Fluctuation mechanism of hopping conductivity in semimagnetic semiconductors

A. S. Ioselevich
L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR

(Submitted 29 December 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **43**, No. 3, 148–151 (10 February 1986)

The effect of bound magnetic polarons on the hopping conductivity is analyzed. Fluctuation jumps (without a phonon, caused by magnetization fluctuation which equalizes the energy levels of the free and occupied donors) are more likely to occur than phonon jumps (in which the phonon is absorbed at equilibrium magnetization). The activation energy depends nonmonotonically on the temperature and magnetic field and may even change sign.

In semimagnetic semiconductors, e.g., in a solid solution $Hg_{1-x}Mn_xTe$ or $Cd_{1-x}Mn_xTe$ (see the reviews by Brandt and Moshchalkov[1] and Lyapilin and Tsidil'kovskiĭ[2]) an electron bound on a donor (or a hole bound on an acceptor) polarizes the Mn spins at a distance of $\sim a$ (Bohr radius), forming a bound magnetic polaron (magnetic polarons are discussed in Refs. 3–5).

 0021-3640/86/030188-05$01.00

The magnetic contribution to the binding energy of an electron is usually relatively small, but it may be considerably larger than the temperature T. In this letter we consider such a situation.

The distinguishing features of a bound magnetic polaron is a semimagnetic semiconductor are (1) its ability to ignore (at $x \gtrsim 0.1$ and $T \gtrsim 1$ K) the direct interaction between the Mn spins and (2) a large number of Mn atoms which effectively interact with electrons ($Na^3 \sim 10^1$–10^2 for $x \sim 0.1$, where N is the Mn concentration).

The effect of a bound magnetic polaron on the hopping conductivity of a magnetic semiconductor was studied by Kasuya and Yanase[5] (see also Refs. 6 and 7). In hopping from one site, around which it manages to polarize the spins (and hence lower its energy by the amount E), to another site where the spins are not polarized, the electron absorbs a phonon with an energy E. In the case of a mechanism of this sort, the magnetic contribution ϵ_3 to the activation energy of the hopping conductivity is E. We will show that there is another mechanism which accounts for a considerably smaller ϵ_3 and we will analyze this mechanism in application to semimagnetic semiconductors.

Let us consider two donors, one of which (i) has an electron and the other (j) does not. The distance between them is $r_{ij} \gg a$. Near each donor there are Mn atoms with a spin $s = 5/2$. For brevity, we call them i spins and j spins, respectively. The entire system, which is placed in a magnetic field H (directed along the z axis), interacts with the heat sink (phonons). The large parameter $Na^3 \gg 1$ allows only the z components of the spins to be taken into account and allows the continuous variables to be introduced: the local spin density $N(\mathbf{r})$ and the local projection $m(\mathbf{r}) = \langle s^z \rangle / s$. The electron energy shift in the i donor in the first order in the exchange interaction can then be written

$$E_i\{m_i\} = \epsilon_i - \int d\mathbf{r} N_i(\mathbf{r}) J(\mathbf{r}) m_i(\mathbf{r}), \qquad (1)$$

and the free energy of the system is $F_i^{(1)}\{m_i\} + F_j^{(0)}\{m_j\}$, where $F_i^{(1)} = F_i^{(0)} + E_i$, and

$$F_i^{(0)} = \int d\mathbf{r} N_i(\mathbf{r}) \{ -J_H m_i(\mathbf{r}) - TS(m_i(\mathbf{r})) - F_0 \} . \qquad (2)$$

Here ϵ_i is a random shift of the level of a nonmagnetic nature, $J(\mathbf{r}) = (s/2) J |\psi(\mathbf{r})|^2$, J is the exchange interaction constant, ψ is the unperturbed wave function of an electron, $J_H = s\mu_0 g H$, $S(m)$ is the local entropy (per spin), and F_0 is chosen in such a way that $\overline{F}_i^{(0)} \equiv 0$. The superscript (1) means that the given donor is occupied and the superscript (0) means that it is not occupied. The superior bar denotes equilibrium value.

