Interference mechanism of magnetoresistance in variable range hopping: the effect of paramagnetic electron spins.

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Abstract.
The work is aimed to modify the conventional approach to interference magnetoresistance for the situation when there is an admixture of free spins. We considered the system with arbitrary probability \( P_{\text{free}} \) of electron spin to be free. We studied analytically and numerically both negative interference magnetoresistance and positive magnetoresistance due to spin ordering in magnetic field. We obtained the expression for magnetoresistance for two limiting cases corresponding to small and large number of scatterers in the hopping act. For both cases we obtained the explicit expressions for the dependence of the magnetoresistance on temperature and \( P_{\text{free}} \). Our results are in semiquantitative agreement with experiment.

1. Introduction
At low temperature the conductivity in semiconductors with compensation is supported by hopping of the carriers between the localized states on the impurities. With low enough temperature the characteristic act of hopping occurs not between the neighboring impurities but between the closest impurities lying in the thin energy strip around the Fermi level. This phenomena is known as variable range hopping conductivity [1].

It is known that at weak magnetic fields \( (H \leq 1 \, \text{T}) \) the semiconductors in variable range hopping regime display negative magnetoresistance that appears to be linear in the magnetic field. This phenomena was first understood by Nguyen, Shklovskii and Spivak [2] (for detailed review see [3]). It is related to the interference. During the hop electron scatters on the impurities that are outside of the conduction strip. So the resulting hopping amplitude is the sum of different tunneling paths, which interfere among themselves. The nature of hopping conductivity is such that destructive interference is strongly emphasized and thus the interference contribution leads to a decrease of the conductivity. The magnetic field suppresses the interference and leads to the negative magnetoresistance.

The theory of interference magnetoresistance [3] was based on the model of spinless electrons. This model can be justified when all electron spins are frozen, for example, by the exchange interaction. In [3] it was stated that there is no interference effect on the magnetoresistance when all electron spins are free. However this statement lacks the solid theoretical proof. Also there were no discussion of the system in which some spins are frozen and some are free. So
there remains a question "how many free spins one should have to suppress the interference magnetoresistance".

Then in [4] it was also argued that the admixture of free spins leads to additional positive magnetoresistance due to spin ordering in the magnetic field. However no detailed consideration of this mechanism of magnetoresistance was made. For example, its detailed temperature dependence remains unknown.

There are two different limits for the theory of interference magnetoresistance. In [2, 3] the system with large number of scatterers in the hopping act was considered. In our work we call such a situation "the case of long hops". For this model only qualitative results were obtained in [2, 3]. Later it was shown in [5, 6] that in many occasions the characteristic number of scatterers is small. Most hopping acts occur without scattering, and to consider interference magnetoresistance one can take into account only hopping acts with a single scatterer. We will call this situation "the case of short hops". For short hops and spinless electron problem [5, 6] gives quantitative results for magnetoresistance.

There were several attempts [7, 8, 9] to make a quantitative theory for long hops. However, to our opinion, all these works do not pay sufficient attention to the dispersion of scatter energies. We will discuss this detail later. We also note that the existing theory of interference contribution to magnetoresistance is not sufficient to describe existing experimental data. For example there were observations of the suppression of negative magnetoresistance [10, 11] at low temperature that can not be described with conventional theory.

The goal of the present study is to develop a theory of interference contribution to magnetoresistance that explicitly takes into account the admixture of free spins. We consider two general problems. The first is to what extent the interference magnetoresistance is suppressed when some spins are free. The second is to study the spin ordering magnetoresistance.

The important feature for our consideration is the spin structure of frozen spins in impurity band. We assume that frozen spins form the so called Bhatt-Lee phase [12].

The common way to treat hopping conductivity is to introduce the Miller and Abrahams network of effective resistors. Within the framework of such an approach one calculates the mean hopping rate between the pairs of hopping impurities \( \Gamma_{ij} \). The effective conductance between this impurities is \( R_{ij} = T/e^2 \Gamma_{ij} \propto \exp(\xi_{ij}) \). Here \( \xi_{ij} \) is the logarithm of resistance. Then with percolation theory one can estimate the critical (percolation) value \( \xi_c \). The resistivity of the whole system is then proportional to \( \propto \exp(\xi_c) \). The magnetoresistance can be calculated as (see [3])

\[
\ln \left( \frac{R(H)}{R(0)} \right) = -\left\langle \ln \frac{\Gamma_{ij}(H)}{\Gamma_{ij}(0)} \right\rangle. \tag{1}
\]

Here \( H \) is the magnetic field. The averaging is taken over pairs of impurities that correspond to critical resistors (i.e. with \( \xi_{ij} = \xi_c \)).

2. Short hops

Let us first discuss the situation when the characteristic number of scatterers in a hopping act is small. The interference magnetoresistance in this case is controlled by the hopping resistors with one intermediate impurity. As it was shown in [6], this situation (of "short hops") corresponds to many typical experimental realizations. The opposite situation is the case of "long hops" when the characteristic hopping resistor contains many scattering impurities.

