Low-temperature resistivity of double-exchange interaction systems

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We studied the double-exchange interaction. The Hamiltonian derived consists of the hoppings of charged fermions and Schwinger bosons. This gives a very simple and clear picture. We also calculated the resistivity with the new Hamiltonian and found that the resistivity is proportional to the square of temperature, if temperature is much lower than the Curie temperature.

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Perovskite manganites^{1,2} ($\text{La}_{1-x}\text{A}_x\text{MnO}_3$, A = divalent elements, x = doping concentration) exhibit many interesting physical phenomena, including metal-insulator phase transition, various magnetic phases (ferromagnetism, antiferromagnetism, and paramagnetism), charge ordering, orbital ordering, and Jahn-Teller effect. The most prominent one, in our opinion, is the close relation between magnetism and transport properties, the colossal magnetoresistance and the interplay between magnetic phase transition and metal-insulator transition. The double-exchange (DE) interaction proposed by Zener³ gave a qualitative explanation. The localized spins of Mn ions interact with each other via the motion of conduction electrons. The spins of conduction electrons are coupled to the localized spin and thus, form energy levels according to Hund's rules. Ferromagnetism facilitates the motion of conduction electrons and lowers the kinetic energy. Anderson and Hasegawa⁴ built a physical model and performed some calculation that combined with de Gennes's elaboration⁵ gave an insightful picture of the systems. The next major progress came from Kubo and Ohata's paper.⁶ They used a projection method to project out the lowest-energy states according to Hund's rule and did the calculation only in these states, thereby preserved the most important physics. Furukawa⁷ used another approach. He solved the infinite-dimension Kondo lattice model to gain some understanding of the double-exchange interaction. But treating DE remains a difficult task. There is no controlled perturbation to bring forth reliable results. The inadequacy of analytical calculation is manifest on, for example, resistivity. Experiment data⁸ showed that the resistivity has T^2 dependence at temperature much lower than the Curie temperature. A more detailed study⁹ found certain deviation. It showed that the T^2 dependence of resistivity disappears below, say 40 K. The authors attributed the T^2 dependence to one-magnon process with shrinking minority-spin band. However, if the minority-spin band shrinks with decreasing temperature, the resistivity should decrease faster than T^2 . Additionally, 40 K is an energy scale much smaller than the band gap between majority- and minority-spin electrons. Their results need to more investigation. In any case, it is clear that the resistivity is closely related to magnetism and exhibits predominantly a T^2 behavior that can be explained by one-magnon scattering.

Since the motion of electrons may be affected by phonons¹⁰ or superexchange interaction to form polarons¹¹ or magnetic polarons under the condition of small doping,¹² we

considered the simplest situation where double exchange dominates, i.e., intermediate doping concentration, $0.2 \leq x \leq 0.5$, at low temperature. In this case, Kubo and Ohata's calculation⁶ produced a $T^{9/2}$ behavior. Furukawa's calculation¹³ was based on the infinite-dimension Kondo lattice. The resulting resistivity was given as a function of magnetization and hence, cannot be compared directly with experiments. Wang and Zhang¹⁴ gave a resistivity of $T^{2.5}$ dependence by assuming that there are localized electron states of minority spin and thus, rendering the spin-flip scattering possible. However, a spin-polarized experiment showed¹⁵ that spin polarization is near 100% at low temperature. In this paper, we gave the DE system a simple and clear picture and showed that DE alone gives the resistivity proportional to T^2 .

The main ingredients of the double-exchange interaction systems are conduction electrons and localized spins. Each Mn ion possesses a localized spin with $s = 3/2$ ($s = 2$ in the hole picture). The spins of conduction electrons are coupled to the localized spins. The coupling energy is dictated by Hund's rules. Therefore, the model Hamiltonian has the form

$$H = -t \sum_{i,j,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \frac{J}{2} \sum_i \mathbf{S}_i \cdot \boldsymbol{\sigma}_i, \quad (1)$$

where c_j is the hole annihilation operator, i and j are nearest neighbors, and $\mathbf{S}_i$ and $\boldsymbol{\sigma}_i/2$ represent the spins of Mn^{+3} ($s = 2$) (to be referred as the localized spin) and the spin of a conduction hole, respectively. We use the hole picture because we are interested in the region where the doping concentration x is less than 0.5. The Hund's coupling energy J is greater than the kinetic energy t of charge carriers and hence, cannot be treated perturbatively. In order to circumvent this difficulty, Kubo and Ohata,⁶ applying the method of Harris and Lange,¹⁶ proposed the following Hamiltonian:

