Temperature dependence of the resistivity in the double-exchange model

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The resistivity around the ferromagnetic transition temperature in the double-exchange model is studied by the Schwinger-boson approach. The spatial spin correlation responsible for scattering of conduction electrons are taken into account by adopting the memory function formalism. Although the correlation shows a peak lower than the transition temperature, the resistivity in the ferromagnetic state monotonically increases with increasing temperature due to a variation of the electronic state of the conduction electron. In the paramagnetic state, the resistivity is dominated by the short-range correlation of scattering and is almost independent of the temperature. It is attributed to a cancellation between the nearest-neighbor spin correlation, the fermion bandwidth, and the fermion kinetic energy. This result implies the importance of the temperature dependence of the electronic states of the conduction electron as well as the localized spin states in both ferromagnetic and paramagnetic phases. [S0163-1829(99)08313-7]

The recent discovery of colossal magnetoresistance[1–4] (CMR) has revived interest in perovskite manganites such as $La_{1-x}Sr_xMnO_3$. It is widely accepted that significant changes in the transport properties, as well as CMR, are observed around the transition between the ferromagnetic phase and the paramagnetic one. More than 40 years ago, Zener[5] proposed a double-exchange (DE) interaction to explain the correlation between electrical conduction and the ferromagnetism, in which the spin of a conduction electron and a localized core spin ($\vec{S}$) on the same site are strongly coupled by Hund's rule. Since the hopping amplitude of the electron to the neighboring sites is maximum when the two neighboring core spins are parallel, the ferromagnetic metallic state is achieved by gaining the kinetic energy of the conduction electron.[5–7] These concepts were settled as the so-called DE model and the magnetic and transport properties in this model have been investigated intensively and extensively.

One of the main interests in this research field is the temperature dependence of the electrical resistivity. The resistivity in the DE model was studied in a mean-field theory by Kubo and Ohata,[8] and similar results have been reproduced by a dynamical mean-field theory by Furukawa.[9] In these calculations, however, the spatial correlation of the core spins is not included properly, although it is pointed out that it plays a crucial role in the electric transport near the Curie temperature (T_C).[10,11] The short-range spin correlation was only considered in Ref. 8, and the spatial correlation was neglected in Ref. 9, where the dynamical fluctuation was taken into account. Millis *et al.* discussed a possibility that the behavior of the resistivity is greatly modified when the spatial correlation of the core spins is properly taken into account.[12] They showed that the resistivity is still increased below T_C with decreasing the temperature. Being based on the calculated results which disagree with the experimental one, they concluded that the additional gradients, such as the Jahn-Teller effect, are necessary to reproduce the observed behaviors.

In this paper, we calculate the temperature dependence of the resistivity in the DE model by the Schwinger boson approach. In order to include the effects of the spatial correlation of the core spins properly, we adopt the memory function formalism which was also used in Ref. 12. In addition, the temperature dependence of the electronic structure is determined self-consistently together with that of the core spins. The calculated resistivity monotonically decreases with decreasing temperature in the ferromagnetic states and does not show a peak below T_C, although the spin correlation has its maximum at $T < T_C$.

The Hamiltonian of DE model in the limit of strong Hund's coupling is given by the Schwinger-boson representation as follows:

$$\mathcal{H} = -\frac{t}{2S_R} \sum_{\langle ij \rangle \sigma} [b_{i\sigma}^\dagger b_{j\sigma} f_i^\dagger f_j + \text{H.c.}] \tag{1}$$

with the local constraint $\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma} - f_i^\dagger f_i = 2S$ at every lattice site i. Here, $b_{i\sigma}(\sigma = \uparrow, \downarrow)$ is a boson and f_i is a spinless fermion operator, $S_R = S + (1-x)/2$,[13–15] and x is the doping concentration of holes ($\langle f_i^\dagger f_i \rangle = 1-x$). We shall exclusively consider the case of $S = \frac{3}{2}$. A transition at T_C from a ferromagnetic state to a paramagnetic state (described as the Bose condensation of Schwinger bosons) was investigated by using a mean-field Hamiltonian[14]

$$\mathcal{H}_{\text{MF}} = -\frac{Bt}{S_R} \sum_{\langle ij \rangle} [f_i^\dagger f_j + \text{H.c.}] - \frac{Dt}{2S_R} \sum_{\langle ij \rangle \sigma} [b_{i\sigma}^\dagger b_{j\sigma} + \text{H.c.}] \tag{2}$$

