Temperature dependences of resistivity and magnetoresistivity for half-metallic ferromagnets

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Peculiarities of transport properties of three- and two-dimensional half-metallic ferromagnets are investigated, which are connected with the absence of spin-flip scattering processes. The temperature and magnetic field dependences of resistivity in various regimes are calculated. The resistivity is proportional to $T^{9/2}$ for $T < T^*$ and to $T^{7/2}$ for $T > T^*$, $T^*$ being the crossover temperature for longitudinal scattering processes. The latter scale plays also an important role in magnetoresistance. The contribution of non-quasiparticle (incoherent) states to the transport properties is discussed. It is shown that they can dominate in the temperature dependence of the impurity-induced resistivity and in the tunnel junction conductivity.

I. INTRODUCTION

Half-metallic ferromagnets (HMF) [1,2] attract now a growing attention of researchers, first of all, because of their importance for “spintronics”, or spin-dependent electronics [3]. HMF have metallic electronic structure for one spin projection (majority- or minority-spin states), but for the opposite spin direction the Fermi level lies in the energy gap [1]. Therefore the corresponding contributions to electronic transport properties have different orders of magnitude, which can result in a huge magnetoresistance for heterostructures containing HMF [2]. A discovery of the half-metallic ferromagnetism in colossal magnetoresistance (CMR) materials like $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ [5] has increased considerably the interest in this topic. Transport properties of HMF are the subject of numerous experimental investigations (see, e.g., recent works for CrO$_2$ [6] and NiMnSb [7], and the reviews [2,8,9]). At the same time, the theoretical interpretation of these results is still a problem.

As for electronic scattering mechanisms, the most important difference between HMF and “standard” itinerant electron ferromagnets like iron or nickel is the absence of one-magnon scattering processes in the former case [2]. Two-magnon scattering processes have been considered many years ago for both the broad-band case (weak $s-d$ exchange interaction) [10] and narrow-band case (“double exchange model”) [11]. The obtained temperature dependence of the resistivity have the form $T^{7/2}$ and $T^{9/2}$, respectively. At low enough temperatures the first result fails and should be replaced by $T^{9/2}$ as well [12]: the reason is the compensation of the transverse and longitudinal contributions in the long-wavelength limit which is a consequence of the rotational symmetry of the $s-d$ exchange Hamiltonian [13,14].

Up to now there are no results which describe in the whole temperature region the resistivity of HFM and especially its magnetic-field dependence which is most interesting from the experimental point of view. Such expressions are obtained in Sect.2. Apart from three-dimensional case studied before [11,12] we consider also two-dimensional HMF keeping in mind, e.g., layered CMR compounds like $\text{LaSr}_2\text{MnO}_7$ (for a review see Ref. [1]) which are almost half-metallic according to the recent band-structure calculations [11].

Owing to peculiar band structure of HFM, an important role belongs to incoherent (non-quasiparticle) states which occur near the Fermi level because of correlation effects [2]. In Sect.3 we treat the corresponding contributions to resistivity and discuss tunneling phenomena in HMF.

II. RESISTIVITY AND MAGNETORESISTIVITY

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

$$
\mathcal{H} = \sum_{k\sigma} f^+_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{qk} I_{k,k+q} \sum_{\alpha\beta} S^+_{qk\alpha\beta} \sigma_{\alpha\beta} c_{k-q\beta} - \sum_{q} J_q S_q S_{-q} \quad (1)
$$
where \( c_{\mathbf{k}\sigma}^\dagger \), \( c_{\mathbf{k}\sigma} \) and \( S_{\mathbf{q}} \) are operators for conduction electrons and localized spins in the quasimomentum representation, the electron spectrum \( t_\mathbf{k} \) is referred to the Fermi level \( E_F \), \( J_{k,k+q} \) is the \( s-d(f) \) exchange parameter which will be put for simplicity \( \mathbf{k} \)-independent, \( \sigma \) are the Pauli matrices. In the spin-wave region we have

\[
\mathcal{H} = \mathcal{H}_0 - I(2S)^{1/2} \sum_{\mathbf{kq}} (c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} b_{\mathbf{q}\sigma}^\dagger + h.c.) + I \sum_{\mathbf{kqps}} \sigma c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{p}\sigma} b_{\mathbf{q}\sigma}^\dagger b_{\mathbf{p}\sigma}
\]  

(2)

The zero-order Hamiltonian includes non-interacting electrons and magnons,

\[
\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}\sigma}^\dagger b_{\mathbf{q}\sigma},
\]  

(3)

\[
E_{\mathbf{k}\sigma} = t_\mathbf{k} - \sigma \Delta / 2, \omega_{\mathbf{q}} = 2S(J_0 - J_\mathbf{q}),
\]  