In the case of short hops each resistor of interest has either a scatterer with an electron with frozen spin, a free scatterer without an electron or a scatterer with a free electron spin. The contributions of these resistors are additive (1). The first two types of resistors can be described with the spinless electron theory. For short hops this theory is a rigorous one (see [5, 6]). Its
has a following result
\[ \ln \frac{R(H)}{R(0)} \propto -r_h^{2+d/2} H, \] (2)
where \( r_h \) is the mean hopping distance and \( d \) is the system dimensionality. The dependence on \( r_h \) controls the temperature dependence of magnetoresistance as \( r_h \propto T^{-1/(d+1)} \) for the Mott conductivity and \( r_h \propto T^{-1/2} \) for Efros-Shklovskii conductivity over Coulomb gap states.

So we have to estimate only the contribution of the hopping resistors with free electron spins. For this resistors it is important to note that \( \Gamma_{ij} \) corresponds to time average of the hopping acts. To calculate it one should take into account that sometimes the tunneling electron has the same direction as the spin on the scatterer and sometimes their directions are opposite. There are always two tunneling paths in this system: one that includes the scatterer and one that does not contain it. If the spins of the sites involved have the same direction, the corresponding paths interfere, otherwise they do not interfere. So we can write the following expression for \( \Gamma_{ij} \) for free intermediate spin
\[ \Gamma_{ij} \propto P_{\uparrow\uparrow} |J_1 + J_2 e^{i\phi}|^2 + (1 - P_{\uparrow\uparrow}) \left( |J_1|^2 + |J_2|^2 \right). \] (3)
Here \( P_{\uparrow\uparrow} \) is the probability for the two spins to have the same direction. It depends on the magnetic field as the magnetic field aligns free spins. \( J_1 \) and \( J_2 \) are, correspondingly, the amplitudes of tunneling path that does not contain the intermediate impurity and the one that includes it. \( \varphi = H S / \Phi_0 \) is the phase difference between this paths. \( S \) is the area between the paths and \( \Phi_0 \) is the magnetic flux quantum.

To get the expression for magnetoresistance one should substitute (3) into (1) and perform the averaging. The resulting magnetoresistance is quadratic on \( H \). There are many magnetoresistance mechanisms that give the quadratic field dependence (not necessary related to interference) so we keep only one term in this magnetoresistance that has unusually strong temperature dependence and thus can be discriminated from other mechanisms (for example from wavefunction shrinkage magnetoresistance). It is the spin ordering term
\[ \propto P_{\text{free}} n r_h (r_h a)^{(d-1)/2} \left( \frac{\mu_B g H}{T} \right)^2. \] (4)
Here \( n \) is the impurity concentration. \( P_{\text{free}} \) is the relative part of the scattering impurities that has an electron with free spin. For three-dimension system with Mott conductivity this term depends on temperature as \( \propto T^{-5/2} \). To compare the temperature dependence of wavefunction shrinkage magnetoresistance it is \( \propto T^{-3/4} \).

To summarize the results of this section let us combine the different contributions to magnetoresistance:
\[ \ln \frac{R(H)}{R(0)} \propto -C_1 (1 - P_{\text{free}}) r_h^{2+d/2} H + C_2 P_{\text{free}} n r_h (r_h a)^{(d-1)/2} \left( \frac{\mu_B g H}{T} \right)^2, \] (5)
where \( C_1 \) and \( C_2 \) are constants independent on temperature and magnetic field.

3. Long hops.
Let us now discuss the case of long hops. In this case there is an exponentially large number of tunneling paths (even without backscattering), \( 2^N \), where \( N \) is the number of scatterers.

There where previous studies of interference magnetoresistance in the long hops case at least for spinless electrons (see e.g. \[7, 8, 9\]). However to our opinion these studies underestimate the dispersion of the tunneling path amplitudes \( J_i \). Some of the works adopt the model when
there is no dispersion of $|J_i|$ (the tunneling path amplitudes differs only with sign). Some adopts the model when the distribution of $J_i$ is the one with zero mean value and the dispersion of normalized tunneling amplitudes of the order of unity.

However we argue that the tunneling path amplitudes actually has an exponentially broad log-normal distribution. The amplitude of some tunneling path $i$ can be expressed as

$$J_i = I_{0,k_1} \prod_{k(i)}^ {N_i+1} \frac{I_{k-1,k}}{E_k}.$$ \hspace{1cm} (6)

Here the index $k(i)$ enumerates the scattering impurities that participate in the tunneling path $i$. $N_i$ is a number of this impurities. Usually $N_i \sim N/2$, where $N$ is the total number of scatterers in the resistor.

So the path amplitude is the product of a large number of random terms. Due to the central limit theorem it is distributed with a log-normal law with dispersion that increases exponentially with $N$. Actually it is an exponentially broad distribution. This fact can be also confirmed with computations (see fig. 1 (a)).

One of the properties of the log-normal distribution is the fact that the mean value is exponentially larger then the value corresponding to the maximum of distribution density. So the sum of a large number of these paths (for example the net tunneling amplitude that controls $\Gamma_{ij}$) is controlled by a small number of the summands. We call the paths corresponding to these summands as "significant paths". On fig. 1 we show that the relative number of this paths is exponentially small.

