MAGNETORESISTANCE IN ANDERSON-LOCALIZED REGIME*

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Magnetoresistance in the Anderson-localized regime is calculated by the percolation method, with a particular purpose of investigating the effects of electron-electron interaction on it. It is predicted that the interplay of the intrastate interaction and the energy dependence of localization lengths gives rise to the competition of positive and negative contributions in the field dependence of the magnetoresistance. Further, combined with the interstate interactions, the temperature change in the magnetoresistance of 1T-TaS_2 and its alloy systems is explained satisfactorily. Finally the correlation of the interaction effects on the variable range hopping in the absence and presence of a magnetic field is clarified.

1 Introduction

Electron-electron interaction effects on hopping conduction in localized regime have been studied for many years. Many authors have studied the effect of direct Coulomb interaction between localized states [1,2]. Yamaguchi, Aoki and Kamimura [3], however, have pointed out that the intrastate interaction within an Anderson localized state is the most important interaction in strongly localized regime. Thus the model Hamiltonian in the first approximation can be written as

$$H = \sum_{\alpha\sigma} \varepsilon_{\alpha\sigma} n_{\alpha\sigma} + (1/2) \sum_{\alpha\sigma} U_\alpha n_{\alpha\sigma} n_{\alpha-\sigma} , \tag{1}$$

where we adopt the transfer diagonal representation in which transfer terms between impurity sites are diagonalized, and $\varepsilon_{\alpha\sigma}$, U_α and $n_{\alpha\sigma}$ represent one-electron energy, the intrastate interaction energy and a number operater of state α with spin σ ,respectively. We presuppose that states α are localized in the Anderson sense, and further assume a constant value for U_α and a uniform distribution of $\varepsilon_{\alpha\sigma}$ with a density of states ν .

Based on the Hamiltonian (1), Kurobe and Kamimura [4] recently developed the theory of variable range hopping in the presence of the intrastate interaction. In the present paper, we will derive the d.c. conductivity in the presence of a magnetic field for the variable range hopping regime by the method of percolation and clarify an effect of the intrastate interaction on magnetoresistance. Further, we attempt to include some of the interstate interaction effects.

2 Variable Range Hopping Conduction in the presence of Intrastate Interaction

In this section we calculate the resistivity due to one-electron hop assisted by one-phonon, paying special attention to effects of intrastate interaction.

In the presence of the intrastate interaction there exist three electronic states for each Anderson localized state, i.e. unoccupied (UO) state, singly occupied (SO) state and doubly occupied (DO) state. SO states are found just below the Fermi level down to the intrastate interaction energy and carry free spins, whereas DO states are to be found deeper in energy and are spin singlets. Accordingly, there exist the following four different kinds of hopping processes as is shown in Fig.1:

(1) hopping processes from an SO to a UO state, (2) those from an SO state to an SO state,
(3) those from a DO state to a UO state, and (4) those from a DO state to an SO state.

Total hopping rate from a localization center of α state to that of β state $\tilde{\Gamma}_{\alpha\beta}$ is the sum of the hopping rates of the four processes. Assuming that each state is statistically independent of each other, each hopping rate $\Gamma_{\alpha\beta}^{(\ell)}$ (ℓ=1 to 4) is the product of the electron occupation probability and an intrinsic hopping rate $\gamma_{\alpha\beta}^{(\ell)}$. We assume the intrinsic hopping rate similar to those given by Miller and Abrahams [5].

$$\begin{aligned} \gamma_{\alpha\beta}^{(\ell)} &\propto \exp[-2R_{\alpha\beta}/\xi^{(\ell)} - \Delta\varepsilon^{(\ell)}/k_B T], \quad (\Delta\varepsilon^{(\ell)}>0), \\ &\propto \exp[-2R_{\alpha\beta}/\xi^{(\ell)}], \quad (\Delta\varepsilon^{(\ell)}<0). \end{aligned} \tag{2}$$

In the presence of the intrastate interaction, however, the localization length of DO state $\xi_2(\varepsilon)$ is different from that of SO states $\xi_1(\varepsilon)$ [6]. Therefore we take the larger of the two in the hopping processes ℓ=2 and 3 in which cases the localization length is different before and after the hopping [7].

