On the theory of electroconductivity of narrow-band antiferromagnetics

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Abstract. A possible explanation for the electroconductivity activation energy temperature dependence observed in transition metal oxides is proposed. The activation energy according to our approach is determined by the mobility edge position in the conduction (valence) band. The dependence of the mobility edge on the magnetic order is obtained. Hence the magnetic order temperature dependence determines the activation energy temperature dependence.

1. Introduction

It is widely accepted that such transition metal oxides as NiO, CoO and MnO are Mott insulators [1]. The theoretical description of these materials is traditionally based on a half-filled Hubbard model, where there is a lower, completely filled band and an upper, empty the band with the correlation gap between. The conduction in these materials is usually due to the carriers which are activated from the impurity levels. Further on we shall consider the electron in the conduction band (the problem of the hole in the valence band is equivalent). The compounds in question are also antiferromagnetics, and the magnetic order has a strong influence on their electrical properties. This influence manifests itself in the temperature dependence of the electroconductivity activation energy, the latter being larger in the antiferromagnetic phase than in the paramagnetic. We propose a possible explanation for the temperature dependence observed.

2. Hamiltonian and theoretical formulation

We accept the narrow-band model, i.e. we suppose that the Coulomb repulsion is much larger than the hopping integral. For the description of such a situation in [2] the adiabatic approximation was used based on the fact that the characteristic electronic frequencies are much larger than the characteristic spin subsystem frequencies and lead to the

decoupling of spin and charge degrees of freedom. The charge carrier in such an approximation is described by the Green function which may be written in the form:

$$\langle G(E)\rangle_T = \sum_{\{s\}} P_s \langle \Psi_s | C(E - H)^{-1} C^+ | \Psi_s \rangle \tag{1}$$

where H is a one-electron Hamiltonian

$$H = t \sum_{\substack{\langle ff'\rangle \\ \sigma}} C_{f\sigma}^+ C_{f'\sigma}. \tag{2}$$

The lattice is supposed to be cubic for simplicity and the hopping takes place only between the nearest neighbours. In equation (1) Ψ_s is the wave-function which describes an arbitrary configuration which participates in the mixed state of the spin subsystem and P_s is the statistical weight of such a configuration determined by the temperature.

When describing the conductivity of such systems (they have been analysed more than once in the framework of the s–d model [3]) it was often supposed that the current is carried by the electrons activated from the impurity levels to the band edge, and this edge was obtained in some kind of effective medium approximation. The dependence of the edge position on magnetic order and hence on temperature was associated with the observed electroconductivity activation energy temperature dependence.

However in [4] it was noted that this approach can be improved. After the adiabatic approximation is postulated the problem is equivalent to that of the electron in a static potential. Then we may use the concepts introduced for the description of the disordered system's conductivity, in particular Anderson localization theory. According to this theory the disorder leads to the existence of a mobility edge E_c, i.e. the energy which separates localized states from the conducting ones. When the Fermi level E_F lies below the mobility edge the current is carried by the electrons activated from the Fermi level above the mobility edge. Hence for the activation energy Δ we obtain:

$$\Delta = E_c - E_F. \tag{3}$$

We suppose that the Fermi level is fixed by the impurities and does not depend upon temperature. The mobility edge does depend upon the magnetic order and hence upon temperature. Our task is to find this temperature dependence.

Consider the following: according to Anderson localization theory (see e.g. [5]) the diagonal in site representation matrix element of the random (unaveraged) Green function is:

$$G(E) = \langle \Psi_s | C_{1\sigma} (E - H)^{-1} C_{1\sigma}^+ | \Psi_s \rangle \tag{4}$$

which is equivalent to the following power series:

$$G(E) = \sum_L (t^L/E^{L+1}) \sum \left\langle \Psi_s \left| \left(\prod_{i=1}^{L} \hat{\mathbf{A}}_i \right)_{\sigma\sigma} \right| \Psi_s \right\rangle = \sum_L G^{(L)} \tag{5}$$

where the following notation is introduced:

$$\hat{\mathbf{A}}_i = \begin{pmatrix} 1/2 + S_i^z & \sqrt{2} S_i^+ \\ \sqrt{2} S_i^- & 1/2 - S_i^z \end{pmatrix}.$$

In (5) $G^{(L)}$ is the sum over all paths on the lattice with L steps starting and ending at site

1. To each intermediate site i there corresponds a matrix $\hat{\mathbf{A}}_i$. Each item in $G^{(L)}$ is the averaged product of these matrices multiplied by t^L/E^{L+1}.

