Im}\, F^{\downarrow}_{kp}(E)\\ &= -U\frac{N_p(n_{k+p\downarrow} - n_{k\uparrow}) + n_{k+p\downarrow}(1 - n_{k\uparrow})}{t_{k+p\downarrow} - t_{k\uparrow} - \omega_p}\\ &\equiv -UB(k+p\downarrow, k\uparrow, p, \omega_p).\end{aligned} \tag{2.25}$$

Neglecting H_{int} in the equation of motion for the Green function in (2.24), calculating the average $\langle[X, X^{+}]\rangle$ with the use of (2.11) and substituting (2.25), we obtain

$$\begin{aligned}\Pi_q(\omega) = U^2 \sum_{kp} \left(\frac{t_{k+q} - t_k}{t_{k+q} - t_k + \Delta - \omega}\right)^2 &[B(k\uparrow, k+q-p\uparrow, p, \omega_p - \omega)\\ &+ B(k+p\downarrow, k+q\downarrow, p, \omega_p - \omega) - B(k+p\downarrow, k\uparrow, p, \omega_p)\\ &- B(k+q\downarrow, k+q-p\uparrow, p, \omega_p)].\end{aligned} \tag{2.26}$$

Now we carry out a more careful calculation for a saturated ferromagnet at $T = 0$. In that case we may neglect the second term in (2.21). Similar to (2.14) we derive

$$(\omega - t_{k+q-p} + t_k - \omega_p)L_{kqp}(\omega) = U(1 - n_{k+q-p\uparrow}) \times \left(n_{k\uparrow} G_q(\omega) - n_\uparrow M_{kq}(\omega) + \sum_r L_{kqr}(\omega)\right). \tag{2.27}$$

Solving the system (2.17), (2.19) and (2.27) we obtain

$$G_q(\omega) = \left(2\langle S^z\rangle - \sum_k \frac{(t_{k+q} - t_k)n_{k\uparrow}}{t_{k+q} - t_k + 2\langle S^z\rangle U^{\text{ef}}_{kq}(\omega) - \omega}\right) \times \left(\omega - \sum_k U^{\text{ef}}_{kq}(\omega)\frac{(t_{k+q} - t_k)n_{k\uparrow}}{t_{k+q} - t_k + 2\langle S^z\rangle U^{\text{ef}}_{kq}(\omega) - \omega}\right)^{-1} \tag{2.28}$$

$$U^{\text{ef}}_{kq}(\omega) = U\left(1 - U\sum_p \frac{1 - n_{k+q-p\uparrow}}{\omega - t_{k+q-p} + t_k - \omega_p}\right)^{-1}. \tag{2.29}$$

The expression for the magnon frequency following from (2.28) coincides with the corresponding exact result in the s–d exchange model of a ferromagnetic semiconductor with $I > 0$ [13–15]. Thus we see that the Hubbard model yields results similar to those given by the s–d model with $I > 0$. However, such a situation takes place only for band fillings that are not too large. Indeed, the almost-half-filled Hubbard model with $U \to \infty$ is equivalent to the s–d model with $S = \frac{1}{2}$, $I \to -\infty$ and small conduction electron concentration [16]. In that case, equation (2.28) is not quite satisfactory since it does not yield Nagaoka's [17] result for the magnon frequency [13, 15, 16].

3. Electron spectrum and occupation numbers

The real parts of equations (2.12) and (2.13) determine the corrections to one-electron energies. Here we treat only the magnon contribution (many-electron contributions are considered below). Taking into account the relation

$$\langle S^z \rangle = S_0 - \sum_p N_p \tag{3.1}$$

where S_0 is the saturation magnetisation, we obtain (cf [10])

$$\delta\Sigma_k^\sigma(E) = \sigma U \sum_q \frac{E - t_{k+q,\sigma} + \sigma\omega_q}{E - t_{k+q,-\sigma} + \sigma\omega_q} N_q \tag{3.2}$$

$$\delta E_k^\sigma(T) = \mathrm{Re}\, \delta\Sigma_k^\sigma(t_{k\sigma}) = \sum_q A_{kq}^\sigma N_q \propto (T/T_c)^{5/2} \tag{3.3}$$

with A_{kq}^σ being the electron–magnon scattering amplitude:

$$A_{kq}^\sigma = \sigma U (t_{k+q} - t_k)/(t_{k+q} - t_k + \sigma\Delta) \to 0 \qquad (q \to 0). \tag{3.4}$$

The one-electron damping is obtained by calculating higher-order contributions to Σ similar to (2.26) (see also [10]). We have

$$\begin{aligned} \gamma_k^\sigma(T) = \pi \sum_{pq} (A_{kq}^\sigma)^2 [N_q(1 + N_p) + n_{k+q-p}(N_p - N_q)] \\ \times \delta(t_k - t_{k+q-p} + \sigma\omega_q - \sigma\omega_p) \end{aligned} \tag{3.5}$$

$$\gamma_k^\sigma(T) \propto \begin{cases} kT^{7/2} & |\eta_{k\sigma}| \ll T \quad (\eta_{k\sigma} = t_{k\sigma} - E_F) \\ k^3 T^{5/2} & |\eta_{k\sigma}| \gg T \quad |\eta_{k\sigma}| > \omega_{2k} \\ k|\eta_{k\sigma}| T^{5/2} & |\eta_{k\sigma}| \gg T \quad |\eta_{k\sigma}| < \omega_{2k}. \end{cases}$$

Expanding the Dyson equation (2.5) we obtain for the density of states

$$\begin{aligned} N_\sigma(E) = -\frac{1}{\pi} \mathrm{Im} \left(\sum_k G_k^\sigma(E) \right) \simeq \rho_\sigma(E) - \sum_k \delta'(E - t_{k\sigma}) [\mathrm{Re}\, \Sigma_k^\sigma(E) - U n_{-\sigma}] \\ - \frac{1}{\pi} \sum_k \frac{\mathrm{Im}\, \Sigma_k^\sigma(E)}{(E - t_{k\sigma})^2} \end{aligned} \tag{3.6}$$

$$\rho_\sigma(E) = \sum_k \delta(E - t_{k\sigma}). \tag{3.7}$$

The third term in (3.6), arising from a branch of the self-energy, describes the non-quasiparticle state contribution $\delta N_\sigma(E)$. The latter does not vanish in the energy region, corresponding to the subband with the opposite spin projection $-\sigma$. At $T = 0$, as follows from (2.12) and (2.13), $\delta N_\sigma(E)$ varies sharply near E_F and is non-zero above E_F for $\sigma = \downarrow$ and below E_F for $\sigma = \uparrow$ (cf [10, 18]). Remember that we consider only the contribution of the collective magnon mode to the spectral density (2.10). The contribution of the Stoner excitations (which is absent in the saturated case) gives, generally speaking, a double-sided non-quasiparticle correction, but in any case $\delta N_\sigma(E_F, T=0) = 0$ [18].

Now we calculate the electron occupation numbers

$$\langle c^+_{k\uparrow} c_{k\uparrow}\rangle = -\frac{1}{\pi}\int \mathrm{d}E f(E)\,\mathrm{Im}\, G^\uparrow_k(E) = f(t_k + \mathrm{Re}\,\Sigma^\uparrow_k(t_{k\uparrow}))$$

$$+ U\Delta \sum_p \frac{N_p(n_{k+p\downarrow} - n_{k\uparrow}) + n_{k+p\downarrow}(1-n_{k\uparrow})}{(t_{k+p\downarrow} - t_{k\uparrow} - \omega_p)^2} \tag{3.8}$$

$$\langle c^+_{k\downarrow} c_{k\downarrow}\rangle = f(t_k + \mathrm{Re}\,\Sigma^\downarrow_k(t_{k\downarrow}))$$

$$- U\Delta \sum_p \frac{N_p(n_{k\downarrow} - n_{k-p\uparrow}) + n_{k\downarrow}(1-n_{k-p\uparrow})}{(t_{k-p\uparrow} - t_{k\downarrow} + \omega_p)^2}. \tag{3.9}$$

Retaining only magnon contributions up to $T^{3/2}$ we get

$$\langle c^+_{k\sigma} c_{k\sigma}\rangle \simeq n_{k\sigma}(S_0 + \langle S^z\rangle)/2S_0 + n_{k,-\sigma}(S_0 - \langle S^z\rangle)/2S_0 \tag{3.10}$$

with $\langle S^z\rangle$ defined by (3.1). Thus, despite the presence of the spin splitting Δ, electron occupation numbers have a strong $T^{3/2}$ dependence rather than an exponential one. This dependence arises because of thermal magnon emission and absorption. The role of such processes in the temperature dependence of conduction electron spin polarisation $P(T)$ of ferromagnetic semiconductors was discussed in [10, 19, 20]. Formally, the law $P(T) \propto \langle S^z\rangle$ is due to the strong temperature dependence of the Green function residues and to the occurrence of the non-quasiparticle states, owing to electron–magnon scattering, in 'alien' spin subbands.