$$H = -t \sum_{i,j,\alpha,\beta} c_{i\alpha}^\dagger (P_i P_j)_{\alpha\beta} c_{j\beta}, \quad (2)$$

where

$$P_i = \frac{s - \mathbf{S}_i \cdot \boldsymbol{\sigma}_i}{2s + 1}. \quad (3)$$

Equation (2) describes the hopping of the holes between Mn^{+3} and Mn^{+4} sites. The projection operators impose constraints on holes. Hoppings can only occur at those sites

where the sum of localized spin and the spin of the hole is equal to $3/2$. This way one can avoid dealing with the Hund's coupling. Nevertheless, Eq. (2) is still a complicated Hamiltonian.

The Hamiltonian can be written in the following form after straightforward expansion:

$$H = -\frac{t}{(2s+1)^2} \sum_{\mathbf{i}, \mathbf{j}} \{ [c_{\mathbf{i}\downarrow}^\dagger (s + S_{\mathbf{i}z}) - c_{\mathbf{i}\uparrow}^\dagger S_{\mathbf{i}-}] \times [(s + S_{\mathbf{j}z}) c_{\mathbf{j}\downarrow} - S_{\mathbf{j}+} c_{\mathbf{j}\uparrow}] + [c_{\mathbf{i}\uparrow}^\dagger (s - S_{\mathbf{i}z}) - c_{\mathbf{i}\downarrow}^\dagger S_{\mathbf{i}+}] \times [(s - S_{\mathbf{j}z}) c_{\mathbf{j}\uparrow} - S_{\mathbf{j}-} c_{\mathbf{j}\downarrow}] \}. \quad (4)$$

We applied the slave-fermion method to separate the spin and charge:

$$c_{\mathbf{j}\uparrow} = \alpha_{\mathbf{j}} f_{\mathbf{j}} \quad (5a)$$

and

$$c_{\mathbf{j}\downarrow} = \beta_{\mathbf{j}} f_{\mathbf{j}}, \quad (5b)$$

where $f_{\mathbf{j}}$ is the spinless fermion operator with charge e and $\alpha_{\mathbf{j}}(\beta_{\mathbf{j}})$ is the spin-up (spin-down) spinon operator. Now the Hamiltonian has the form

$$H = \frac{-t}{(2s+1)^2} \sum_{\mathbf{i}, \mathbf{j}} f_{\mathbf{i}}^\dagger \{ [\beta_{\mathbf{i}}^\dagger (s + S_{\mathbf{i}z}) - \alpha_{\mathbf{i}}^\dagger S_{\mathbf{i}-}] \times [(s + S_{\mathbf{j}z}) \beta_{\mathbf{j}} - S_{\mathbf{j}+} \alpha_{\mathbf{j}}] + [\alpha_{\mathbf{i}}^\dagger (s - S_{\mathbf{i}z}) - \beta_{\mathbf{i}}^\dagger S_{\mathbf{i}+}] \times [(s - S_{\mathbf{j}z}) \alpha_{\mathbf{j}} - S_{\mathbf{j}-} \beta_{\mathbf{j}}] \} f_{\mathbf{j}}. \quad (6)$$

It is still a complicated Hamiltonian. We used the Clebsch-Gordan coefficients,

$$|s-1/2, m-1/2\rangle = \sqrt{\frac{s+m}{2s+1}} |s, m\rangle |\downarrow\rangle - \sqrt{\frac{s-m+1}{2s+1}} |s, m-1\rangle |\uparrow\rangle, \quad (7a)$$

$$|s-1/2, m+1/2\rangle = \sqrt{\frac{s+m+1}{2s+1}} |s, m+1\rangle |\downarrow\rangle - \sqrt{\frac{s-m}{2s+1}} |s, m\rangle |\uparrow\rangle, \quad (7b)$$

and the fact that α and β annihilate $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively, to reach the following relations:

$$[(s + S_z) \beta - S_+ \alpha] |s-1/2, m-1/2\rangle = \sqrt{(2s+1)(s+m)} |s, m\rangle, \quad (8a)$$

and

$$[(s - S_z) \alpha - S_- \beta] |s-1/2, m+1/2\rangle = -\sqrt{(2s+1)(s-m)} |s, m\rangle. \quad (8b)$$