(4)

with \( \Delta = 2IS \) being the spin splitting which is included in \( \mathcal{H}_0 \). \( b_{\mathbf{q}\sigma}^\dagger, b_{\mathbf{q}\sigma} \) are the Holstein-Primakoff boson operators. In the half-metallic case the spin-flip processes do not work in the second order in \( I \) since the states with one spin projection only are present at the Fermi level. At the same time, we have to consider the renormalization of the longitudinal processes in higher orders in \( I \) (formally, we have to include the terms up to the second order in the quasiclassical small parameter \( 1/S \)). To this end we eliminate from the Hamiltonian the terms which are linear in the magnon operators by using the canonical transformation [13], \( \mathcal{H} = e^U \mathcal{H} e^{-U} \) with

\[
U = -I(2S)^{1/2} \sum_{\mathbf{kq}} \frac{c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} b_{\mathbf{q}\sigma}^\dagger}{t_\mathbf{k}+\mathbf{q} - t_\mathbf{k} + \Delta} - h.c.
\]  

(5)

Then we obtain the effective Hamiltonian

\[
\tilde{\mathcal{H}} = \mathcal{H}_0 + \frac{1}{2} \sum_{\mathbf{kqps}} (\mathcal{A}_{\mathbf{kq}}^\sigma + \mathcal{A}_{\mathbf{kq}\mathbf{ps}}^\sigma) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{p}\sigma} b_{\mathbf{q}\sigma}^\dagger b_{\mathbf{p}\sigma}
\]  

(6)

Here

\[
\mathcal{A}_{\mathbf{kq}}^\sigma = \sigma I \frac{t_\mathbf{k}+\mathbf{q} - t_\mathbf{k}}{t_\mathbf{k}+\mathbf{q} - t_\mathbf{k} + \sigma \Delta}
\]  

(7)

is the \( s-d \) scattering amplitude which vanishes at \( q \to 0 \) and thereby takes properly into account the rotational symmetry of electron-magnon interaction. More general interpolation expression for the effective amplitude which does not assume the smallness of \( |I| \) or \( 1/S \) was obtained in Ref. [14] by a variational approach; it does not differ qualitatively from simple expression (7). In the case of a considerably \( \mathbf{k} \)-dependent exchange parameter, which may be relevant for real itinerant magnets including HFM, one has in (3)

\[
\mathcal{A}_{\mathbf{kq}}^\sigma \to \mathcal{A}_{\mathbf{kqp}}^\sigma = \sigma I_{\mathbf{k},\mathbf{k}+\mathbf{q}-\mathbf{p}} - \frac{2|I_{\mathbf{k},\mathbf{k}+\mathbf{q}}^2 S}{t_\mathbf{k}+\mathbf{q} - t_\mathbf{k} + \sigma S(t_\mathbf{k}+\mathbf{q},k+\mathbf{q} + I_{\mathbf{k},\mathbf{k}})}
\]  

(8)

The most general and rigorous method for calculating the transport relaxation time is the use of the Kubo formula for the conductivity \( \sigma_{xx} \) [16]

\[
\sigma_{xx} = \beta \int_0^\beta d\lambda \int_0^\infty dt \exp(-\varepsilon t) \langle j_x(t+i\lambda) j_x \rangle
\]  

(9)

where \( \beta = 1/T, \varepsilon \to 0 \),

\[
j = -e \sum_{\mathbf{k}\sigma} \mathbf{v}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}
\]

is the current operator, \( \mathbf{v}_{\mathbf{k}\sigma} = \partial E_{\mathbf{k}\sigma} / \partial \mathbf{k} \) is the electron velocity. Representing the total Hamiltonian in the form \( \mathcal{H} = \mathcal{H}_0 + \mathcal{H}' \), the correlator in (9) may be expanded in the perturbation \( \mathcal{H}' \) [17]. In the second order we obtain for the electrical resistivity

\[
\rho_{xx} = \sigma_{xx}^{-1} = \frac{T}{(J_2)^2} \int_0^\infty dt \langle [j_x(\mathcal{H}'(t)], j_x, \mathcal{H}'(t)] \rangle
\]  

(10)
where $\mathcal{H}'(t)$ is calculated with the Hamiltonian $\mathcal{H}_0$. Provided that the perturbation Hamiltonian has the form

$$\mathcal{H}' = \sum_{kk'\sigma\sigma'} \hat{W}_{kk'}^{\sigma\sigma'} \hat{c}_{k\sigma} \hat{c}_{k'\sigma'}$$

we obtain

$$\rho_{xx} = \frac{T}{2(J^2)} \int_{-\infty}^{\infty} dt \langle \hat{W}_{kk'}^{\sigma\sigma'}(t)\hat{W}_{k'k}^{\sigma\sigma'} \rangle \exp[i(E_{k\sigma} - E_{k'\sigma'})t]$$

with

$$\langle j_0^2 \rangle = \frac{e^2}{\tau} \sum_{k\sigma} (\nu_k^2)^2 n_{k\sigma}(1 - n_{k\sigma})$$

This approach is equivalent to the solution of the Boltzmann transport equation by the variational method [18].