4. Spin-wave spectrum and damping

Within the RPA (see (2.22) and (2.23)), we have for the magnon frequency

$$\omega_q = \Omega_q(0) = \sum_{k\sigma} A^\sigma_{kq} n_{k\sigma}$$

$$\omega_{q\to 0} = D_{\alpha\beta} q_\alpha q_\beta \tag{4.1}$$

$$D_{\alpha\beta} = \frac{U}{\Delta}\sum_k \left(\frac{\partial^2 t_k}{\partial k_\alpha \partial k_\beta}(n_{k\uparrow} + n_{k\downarrow}) - \frac{1}{\Delta}\frac{\partial t_k}{\partial k_\alpha}\frac{\partial t_k}{\partial k_\beta}(n_{k\uparrow} - n_{k\downarrow})\right). \tag{4.2}$$

For weak itinerant ferromagnets ($\Delta \ll E_F$, U) we obtain from (4.2)

$$D_{\alpha\beta} = \frac{U\Delta}{4}\sum_k \left(\frac{\partial^2 t_k}{\partial k_\alpha\, \partial k_\beta}\frac{\partial^2 n_k}{\partial t_k^2} + \frac{1}{6}\frac{\partial t_k}{\partial k_\alpha}\frac{\partial t_k}{\partial k_\beta}\frac{\partial^3 n_k}{\partial t_k^3}\right) \tag{4.3}$$

i.e. the spin-wave stiffness constant $D \propto \Delta$ (cf [21]).

The magnon damping in the RPA reads

$$\gamma^{(1)}_q(\omega) = -\mathrm{Im}\,\Omega_q(\omega) \simeq \pi U\Delta\omega \sum_k \left(-\frac{\partial n_{k\uparrow}}{\partial t_{k\uparrow}}\right)\delta(\omega - t_{k+q\downarrow} + t_{k\uparrow})$$

$$\gamma^{(1)}_q \equiv \gamma^{(1)}_q(\omega_q) \simeq \pi U\Delta\omega_q \rho_\uparrow(E_F)\rho_\downarrow(E_F)\theta(\omega_q - \omega_-) \tag{4.4}$$

with $\theta(x)$ the step function. Here ω_- is the threshold frequency which is determined by the condition for entering into the Stoner continuum, $\omega_- = \omega_{q_0}$ where q_0 is the minimal (in k) solution to the equation $t_{k+q_0\downarrow} = t_{k\uparrow} = E_F$. For a weak itinerant ferromagnet we have

$$q_0 = k_{F\uparrow} - k_{F\downarrow} \qquad \omega_- = D(k_{F\uparrow} - k_{F\downarrow})^2 \propto \Delta^3.$$

In that case, the contribution of the spin Green function branch may be approximately considered to be that of a paramagnon pole at imaginary ω. The scale $\omega_- \sim T^* \simeq T_c^2/E_F$ is the borderline of two temperature regions: the contributions of spin waves dominate at $T < T^*$, and those of paramagnons at $T > T^*$ [21]. Note that the same estimation $\omega_- \sim T_c^2/E_F$ holds in the s–d model with indirect RKKY exchange where

$$D \sim T_c/S \sim I^2S/E_F \qquad k_{F\uparrow} - k_{F\downarrow} \propto IS/E_F.$$

The damping (4.4) vanishes at small q, and for a saturated ferromagnet in the whole Brillouin zone. For such cases, the magnon damping is given by the imaginary part of (2.26):

$$\gamma_q^{(2)}(\omega) = \pi \sum_{kp\sigma} (A_{kq}^{\sigma})^2 (n_{k\sigma} - n_{k+q-p,\sigma}) \times [N_p - N_B(\omega_p - \omega)]\delta(\omega - \omega_p + t_k - t_{k+q-p}). \tag{4.5}$$

Integration in the case of an isotropic electron spectrum gives [14, 22]

$$\gamma_q^{(2)} = \frac{v_0^2 q^4}{12\pi^3(2S_0)^2} \sum_\sigma k_{F\sigma}^2 \begin{cases} \omega_q/35 & T \ll \omega_q \\ (T/4)(\ln(T/\omega_q) + \frac{5}{3}) & T \gg \omega_q \end{cases} \tag{4.6}$$

with v_0 the lattice cell volume.

The quantity (4.5) determines the contribution of two-magnon processes to the longitudinal nuclear relaxation rate:

$$\delta\frac{1}{T_1} = -\frac{A^2T}{2\pi\omega_n}\,\mathrm{Im}\left(\sum_q \delta G_q(\omega_n)\right) = \frac{\langle S^z\rangle A^2 T}{\pi\omega_n}\sum_q \frac{\gamma_q^{(2)}(\omega_n)}{\omega_q^2}$$
$$= \frac{A^2}{4\langle S^z\rangle}\sum_{kqp\sigma}\frac{\omega_p}{\omega_q^2}(t_{k-q} - t_k)^2 N_p(1+N_p)\left(-\frac{\partial n_{k\sigma}}{\partial t_{k\sigma}}\right)\delta(t_k - t_{k-q+p} + \omega_p) \tag{4.7}$$

where $\omega_n \ll T$ is the NMR frequency and A is the hyperfine interaction. The integration gives [23]

$$\delta\frac{1}{T_1} = \frac{12\pi^{1/2}}{\langle S^z\rangle}\frac{T^{5/2}}{D^{7/2}}\left(\frac{v_0}{16\pi^2}\right)^3 \tfrac{3}{2}\zeta \sum_\sigma k_{F\sigma}^2. \tag{4.8}$$

The contribution (4.8) is particularly important in HFMs where the linear Korringa contribution

$$\frac{1}{T_1} = \frac{A^2T\langle S^z\rangle}{\pi\omega_n}\sum_q \frac{\gamma_q^{(1)}(\omega_n)}{\omega_q^2} \propto T\rho_\uparrow(E_F)\rho_\downarrow(E_F) \tag{4.9}$$

is absent (see section 9).

Consider the temperature dependence of the spin-wave stiffness. The usual $T^{5/2}$ correction may be obtained similar to the case of the s–d model [14] (see also [16]). Here we treat the correction owing to the real part of $\Pi_q(\omega)$ (2.26):

$$\delta D_{\alpha\beta} = (2S_0)^{-2} \sum_{kp} \frac{\partial t_k}{\partial k_\alpha} \frac{\partial t_k}{\partial k_\beta} \left(\frac{n_{k\uparrow}(1-n_{k-p\uparrow})}{t_k - t_{k-p} - \omega_p} + \frac{n_{k+p\downarrow}(1-n_{k\downarrow})}{t_{k+p} - t_k - \omega_p} \right.$$
$$\left. - \frac{n_{k+p\downarrow}(1-n_{k\uparrow})}{t_{k+p\downarrow} - t_{k\uparrow} - \omega_p)} - \frac{n_{k\downarrow}(1-n_{k-p\uparrow})}{t_{k\downarrow} - t_{k-p\uparrow} - \omega_p} \right). \tag{4.10}$$

For parabolic spectra $t_k = k^2/2m$, $\omega_q = q^2$ integration gives

$$\delta D = \left(\frac{\pi v_0 T}{12 S_0 m}\right)^2 \frac{1}{D} \left[\sum_\sigma \rho_\sigma^2(E_F) \ln\left(\frac{T}{4Dk_{F\sigma}^2}\right) \right.$$
$$\left. - 2\rho_\uparrow(E_F)\rho_\downarrow(E_F) \ln\left(\frac{\max(\omega_-, T)}{\omega_+}\right)\right] \tag{4.11}$$

$$\omega_\pm = D(k_{F\uparrow} \pm k_{F\downarrow})^2 \qquad \rho_\sigma(E_F) = m v_0 k_{F\sigma}/2\pi^2. \tag{4.12}$$

The $T^2 \ln T$ correction to D, as well as the $T^{5/2}$ contribution to $1/T_1$, were firstly obtained in [16] for a saturated Hubbard ferromagnet with $U \to \infty$. The result (4.11) holds for the s–d model ($S_0 \to S$). For $\omega_- \ll T \ll \omega_+$ we have

$$\delta D = (m v_0 T/12 m S_0)^2 (1/D) [\rho_\uparrow(E_F) - \rho_\downarrow(E_F)]^2 \ln(T/\omega_+). \tag{4.13}$$

For a weak itinerant ferromagnet one obtains

$$\delta D = [v_0^2 k_F^2 T^2 / 72\pi^2 (2S_0)^2 D] \ln(T/T^*) \qquad (T \ll T^*). \tag{4.14}$$

The correction (4.11) dominates over corrections owing to the temperature dependence of the Fermi functions in (4.2) (cf [16]).