Figure 1. (a) — distribution of absolute values of tunneling path amplitudes $J_i$. Points are computed values, line is the approximation with log-normal law. (b) — the relative part of significant path versus scatterers number.

To understand the interference effects in the case of long hops one should understand the nature of the significant paths. The numerical computations show that these paths are similar to each other in some way. This fact is related to the dispersion of spatial locations and of energies of the scatterers. One can see from (6) that the inclusion of some scatterer $j$ into the tunneling path is equivalent to the multiplication of path amplitude by the factor

$$\mu_j = \frac{I_{j-j}I_{j,j+}}{I_{j-j}+E_j}.$$ \hspace{1cm} (7)

Here $j-$ is the previous (to $j-th$) scatterer included into the path under consideration. $j+$ is the closest scatterer after $j-th$ included into the path. $I_{ij}$ is the energy overlap integral. $E_j$ is the energy of scatterer $j$ measured from the Fermi level.

Strictly speaking $\mu_j$ depends not only on the characteristics of scatterer $j$ but also on the rest of the tunneling path. However basing on the typical values of energy and position of the scatterer one can estimate $\mu_j$ for a characteristic path. Let the overlap integrals have the form
\[ I_{ij} = I_0 \exp(-r_{ij}/a). \] Also we assume that all considered scattering impurities lie in a thin strip around direct tunneling line. Then \( \mu_j \) for the characteristic path can be estimated as

\[
\mu_j = \exp \left( -\frac{\rho_j^2}{a r_{nn}} \right) I_0 E_j. \tag{8}
\]

Here \( \rho_j \) is the distance of scatterer \( j \) from the tunneling line. \( r_{nn} \) is the typical distance between impurities included into the tunneling path.

With above arguments all scatterers can be separated into three groups. First there are scatterers with \( |\mu_j| \ll 1 \). These scatterers are not included into the significant paths (at least into most of them) as inclusion of this impurities make tunneling path amplitude smaller. All impurities that are far from tunneling line fall into this group. In our work we call this impurities irrelevant. They can easily be excluded from consideration. Then there are impurities with \( \mu_j \gg 1 \). Such impurities are included into most significant paths because they significantly increase the path amplitude. We call these impurities the backbone ones. Finally there are impurities with \( \mu_j \sim 1 \) that do not fall into the previous groups. We call them the interference impurities.

We made numerical computations to find whether the backbone impurities really exist in the system. We considered the distribution density of impurity energy to be constant within the interval \(-I_0 < E_j < I_0\). The computations show that the backbone impurities exist in the system. Their number is comparable to the number of interference scatterers and their ratio seems to be independent on hopping distance and impurity concentration.

To go further we adopt the simple model that is valid when any two interference scatterers are separated from each other by at least one backbone impurity. In this case one can express the typical significant path amplitude as a product of factors corresponding to different scatterers. With this expansion one can get the following expression for magnetoresistance in the long hop limit

\[
\ln \frac{R(H)}{R(0)} \propto (n r_h \rho_{\text{max}}^{d-1}) \left( C_1 (1 - P_{\text{free}}) r_b^{2+d/2} H + C_2 P_{\text{free}} n r_b (\mu_j g H T)^{1/2} \frac{1}{T} \right)^2. \tag{9}
\]

Here \( \rho_{\text{max}} \sim (a/n)^{1/d+1} \) is the width of the area where one can find backbone or interference scatterer, \( r_b \sim (1/a + d/n)^{2+d/d+1} \) is the characteristic distance between neighbor backbone impurities. The expression in the first brackets is the characteristic number of scatterers in the hopping act; the expression in the second ones is equal to magnetoresistance in the case of short hops when the real hopping length \( r_h \) is substituted by the distance between backbone impurities \( r_b \).

There is a negative magnetoresistance that is linear on \( H \), \( r_h \) and \((1 - P_{\text{free}})\). And also there is a positive quadratic magnetoresistance due to the alignment of the spins that has strong temperature dependence. On fig. 2 we compare these results with our computations (that include all intermediate impurities and tunneling paths). One can see that analytic results are in good agreement with computations.

4. Discussion

Let us compare our results with experimental data observed in [10, 11]. This experiments show the unusual magnetoresistance dependence on temperature, namely, the suppression of negative magnetoresistance at low temperatures. The spin mechanisms of magnetoresistance was suggested to understand this phenomena in [11], however no detailed theory of this mechanisms was given.

On figure 3 we compared the experimental data with theoretical result (9). One can see that there is a good semiquantitative agreement with experiment.
To conclude, we generalize the theory of interference effects on the magnetoresistance in hopping conductivity to include the contribution of scatterers with free electron spins. We considered both the cases of short hops and long hops. For the case of long hops we developed a new approach to the problem of interference magnetoresistance that relies upon the dispersion of scatterer energies $E_j$. Our theory is in semiquantitative agreement with experimental data on magnetoresistance in GaAs – AlGaAs 2D structures.

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