

Rapid Note

Localization and dephasing driven by magnetic fluctuations in low carrier density colossal magnetoresistance materials

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Abstract. Localization and dephasing of conduction electrons in a low carrier density ferromagnet due to scattering on magnetic fluctuations is considered. We claim the existence of the “mobility edge”, which separates the states with fast diffusion and the states with slow diffusion; the latter is determined by the dephasing time. When the “mobility edge” crosses the Fermi energy a large and sharp change of conductivity is observed. The theory provides an explanation for the observed temperature dependence of conductivity in ferromagnetic semiconductors and manganite pyrochlores.

PACS. 75.50.Pp Magnetic semiconductors – 75.70.Pa Giant magnetoresistance – 72.10.-d Theory of electronic transport; scattering mechanisms – 72.10.Di Scattering by phonons, magnons, and other nonlocalized excitations

1 Introduction

Colossal magnetoresistance (CMR) materials attract nowadays considerable interest, associated mostly with the properties of double-exchange manganite perovskites [1]. Class of CMR materials, however, is much wider and includes, in particular, magnetic semiconductors [2] and manganite pyrochlores [3]. All these materials are characterized by strong interaction between the localized spins and itinerant charge carriers. In all these materials CMR is associated with the sharp increase of the resistivity when the temperature T approaches the Curie temperature T_c . However, taking into account the large variety of the materials involved and diverse manifestations of the effect, it is difficult to expect that any single theory can provide a universal explanation of the phenomena.

We concentrate on low carrier density materials (magnetic semiconductors and manganite pyrochlores), where the carriers do not affect the spin-spin interaction, and magnetic d - or f -ions interact mainly *via* ferromagnetic direct exchange (super-exchange). These materials being deficient in chalcogen (oxygen) or being properly doped, have at low temperatures quasi-metallic conductivity. When the temperature approaches T_c they undergo the metal-insulator transition.

In the previous publications [4–6] we suggested, that such behavior of the conductivity is due to Anderson localization of the carriers driven by spin fluctuations of magnetic ions. We considered the spin fluctuations as *static*; hence the scattering of electrons by the fluctuations can be treated as elastic, and hence it leads to the existence of the mobility edge E_c . (This mechanism is close to the phonon scattering induced electron localization [7,8].) When the temperature increases, so does the scattering intensity, which leads to the upward motion of the mobility edge. The temperature at which the mobility edge crosses the Fermi level is identified with the temperature of the metal-insulator transition (MIT). This view point on temperature-induced MIT has also been recognized and legitimated in several recent publications [9–11].

In this paper we consider the influence of the dynamics in the spin subsystem on the transition by developing an idea suggested in reference [12]

2 Hamiltonian and approximations

The Hamiltonian of the system has the form

$$H = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} - \frac{I}{N} \sum_{\mathbf{k}\mathbf{q}\sigma\sigma'} \mathbf{S}_{\mathbf{q}} \sigma_{\sigma\sigma'} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q}\sigma'} + H_M, \quad (1)$$

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where $E_{\mathbf{k}}$ is the bare electron spectrum, $c_{\mathbf{k},\sigma}^\dagger$, $c_{\mathbf{k},\sigma}$ are the electron creation and annihilation operators, I is the parameter of Hund exchange between the electrons and localized spins, $\mathbf{S}_{\mathbf{q}}$ is the Fourier components of the spin density, σ is the vector of the Pauli spin matrices and H_M is the direct exchange interaction described by superexchange integral $J(\mathbf{Q})$.

Let us state the relations between the parameters of the problem. We consider the case of wide conduction band $W \gg 2IS$, where $W \sim 1/ma^2$ is the width of the conduction band (a is the lattice constant and m is the electron mass), S is the spin of magnetic ion. This inequality is certainly applicable to such magnetic semiconductors as EuO and EuS [13]. For manganite pyrochlores we do not have strong inequality [14], but we believe that the approximation still works in this case, at least semi-quantitatively¹. Due to low carrier density considered (not in excess of 10^{-19} cm^{-3}), the Fermi energy E_F is at least an order of magnitude less than $2IS$ (which is larger than 0.5 eV in the materials considered [13,14]). We consider ferromagnetic phase and temperatures such that the spin splitting of the conduction band is larger than E_F (estimations show, that this will be true up to the temperatures very close to T_c). All our assumptions can be thus reduced to inequalities

$$\begin{aligned} W &\gg 2IS \\ 2I\overline{S^z} &\gg E_F \gg T, \end{aligned} \quad (2)$$

where $\overline{S^z}$, is the average spin of magnetic ion.