5. The magnetisation

Consider the magnetisation $\langle S^z \rangle$. We have

$$\langle S^z \rangle = \frac{n}{2} - \sum_q \langle S_{-q}^- S_q^+ \rangle - \langle n_{i\uparrow} n_{i\downarrow} \rangle. \tag{5.1}$$

The first average involved in (5.1) is calculated via the spectral representation of the RPA Green function (2.22) and (2.23) ($\Pi \to 0$):

$$\langle S_{-q}^- S_q^+ \rangle = \langle S_{-q}^- S_q^+ \rangle_{\text{pole}} + \langle S_{-q}^- S_q^+ \rangle_{\text{bc}} \tag{5.2}$$

$$\langle S_{-q}^- S_q^+ \rangle_{\text{pole}} = 2S_0 N_q \qquad (q < q_0) \tag{5.3}$$

$$\langle S_{-q}^- S_q^+ \rangle_{\text{bc}} = \frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{N_B(\omega)(\Delta - \omega)\gamma_q^{(1)}(\omega)}{U\{[\omega - \operatorname{Re}\Omega_q(\omega)]^2 + [\gamma_q^{(1)}(\omega)]^2\}}$$
$$= \sum_k \frac{(t_{k+q} - t_k)^2 n_{k+q\downarrow}(1-n_{k\uparrow})}{(t_{k+q\downarrow} - t_{k\uparrow} - \omega_q)^2 + [\gamma_q^{(1)}(t_{k+q\downarrow} - t_{k\uparrow})]^2} \qquad (q > q_0). \tag{5.4}$$

We have used in (5.4) the identity

$$N_B(t_{k+q\downarrow} - t_{k\uparrow})(n_{k\uparrow} - n_{k+q\downarrow}) = n_{k+q\downarrow}(1 - n_{k\uparrow}).$$

The true Bloch spin-wave contribution is given by (3.1), since magnons are bosons, and every magnon decreases the magnetisation by unity. Equations (5.1) and (5.3) do not agree with (3.1). The situation may be improved by allowing branch contributions. For example, taking into account in (5.4) (with $n_{k\sigma} \to \langle c^+_{k\sigma} c_{k\sigma} \rangle$) the temperature dependence of occupation numbers (3.10) we obtain

$$\delta\langle S^z\rangle_{\rm sw} = \delta\langle S^z\rangle_{\rm pole} + \delta\langle S^z\rangle_{\rm bc} = -\sum_q N_q \bigg[2S_0 + \frac{1}{2S_0} \times \sum_{kk'} \frac{(t_{k'} - t_k)^2 (n_{k\uparrow} - n_{k\downarrow})}{(t_{k'\downarrow} - t_{k\uparrow} - \omega_{k-k'})^2} (1 - n_{k'\uparrow} + n_{k'\downarrow})\bigg] \simeq -\sum_q N_q \tag{5.5}$$

where we have neglected the spin splitting in the denominator. Considerable contributions to the Bloch term arise also from the branch cut corresponding to the damping (4.5) (cf the case of a saturated ferromagnet [16]).

In the semi-phenomenological manner, it is suitable to introduce 'magnon' operators which satisfy on the average the Bose commutation relations $b_q = (2S_0)^{-1/2} S^+_q$, $b^+_q = (2S_0)^{-1/2} S^-_{-q}$:

$$\delta\langle S^z\rangle = -\sum_q \langle b^+_q b_q\rangle = -\frac{1}{2S_0}\sum_q \langle S^-_{-q} S^+_q\rangle. \tag{5.6}$$

We shall demonstrate in section 6 that such a way of calculating the electron correction to $\langle S^z\rangle$ is in agreement with that using the differentiation of the free energy. At $T = 0$ ($N(\omega) = -\theta(-\omega)$), integrating over ω in (5.4) yields

$$\delta\langle S^z\rangle \simeq -\frac{1}{\pi}\sum_q \frac{\gamma^{(1)}_q}{\omega_q} \ln\left(\frac{W}{\omega_q}\right) \tag{5.7}$$

with W being of the order of the band width. Such a contribution was found in the s–d(f) model [9]. At $T < \omega_-$, neglecting the damping and using the parabolic isotropic spectra, we get

$$\delta\langle S^z\rangle_{\rm el} \simeq -U\Delta \sum_{kk'} \frac{n_{k'\downarrow}(1 - n_{k\uparrow})}{(t_{k'\downarrow} - t_{k\uparrow} - \omega_{k-k'})^2} = -\left(\frac{mv_0}{2\pi^2}\right)^2 \frac{U\Delta}{4D}\left[\omega_+ \ln\left(\frac{W}{\omega_+}\right) - \omega_- \ln\left(\frac{W}{\omega_-}\right) + \frac{2\pi^2}{3} T^2 \left(\frac{1}{\omega_-} - \frac{1}{\omega_+}\right)\right]. \tag{5.8}$$

For a weak ferromagnet we obtain from (5.8) a correction of the order of $(T/T_c)^2$, in agreement with the result of the self-consistent renormalisation (SCR) theory [2, 24].

Unlike the s–d model, for the Hubbard model the interaction parameter U is not small, and the damping cannot be neglected. However, at low T this influences numerical factors only. On the contrary, at high $T \gg \omega_-$ the integral is determined by the contribution of small ω, q:

$$q \propto |\omega|^{1/3} = |t_{k+q\downarrow} - t_{k\uparrow}|^{1/3} \qquad \gamma_q(\omega) \propto \Delta\omega/q \tag{5.9}$$

$$\delta\sum_q \langle S^-_{-q} S^+_q\rangle_{\rm el} \simeq \Delta^2 \sum_{kq} \frac{n_{k+q\downarrow}(1 - n_{k\uparrow})}{(Dq^2)^2 + A^2\Delta^2(t_{k+q\downarrow} - t_{k\uparrow})^2/q^2} \sim \int {\rm d}\varepsilon\, {\rm d}\varepsilon' \frac{f(\varepsilon')[1 - f(\varepsilon)]}{|\varepsilon - \varepsilon'|^{2/3}} \propto \left(\frac{T}{E_{\rm F}}\right)^{4/3}. \tag{5.10}$$

Then we obtain from (5.1) (without introducing the factor $(2S_0^-)^{-1}$) the $T^{4/3}$ contribution to the magnetisation (cf [2, 21, 24]). Thus our approach does not yield a unified picture of the T-dependence of $\langle S^z \rangle$. On the other hand, use of the full SCR theory is not inevitable for obtaining the T^2 and $T^{4/3}$ corrections themselves.

6. Thermodynamic properties

Consider the renormalisation of electronic specific heat owing to many-electron contributions. At $T = 0$, integration in (2.12) and (2.13) gives

$$\mathrm{Re}\,\Sigma^{\sigma}(\mathrm{K}_{\mathrm{F}\sigma}, E) \simeq -U\Delta \frac{\rho_{-\sigma}(E_{\mathrm{F}})}{\omega_+ - \omega_-} \sum_{\alpha=\pm} \alpha(E - \omega_\alpha) \ln \left| \frac{E - \omega_\alpha}{W} \right| . \tag{6.1}$$

Then the inverse residue of the electron Green function, determining the effective-mass renormalisation, reads

$$\begin{aligned} Z_\sigma^{-1}(k_{\mathrm{F}\sigma}, E) &= 1 - (\partial/\partial E)\,\mathrm{Re}\,\Sigma^{\sigma}(k_{\mathrm{F}\sigma}, E) \\ &= 1 + U\Delta[\rho_{-\sigma}(E_{\mathrm{F}})/(\omega_+ - \omega_-)] \ln|(E - \omega_+)/(E - \omega_-)| . \end{aligned} \tag{6.2}$$

At low $T \ll \omega_-$ we have for the coefficient of the linear term in the specific heat $C(T)$

$$\begin{aligned} \gamma_\sigma = \gamma_\sigma^{(0)}/Z_\sigma(k_{\mathrm{F}\sigma}, E_{\mathrm{F}}) &= (\pi^2/3)\rho_\sigma(E_{\mathrm{F}}) \\ &\times \{1 + U\Delta[\rho_{-\sigma}(E_{\mathrm{F}})/(\omega_+ - \omega_-)] \ln(\omega_+/\omega_-)\} . \end{aligned} \tag{6.3}$$

An analogous result for the s–d model was obtained in [9]. For weak itinerant ferromagnets,

$$\ln(\omega_+/\omega_-) \simeq -2 \ln \alpha \qquad 0 < \alpha = UN(E_{\mathrm{F}}) - 1 \ll 1$$

and equation (6.3) describes the paramagnon enhancement of specific heat [2, 7, 21], the numerical factor being inexact because longitudinal spin fluctuations and vortex corrections are neglected. On the other hand, our consideration is not restricted to the case of very weak ferromagnets.