The derivation should be confined to the subspace of two kinds of states, namely spin s and spin $s-1/2$ due to the projection operators. Thus, Eq. (6) is equivalent to

$$H = \frac{-t}{2s+1} \sum_{\mathbf{i}, \mathbf{j}, m_i, m_j} f_{\mathbf{i}}^\dagger [\sqrt{(s+m_i)(s+m_j)} |s-1/2, m_i-1/2\rangle_{\mathbf{i}} |s, m_j\rangle_{\mathbf{j}} \langle s-1/2, m_j-1/2|_{\mathbf{i}} \langle s, m_i| + \sqrt{(s-m_i)(s-m_j)} |s-1/2, m_i+1/2\rangle_{\mathbf{i}} |s, m_j\rangle_{\mathbf{j}} \langle s-1/2, m_j+1/2|_{\mathbf{i}} \langle s, m_i|] f_{\mathbf{j}}, \quad (9)$$

where m_i and m_j run over all the possible values and $|s, m_j\rangle_{\mathbf{j}}$ denotes the state at site $\mathbf{j}$. The first term in Eq. (9) denotes the hoppings of spin-down holes from site $\mathbf{j}$ to site $\mathbf{i}$. The total spin at site $\mathbf{j}$ changes from $s-1/2$ to s , and that at site $\mathbf{i}$ changes from s to $s-1/2$. The second term is for spin-up holes. We can further simplify the Hamiltonian with the Schwinger boson method.¹⁷

$$|s, m\rangle = \frac{(A^\dagger)^{s+m}}{\sqrt{(s+m)!}} \frac{(B^\dagger)^{s-m}}{\sqrt{(s-m)!}} |0, 0\rangle. \quad (10)$$

The Schwinger bosons can be used to construct spin states. In particular,

$$A^\dagger |s-1/2, m-1/2\rangle = \sqrt{s+m} |s, m\rangle, \quad (11a)$$

and

$$B^\dagger |s-1/2, m+1/2\rangle = \sqrt{s-m} |s, m\rangle. \quad (11b)$$

Obviously, $A^\dagger$ and $B^\dagger$ are equivalent to $\sqrt{s+m} |s, m\rangle \langle s-1/2, m-1/2|$ and $\sqrt{s-m} |s, m\rangle \langle s-1/2, m+1/2|$, respectively, in the subspace of spin states s and $s-1/2$. Finally, the Hamiltonian can be written simply as

$$H = -\frac{t}{2s+1} \sum_{\mathbf{i}, \mathbf{j}} f_{\mathbf{i}}^\dagger (A_{\mathbf{i}} A_{\mathbf{j}}^\dagger + B_{\mathbf{i}} B_{\mathbf{j}}^\dagger) f_{\mathbf{j}} \quad (12)$$

with the constraint coming from applying slave-fermion and Schwinger boson methods

$$A_{\mathbf{j}}^\dagger A_{\mathbf{j}} + B_{\mathbf{j}}^\dagger B_{\mathbf{j}} + f_{\mathbf{j}}^\dagger f_{\mathbf{j}} = 2s. \quad (13)$$

Equations (12) and (13) give a simple and clear picture of the double-exchange interaction. First of all, we found that the spins of holes were coupled with localized spins and lost their identities. The total spin represented by Schwinger bosons at each site is a more suitable description of the system. Second, the hopping of a hole should be viewed as

hoppings of a fermion and a Schwinger boson. The motions of fermions have two channels, namely, exchanging Schwinger boson A and B . The kinetic-energy gain of fermions is of the order $zt(s \pm \langle S_z \rangle)/(2s+1)$ for channels A and B , respectively. Here z is the coordination number. In the ferromagnetic states, with $\langle S_z \rangle > 0$, channel A is more favorable because of the abundance of A bosons.

There are important differences between the present picture and that given by the mean-field approximation of Eqs. (1) and (2). The kinetic-energy gain by the mean-field approximation is $zt(s \pm \langle S_z \rangle)^2/(2s+1)^2$, smaller than the one given above. More importantly, the mean-field approximation gives separated spin-up and spin-down bands. As a result, there is only one type of charge carriers (spin-down holes if $\langle S_z \rangle > 0$) at low temperature. In the present picture, both spin-up and spin-down holes exist in each channel, even at absolute zero, as shown clearly by Eq. (6).