In the HFM situation the band states with one spin projection only, $\sigma = \text{sign} I$, are present at the Fermi level [2]. Below we consider the case $I > 0$, $\sigma = +$ and omit the spin indices in the electron spectrum. We find from Eq.(12) the following expression for the transport relaxation time $\tau$ defined by $\sigma_{xx} = e^2 (\langle (v^2)^2 \rangle \tau$

$$\frac{1}{\tau} = \frac{\pi}{4T} \sum_{kk'q}(\nu_k^2 - \nu_{k'}^2)^2(A_{kq}^{\uparrow} + A_{k'q-k+k}^{\uparrow})N_q(1 + N_{q-k+k})$$

$$\times n_k(1 - n_{k'})\delta(t_{k'} - t_k - \omega_q + \omega_{q-k+k}) \sum_k (\nu_k^2)^2 \delta(t_k)$$

where $N_q$ and $n_k$ are the Bose and Fermi functions. A similar expression has been derived first in Ref. [10], but with the replacement of the effective amplitude just by $I$. After some transformations we obtain

$$\frac{1}{\tau} = \pi I^2 \sum_{kk'q}(\nu_k^2 - \nu_{k'}^2)^2 \delta(t_k)\delta(t_{k+q-p})(1 + N_q(1 + N_p) \left(\frac{\omega_k + \Delta}{\omega_q + \Delta}\right)^2 \frac{\beta(\omega_p - \omega_q)}{\exp \beta \omega_p - \exp \beta \omega_q} \sum_k (\nu_k^2)^2 \delta(t_k)$$

Averaging over the angles of the vector $k$ leads to the result $1/\tau \propto I^2 \Lambda$ with

$$\Lambda = \sum_{pq} f_{pq} \frac{\beta(\omega_p - \omega_q)\|p - q\|}{\exp \beta \omega_p - \exp \beta \omega_q} (1 + N_q(1 + N_p)$$

where $f_{pq} = 1$ for $p, q \gg q_0$ and

$$f_{pq} = \frac{[p \times q]^2}{(p - q)^2 q_0^2} \quad (p, q \ll q_0).$$

The wavevector $q_0$ determines the boundary of the region where $q$-dependence of the amplitude become important, so that $t(k + q) - t(k) \simeq \Delta$ at $q \simeq q_0$. In the case $q < q_0$ the simple perturbation theory fails and we have to take into account the spin splitting by careful collecting the terms of higher orders in $I$. In the simple one-band model of HMF where $E_F < \Delta$ one has $q_0 \sim \sqrt{\Delta/W}$ ($W$ is the conduction bandwidth, lattice constant is put to unity) [13]. Generally speaking, $q_0$ may be sufficiently small provided that the energy gap is much smaller than $W$, which is the case for real HMF systems. A “crossover” wavevector may exist in principle even for the narrow-band case (where, instead of spin splitting, the spin subbands have different widths) provided that the Fermi level is close to the gap edge for the spin projection $-\sigma$.

The quantity $q_0$ determines a characteristic temperature and energy scale

$$T^* = D q_0^2 \propto D(\Delta/W)$$

where $D \propto T_C/S$ is the spin-wave stiffness defined by $\omega_{q\rightarrow 0} = D q^2$, $T_C$ is the Curie temperature. Note that in the case of an usual ferromagnetic metal the scale for existence of one-magnon processes is smaller, $T^*_1 \propto D(\Delta/W)^2$.