Let us calculate the corresponding contribution to the entropy $S(T)$ using the well known identity

$$(\partial n/\partial T)_\mu = (\partial S/\partial \mu)_T \tag{6.4}$$

where μ is the chemical potential. Substituting (3.6) into the relation

$$n_\sigma = \int_{-\infty}^{\infty} \mathrm{d}E\, f(E) N_\sigma(E)$$

we obtain the contributions

$$\delta n = \delta n_\uparrow + \delta n_\downarrow = \frac{\partial}{\partial \mu}\left(U\Delta \sum_{kq} \frac{n_{k+q\downarrow}(1 - n_{k\uparrow})}{t_{k\uparrow} - t_{k+q\downarrow} + \omega_q} \right) \tag{6.5}$$

$$\delta S(T) = \frac{\partial}{\partial T}\left(U\Delta \sum_{kq} \frac{n_{k+q\downarrow}(1 - n_{k\uparrow})}{t_{k\uparrow} - t_{k+q\downarrow} + \omega_q} \right) . \tag{6.6}$$

For parabolic spectra we have

$$\begin{aligned} \delta S(T) &= \frac{U\Delta}{2(\omega_+ - \omega_-)} \rho_\uparrow(E_{\mathrm{F}})\rho_\downarrow(E_{\mathrm{F}}) \\ &\times \frac{\partial}{\partial T} \int \mathrm{d}\varepsilon\, \mathrm{d}\varepsilon' \frac{\partial f(\varepsilon)}{\partial \varepsilon} \frac{\partial f(\varepsilon')}{\partial \varepsilon'} (\varepsilon - \varepsilon')^2 \ln \left| \frac{\varepsilon - \varepsilon' + \omega_+}{\varepsilon - \varepsilon' + \omega_-} \right| . \end{aligned} \tag{6.7}$$

To logarithmic accuracy,

$$\begin{aligned} \delta S(T) = \delta C(T) = -2\delta F_{\mathrm{el}}(T)/T &= [2U\Delta/(\omega_+ - \omega_-)]\rho_\uparrow(E_{\mathrm{F}})\rho_\downarrow(E_{\mathrm{F}})(\pi^2/3)T \\ &\times \ln[\omega_+/\max(\omega_-, T)] \end{aligned} \tag{6.8}$$

with $F_{el}(T)$ the corresponding contribution to the free energy. If a 'direct' exchange interaction H_d is present (in particular, for the s–d model), the result (6.8) is definitely valid both at $T < \omega_-$ and at $T > \omega_-$. For weak itinerant ferromagnets at $T > \omega_-$, it is important that for $\omega > \omega_-$ the approximation $\omega_q = Dq^2$ does not work, and it is suitable to use the estimation $\omega_q = \omega_- = \text{constant}$. Then we obtain from (6.6)

$$\delta F_{el}(T) \propto -T^2 N(E_F) \ln(W/T) \qquad (T > \omega_-) \tag{6.9}$$

in qualitative agreement with [2, 21].

The singular correction to the free energy may be also obtained by integrating over 'effective' Heisenberg exchange parameters, as was done for the s–d model [9]. We have for $T \ll \omega_-$

$$F_{el} \simeq \sum_q \omega_q \delta\langle b_q^+ b_q \rangle_{el} = \frac{1}{2S_0} \sum_q \omega_q \delta\langle S_{-q}^- S_q^+ \rangle_{bc}$$

$$\simeq U\Delta \sum_{kq} \frac{n_{k+q\downarrow}(1 - n_{k\uparrow})}{t_{k\uparrow} - t_{k+q\downarrow} + \omega_q} \equiv F_{el}(0) + \delta F_{el}(T) \tag{6.10}$$

$$F_{el}(0) \simeq \frac{1}{\pi} \sum_q \gamma_q^{(1)} \ln\left(\frac{W}{\omega_q}\right) \simeq \frac{1}{8D} \left(\frac{mv_0}{2\pi^2}\right)^2 \left[\omega_-^2 \ln\left(\frac{W}{\omega_-}\right) - \omega_+^2 \ln\left(\frac{W}{\omega_+}\right)\right]. \tag{6.11}$$

Adding to the Hamiltonian the interaction $-hS^z$ with external magnetic field so that

$$t_{k\sigma} \to t_{k\sigma} - \tfrac{1}{2}\sigma h \qquad \omega_q \to \omega_q + h$$

using the identity

$$(\partial\langle S^z \rangle/\partial T)_h = (\partial S/\partial h)_T \tag{6.12}$$

and picking out the singular contribution, we obtain

$$\delta\langle S^z \rangle_{el} = \frac{\partial}{\partial h}\left(U\Delta \sum_{kq} \frac{n_{k+q\downarrow}(1 - n_{k\uparrow})}{t_{k\uparrow} - t_{k+q\downarrow} + \omega_q} \right)_{h=0} \simeq -U\Delta \sum_{kq} \frac{n_{k+q\downarrow}(1 - n_{k\uparrow})}{(t_{k\uparrow} - t_{k+q\downarrow} + \omega_q)^2} \tag{6.13}$$

in agreement with (5.8). Note that the correction (6.13) cannot be obtained directly from (3.8) and (3.9) since the contributions of the last terms in these equations are cancelled by the terms with derivatives of Fermi functions.

The spin-wave contribution to the free energy reads (cf [23])

$$\delta F_{sw} = -\tfrac{2}{3}\delta\langle H \rangle_{sw}$$

$$\delta\langle H \rangle_{sw} = \sum_q \omega_q N_q = \sum_{k\sigma} \delta E_k^\sigma(T) n_{k\sigma} = \sum_{kq\sigma} A_{kq}^\sigma n_{k\sigma} N_q = \frac{3v_0}{16\pi^{3/2}} \tfrac{5}{2} \zeta \frac{T^{5/2}}{D^{3/2}}. \tag{6.14}$$

Using (6.8), (6.9) and (6.14) we can calculate and compare corrections to various physical quantities. This may be done most clearly for the case of a weak itinerant ferromagnet where

$$D \sim \Delta \sim \omega_+ \propto \alpha^{1/2} \qquad T^* \sim \omega_- \propto \alpha^{3/2} \qquad T_c \propto \alpha^{3/4}.$$

For example, for elastic moduli $C_{ik} = \partial^2 F/(\partial u_i \, \partial u_k)$ (u_i are corresponding deformations), selecting the most singular (in α) contributions gives

$$\delta(C_{ii})_{el} \propto -(T/E_F)^2 \{\partial[\ln N(E_F)]/\partial u_i\}^2 \alpha^{-2} \propto -(T/T_c)^2 \alpha^{-1/2} \qquad (T < T^*)$$

$$\delta(C_{ii})_{sw} \propto -(T/E_F)^{5/2}\{\partial[\ln N(E_F)]/\partial u_i\}^2\alpha^{-11/4}$$
$$\propto -(T/T_c)^{5/2}\alpha^{-7/8} \qquad (T < T^*) \tag{6.15}$$

(if $\partial[\ln N(E_F)]/\partial u_i = 0$ owing to symmetry, the singularity is weakened by one power of α). At $T \simeq T^*$, $\delta(C_{ii})_{el,sw}/C_{ii} \sim -T_c/E_F$ and the corresponding correction to the velocity of sound may be appreciable.