To begin with Kubo and Ohata's Hamiltonian⁶ is of great importance. This way we are able to consider only those states with total spin 2 and 3/2, and give a rigorous derivation. Khaliullin and Kilian¹⁸ started from the Hamiltonian in Eq. (1). As a result, they should have treated Hund's coupling [the second term of Eq. (1)] properly and accounted for the states of total spin $(s-1)=1$. Their mapping would have been very complicated. For example, there should have been additional terms such as $\hat{c}_{i\alpha}^\dagger \hat{c}_{j\beta} D_{is} D_{js}^\dagger$ in their Hamiltonian, and the Hund's coupling should elevate the energy of this term. Hence, their approach is an approximated mapping.

A more convenient form for later calculation is

$$H = -\frac{1}{N(2s+1)} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{q}} E_{\mathbf{k}-\mathbf{p}-\mathbf{q}} f_{\mathbf{k}-\mathbf{q}}^\dagger (A_{\mathbf{p}} A_{\mathbf{p}+\mathbf{q}}^\dagger + B_{\mathbf{p}} B_{\mathbf{p}+\mathbf{q}}^\dagger) f_{\mathbf{k}} \quad (14)$$

where

$$E_{\mathbf{k}} = t \sum_{nn} e^{i\mathbf{k} \cdot \mathbf{R}_{nn}} \quad (15)$$

and the summations are over nearest neighbors (nn). Applying the mean-field approximation, we found the energies of fermions and bosons:

$$\varepsilon_{\mathbf{k}} = -\frac{1}{N(2s+1)} \sum_{\mathbf{p}} E_{\mathbf{k}+\mathbf{p}} \langle A_{\mathbf{p}} A_{\mathbf{p}}^\dagger + B_{\mathbf{p}} B_{\mathbf{p}}^\dagger \rangle, \quad (16)$$

and

$$\omega_{\mathbf{q}} = -\frac{1}{N(2s+1)} \sum_{\mathbf{k}} E_{\mathbf{k}+\mathbf{q}} \langle f_{\mathbf{k}}^\dagger f_{\mathbf{k}} \rangle, \quad (17)$$

Readers should not be worried about the negative energies of bosons and fermions. We can shift the origin in $\mathbf{k}$ space and the zero point of energy to make them "normal." The effective mass of bosons is of the order of $(2s+1)\hbar^2/xta^2$, while that of fermions is $\hbar^2/ta^2$ with a being the lattice constant. Note that x and $(2s+1)$ are, respectively, the density of fermions and bosons. Since the bosons are more dense, the fermions have greater kinetic energy. From the point of view

of bosons (fermions), they are able to move because of the presence of fermions (bosons). The bosons (fermions) interact with each other indirectly through the media of fermions (bosons). The bosons and fermions are the counterpart of each other. Of course, we can further combine a fermion with a boson to form a new fermion, a special kind of magnetic polaron. But it seems this way we cannot gain more insight.

One final comment is that the bosons A or B are different from the conventional spin waves. In order to calculate the spin-wave properties, the propagator $\langle \hat{T}A(t)B^\dagger(t)BA^\dagger \rangle$, instead of $\langle \hat{T}A(t)A^\dagger \rangle$ or $\langle \hat{T}B^\dagger(t)B \rangle$ should be calculated. This is, of course, due to the relations $S_+ = A^\dagger B$ and $S_- = AB^\dagger$. At low temperature, certain approximations, such as that in Ref. 18, can be made to simplify calculation.

Now the resistivity is calculated. We consider only the channel of A bosons. It is the main contributor of current at low temperature. The following approach is same as the Boltzmann equation. We preferred it because the collision term comes out of it naturally. Using the Langevin equation of holes,^{19,20} we found the resistivity

$$\rho(\omega) = \frac{1}{ne^2} \left(i m \omega + \frac{1}{N\hbar} \omega \int_0^\infty e^{-i\omega t} \langle [F, F(t)] \rangle dt \right), \quad (18)$$

where $\langle [F, F(t)] \rangle$ is the thermal average of the force commutator. Hence the dc resistivity is given by

$$\rho = \frac{2\pi\hbar}{Nne^2k_B T} \sum_{n,m} e^{-\beta E_n} F_{nm} F_{mn} \delta(E_{mn}). \quad (19)$$