Because of the interaction with the heat sink, the spin system is characterized by a finite longitudinal relaxation time, τ_{sl}. We assume $\tau_{sl} \ll \tau_{\text{hop}}$—the lifetime of the electron on the donor. The i spins will then have time to reach an equilibrium corresponding to $\overline{F}_i^{(1)}$ and the j spins will have time to reach an equilibrium corresponding to $\overline{F}_j^{(0)}$ ($\equiv 0$). The equilibrium $\overline{m}_{i,j}(\mathbf{r})$ can be expressed in terms of the Brillouin function B_s

$$\overline{m}_i(\mathbf{r}) = \overline{m}^{(1)} = B_s[(J_H + J(\mathbf{r}))/T], \quad \overline{m}_j(\mathbf{r}) = \overline{m}^{(0)} = B_s(J_H/T) \qquad (3)$$

$E_i^{(1)}$ and $E_j^{(0)}$ are found by substituting (3) into (1), and the free equilibrium energy is

$$\overline{F}_i^{(1)} = \epsilon_i - T\int d\mathbf{r} N_i(\mathbf{r}) \ln \left\{ \frac{\mathrm{sh}\left(\frac{2s+1}{2s}\frac{J_H+J(\mathbf{r})}{T}\right)\mathrm{sh}\left(\frac{1}{2s}\frac{J_H}{T}\right)}{\mathrm{sh}\left(\frac{1}{2s}\frac{J_H+J(\mathbf{r})}{T}\right)\mathrm{sh}\left(\frac{2s+1}{2s}\frac{J_H}{T}\right)} \right\} . \tag{4}$$

If the electron executes a jump $i \to j$ when the i and j spins are in an equilibrium configuration, it will absorb (emit) a phonon with an energy $\overline{\Delta}_{ij} = \overline{E}_j^{(0)} - \overline{E}_i^{(1)}$. If $\overline{\Delta}_{ij} > 0$, the probability for such a process (we call it a phonon jump) is $\overline{P}_{ij} \propto \exp(-\overline{\Delta}_{ij}/T)$. However, $m_i(\mathbf{r})$ and $m_j(\mathbf{r})$ may fluctuate and $E_i\{m_i\} - E_j\{m_j\}$ may decrease. The jump frequency is proportional to the product of the fluctuation probability and the probability for the absorption (emission) of a phonon, so that within exponential error $P_{ij} \propto \exp(-\Delta_{ij}/T)$, where

$$\Delta_{ij} = \min_{m_i, m_j} \{F_i^{(1)}\{m_i\} + F_j^{(0)}\{m_j\} + \|E_j\{m_j\} - E_i\{m_i\}\|\} - \overline{F}_i^{(1)} , \tag{5}$$

where $\|x\| = x$ for $x > 0$ and $\|x\| = 0$ for $x < 0$. Minimization leads to the following physical picture. 1) If $\overline{E}_i^{(1)} > \overline{E}_j^{(0)}$, we have a phonon jump [in which a phonon is emitted; Fig. 1(a)]. This is a nonactivating process: $\Delta_{ij} = 0$. 2) if $\overline{E}_i^{(1)} < \overline{E}_j^{(0)}$ but $\overline{E}_i^{(0)} > E_j^{(1)}$, this process will occur with fluctuations and without a phonon. The maximum fluctuation corresponds to $E_i\{m_i\} = E_j\{m_j\}$, and the electron undergoes a resonant tunneling [Fig. 1(b)]. We call these jumps fluctuation jumps. 3) If $\overline{E}_i^{(0)} < \overline{E}_j^{(1)}$, we will have a mixed fluctuation-phonon jump [Fig. 1(c)]. In this case we have $\Delta_{ij} = \overline{F}_j^{(1)} - \overline{F}_i^{(1)}$.