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The percolation calculation [8] in the presence of the intrastate correlation gives the following result for the temperature dependence of resistivity [4].

$$\rho \propto \exp(T_0/T)^{1/4} \tag{3}$$

where

$$T_0 = \frac{13.6}{k_B \nu} \frac{\xi_1^3+3\xi_2^3}{(\xi_1^3+\xi_2^3)^2+4\xi_2^6}, \tag{4}$$

and ν is the density of states at the Fermi level. The energy dependence of the localization lengths ξ_1 and ξ_2 is neglected here, and ξ_2 is taken to be larger than ξ_1. This result shows that the Mott's quarter law still holds even in the presence of the intrastate correlation, but with prefactor T_0 which now depends on the two types of the localization lengths ξ_1 and ξ_2, brought about by the intrastate interaction.

3 Magnetoresistance

Although the intrastate interaction does not change the temperature dependence of the resistivity, the electron-electron interactions in the Anderson localized states play an essential role in the magnetoresistance. In 3-1 it is shown that the intrastate interaction gives positive contribution to magnetoresistance, when one takes into account the change of the electron occupation probability due to a magnetic field. Negative contribution to magnetoresistance is due to the energy dependence of the localization lengths [9] and this is discussed in the latter subsection.

3-1 Positive Contribution

When a magnetic field is applied, the spins of SO states become parallel to the field. Therefore, the probability of finding a pair of SO states with antiparallel spins becomes smaller with increasing a magnetic field, and the hopping processes from SO to SO states become suppressed because a state cannot accomodate two electrons of the same spin. The processes from DO to UO states also become suppressed because they are connected to the SO to SO processes by the detailed balance. On the other hand, the remaining two types of processes are scarecely affected by a magnetic field. Consequently, the magnetoresistance is positive and saturates above a certain magnetic field where only the two types of proceses contribute to the variable range hopping conduction. We can calculate the magnetoresistance in the percolation method described in ref.[4], and the results in three dimensional case are shown in Fig.2 for various temperatures with parameter values shown in the figure. Here, the localization lengths are assumed constant.

The saturation value of the positive magnetoresistance can be obtained from the ratio of the resistivity due only to processes (1) and (4) in Fig.1 to that due to all the four processes:

$$\frac{\Delta\rho(H)}{\rho(0)} = \exp\left[\left(\frac{13.6}{\nu k_B T}\right)^{1/4}\left\{\left(\frac{\xi_1^3+\xi_2^3}{\xi_1^6+\xi_2^6}\right)^{1/4} - \left(\frac{\xi_1^3+3\xi_2^3}{(\xi_1^3+\xi_2^3)^2+4\xi_2^6}\right)^{1/4}\right\}\right] - 1. \tag{5}$$

From the saturation value (5), it is concluded that the positive contribution becomes larger as the temperature, the density of states or the localization lengths decreases. This is also true for T_0 in eq.(4) which characterizes the variable range hopping without a magnetic field. Therefore, we can infer that a material which shows a large T_0 should show a large positive magnetoresistance.

3-2 Negative Contribution

In the SO to UO processes, the state energy of both the initial and final states lie in the vicinity of the Fermi level (Fig.1). In a magnetic field, the spins of SO states become parallel to the field, and the one-electron energy for a parallel spin ε becomes $\varepsilon = \varepsilon_\alpha - \mu_B H$, so that the corresponding ε_α at E_F is raised to $\varepsilon_\alpha = E_F + \mu_B H$. As the localization length increases with ε_α, the hopping rate increases with a magnetic field, and the magnetoresistance becomes negative. This change of the envelope function for up and down spins can be included in the percolation calculation. Combining these two effects, the magnetoresistance can be written conventionally in the following form:

$$\Delta\rho(H)/\rho(0) = N(H) + P(H) \tag{6}$$

where N(H) and P(H) represent negative and positive parts of the magnetoresistance, respectively.