Since the total momentum is $\sum c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\downarrow} \hbar \mathbf{k}$, the force is

$$F_x = -\frac{i}{\sqrt{N}} \sum_{\mathbf{k}, \mathbf{q}} \frac{(s + \langle S_z \rangle) E_{\mathbf{k}} k_x}{2s+1} (f_{\mathbf{p}}^\dagger A_{\mathbf{p}-\mathbf{k}} c_{\mathbf{k}\downarrow} - c_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{p}} A_{\mathbf{p}-\mathbf{k}}^\dagger), \quad (20)$$

where we have made the approximation of replacing S_z by its thermal average. Substituting Eq. (20) into Eq. (19), we found

$$\rho = \frac{2\pi\hbar}{N^2 ne^2 k_B T} \sum_{\mathbf{k}, \mathbf{p}} \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} + \omega_{\mathbf{p}-\mathbf{k}}) n_f(\mathbf{k}) [1 - n_f(\mathbf{p})] \times n_b(\mathbf{p}-\mathbf{k}) \left| \frac{(s + \langle S_z \rangle) E_{\mathbf{k}}}{2s+1} \right|^2 \mathbf{k} \cdot (\mathbf{k}-\mathbf{p}), \quad (21)$$

where n_f and n_b are the distribution functions of fermions and Schwinger bosons, respectively. Here we have made the approximation of using the distribution function of charged fermions in place of that of spin-down holes. It will not cause any significant error at low temperature because their effective masses are very similar.

Now Eq. (21) has the form of one-magnon scattering,^{21,22} and the resistivity is expected to be proportional to T^2 . Nonetheless, we provided a brief analysis. The factor $n_f(\mathbf{k}) \times [1 - n_f(\mathbf{p})]/k_B T$ gives a factor of density of states at Fermi level. It is independent of temperature. The factor $n_b(\mathbf{p}-\mathbf{k})$ imposes a restriction $D(\mathbf{p}-\mathbf{k})^2 < k_B T$, where D is the spin-

wave stiffness, $\mathbf{k} \cdot (\mathbf{k} - \mathbf{p})$ is the result of excluding forward scattering. It can be written as $2k_F^2 \sin^2(\theta/2)$, where θ is the angle between $\mathbf{k}$ and $\mathbf{p}$. Therefore, $\theta < \sqrt{k_B T / D k_F^2}$. The integration over θ gives

$$\rho \approx \frac{3\hbar (ak_F)^6 (s + \langle S_z \rangle)^2}{8\pi e^2 k_F (2s + 1)^2} \left(\frac{k_B T}{D k_F^2} \right)^2. \quad (22)$$

We note that the spin stiffness and the factor $(s + \langle S_z \rangle)^2$ decrease with increasing temperature. Their variation tend to cancel each other. Hence, we can use their values at the low-temperature limit: $D = xta^2/(2s + 1)$, and $\langle S_z \rangle = s$. Assuming $x = 1/3$ and the Fermi energy is equal to 0.7 eV, we found that $\rho \cong 8 \text{ n } \Omega \text{ cm T}^2/\text{K}^2$. This agrees with the experimental result⁹ in order of magnitude.

We give a clear picture of the system. An essential element is that the spins of holes are combined with the localized spins. The states of total spin contain both spin-up and spin-down holes [see Eq. (6)]. Therefore, spin flipping of holes does not cost finite amount of energy. The resistivity is calculated accordingly. It has the expression of one-magnon process and has a T^2 dependence. This picture is vastly different from that given by the mean-field approximation of Eq. (1) or (2). The mean-field approximation gives a band

gap between spin-down holes and spin-up holes. At low temperature, the spin-up band is empty. It costs finite amount of energy to flip a spin. Hence, the one-magnon mechanism is frozen at low temperature. Kubo and Ohata's calculation⁶ on resistivity (proportional to $T^{9/2}$) did contain the one-magnon process. However, its contribution is negligible due to the reason given above. Their resistivity comes mainly from the two-magnon process. Its magnitude is much smaller than the experimental value and that given here. In conclusion, we transformed the double-exchange interaction into a simple form. The resistivity from this picture has the correct temperature dependence and magnitude. This again shows that the magnetic and transport properties are closely related in manganites.

It was pointed out to us after we finished this work that the Schwinger boson method had been applied to this problem.¹⁸ We think that our approach is more rigorous. The Hund coupling term in Eq. (1) had been taken care of properly. The spins of conduction holes combined naturally with localized spins and represented by Schwinger bosons.

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