Consider the temperature dependence of a local moment on a site

$$\langle S_i^2\rangle = \tfrac{3}{4}n - \tfrac{3}{2}N_2 \qquad N_2 = \langle n_{i\uparrow} n_{i\downarrow}\rangle \tag{6.16}$$

where the number of doubly occupied sites (doubles) may be determined using the Hellman–Feynman theorem $N_2 = \partial F/\partial U$. We have from (6.8) and (6.14)

$$\delta\langle S^2\rangle_{el} \propto -(T/\Delta)^2 \qquad (T < T^*) \tag{6.17}$$

$$\delta\langle S^2\rangle_{sw} = -(9v_0/32\pi^{3/2})(T/D)^{5/2}(\partial D/\partial U) \propto -(T/\Delta)^{5/2}\alpha^{-1/2} \tag{6.18}$$

so that at $T < T^*$ the electron contribution dominates over the spin-wave contribution (the latter was discussed in [25]). At $T > T^*$, the electron contribution to the free energy (6.9) is weakly U dependent, and the main contribution to $\langle S^2\rangle$ comes from (5.10) and is positive:

$$\delta\langle S^2\rangle = \delta\sum_q \langle S_{-q}^- S_q^+\rangle_{el} \propto (T/E_F)^{4/3}. \tag{6.19}$$

Thus the amplitude of the local moment may have a minimum at $T \sim \omega_- \sim T^*$.

7. Electron Green functions in a narrow-band Hubbard ferromagnet

Here we consider the Hubbard model with strong electron correlations in the representation of Hubbard's many-electron operators [5]:

$$X_i^{\alpha\beta} = |i\alpha\rangle\langle i\beta| \qquad X_i^{\alpha\beta}X_i^{\gamma\varepsilon} = \delta_{\beta\gamma}X_i^{\alpha\varepsilon} \tag{7.1}$$

$$c_{i\sigma}^{+} = X_i^{\sigma 0} + \sigma X_i^{2-\sigma} \qquad H_{int} = U\sum_i X_i^{22} \tag{7.2}$$

where $|i\alpha\rangle$ ($\alpha = 0, \sigma, 2$) are the states, corresponding to the empty, singly occupied and doubly occupied sites, respectively. We treat the case where $U \to \infty$, $n < 1$, so that the doubly occupied states are absent. The Hamiltonian (2.1) takes the form

$$H = \sum_{k\sigma} \varepsilon_k X_{-k}^{0\sigma} X_k^{\sigma 0} \qquad \varepsilon_k \equiv -t_k \tag{7.3}$$

and describes the motion of current carriers—holes—in the system of local moments—singly occupied sites.

First we calculate the electron Green function

$$\tilde{G}_k^{\sigma}(E) = \langle\langle X_k^{\sigma 0} | X_{-k}^{0\sigma}\rangle\rangle_E \tag{7.4}$$

within the $1/z$-expansion [3, 23] starting from the Hubbard-I approximation [1]. We have

$$(E - \varepsilon_{k\sigma})\tilde{G}_k^{\sigma}(E) = n_0 + n_\sigma + \sum_q \varepsilon_{k-q}\tilde{F}_{kq}^{\sigma}(E) \tag{7.5}$$

$$\varepsilon_{k\sigma} = \varepsilon_k(n_0 + n_\sigma) \qquad n_\alpha = \langle X_i^{\alpha\alpha}\rangle \tag{7.6}$$

$$\tilde{F}^{\sigma}_{kq}(E) = \langle\langle X^{\sigma-\sigma}_{q} X^{-\sigma 0}_{k-q} | X^{0\sigma}_{-k} \rangle\rangle_E. \tag{7.7}$$

We neglect the contribution of longitudinal spin fluctuations which is not important at low temperatures. Carrying out the simplest decoupling in the equation of motion for the Green function (7.7) we obtain to first order in $1/z$

$$\tilde{G}^{\sigma}_{k}(E) = \left(n_0 + n_\sigma + \sum_q \varepsilon_{k-q} \frac{\langle S^{\sigma}_{q} S^{-\sigma}_{-q}\rangle + \langle X^{0-\sigma}_{q-k} X^{-\sigma 0}_{k-q}\rangle}{E - \varepsilon_{k-q,-\sigma} - \sigma\omega_q}\right)$$
$$\times \left(E - \varepsilon_{k\sigma} - \sum_q \varepsilon_{k-q} \frac{\varepsilon_k \langle S^{\sigma}_{q} S^{-\sigma}_{-q}\rangle - (\varepsilon_{k-q} - \varepsilon_k)\langle X^{0-\sigma}_{q-k} X^{-\sigma 0}_{k-q}\rangle}{E - \varepsilon_{k-q,-\sigma} - \sigma\omega_q}\right)^{-1} \tag{7.8}$$

where, in the Hubbard-I approximation,

$$\langle X^{0\sigma}_{-k} X^{\sigma 0}_{k}\rangle = (n_0 + n_\sigma) f(\varepsilon_{k\sigma}). \tag{7.9}$$

At low temperatures we derive (cf (3.3) and (3.4))

$$\delta E^{\sigma}_{k}(T) = \sum_q A^{\sigma}_{kq} N_q \qquad A^{\sigma}_{kq} = \frac{\sigma\varepsilon_k(\varepsilon_{k+q} - \varepsilon_k)}{\varepsilon_{k\sigma} - \varepsilon_{k+q,-\sigma}}. \tag{7.10}$$

It is easy to prove that the magnon frequency (see [3]) is expressed, similar to (4.1), in terms of the electron–magnon scattering amplitude (7.10).

For finite U, the calculations are carried out in a similar way by using the Bogoliubov u–v transformation to new operators corresponding to the Hubbard subbands [1]

$$E^{\sigma}_{k1,2} = \tfrac{1}{2}(t_k + U \mp \varepsilon^{\sigma}_{k}) \qquad \varepsilon^{\sigma}_{k} \equiv [U^2 + t_k^2 + 2Ut_k(2n_{-\sigma} - 1)]^{1/2}. \tag{7.11}$$

To first order in $1/z$ one obtains [23]

$$A^{i\sigma}_{kq} = \left(\sigma U t_k (t_{k+q} - t_k) \Big/ \prod_{j=1,2} (E^{\sigma}_{ki} - E^{-\sigma}_{k+qj})\right)$$
$$\times \left(1 + (-1)^i \frac{t_k + U(2n_{-\sigma} - 1)}{\varepsilon^{\sigma}_{k}}\right). \tag{7.12}$$

The spectrum (7.11) yields four subbands in the ferromagnetic region. One may expect that higher orders in $1/z$ modify the structure of the Green functions, so that some branches of the electron spectrum become ill defined and describe non-quasi-particle states (formally, some denominators are replaced by resolvents). For example, equations (2.5) and (2.15) give correctly the atomic limit ($t_k \equiv 0$), as the Hubbard-I approximation does [8].

An accurate calculation may be carried out in the case of small hole concentrations $c = n_0$ (saturated ferromagnetic state [17]) and low temperatures. We have [16, 26]

$$\tilde{G}^{\uparrow}_{k}(E) = \left(1 - \sum_q N_q\right)\left(E - \varepsilon_k - \sum_q \varphi_{kq}(E) N_q\right)^{-1} \qquad \varphi(q \to 0) \to 0$$

so that, at $T = 0$, spin-up electrons propagate freely:

$$\langle X^{0+}_{-k} X^{+0}_{k}\rangle = f(\varepsilon_k) \equiv n_k \qquad \delta\varepsilon_k(T) \propto T^{5/2}.$$

The situation is more interesting for the 'spin-down' Green function. Using the kinematical relations (7.1) we obtain

$$\tilde{G}^{\downarrow}_{k}(E) = \sum_q \tilde{F}^{\downarrow}_{kq}(E) \tag{7.13}$$

$$(E - \varepsilon_{k-q})\tilde{F}^{\downarrow}_{kq}(E) = N_q + n_{k-q} + \sum_{pr} \langle\langle (\varepsilon_{k-q+r} - \varepsilon_{k-q-p+r}) X_q^{-+} X_p^{-+} X_{-r}^{+-} X_{k-p+r-q}^{+0} + (\varepsilon_r - \varepsilon_{r+q}) X_{-r}^{0+} X_{r+q-p}^{-+} X_p^{+0} X_{k-q}^{+0} | X_{-k}^{0-} \rangle\rangle_E. \qquad (7.14)$$

After decoupling, we derive the integral equation

$$(E - \varepsilon_{k-q} - \delta\varepsilon_{k-q}(T) + \omega_q]\,\tilde{F}^{\downarrow}_{kq}(E) = (n_{k-q} + N_q) \times \left(1 - \sum_p (\varepsilon_{k-p} - \varepsilon_k)\tilde{F}^{\downarrow}_{kp}(E)\right) \qquad (7.15)$$

where, to first order in $1/z$,

$$\delta\varepsilon_k(T) = \sum_q (\varepsilon_{k-q} - \varepsilon_k) N_q \qquad \omega_q = \sum_k (\varepsilon_{k-q} - \varepsilon_k) n_k. \qquad (7.16)$$

Solving (7.15) we obtain

$$\tilde{G}^{\downarrow}_k(E) = \{E - \varepsilon_k + [\tilde{G}^{0\downarrow}_k(E)]^{-1}\}^{-1} \qquad (7.17)$$

$$\tilde{G}^{0\downarrow}_k(E) \equiv \sum_q \frac{N_q + n_{k-q}}{E - \varepsilon_{k-q} + \omega_q}. \qquad (7.18)$$

Note that (7.17) coincides with (2.5) and (2.15) for $U \to \infty$ if we make the 'particle–hole' transformation. An expression, similar to (7.17), was derived in [27] using the diagram technique for X-operators.