Let us apply the present theory of the magnetoresistance to two-dimensional disordered systems, with the purpose of explaining peculiar feature of magnetoresistance observed in 1T-TaS_2 [10] and its alloy systems [11]. Assuming that the localization lengths depend on the state energy ε_α in the following way

$$\xi_1(\varepsilon_\alpha) = (1/2)\xi_2(\varepsilon_\alpha) \propto (E_c - \varepsilon_\alpha)^{-1}, \tag{7}$$

and choosing the values of the parameters to be $(E_c-E_F) = 1.0$ meV, $U = 1.7$ meV, $\nu = 5.3\times10^{14}/cm^2\cdot eV$ and $\xi_1(E_F) = 100$ A, we have calculated the magnetoresistance. The results are shown by the curves of 1K and 0.6K in Fig.3. Magnetoresistance increases linearly in a weak field, changes to decrease with further increasing a field due to the saturation of the positive contribution, and then the negative contribution overwhelms the positive one in the high field region.

It was shown [12,13] that interstate interactions lead to the ferro- or antiferromagnetic interactions among SO states and are the origin of the Schottky type anomaly in the specific heat at very low temperatures. The spin-spin interaction between the two SO states of SO to SO processes is antiferromagnetic, because the two states differ in energy by just the intrastate interaction energy in which case the kinetic-type exchange interaction is dominant. As the spins of SO states are locked by the antiferromagnetic interaction, the SO to SO and DO to UO processes do not get suppressed by a magnetic field and we expect that the only negative contribution appears in the magnetoresistance at very low temperatures. This is shown in Fig.3 by the curves 0.1K and 0.4K.

The calculated result of field dependence and temperature change of magnetoresistance is in qualitative agreement with the experiment [10]. Furthermore, when T_0 is increased by doping Se, a larger positive magnetoresistance is observed [11] also in agreement with the present theory.

4 Conclusion

We have investigated the effect of electron-electron interaction on the variable range hopping conduction. In the absence of a magnetic field, intrastate interaction does not change the Mott's law of temperature dependence though the prefactor T_0 now depends on two kinds of localization lengths ξ_1 and ξ_2. In the presence of a magnetic field, intrastate interaction gives positive contribution to the magnetoresistance through the suppression of two types of hopping processes. Combined with the negative contribution due to energy dependence of localization lengths and interstate interactions, we have explained successfully the so far puzzling features of the magnetoresistance observed in two-dimensional $1T\text{-}TaS_{2-x}Se_x$ systems.

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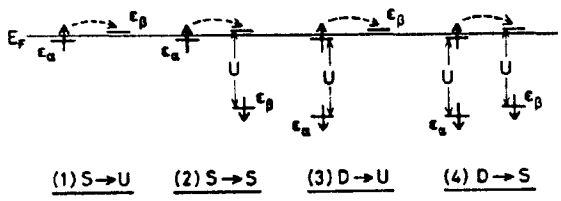

Fig.1 Four kinds of hopping processes in the presence of the intrastate interaction.

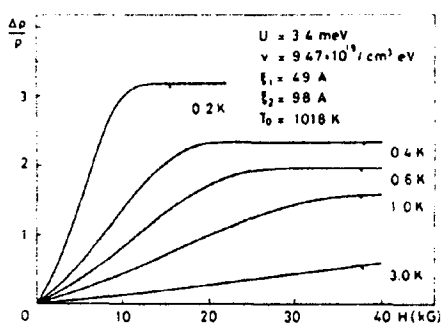

Fig.2 Positive part of magnetoresistance.

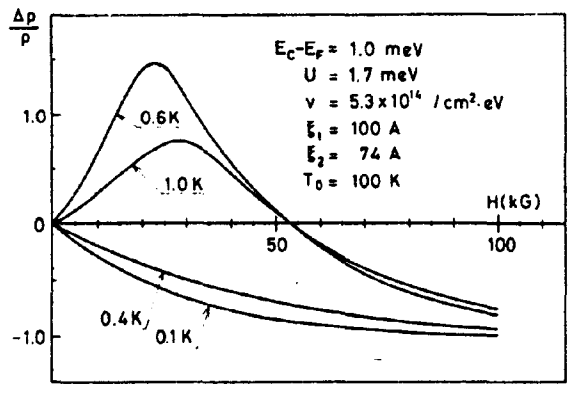

Fig.3 Calculated magnetoresistance of $1T\text{-}TaS_2$.