with a global constraint

$$\left\langle \sum_\sigma b_{i\sigma}^\dagger b_{i\sigma} \right\rangle = 2S_R, \tag{3}$$

where B and D are given by $\frac{1}{2}\sum_\sigma \langle b_{i\sigma}^\dagger b_{j\sigma} \rangle$ and $\langle f_i^\dagger f_j \rangle$, respectively, and both are determined self-consistently. This
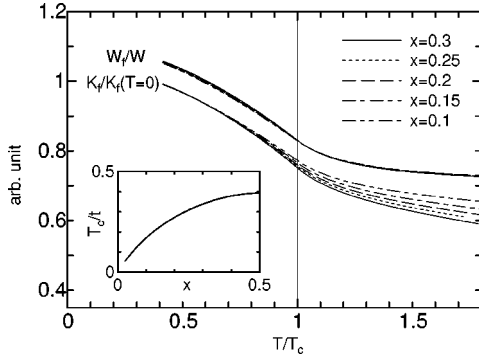
FIG. 1. The fermion bandwidth normalized by bare bandwidth (W_f/W) and the fermion kinetic energy normalized by the zero-temperature value [$K_f/K_f(T=0)$] as a function of T/T_C for several doping concentrations. The inset shows the transition temperature from a ferromagnetic state to a paramagnetic state as a function of the doping concentration.

mean-field treatment, however, leads to an additional transition at slightly higher temperature than T_C (about $1.4T_C$) into an artifact state in which $B=D=0$.[15] As a result, above T_C the fermion bandwidth ($W_f \equiv 12Bt/S_R$) rapidly decreases. This decrease obviously causes a misleading diverging increase of the resistivity.

In the present study, we assume that Eq. (2) itself has a suitable form as a mean-field Hamiltonian, but in order to avoid the difficulty mentioned above, the fermion bandwidth B is determined as

$$
\begin{aligned}
B &\equiv \frac{1}{2}\left\langle \sqrt{\left|\sum_\sigma b_{i\sigma}^\dagger b_{j\sigma}\right|^2} \right\rangle \\
&= \frac{S_R}{\sqrt{2}}\left\langle \sqrt{1+\left(\frac{1}{2S_R^2}\sum_{\sigma\sigma'} b_{i\sigma}^\dagger b_{i\sigma'} b_{j\sigma'}^\dagger b_{j\sigma} -1\right)+\frac{1}{S_R}} \right\rangle \\
&\approx \frac{S_R}{\sqrt{2}}\left[\frac{1}{2}+\frac{1}{4S_R^2}\sum_{\sigma\sigma'}\langle b_{i\sigma}^\dagger b_{i\sigma'} b_{j\sigma'}^\dagger b_{j\sigma}\rangle\right]
\end{aligned} \tag{4}
$$

together with

$$
D \equiv \langle f_i^\dagger f_j\rangle \tag{5}
$$

in a self-consistent manner. Here, we ignore the Berry's phase in the electron hopping and use the fact that $\sum_{\sigma\sigma'} b_{i\sigma}^\dagger b_{i\sigma'} b_{j\sigma'}^\dagger b_{j\sigma} \to 2S_R^2$ in the high-temperatures limit. The approximation in Eq. (4) corresponds to the expansion with respect to $\vec{S}_i\cdot\vec{S}_j$. It should be noted that the fermion bandwidth obtained in Eq. (4) remains finite for $T\to\infty$ as expected, while $\frac{1}{2}\sum_\sigma\langle b_{i\sigma}^\dagger b_{j\sigma}\rangle$ characterizing a nearest-neighbor magnetic correlation (denoted by C) vanishes for $T\to\infty$ in this model. Therfore, the behavior obtained in the above formulas is physically reasonable.

The Curie temperature (T_C) in this model as a function of the doping concentration is shown in the inset of Fig. 1. Since T_C is determined by Eq. (3), the results are essentially independent on the formula of B and are the same as those in Ref. 14. The transition temperature is scaled independent on x by D as $T_C/t\approx 2.5D$.