Equation (7.18), yielding $\tilde{G}^{\downarrow}$ to lowest order in c, was obtained in [16, 26]. Electron states described by (7.18) have a pure non-quasiparticle nature. A similar situation takes place for the full Green function (7.17) since at small c it has no poles below E_F on the real axis. The corresponding distribution function, $\langle X^{0-}_{-k} X^{-0}_{k} \rangle \simeq c$, is weakly k dependent. As follows from the general consideration of the electric field action on a many-electron system [28], states with such a property transfer no current. The non-quasiparticle states do not contribute to the density of states on E_F at $T = 0$:

$$N_{\downarrow}(E) \simeq \sum_q n_{k-q}\,\delta(E - \varepsilon_{k-q} + \omega_q) \propto (E_F - E)^{3/2}\theta(E_F - E) \qquad (7.19)$$

for $E_F - E \ll \bar{\omega}$. At the same time, they give a contribution to the γT-term in the specific heat (see the next section). Similar properties (except the condition $\delta N(E_F) = 0$) were postulated by Anderson for spinons (neutral fermion excitations in the resonating-valence-bond state without magnetic order) which, according to [29], may be described by a Green function with zero residue. In fact, we have demonstrated the existence of such excitations in a narrow-band Hubbard ferromagnet.

With increasing c, the Green function (7.18) acquires a real pole below E_F (similar to that describing spin-polaron states in the s–d model [11–13]), and the saturated ferromagnetic state is destroyed [8]. A conclusion about an antiferromagnetic instability was put forward in [27]. According to considerations in [3], ferromagnetism is preserved up to $c \simeq 1$, but becomes unsaturated, the nature of spin-down states being changed, so that they are roughly described by the Hubbard-I approximation (7.6), i.e. they form narrowed quasiparticle bands. Near the instability, the effective mass of the quasiparticles that arise may be very large owing to the logarithmic divergence of the quantity $\tilde{G}^{0\downarrow}_k(E)$. Such a mechanism was proposed in [30, 31] to explain the experimental data on the specific heat of $CeSi_x$.

8. Non-quasiparticle contributions to specific heat: ferrospinons

As follows from the above consideration, branch cuts of the electron Green functions, as well as their poles, play an important role in the thermodynamic and magnetic properties of conducting ferromagnets. The theory of a ferromagnetic Fermi liquid [32], like the usual Fermi-liquid theory [33], is restricted to an explicit consideration of pole (quasiparticle) contributions, non-quasiparticle contributions being assumed to result in renormalisations of $N(E_F)$ and Fermi-liquid parameters only. We shall demonstrate that non-quasiparticle contributions of quite a different type occur in the electronic specific heat of a conducting ferromagnet.

Firstly, such contributions were found in the anisotropic s–d model of a (pseudo) ferromagnet [18]. Here we reproduce this result using equation (6.4). We have

$$\frac{\partial n_\sigma}{\partial T} = \frac{\partial}{\partial T}\left(\int_{-\infty}^{\infty} \mathrm{d}E f(E) N_\sigma(E)\right) = \int_{-\infty}^{\infty} \mathrm{d}E \frac{E}{T}\frac{\partial f(E)}{\partial E} N_\sigma(E) + \int_{-\infty}^{\infty} \mathrm{d}E f(E) \frac{\partial N_\sigma(E)}{\partial T}. \tag{8.1}$$

The first term in (8.1) yields the usual result

$$S_\sigma(T) = C_\sigma(T) = (\pi^2/3) N_\sigma(E_F) T. \tag{8.2}$$

The second term is due to the temperature dependence of the density of states. Substituting (2.12) and (2.13) into the last term of (3.6) we derive

$$\delta\left(\frac{\partial n_\sigma}{\partial T}\right) = 2I^2 \langle S^z \rangle \sum_{kq} \frac{\sigma f(t_{k+q,-\sigma} - \sigma\omega_q)}{(t_{k+q,-\sigma} - t_{k\sigma} - \sigma\omega_q)^2} \frac{\partial}{\partial T} n_{k+q,-\sigma} \tag{8.3}$$

(For the Hubbard model, $I \rightarrow U > 0$.) At low $T, f(t_{k+q\downarrow} - \omega_q) \rightarrow 1$ and $f(t_{k+q} + \omega_q) \rightarrow 0$. Thus non-quasiparticle states with $\sigma = \downarrow$ do not contribute to the γT-term since they are empty at $T = 0$. For $\sigma = \uparrow$ we get

$$\delta\left(\frac{\partial n_\uparrow}{\partial T}\right) = \frac{2\pi^2}{3} I^2 \langle S^z \rangle \frac{\partial}{\partial \mu}\left(\rho_\downarrow(\mu) \sum_k (t_{k\uparrow} - \mu)^{-2}\right)_{\mu = E_F} \tag{8.4}$$

$$\delta S_\uparrow = \delta C_\uparrow = \frac{2\pi^2}{3} T I^2 \langle S^z \rangle \rho_\downarrow(E_F) \sum_k (t_{k\uparrow} - E_F)^{-2}. \tag{8.5}$$

The result (8.5) may seem to be striking, since it is not clear why the general and apparently strict proof of equation (8.2) [33] is not valid for a ferromagnetic state. In fact, the presence of the energy spectrum splitting plays an essential role in our calculations. Also, temperature effects are taken into account in each thermodynamic potential diagram for one Green function only in [33]. At the same time, we have considered terms with products of Fermi functions at close energies.

Selecting the non-quasiparticle contribution is most unambiguous for a saturated ferromagnet. In the s–d model with $I < 0$ (where $\sigma = \downarrow$ corresponds to the lower-spin subband, and $\rho_\uparrow(E_F) = 0$), equation (8.5) yields the only contribution of minority states to the γT-term. In the s–d model with $I > 0$ and the Hubbard model ($\rho_\downarrow(E_F) = 0$), non-quasiparticle contributions to the specific heat are absent. In the non-saturated case, the consideration is more difficult since the density of states below E_F with a given spin projection contains contributions of both poles and branch cuts.

The situation in the Hubbard ferromagnet changes if we consider an almost-half-filled band with strong correlations. Then we have to introduce the 'hole' representation (or the 'double' representation for $n > 1$), and the Hubbard model has properties similar to those of the s–d model with $I < 0$, unlike the 'broad-band' Hubbard model (see section 2). The non-quasiparticle hole states (described by the creation operators X^{0-}_{-k}) are occupied, and in the saturated state case they are the only minority states contributing to γ, since the Green function (7.4) with $\sigma = \downarrow$ has no poles below the hole Fermi level.

First we consider the non-quasiparticle contribution to C using the Green function (7.8). We have

$$\delta C_{\downarrow} = \frac{\partial}{\partial T}(\delta\langle H - \mu n_0\rangle) = \frac{\partial}{\partial T}\left[\sum_k \left(\varepsilon_k - \frac{\mu}{n_0 + n_-}\right)\right.$$

$$\left.\times \int_{-\infty}^{\infty} \mathrm{d}E f(E) \left(-\frac{1}{\pi}\operatorname{Im}\delta\tilde{G}_k^{\downarrow}(E)\right)\right] \tag{8.6}$$

$$\delta\tilde{G}_k^{\downarrow}(E) = \sum_q \varepsilon_{k-q} \frac{(E - \varepsilon_{k-q\downarrow})(n_0 + n_+) f(\varepsilon_{k-q\uparrow})}{(E - \varepsilon_{k-q\uparrow} - \omega_q)(E - \varepsilon_{k\downarrow})^2}. \tag{8.7}$$

The factor $(n_0 + n_-)^{-1}$ of the chemical potential μ of holes is introduced to compensate violation of kinematical relations in the Hubbard-I approximation. Integration gives

$$\delta C_{\downarrow} = \frac{4\langle S^z\rangle(n_0 + n_+)}{T(n_0 + n_-)} \sum_{kq} \frac{\varepsilon_q^2(\varepsilon_{k\downarrow} - \mu)^2(\varepsilon_{q\uparrow} - \mu)^2}{(\varepsilon_{k\downarrow} - \varepsilon_{q\uparrow})^3}\left(-\frac{\partial f(\varepsilon_{q\uparrow})}{\partial\varepsilon_{q\uparrow}}\right)$$

$$\simeq \frac{4\langle S^z\rangle\mu^2}{(n_0 + n_-)(n_0 + n_+)^2}\frac{\pi^2}{3}N_{\uparrow}(E_{\mathrm{F}})T\sum_k \frac{1}{(\varepsilon_{k\downarrow} - \mu)^2} \tag{8.8}$$

which is reminiscent of equation (8.5).