Cases 1) and 3) are characteristic for a situation in which E_i is determined primarily by the nonmagnetic component ϵ_i. Let us consider the opposite situation, a more interesting one, in which the magnetic-polaron shift is greater than the spread of levels, W:

$$|\overline{E}_i^{(1)} - \overline{E}_i^{(0)}| \gg |\overline{E}_i^{(1)} - \overline{E}_j^{(1)}| \sim W. \tag{6}$$

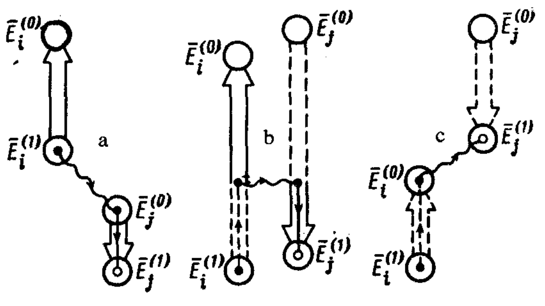

FIG. 1. Energy scheme of the $i \to j$ transition. Dashed line—Fluctuation; solid line—relaxation; wavy line—electron tunneling with absorption (emission) of a phonon or without it.

Fluctuation jumps are typical in this case, and in a homogeneous approximation (i.e., one in which we set $N_i(\mathbf{r}) = N_j(\mathbf{r}) = N$ and $\epsilon_i = \epsilon_j = 0$ and omit the subscripts i and j) we can easily derive the following expression from (5):

$$\Delta = 2\overline{F}^{(1/2)} - \overline{F}^{(1)}, \tag{7}$$

where $\overline{F}^{(1/2)}$ differs from $\overline{F}^{(1)}$ because of the substitution $J(\mathbf{r}) \to \frac{1}{2}J(\mathbf{r})$.

We assume that there is no external field ($J_H = 0$). At a high temperature ($\widetilde{J} = J/a^3 \ll T$) we then find from (7) an unusual temperature dependence for the hopping resistivity ρ:

$$\rho \propto \exp\left\{\frac{s+1}{12s} C(Na^3)(\widetilde{J}/T)^2\right\}, \tag{8}$$

where C depends on ψ. The activation energy is only one-fourth of the activation energy of phonon hops: $\Delta = -\overline{F}^{(1)}/2 = -\overline{E}^{(1)}/4 = \overline{\Delta}/4$. This ratio also holds for a strong lattice polaron effect (see Ref. 6), although the susceptibility $\chi \propto T^{-1}$ in the magnetic case, so that the temperature dependence is different from that in the lattice effect.

At a low temperature ($T \ll \widetilde{J}$) we have $\Delta/T = \ln(2s+1)N\widetilde{a}^3$, where $\widetilde{a} \gtrsim a$ is the size of the region in which the spins are polarized. The quantity Δ/T is essentially independent of T for obvious reasons: At $T \ll \widetilde{J}$ all i spins are compressed by a strong exchange field and cannot fluctuate. In contrast, the j spins, unaffected by the field, fluctuate freely, so that at $T \ll \widetilde{J}$ all the fluctuation is concentrated on the j spins and its probability is determined by the entropy and does not depend on T. For phonon jumps we have $\overline{\Delta}/T = Na^3\widetilde{J}/T \gg \Delta/T$. The T independence of Δ/T is valid only in a homogeneous approximation. The random inhomogeneity of $\overline{F}_i^{(1)}$ must be taken into account in order to obtain the correct temperature dependence of ρ at $T \ll \widetilde{J}$. Assuming, in accordance with (6), that $|\overline{F}_i^{(1)} - \overline{F}_j^{(1)}| \ll |\overline{F}^{(1)}|$ and carrying out standard calculations (see Ref. 8), at $T \ll \widetilde{J}$ we find

$$\rho \propto \exp\{\ln(2s+1)N\widetilde{a}^3 + \xi W/T\}, \tag{9}$$

where $\xi \sim 1$ depends on the degree of cancellation. The quantity W consists of two components: a magnetic component (W_m), which is associated with the fluctuations of the number of spins along the Bohr radius, and a nonmagnetic component ($W_0 \sim |\epsilon_i|$), which is associated with the fluctuations of the composition and random fields of the charged impurities. For $Na^3 \gg 1$ the magnetic fluctuations are Gaussian, so that $W_m \sim (Na^3)^{-1/2}|\overline{F}^{(1)}| \sim (Na^3)^{1/2}\widetilde{J}$. If $W_m \gg W_0$, then $W = W_m$ and ξ can be calculated explicitly.