The temperature dependences of the fermion bandwidth normalized by a bare bandwidth ($W=12t$) are plotted in Fig. 1. At the transition temperature, the bandwidth does not directly depend on the doping concentration (it depends on x only through S_R). This is because both the chemical potential and the condensate density of bosons are zero, and Dt/T_C, which is independent of x, is only a parameter in Eq. (4).[17] Further, W_f/W approaches $1/\sqrt{2}$ in an infinite temperature limit. As a result, the behavior of the fermion bandwidth as a function of T/T_C is almost universally independent of x. On the other hand, the behavior of the kinetic energy of the fermion ($K_f\equiv Bt\langle f_i^\dagger f_j\rangle/S_R$) as a function of T/T_C (Fig. 1) changes depending on x. It is important that the bandwidth varies even in the disordered-spin regime of $T>T_C$. This behavior agrees well with the result in Ref. 16. In fact, the bandwidth at T_C is 1.16 times bigger than that in the $T\to\infty$ limit.

The resistivity as a function of the temperature is calculated by the memory function method,[18,19] where the lowest order fluctuation from the mean field can be included automatically. In this lowest-order perturbational treatment, a static approximation for Schwinger bosons is appropriate. This is because the bandwidth of Schwinger bosons is much smaller than that of the fermion ($D\ll B$) and the effects of the quantum fluctuation of bosons can be negligible for $T\gtrsim 0.5T_C$ where $Dt/(2S_RT)\ll 1$. The memory function is evaluated to leading order in $1/S_R$, and thus, the resistivity is written as

$$
\rho = \frac{\hbar^2 a}{2e^2 K_f\tau}, \tag{6}
$$

with

$$
\begin{aligned}
\frac{1}{\tau} = \frac{\pi t^4}{8\hbar K_f S_R^4}\sum_i \Gamma(\vec{R}_i)\frac{1}{N^2}\sum_{p_1 p_2}\left(-\frac{\partial f(\varepsilon_{\vec{p}_1})}{\partial\varepsilon_{\vec{p}_1}}\right)\delta(\varepsilon_{\vec{p}_1}-\varepsilon_{\vec{p}_2}) \\
\times(e^{i\kappa_x}-1)(e^{-i\kappa_x}-1)e^{-i\vec{\kappa}\cdot\vec{R}_i},
\end{aligned} \tag{7}
$$

where $\Gamma(\vec{R}_i)$ represents the spatial spin correlation defined as

$$
\Gamma(\vec{R}_i) \equiv \sum_{\sigma\sigma'\rho\rho'}\langle b_{0\sigma}^\dagger b_{x\sigma} b_{x\sigma'}^\dagger b_{0\sigma'} b_{i\rho}^\dagger b_{i+x\rho} b_{i+x\rho'}^\dagger b_{i\rho'}\rangle. \tag{8}
$$

Here, $f(\varepsilon_{\vec{p}})$ is the Fermi distribution function of the spinless fermion, $\vec{\kappa}=\vec{p}_1-\vec{p}_2$ is the momentum transfer of the fermion due to scattering, and the average $\langle\dots\rangle$ is evaluated by the mean-field Hamiltonian in Eq. (2). The same expression given by spin variables has been derived in Ref. 12. It should be noted that in this model the actual value of the resistivity in units of ha/e^2 does not depend on that of t. This is because $\varepsilon_{\vec{p}}$ and K_f are scaled by t, and τ is scaled by $1/t$; thus, $K_f\tau$ becomes independent of t.

Results of the calculated resistivity (ρ) are shown in Fig. 2 as a function of the temperature (T) for several doping concentrations. The resistivity monotonically increases with increasing T in a ferromagnetic state for all doping concentrations. In a paramagnetic state, the resistivity still weakly increases, i.e., metallic for $x<0.2$. In the case of $x=0.2$ to 0.25, the T dependence almost vanishes for $T\gtrsim 1.2T_C$. For a
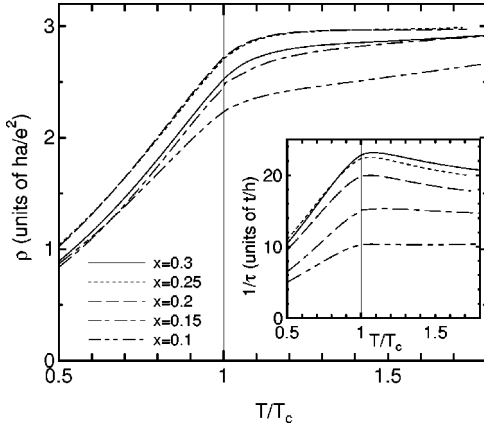
FIG. 2. Calculated resistivity as a function of T/T_C for several doping concentrations. The results for $x=0.2$ and $x=0.25$ are almost the same and are overlapping. The corresponding inverse relaxation time $(1/\tau)$ is shown in the inset.