In the paramagnetic state, non-quasiparticle contributions to the Green function (7.8), containing Fermi functions, vanish to first order in $1/z$. Formally, this is due to the structure of the Hubbard-I spectrum (7.11): at $U \to \infty$, $E_k \propto t_k$, and the energy denominators are cancelled. At $U \neq \infty$, such contributions do occur in the paramagnetic state [23], so that the Hubbard splitting (which contradicts the Fermi-liquid theory) may result in non-quasiparticle terms in the specific heat, too.

As we noted in section 7, states corresponding to branch cuts of electron Green functions possess properties similar to those of Anderson's spinons. Now we consider an interesting case when the non-quasiparticle states (we call them ferrospinons) make the dominant contribution to specific heat. We use equation (7.17), expanding it in $\tilde{G}^{0\downarrow}$. A non-zero contribution arises in the third order:

$$\delta C_{\downarrow}^{(3)}(T) = \frac{\partial}{\partial T}\left[\sum_k (\varepsilon_k - \mu)\int_{-\infty}^{\infty}\mathrm{d}E f(E)\left(-\frac{1}{\pi}\operatorname{Im}\{(E - \varepsilon_k)^2[\tilde{G}_k^{0\downarrow}(E)]^3\}\right)\right]$$

$$\simeq \frac{\partial}{\partial T}\left(\sum_{kpqr}\frac{3(\varepsilon_k - \mu)(\varepsilon_k - \varepsilon_q)^2 n_q n_p n_r}{(\varepsilon_q - \varepsilon_p + \omega_{k-p} - \omega_{k-q})(\varepsilon_q - \varepsilon_r + \omega_{k-r} - \omega_{k-q})}\right). \tag{8.9}$$

Exact calculation of the integral (8.9) for concrete spectra ε_k, ω_q is very difficult. We estimate (8.9) by putting $\omega_q = 0$ and cutting divergences that arise at the mean magnon frequency:

$$\bar{\omega} \sim D k_F k \propto c^{4/3} \qquad (k \sim v_0^{-1/3}, \quad k_F \propto c^{1/3}, \quad D \propto c).$$

Then we have

$$\delta C_\downarrow(T) \simeq 12\pi^2 T[\rho^3(E_F)/\bar{\omega}] \ln(W/\bar{\omega}) \sum_k (\varepsilon_k - \mu)^3. \tag{8.10}$$

$$\gamma_\downarrow \propto c^{-1/3} \ln c^{-1} \qquad \gamma_\downarrow \gg \gamma_\uparrow \propto \rho(E_F) \propto c^{1/3}. \tag{8.11}$$

Higher orders in $\tilde{G}^{0\downarrow}$ do not change the result (8.11) since they contain extra factors of order $c^{1/3} \ln c$:

$$\delta C_\downarrow^{(l)}(T) \propto l(l+1)\bar{\omega}^{-1}[\rho(E_F) \ln \bar{\omega}]^{l+1} \sum_k (\varepsilon_k - \mu)^l. \tag{8.12}$$

Thus we obtain an enhancement of the γT-term by a factor of the order of $c^{-2/3} \ln(1/c)$. This enhancement is somewhat weaker than that found by the Gutzwiller method for the paramagnetic state: $\gamma/\gamma_0 \propto 1/c$ [34]. We see that the ferrospinon contribution dominates in the specific heat of a saturated ferromagnet at small c.

9. Discussion of experimental data on half-metallic ferromagnets: spin polarisation and longitudinal nuclear relaxation rate

An important class of itinerant-electron ferromagnets is constituted by HMFs, where the Fermi level for minority spin states lies in the energy gap. To this class belong the Mn-based Heusler alloys NiMnSb, PtMnSb and CoMnSb [4, 35–37], and possibly UNiSn [38] and (according to electronic-structure calculation [39]) chromium dioxide CrO_2 which is widely used in magnetic recording. PtMnSb and UNiSn are promising from the technical point of view owing to their very high magneto-optical Kerr effect, which is intimately related to their electronic structure [35]. FeMnSb and Fe_3O_4 are half-metallic ferrimagnets [37]. In the ferrimagnet Mn_4N, $\rho_\downarrow(E_F) = 0$ for the Mn(I) position and $\rho_\downarrow(E)$ has a deep minimum at E_F for the Mn(II) position [40]. In Fe–Co alloys, which provide the basis of modern soft magnetic materials and are important in connection with the problem of obtaining largest saturation magnetisation, $\rho_\downarrow(E_F) \ll \rho_\uparrow(E_F)$ [41], so that they are close to HMFs.

The results obtained in the present paper demonstrate that the case of a HMF is very convenient for selecting non-quasiparticle contributions. Consider the available experimental data from this point of view.

An interesting question is that of the spin polarisation of conduction electrons in a HMF. According to the naive Stoner picture, $P(E_F) = 100\%$ at temperatures small in comparison with spin splitting, i.e. up to $T = T_c$. Experimental data on spin-resolved threshold photoemission in the Mn-based Heusler alloys yield $P(E_F) \simeq 50\%$ [42]. Data on resistivity and Hall effect in the Heusler alloys [36] show that $P(E_F)$ is strongly T dependent and behaves roughly as the magnetisation $\langle S^z \rangle$. A conclusion was put forward in [36] that the latter fact indicates that Heusler alloys should be described by a strong-coupling model. As follows from our consideration of the electron–magnon interaction (section 3), the dependence $P(T) \propto \langle S^z \rangle$ takes place for arbitrary coupling, both for the Hubbard model (where it is physically lucid since the current carriers form at the same time magnetic moments) and for the s–d model (where the current carriers and magnetic moments belong to different energy bands) [10, 20], and is related to the occurrence of minority non-quasiparticle states at E_F and to a decrease in the residue of the majority Green function with increasing T.

The question concerning depolarisation of conduction electrons in a HMF at $T = 0$ is more complicated. Depolarisation may be found by photoemission measurements provided that occupied non-quasiparticle states are present near E_F, which takes place in the s–d model with the antiferromagnetic exchange interaction ($I < 0$) [10]. (For $I > 0$, the non-quasiparticle states are empty and may be observed by inverse photoemission measurements.) In the broad-band Hubbard model, at $T = 0$ the non-quasiparticle states lie above E_F (section 3), so that depolarisation is absent. However, in the narrow-band limit ($U \to \infty$) the situation changes. Consider the almost-half-filled band with $n > 1$, $c = N_2 = n - 1 \ll 1$. Then the current carriers are spinless doubles, and spin-up and spin-down electrons may be 'pulled out' from the occupied states with equal probability. On the other hand, empty states may be filled, according to the Pauli principle, only by spin-down electrons [26]. These conclusions are confirmed by the calculation of the electron Green functions (cf section 7):

$$N_{\downarrow}(E) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{d}E\, f(E)\, \mathrm{Im}\left(\sum_k \langle\langle X_k^{+2} | X_{-k}^{2+} \rangle\rangle_E\right) = \sum_k \delta(E - t_k)$$

$$N_{\uparrow}(E) = \sum_k f(t_{k+q})\delta(E - t_{k+q} + \omega_q) \simeq \begin{cases} N_{\downarrow}(E) & E < E_F \\ 0 & E > E_F \end{cases}$$

in agreement with the sum rules

$$\sum_k \langle X_{-k}^{2+} X_k^{+2} \rangle = \sum_k \langle X_{-k}^{2-} X_k^{-2} \rangle = \langle X_i^{22} \rangle = c.$$

Thus the spin polarisation is absent below E_F except for the narrow layer of order $\bar{\omega}$, and experiments with a fairly low energy resolution would demonstrate a small spin polarisation. Realistic values of model parameters are intermediate, so that a deviation $P(T = 0)$ from 100% is not surprising.