Let us consider the magnetoresistance. It is clear that at $J_H \gg T$ both the i spins and the j spins are equally ordered and the magnetic polaron effect is suppressed. In this case $\rho \propto \exp(\xi W/T)$, irrespective of the relationship between $\widetilde{J}$ and T. In the case of weak fields ($J_H \ll T$), there are two possibilities: If J_H and $\widetilde{J} \ll T$, the effect of the field is slight, and the J_H-dependent correction to Δ/T is on the order of $Na^3 J_H \widetilde{J}^3/T^4$. If, on the other hand, $J_H \ll T \ll \widetilde{J}$, the activation energy

$$\epsilon_3 = \xi W - N\widetilde{a}^3 J_H$$

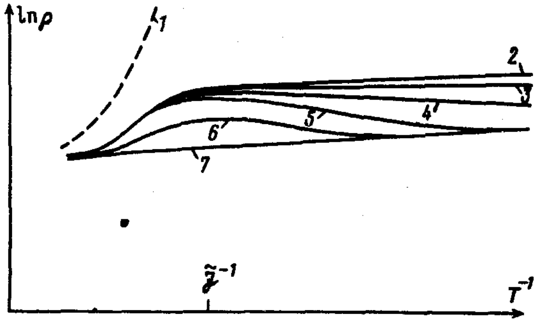

FIG. 2. Temperature dependence of the resistivity in the hopping region. 1—Phonon jumps ($J_H = 0$); fluctuation jumps: 2—$J_H = 0$; 3, 4, 5,—$J_H \ll \tilde{J}$; 6—$J_H \sim \tilde{J}$; 7—$J_H \gg \tilde{J}$.

will decrease markedly with increasing field (Fig. 2) and may even become negative if $W/N\tilde{a}^3 < J_H$. If $W_M > W_0$, this situation will occur when $\tilde{J}(Na^3)^{-1/2} < J_H < T < \tilde{J}$. The magnetoresistance found by us is negative, while the typical positive contribution is ignored (see Ref. 8). This contribution, however, does not depend on T, i.e., it does not change the activation energy.

The hopping conductivity in semimagnetic semiconductors was observed in Refs. 7, 9, and 10. It was found that the behavior of $\epsilon_3(T)$ is nonmonotonic[9] and that the negative magnetoresistance depends on T. In a separate paper we will carry out a detailed comparison with experiment and determine the origin of the maximum of the magnetoresistance[7,10] in small fields.

I wish to thank S. I. Gubarev and M. É. Raĭkh for a discussion of the physics of semimagnetic semiconductors.

[1]N. B. Brandt and V. V. Moshchalkov, Adv. Phys. **33**, 193 (1984).
[2]I. I. Lyapilin and I. M. Tsidil'kovskiĭ, Usp. Fiz. Nauk **146**, 35 (1985) [Sov. Phys. Uspekhi **28**, 349 (1985)].
[3]M. A. Krivoglaz, Usp. Fiz. Nauk **111**, 617 (1973).
[4]É. L. Nagaev, Fizika magnitnykh poluprovodnikov (The Physics of Magnetic Semiconductors), Nauka, Moscow, 1979.
[5]T. Kasuya and A. Yanase, Rev. Mod. Phys. **40**, 684 (1968).
[6]N. F. Mott and E. A. Davis, Electronic Processes in Non-Crystalline Materials, Clarendon Press, Oxford (1971) (Russ. transl. Mir, Moscow, 1982).
[7]T. Dietl, J. Antoszewski, and L. Swierkowski, Physica B + C **117–118**, 491 (1983).
[8]B. I. Shkolovskiĭ and A. L. Éfros, Elektronnye svoĭstva legirovannykh poluprovodnikov (Electronic Properties of Doped Semiconductors), Nauka, Moscow, 1979, Secs. 15, 24, 25, and 28.
[9]A. Mycielski and J. Mycielski, J. Phys. Soc. Jpn., Suppl. **A49**, 807 (1980).
[10]J. R. Anderson, W. B. Johnson, and D. R. Stone, J. Vac. Sci. and Techn. **A1**, 1761 (1983).

Translated by S. J. Amoretty