further high doping concentration, $x>0.2$, the resistivity comes to weakly increase again. On the other hand, the corresponding inverse relaxation time $(1/\tau)$ shown in the inset of the figure shows a different T dependence: it decreases in the paramagnetic state for all cases of x. This difference clearly indicates the importance of the T dependence of K_f since $\rho \propto 1/(K_f \tau)$.

These behaviors in the paramagnetic state can be understood in terms of Fisher and Langer's scheme,[11] although it was originally proposed to analyze the electron transport in the transition-metal ferromagnets. The inverse relaxation time in the DE model can be rewritten as[11]

$$\frac{1}{\tau} \propto \frac{D(E_F)^2}{K_f} \sum_i \Gamma(\vec{R}_i) f(\vec{R}_i), \qquad (9)$$

where $f(\vec{R}_i)$ is the decaying oscillatory function, and $D(E_F)$ is the density of states at the Fermi level. In the case of the transition-metal ferromagnets, $\Gamma(0)$ does not depend on T in the paramagnetic state; thus, the temperature-dependent part of the resistivity is wholly determined by $\Gamma(\vec{R}_i)$ for $\vec{R}_i \neq 0$.[11] In the case of the DE model, however, the term with $\vec{R}_i=0$ depends on T through C as

$$\Gamma(0) \sim 8S_R^2(7C^2 + S_R^2) \quad \text{for} \quad S_R \gg 1, \qquad (10)$$

where C is the correlation function between nearest-neighboring spins. It gives a dominant contribution in $1/\tau$. Further, $D(E_F)(\propto 1/W_f)$ and K_f also depend on T; therefore, the temperature dependence of $1/\tau$ and ρ are given by

$$\frac{1}{\tau} \propto \frac{7C^2 + S_R^2}{W_f^2 K_f}, \qquad (11)$$

$$\rho \propto \frac{7C^2 + S_R^2}{W_f^2 K_f^2}. \qquad (12)$$

These quantities for $x=0.3$ are plotted in Fig. 3 and roughly agree with the calculated results shown in Fig. 2. The rounding of the calculated ρ at very close to T_C, however, must come from $\Gamma(\vec{R}_i)$ at $\vec{R}_i \neq 0$.
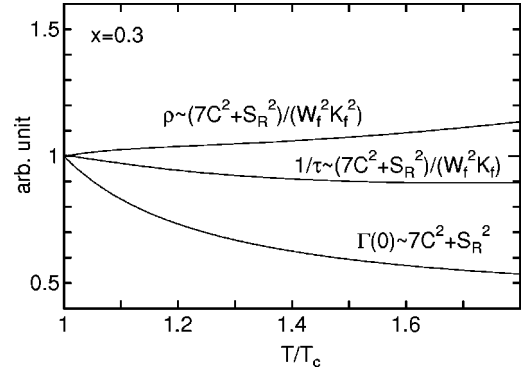

FIG. 3. An approximate temperature dependence of $\Gamma(0)$, $1/\tau$, and ρ obtained by Eqs. (10)–(12), respectively, in the paramagnetic state for $x=0.3$. Each result is normalized by the value at T_C.

It is worth to note that the calculated results in the temperature dependence of the resistivity are different from those in Ref. 12, although the memory function formalism is adopted in both cases. The discrepancy is attributed to the fact that in the present calculation the temperature dependence of the electronic structure, that is, W_f and K_f (shown in Fig. 1), are taken into account, as well as that of $\Sigma_i \Gamma(\vec{R}_i) f(\vec{R}_i)$. In fact, $\Sigma_i \Gamma(\vec{R}_i) f(\vec{R}_i)$ plotted in Fig. 4 shows a peak at $T<T_C$, which is smeared out in the resistivity due to the variation of the electronic structure. The peak structure originates from the process in which bosons in the condensate part are scattered to the noncondensate part, and vice versa.[12] It should be noted that, since the number of condensate bosons is macroscopically large, the lowest order perturbational treatment for such scattering processes might overestimate the scattering amplitude, and the resistivity might become slightly smaller than the present results because of higher-order perturbations. In any case, the resistivity is unlikely to show the peak in the ferromagnetic state.