Recently [43] a striking result has been obtained from the photoemission spectra of CrO_2: no conduction electrons has been found at E_F, in contradiction with metallic conductivity. In our opinion, the most natural explanation of this result is provided by final-state effects: for narrow bands, the photoelectron density of states may differ appreciably from that in the ground state because of the attraction of the electron to the hole that forms (see, e.g., the calculation for Ni [44]). The possible 'polaronic' nature of states at E_F is discussed in [43] as the reason for the above discrepancy. Such a possibility seems to be more exotic but is not excluded near the boundary of the stability of the half-metallic state (see section 7).

One of the direct methods for proving the half-metallic nature of a ferromagnet is investigation of the temperature dependence of the longitudinal nuclear relaxation rate $1/T_1(T)$. For $\rho_{\downarrow}(E_F) = 0$, the linear Korringa contribution (4.9) is absent and the relaxation is due to two-magnon processes which give the $T^{5/2}$ contribution (4.8). Note that the non-quasiparticle electron–magnon scattering states are essentially involved in $\gamma_q^{(2)}(\omega)$ [13] and, therefore, in the contribution to $1/T_1$ (4.8).

Strong deviations from the Korringa law were found in the above-discussed compounds NiMnSb [45] and Mn_4N [46]. For NiMnSb, which is a ferromagnet with $T_c =$

750 K, a dependence of the form $1/T_1 = aT + bT^{3.8}$ was obtained at $T > 250$ K. The modification of the exponent (3.8 instead of 2.5) may be due to the dependences $\langle S^z \rangle (T)$, $D(T)$ in (4.8). The presence of a small linear term might be explained by errors of the band calculation [4] or by the influence of impurities which form minority states near E_F. Thus, NMR experiments may give a further insight into the true nature of the ground state for such ferromagnets as CrO_2.

We see that some non-quasiparticle contributions are most simply observable for HMFs. On the other hand, effects related to the Stoner continuum (e.g. the logarithmic enhancement of specific heat) take place for non-saturated ferromagnets only.

In the light of the results in section 8, careful experimental investigations of specific heat of conducting ferromagnets with strong electron correlations (see, e.g., [47]) would be of great interest.

References

[1] Hubbard J 1963 *Proc. R. Soc.* A **276** 238

[2] Moriya T 1985 *Spin Fluctuations in Itinerant Electron Ferromagnetism* (Berlin: Springer)

[3] Auslender M I, Irkhin V Yu and Katsnelson M I 1988 *Fiz. Metall. Metalloved.* **65** 57; *J. Phys. C: Solid State Phys.* **21** 5521

[4] de Groot R A, Mueller F M, Mueller P G, van Engen P G and Bushow K H J 1983 *Phys. Rev. Lett.* **50** 2427

[5] Hubbard J 1965 *Proc. R. Soc.* A **285** 542

[6] Zubarev D N 1960 *Usp. Fiz. Nauk* **71** 71

[7] Brinkman W F and Engelsberg S 1968 *Phys. Rev.* **169** 417

[8] Hertz J A and Edwards D M 1973 *J. Phys. F: Met. Phys.* **3** 2174
Edwards D M and Hertz J A 1973 *J. Phys. F: Met. Phys.* **3** 2191

[9] Irkhin V Yu and Katsnelson M I 1989 *Z. Phys.* B **75** 67

[10] Auslender M I and Irkhin V Yu 1985 *J. Phys. C: Solid State Phys.* **18** 3533

[11] Methfessel S and Mattis D 1968 *Handbuch der Physik* vol XVIII/1 (Berlin: Springer)

[12] Izyumov Yu A, Kassan-ogly F A and Skryabin Yu N 1974 *Polevye Metody v Teorii Ferromagnetizma* (Moscow: Nauka)

[13] Irkhin V Yu and Katsnelson M I 1985 *Zh. Eksp. Teor. Fiz.* **88** 522 (Engl. Transl. 1985 *Sov. Phys.-JETP* **61** 306)

[14] Auslender M I and Irkhin V Yu 1984 *Z. Phys.* B **56** 301; 1985 *Z. Phys.* B **61** 129

[15] Irkhin V Yu 1987 *Fiz. Metall. Metalloved.* **64** 260

[16] Irkhin V Yu and Katsnelson M I 1985 *J. Phys. C: Solid State Phys.* **18** 4173

[17] Nagaoka Y 1966 *Phys. Rev.* **147** 392

[18] Irkhin V Yu, Katsnelson M I and Trefilov A V 1990 *Physica* C **160** 397

[19] Edwards D M 1983 *J. Phys. C: Solid State Phys.* **16** L327

[20] Auslender M I and Irkhin V Yu 1984 *Solid State Commun.* **50** 1003

[21] Dzyaloshinsky I E and Kondratenko P S 1976 *Zh. Eksp. Teor. Fiz.* **70** 1987

[22] Silin V P and Solontsov A Z 1982 *Fiz. Metall. Metalloved.* **52** 231

[23] Irkhin V Yu and Katsnelson M I 1988 *Fiz. Metall. Metalloved.* **66** 41

[24] Makoshi K and Moriya T 1975 *J. Phys. Soc. Japan* **38** 10

[25] Solontsov A Z 1984 *Fiz. Metall. Metalloved.* **58** 1080

[26] Irkhin V Yu and Katsnelson M I 1983 *Fiz. Tverd. Tela* **25** 3383 (Engl. Transl. 1983 *Sov. Phys.–Solid State* **25** 1947)

[27] Vedyaev A V and Nikolaev M Yu 1985 *Zh. Eksp. Teor. Fiz. Pis'ma Red.* **41** 18
Nikolaev M Yu, Ryzhanova N V, Vedyaev A V and Zubritskii S M 1985 *Phys. Status Solildi* b **128** 513

[28] Vonsovsky S V and Katsnelson M I 1989 *Usp. Fiz. Nauk* **158** 723

[29] Anderson P W 1988 *Proc. Int. School on Physics 'Enrico Fermi' (Varenna, 1987)* (Amsterdam: North-Holland) p

[30] Vedyaev A V, Zubritskii S M and Ryzhanova N V 1988 *Fiz. Metall. Metalloved.* **65** 882

[31] Goodbody S and Edwards D M 1989 *Proc. Int. Conf. on Magnetism (Paris, July 1988)*

[32] Abrikosov A A and Dzyaloshinsky I E 1958 *Zh. Eksp. Teor. Fiz.* **35** 771
[33] Abrikosov A, Gorkov L and Dzyaloshinsky I 1963 *Methods of Quantum Field Theory in Statistical Physics* (New York: Prentice-Hall)
[34] Vollhardt D 1984 *Rev. Mod. Phys.* **56** 99
[35] de Groot R A, Mueller F M, van Engen P G and Bushow K H J 1984 *J. Appl. Phys.* **55** 2151
[36] Otto M J, Feihl H, van Woerden R A M, Wijngaard J, van der Valk P J, van Bruggen C F and Haas C 1987 *J. Magn. Magn. Mater.* **70** 33
[37] de Groot R A and Bushow K H J 1986 *J. Magn. Magn. Mater.* **54–57** 1377
[38] Albers R C, Boring A M, Daalderop G H O and Mueller F M 1987 *Phys. Rev.* B **36** 3661
[39] Schwarz K 1986 *J. Phys. F: Met. Phys.* **16** L211
[40] Matar S, Mohn P, Demazeau G and Siberchicot B 1988 *J. Physique* **49** 1761
[41] Schwarz K, Mohn O, Blaha P and Kübler J 1984 *J. Phys. F: Met. Phys.* **14** 2659
[42] Bona G L, Meier F, Taborelli M, Bucher E and Schmidt P H 1985 *Solid State Commun.* **56** 391
Kisker E, Carbone C, Flipse C F and Wassermann E F 1987 *J. Magn. Magn. Mater.* **70** 21
[43] Kämper K R, Schmitt W, Güntherhodt G, Gambino R J and Ruf R 1987 *Phys. Rev. Lett.* **59** 2788
[44] Anisimov V I, Katsnelson M I, Kurmaev E Z, Liechtenstein A I and Gubanov V A 1981 *Solid State Commun.* **40** 927
[45] Enokiya H 1971 *J. Phys. Soc. Japan* **31** 1037
[46] Matsuura M M 1966 *J. Phys. Soc. Japan* **21** 1886
[47] Mott N F 1974 *Metal–Insulator Transitions* (London: Taylor and Francis)