In the wide conduction band case the electron-spin exchange can be treated as a perturbation, leading to electron scattering. The conduction electrons being fully spin-polarized and spin-flip processes thus being forbidden, the scattering (in the Born approximation) is connected only with the longitudinal spin correlator $\langle \delta S_{\mathbf{q}}^z \delta S_{-\mathbf{q}}^z \rangle$. It is argued [15], that for the wavevector \mathbf{q} small enough ($qa < \text{const}(\overline{S^z})^2$) the correlator is dominated by contribution of weakly interacting spin waves with the dispersion law

$$\omega_{\mathbf{q}} = 2\overline{S^z}[J(0) - J(\mathbf{Q})] \quad (3)$$

and quasi-classical occupation numbers

$$n_{\mathbf{Q}} = \frac{T}{\omega_{\mathbf{Q}}}. \quad (4)$$

As a result the static correlator is [15]

$$\langle \delta S_{\mathbf{q}}^z \delta S_{-\mathbf{q}}^z \rangle = \frac{T^2}{8\overline{S^z}^2 C^2 qa}, \quad (5)$$

where C is the spin stiffness (for nearest-neighbor exchange in a cubic lattice $C \simeq T_c/2S(S+1)$).

¹ We emphasize here the difference between the manganite pyrochlores, which are n-type low carrier density intermediate-band materials, and the manganite perovskites, which are p-type high carrier density narrow-band materials; the latter thus being definitely outside the scope of the theory presented in the paper.

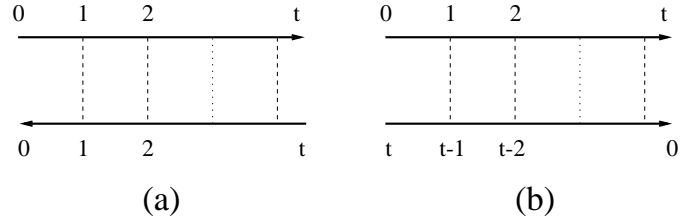


Fig. 1. Diagrams for the Diffuson (a) and the Cooperon (b). Solid line is dressed electron propagator, dashed line connecting times t and t' corresponds to $\Phi_{zz}(t - t')$.

For the transport relaxation time we obtain

$$\begin{aligned} \frac{1}{\tau} &= \frac{2\pi}{N} I^2 \sum_{\mathbf{q}} \langle \delta S_{\mathbf{q}}^z \delta S_{-\mathbf{q}}^z \rangle \frac{\mathbf{k} \cdot \mathbf{q}}{k^2} \delta(E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) \\ &= \frac{ma^2 I^2 T^2}{16\pi \overline{S^z}^2 C^2} \sim \frac{I^2 S(S+1) T^2 S^2}{W T_c^2 \overline{S^z}^2}. \end{aligned} \quad (6)$$

We see that for temperatures high enough, $\tau E_F < 1$. Hence we need some kind of strong scattering theory. As such we shall use the self-consistent localization theory by Vollhard and Wölfle (VW) [16], extended in reference [17] to systems without time-reversal invariance. But first we should calculate the crucial parameter in our approach - the dephasing time τ_φ .

3 Dephasing time

The inverse dephasing time can be defined as the mass of the Cooperon [18,19]. (An alternative, but essentially equivalent view on dephasing see in Ref. [20].) For the Cooperon $C(\mathbf{R}, t)$ we obtain equation

$$\{\partial/\partial t - D\nabla^2 + [f(0) - f(t)]\} C(\mathbf{R}, t) = 0, \quad (7)$$

where

$$f(t) = \frac{2\pi}{N} I^2 \sum_{\mathbf{q}} \Phi_{zz}(\mathbf{q}, t) \delta(E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) \quad (8)$$

and $\Phi_{zz}(\mathbf{q}, t)$ is the temporal longitudinal spin correlator ($\Phi_{zz}(\mathbf{q}, t=0) \equiv \langle \delta S_{\mathbf{q}}^z \delta S_{-\mathbf{q}}^z \rangle$).

Equation (7) can be easily understood if we compare diagrams for the Diffuson and the Cooperon in Figure 1. The Diffuson does not have any mass because of Ward identity. In the case of the Cooperon, the Ward identity is broken: interaction line which dresses single particle propagator is given by static correlator, and interaction line which connects two different propagators in a ladder is given by dynamic correlator. The difference $[f(0) - f(t)]$ shows how strongly the Ward identity is broken and, as we'll see below, determines the mass of the Cooperon. Solving equation (7) we get [21]

$$C(t) = C_{\text{el}}(t) \exp \left\{ \int_0^t [f(t') - f(0)] dt' \right\}, \quad (9)$$

where C_{el} is the Cooperon calculated ignoring the inelasticity of scattering.