When estimating temperature dependences of resistivity one has to bear in mind that each power of $p$ or $q$ yields $T^{1/2}$. At very low temperatures $T < T^*$ small quasimomenta $p, q < q_0$ yield main contribution to the integrals. Averaging the quantity [13] over the angle between the vectors $p$ and $q$ we derive

$$3$$
\[ \Lambda = \frac{8}{15g_0^2} \sum_{pq} \frac{(5p_+^2 - p_2^2)p_2^2}{p_+} \frac{\beta(\omega_p - \omega_q)}{\exp \beta \omega_p - \exp \beta \omega_q} (1 + N_q)(1 + N_p) \]  

(18)

with \( p_+ = \max(p, q), p_- = \min(p, q) \). Then we obtain for the resistivity

\[ \rho(T) \propto (T/T_C)^{5/2} \]  

(19)

Such a dependence was obtained in the narrow-band case (double-exchange model with large \(|I|\)), where the scale \( T^* \) is absent [1], and by the diagram approach in the broad-band case [2]. At the same time, at \( T > T^* \) the function \( f_{pq} \) in Eq. (15) can be replaced by unity to obtain

\[ \rho(T) \propto (T/T_C)^{7/2} \]  

(20)

This result is in agreement with the old works [10].

Now we treat the two-dimensional (2D) situation which may be appropriate for layered manganites like \( \text{La}_{2-x}\text{Ca}_{1+x}\text{Mn}_2\text{O}_7 [9,15] \). At low temperatures we obtain

\[ \rho(T < T^*) \propto (T/T_C)^{7/2} \]  

(21)

At the same time, for \( T > T^* \) we obtain after replacing the scattering amplitude by unity a logarithmically divergent integral which should be cut at \( T^* \). Thus we get

\[ \rho(T > T^*) \propto (T/T_C)^{5/2} \ln(T/T^*) \]  

(22)

To calculate the magnetoresistivity we introduce the gap in the magnon spectrum, \( \omega_{q=0} = Dq^2 + \omega_0 \). Provided that the external magnetic field \( H \) is large in comparison with the anisotropy gap, \( \omega_0 \) is proportional to \( H \). In the 3D case the resistivity at \( T < T^* \) is linear in magnetic field,

\[ \rho(T, H) - \rho(T, 0) \propto -\omega_0 T^{7/2}/T_C^{9/2} \]  

(23)

The situation at \( T > T^* \) is more interesting since the quantity

\[ \frac{\partial \Lambda}{\partial \omega_0} \propto \sum_q q\omega_q N_q(1 + N_q) \sum_p \frac{1}{\omega_p^2} \propto \left( \frac{T}{T_C} \right)^3 \sum_p \frac{1}{\omega_p^2} \]

contains a divergence which is cut at \( \omega_0 \) or \( T^* \). We have at \( T > \omega_0, T^* \)

\[ \delta \rho(T, H) \propto -\frac{T^2 \omega_0}{[\max(\omega_0, T^*)]^{1/2}} \]  

(24)

(of course, at \( T < \omega_0 \) the resistivity is exponentially small). A negative \( H \)-linear magnetoresistance was observed recently in \( \text{CrO}_2 [6] \).

In the 2D case we obtain

\[ \frac{\partial \Lambda}{\partial \omega_0} \propto T^{5/2} \sum_p \frac{\phi(p)}{\omega_p^2} \]  

(25)

where \( \phi(p < q_0) = p^2/q_0^2, \phi(p > q_0) = 1 \). This integral diverges logarithmically at \( \omega_0 \ll T^* \) and as \( \omega_0^{-1} \) at \( \omega_0 \gg T^* \). Taking into account the lower limit cutoff we derive

\[ \delta \rho(T, \omega_0 \ll T^*) \propto -\left( \frac{T}{T_C} \right)^{5/2} \frac{\omega_0}{T^*} \ln \frac{T^*}{\omega_0} \]  

(26)

\[ \delta \rho(T, \omega_0 \gg T^*) \propto -\left( \frac{T}{T_C} \right)^{5/2} \ln \frac{\omega_0}{\max(T, T^*)} \]  

(27)

We see that simple replacement of the electron-magnon scattering amplitude by \( I \) does not enable one to describe correctly magnetoresistance even at \( H > T^* \).
III. NON-QUASIPARTICLE CONTRIBUTIONS TO TRANSPORT PROPERTIES

Now we treat the impurity contributions to transport properties in the presence of potential scattering (they were considered first in Ref. [13], see also Ref. [2]). To second order in the impurity potential $V$ we derive for the electron Green’s function

$$G_{kk’\sigma}(E) = \delta_{kk'} G^{(0)}_{kk\sigma}(E) + V G^{(0)}_{kk\sigma}(E) G^{(0)}_{kk’\sigma}(E) [1 + V \sum_p G^{(0)}_{pp\sigma}(E)]$$

(28)

where

$$G^{(0)}_{kk\sigma}(E) = [E - E_{kk\sigma} - \Sigma_{kk\sigma}(E)]^{-1}$$

(29)

is the exact Green’s function for the ideal crystal. In the second order in $I$ the electron self-energy has the form

$$\Sigma_{kk\sigma}(E) = 2I^2 S \sum_q \frac{f(\sigma E_{kk+q,-\sigma}) + N_q}{E - E_{kk+q,-\sigma} + \sigma \omega_q}$$

(30)

with $f(E)$ the Fermi function.