3. The mobility edge calculation

It has been shown that the mobility edge is the convergence radius for the self-energy modified perturbation theory expansion, where the summation takes place only for the paths which have no self-intersections [5]. Unfortunately, the structure of such series is highly complicated and the convergence radius is very difficult to obtain. There is, however, another approach when an approximate criterion of localization is formulated (see e.g. [6]). In our paper [4], for the analysis of the series of the type (5) a simple approximate criterion was formulated. This consists of identification of the mobility edge with the convergence radius of the series $\Sigma_L \bar{G}^{(L)}$, which is obtained from series (5) when ignoring the path self-intersections. We can use the theorem [7] according to which the series in question converges with probability unity if and only if the series $\Sigma_L \langle \bar{G}^{(L)} \rangle$ and $\Sigma_L \langle \bar{G}^{(L)2} \rangle$ converge, where the brackets mean the average (in our case thermodynamic). We introduce formally a small parameter $1/z$, where z is the number of nearest neighbours. In the leading approximation with respect to $1/z$ the convergence radius of both averaged series coincide with the convergence radius of the series:

$$\langle \bar{G}_A \rangle_T = \sum_L (z^L t^L/E^{L+1}) \left\langle \left\langle \prod_{i=1}^{L} \hat{\mathbf{A}}_i \right\rangle_T \right\rangle_L \tag{6}$$

where the brackets $\langle \ldots \rangle_L$ denote the average over all paths of the length L; the multiplier Z^L is the asymptotic number of the paths when $L \gg 1$.

To calculate the correlator we use the chain approximation due to Kirkwood [8]:

$$\left\langle \left(\prod_{i=1}^{L} \hat{\mathbf{A}}_i \right)_{\sigma\sigma} \right\rangle_T = \left(\prod_{i=1}^{L} \langle \hat{\mathbf{A}}_i \hat{\mathbf{A}}_{i+1} \rangle_T \bigg/ \prod_{i=1}^{L} \langle \hat{\mathbf{A}}_i \rangle_T \right)_{\sigma\sigma}. \tag{7}$$

In the equation (7) we need pay no attention to the multipliers' order, because all the correlators are the diagonal matrices:

$$\langle \hat{\mathbf{A}}_i \rangle_T = \begin{pmatrix} 1/2 + \langle S_i^z \rangle & 0 \\ 0 & 1/2 - \langle S_i^z \rangle \end{pmatrix} \tag{8}$$

and

$$\langle \hat{\mathbf{A}}_i \hat{\mathbf{A}}_{i+1} \rangle_T = \begin{pmatrix} 1/4 + \langle S_i S_{i+1} \rangle & 0 \\ 0 & 1/4 + \langle S_i S_{i+1} \rangle \end{pmatrix}. \tag{9}$$

As a result, for the mobility edge we obtain:

$$|E_c| = \tfrac{1}{2} W (1/4 + \langle S_1 S_2 \rangle)(1/4 - \langle S^z \rangle^2)^{-1/2} \tag{10}$$

where $\langle S^z \rangle$ is the averaged sublattice spin, $\langle S_1 S_2 \rangle$ is the pair correlation function of the nearest-neighbour spins and $W = 2zt$ is the bandwidth the conduction band would have

if all the spins were aligned ferromagnetically. It is worth noting that (10) coincides with the result for the bandwidth which was obtained in [9].

4. Electroconductivity activation energy

Suppose that the electrons are excited from the impurity levels which fix the Fermi level. The temperature dependence of the activation energy defined by the equation

$$\Delta = \tfrac{1}{2}W[1 - (1/4 + \langle S_1 S_2 \rangle)(1/4 - \langle S^z \rangle^2)^{-1/2}] \tag{11}$$

is obvious. At high temperatures ($T \gg T_N$) all the correlators are equal to zero, and for the activation energy we obtain:

$$\Delta = W/4. \tag{12}$$

At $T = 0$, we may suppose that

$$\langle S_1 S_2 \rangle = -\langle S^z \rangle^2. \tag{13}$$

It is necessary to note that even at $T = 0$, $\langle S^z \rangle \neq \pm 1/2$ due to quantum spin fluctuations (e.g. from the spin-wave theory it follows that $1/2 - |\langle S^z \rangle| \simeq 1/z$). Hence the extended states exist even at $T = 0$, and the width of the extended states band as can be seen from (10) is equal to $W(1/4 - \langle S^z \rangle^2)^{1/2}$. For the activation energy at $T = 0$ we obtain:

$$\Delta_{AF} = \tfrac{1}{2}W[1 - (1/4 - \langle S^z \rangle^2)^{1/2}]. \tag{14}$$

Hence we see that if we use the realistic value of the bandwidth $W \simeq 1$ eV the difference between the activation energy in the antiferromagnetic and paramagnetic phases is of the order of 0.1 eV, which agrees with the experimental values [10–12].

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