Using the spin-wave picture described above, we obtain

$$\Phi_{zz}(\mathbf{q}, t) = \frac{1}{N} \sum_{\mathbf{Q}} n_{\mathbf{Q}} n_{\mathbf{Q}+\mathbf{q}} \exp[i(\omega_{\mathbf{Q}+\mathbf{q}} - \omega_{\mathbf{Q}})t]. \quad (10)$$

Performing integration in equation (9) we get

$$C(t) = C_{\text{el}}(t) \exp[-t^3/\tau_{\varphi}^3], \quad (11)$$

where

$$\frac{1}{\tau_{\varphi}^3} = \frac{\pi}{3N^2} I^2 \sum_{\mathbf{Q}\mathbf{q}} n_{\mathbf{Q}} n_{\mathbf{Q}+\mathbf{q}} \delta(E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) (\omega_{\mathbf{Q}+\mathbf{q}} - \omega_{\mathbf{Q}})^2. \quad (12)$$

Calculating the integrals in equation (12) we obtain

$$\frac{1}{\tau_{\varphi}} = \left(\frac{I^2 T^2 (\mathcal{W} - 1) m a^5 k_{\text{F}}^3}{18\pi} \right)^{1/3} \simeq \left(\frac{I^2 T^2 E_{\text{F}}^{3/2}}{W^{5/2}} \right)^{1/3} \quad (13)$$

where \mathcal{W} is the Watson integral. It is worth noting that dephasing time is defined by the second time derivative of $\Phi_{zz}(\mathbf{q}, t)$ at $t = 0$ which can be calculated *via* second moment of corresponding spectral density; the result turns out to be essentially the same as equation (12). So the spin-wave picture, being physical one, is not crucial for obtaining $1/\tau_{\varphi}$.

It should be noticed that the form of equation (11) for the Cooperon is quite general, provided the scatterers are in a ballistic motion, irrespective of whether they are point particles [21], phonons [8], or spin waves, like in our case.

The result for the dephasing time can be understood using simple qualitative arguments. If all the collisions lead to the same electron energy change δE , the dephasing time could be obtained using relation [18]

$$\tau_{\varphi} \delta E \sqrt{\frac{\tau_{\varphi}}{\tau_{\text{out}}}} \sim 2\pi, \quad (14)$$

where $\tau_{\varphi}/\tau_{\text{out}}$ is just the number of scattering acts during the time τ_{φ} (τ_{out} is the extinction time). So in this case

$$\frac{1}{\tau_{\varphi}^3} \sim \frac{(\delta E)^2}{\tau_{\text{out}}}. \quad (15)$$

If we rewrite the formula for the extinction time

$$\frac{1}{\tau_{\text{out}}} = \frac{2\pi}{N} I^2 \sum_{\mathbf{q}} \langle \delta S_{\mathbf{q}}^z \delta S_{-\mathbf{q}}^z \rangle \delta(E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) \quad (16)$$

in the form

$$\frac{1}{\tau_{\text{out}}} = \frac{2\pi}{N^2} I^2 \sum_{\mathbf{Q}\mathbf{q}} n_{\mathbf{Q}} n_{\mathbf{Q}+\mathbf{q}} \delta(E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) \quad (17)$$

and notice that $(\omega_{\mathbf{Q}+\mathbf{q}} - \omega_{\mathbf{Q}})$ is just the energy change of the electron when scattering on a spin wave, we immediately see that equation (12) is just equation (15) with the integration with respect to different collision induced energy changes built in.

4 Conductivity calculation

The time-reversal invariance in the system we are considering is broken for two reasons. First, because we are considering ferromagnetic system, it is naturally to expect that the magnetic field is present in the system. Even more important is that the dephasing itself breaks the time-reversal invariance. We have shown in the previous Section, that due to dephasing the diffusion pole of the particle-particle propagator disappears, although particle-hole propagator still has a diffusion pole, which is guaranteed by particle number conservation. Inserting equation (11) into the self-consistent equations proposed in reference [17], for the (particle-hole) diffusion coefficient D and the particle-particle diffusion coefficient \tilde{D} we obtain system

$$\frac{D_0}{D} = 1 + \frac{1}{\pi\nu} \int_0^{\infty} \sum_{\mathbf{k}} e^{-\tilde{D}(\mathbf{k} + \frac{2e}{c}\mathbf{A})^2 t - t^3/\tau_{\varphi}^3} dt \quad (18)$$

$$\frac{D_0}{\tilde{D}} = 1 + \frac{1}{\pi\nu} \int_0^{\infty} \sum_{\mathbf{k}} e^{-Dk^2 t} dt, \quad (19)$$

where ν is the density of states at the Fermi surface, D_0 is the diffusion coefficient calculated in Born approximation and the momentum cut-off $|\mathbf{k}| < 1/\ell$, where ℓ is the transport mean free path, is implied. The conductivity is connected to the diffusion coefficient in a usual way

$$\sigma = e^2 \nu D. \quad (20)$$

For simplicity, we will make an analysis of self-consistent equations only in the absence of magnetic field ($A = 0$). In our case ($\tau_{\varphi} \gg \tau$), like in the case of purely elastic scattering, the conductivity drastically differs in the regions $E > E_c$ and $E < E_c$, where the mobility edge E_c is obtained from the equation [16]

$$E_c \tau = \sqrt{3/4\pi}. \quad (21)$$

More exactly, we have essentially three regions:

1) metallic region ($E > E_c$) with fast diffusion

$$D \sim D_0, \quad (22)$$

where dephasing is irrelevant;

2) ‘‘dielectric region’’ ($E < E_c$) with slow diffusion

$$D \sim D_0 (k\ell)^2 (\tau/\tau_{\varphi}), \quad (23)$$

determined by the dephasing time;

3) critical region around E_c , ($|E/E_c - 1| \ll (\tau/\tau_{\varphi})^{1/3}$)

$$D \sim D_0 (\tau/\tau_{\varphi})^{1/3}. \quad (24)$$

When the ‘‘mobility edge’’ crosses the Fermi level E_{F} (it is achieved by tuning the temperature) the resistivity changes sharply, which looks like a metal-insulator transition.

If we want to take into account the magnetic field in equation (18), it must be noticed, that the vector potential \mathbf{A} does not commute with the momentum \mathbf{k} . So the equation takes the form

$$\frac{D_0}{D} = 1 + \frac{1}{2\pi\nu} \int_0^\infty \sum_{\varepsilon_\perp} e^{-\varepsilon_\perp t - t^3/\tau_\nu^3} dt \quad (25)$$

where

$$\varepsilon_\perp = \tilde{D} \left[k_H^2 + \frac{4}{l_H^2} \left(N + \frac{1}{2} \right) \right] \quad (26)$$

(l_H is the magnetic length).

5 Discussion

Let us return to equation (12). The electron energy change in a single scattering $\delta E \sim T_c \sqrt{E_F/W} \ll T$, though all the spin waves (with the energies up to $\sim \bar{S}^z T_c/S$) participate in the dephasing. This quasi-elasticity of scattering gives the opportunity to calculate the dephasing time the way we did. (The quasi-elasticity condition holds even better for Eq. (17); in this case only the spin waves with small wave vectors contribute.)

When analyzing explicitly the CMR effect, we should first and most take into account the influence of the magnetic field on the spin disorder. The static spin correlator (in ferromagnetic phase) becomes [15]

$$\langle \delta S_{\mathbf{q}}^z \delta S_{-\mathbf{q}}^z \rangle = \frac{T^2}{4\pi \bar{S}^z C^2 q a} \tan^{-1} \frac{q\xi}{2}, \quad (27)$$

where $\xi \sim a \sqrt{\bar{S}^z C/g\mu_B H}$ is the correlation length. Thus the long wave spin fluctuations are suppressed, which decreases scattering and hence reduce the mobility edge. This mechanism is appropriate for describing CMR effect in magnetic semiconductors [5], and can be applied to manganite pyrochlores (these results will be presented elsewhere).

Second, magnetic field shifts the mobility edge by cutting off the Cooperon (see Eq. (25)). It is appropriate here to explain, why dephasing, which also cuts off the Cooperon, influences the localization in a totally different way. Consider a case of no magnetic field and a simplified version of the self-consistent localization theory, when we ignore the difference between D and \tilde{D} , and also consider the dephasing mechanism which leads to $C(t) = C_{el}(t) \exp[-t/\tau_\varphi]$ time dependence². Then instead of equations (18) and (19) we have a single one

$$\frac{D_0}{D} = 1 + \frac{1}{\pi\nu} \sum_{\mathbf{k}} \frac{1}{Dk^2 + 1/\tau_\varphi}. \quad (28)$$

We see, that due to presence of k^{d-1} in the numerator in this equation, the pole of the Cooperon is of no special

² This happens when the scatterers are in a diffusive motion [21].

importance at $d = 3$. The dephasing leads to the delocalization not because it leads to the disappearance of the diffusion pole, but because there appears in the denominator the term, which does not depend on D .

Consider finally the paramagnetic (PM) phase. In the absence of self-consistent localization theory which takes into account the spin-flip processes, a very rough idea about the localization in the PM phase we can get from the Ioffe-Regel criterium for the position of the mobility edge $\tau E_F \approx 1$. Using the well-known expression for spin-disorder scattering rate at temperatures above, but not too close to, T_c we arrive to two opportunities. For the relatively high Fermi energy $E_F > E_0 \sim I^4 S^4/W^3$ the increase of the temperature above T_c leads to a reverse insulator-metal transition. In the opposite case the system remains in the dielectric phase.

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