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

$$\delta \tau_{imp}^{-1}(E) = -2V^2 \text{Im} \sum_p G^{(0)}_{pp\sigma}(E)$$

(31)

Thus the contributions under consideration are determined by the energy dependence of the density of states $N(E)$ for the interacting system near the Fermi level. The most nontrivial dependence comes from the non-quasiparticle (incoherent) states with the spin projection $-\sigma = -\text{sign} I$, which are present near $E_F$ (Fig.1). They originate from the imaginary part of the electron self-energy $\Sigma_{kk\sigma}(E)$. We obtain at $T = 0$

$$\delta N_{incoh}(E) = 2I^2 S \sum_{kk} f(-\sigma E_{kk+q,\sigma}) \delta(E - E_{kk+q,\sigma} - \sigma \omega_q) / (E_{kk+q,\sigma} - E_{kk,-\sigma})^2$$

(32)

The contribution is asymmetric and vanishes at $E_F$ (Figs.1,2). Near the Fermi level it is determined by the magnon density of states $g(\omega)$ and follows a power law,

$$\delta N_{incoh}(E) \propto \int_0^{\sigma E} d\omega g(\omega) \propto |E|^\alpha \theta(\sigma E) \text{ (} |E| \ll \overline{\omega})$$

(33)

Here $\overline{\omega}$ is the maximum magnon frequency, $\theta(x)$ is the step function, $E$ is referred to $E_F$; we have $\alpha = 3/2$ and $\alpha = 1$ for 3D and 2D cases, respectively. The corresponding correction to resistivity reads

$$\frac{\delta \rho_{imp}(T)}{\rho^2} = -\sigma \delta \rho_{imp}(T) \propto -V^2 \int dE \left( -\frac{\partial f(E)}{\partial E} \right) \delta N_{incoh}(E) \propto T^\alpha$$

(34)

The contribution of the order of $T^\alpha$ with $\alpha \approx 1.65$ (which is not too far from 3/2) has been observed recently in the temperature dependence of the resistivity for NiMnSb [3]. The incoherent contribution to magnetoresistivity is given by

$$\delta \rho_{imp}(T, H) \propto \omega_0 \partial \delta N_{incoh}(\sigma T)/\partial T \propto \omega_0 T^{\alpha - 1}$$

(35)

so that we obtain a temperature-independent term in the 2D case.

The non-quasiparticle states in HMF can be probed also by nuclear magnetic resonance (NMR) since they lead to the unusual temperature dependence for the longitudinal nuclear magnetic relaxation rate, $1/T_1 \propto T^{5/2}$, instead of the T-linear Korringa contribution which is absent in HMF [22,23]. Another useful tool is provided by tunneling phenomena [2], especially by Andreev reflection spectroscopy for a HMF-superconductor tunnel junction [24]. The most direct way is probably the measurement of a tunnel current between two pieces of HMF with the opposite magnetization directions. To this end we consider a standard tunneling Hamiltonian (see, e.g., Ref. [26])

$$H = H_L + H_R + \sum_{kp} (T_{kp} c_{kp}^\dagger c_{kp} + h.c.)$$

(36)
where $H_{L,R}$ are the Hamiltonians of the left (right) half-spaces, respectively, $k$ and $p$ are the corresponding quasi-momenta, and spin projections are defined with respect to the magnetization direction of a given half-space (spin is supposed to be conserving in the “global” coordinate system). Carrying out standard calculations of the tunneling current $I$ in the second order in $T_{kp}$ one has (cf. [26])

$$I \propto \sum_{kqp} |T_{kp}|^2 [1 + N_q - f(t_{p-q})][f(t_k) - f(t_k + eV)]\delta(eV + t_k - t_{p-q} + \omega_q).$$

(37)

where $V$ is the bias voltage. For $T = 0$ one obtains

$$dI/dV \propto \delta N_{\text{incoh}}(eV).$$

(38)

To conclude, we have considered peculiarities of transport properties of half-metallic ferromagnets which are connected with the unusual electronic structure of these systems. Further experimental investigations would be of great importance, especially keeping in mind possible role of HMF for applications [2–4].

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**Figure Captions**

Fig.1. Density of states in a half-metallic ferromagnet with $I > 0$. Non-quasiparticle states with $\sigma = -$ are absent below the Fermi level.

Fig.2. Density of states in a half-metallic ferromagnet with $I < 0$. Non-quasiparticle states with $\sigma = +$ occur below the Fermi level.

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