On the other hand, our results are similar to the previous results by Kubo and Ohata[8] except for the discontinuity in $d\rho/dT$ at T_C. In Ref. 8, only the shortest correlation of scattering ($\vec{R}_i=0$) is included and this is a suitable approximation as discussed above. It should be noted, however, that
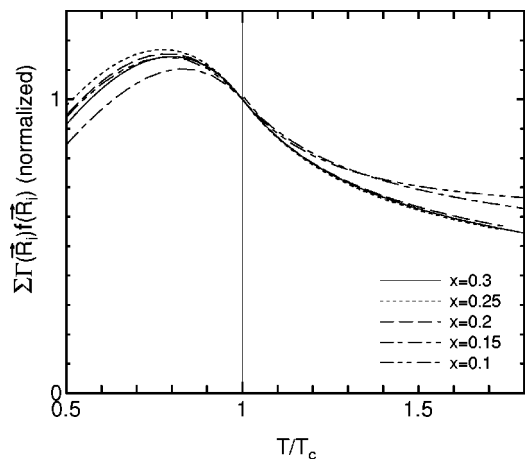

FIG. 4. The temperature dependence of $\Sigma_i \Gamma(\vec{R}_i) f(\vec{R}_i)$ for several doping concentrations. Results are normalized by the value at T_C.

the physical mechanism leading to the weak temperature dependence of the resistivity in the paramagnetic state is completely different. The mechanism is a result of the cancellation between the bandwidth (W_f), the kinetic energy (K_f), and the nearest-neighbor spin correlation (C) in a somewhat complicated manner [Eq. (12)] in our calculations. On the other hand, these quantities used in Ref. 8 are temperature independent in the paramagnetic state. Further, the discontinuity in $d\rho/dT$ at T_C comes from the sudden change of W_f, which is absent in our results since the contribution from $\Gamma(\vec{R}_i)$ with $R_i \neq 0$ is not neglected near T_C and W_f is a smooth function of T. Although our results are also similar to the results by Furukawa,[9] it is likely to be just a coincidence because the spatial correlation of core spins between different sites are neglected and scattering processes responsible for the resistivity are different. It should be noted further that our results qualitatively agree with the recent results by Monte Carlo simulations.[20] For $a = 4$ Å, at T_C, we obtain $\rho \sim 2 \times 10^{-3}$ Ω cm, whose order also agrees with these results.

To conclude, using the Schwinger-boson approach, we have calculated the resistivity in the double-exchange model. In this approach, the fermion bandwidth has been determined by the absolute value of the hopping amplitude giving a physically reasonable temperature dependence in contrast to the conventional Schwinger-boson approach. The resistivity monotonically increases with increasing temperature in the ferromagnetic state, which is different from the previous results in Ref. 12. In the paramagnetic state, the resistivity is dominated by the short-range correlation of scattering. Although the behavior slightly changes depending on the doping concentration, the temperature dependence almost vanishes due to a cancellation between the nearest-neighbor magnetic correlation, the fermion bandwidth, and the fermion kinetic energy. These results imply the importance of the temperature dependence of the electronic structure of the conduction electron in the both ferromagnetic and paramagnetic phases.

The results agree with the experiments for ''higher'' doping concentrations $x \sim 0.3$, where experimentally observed resistivity is relatively low as a whole ($\rho \sim 5 \times 10^{-3}$ Ω cm at T_C) and shows a metallic behavior in the paramagnetic state. For lower concentrations $x \sim 0.2$, however, the experimentally observed singular behavior around the transition temperature and the insulating behavior in the paramagnetic state are not reproduced in our calculations. Other effects might play a crucial role in cooperation with the double-exchange mechanism for the system with such the lower concentration.

[1] K. Chahara, T. Ohono, M. Kasai, Y. Kanke, and Y. Kozono, Appl. Phys. Lett. **62**, 780 (1993).

[2] R. von Helmolt, J. Wecker, B. Holzapfel, L. Schultz, and K. Samwer, Phys. Rev. Lett. **71**, 2331 (1993).

[3] Y. Tokura, A. Urushibara, Y. Moritomo, T. Arima, A. Asamitsu, G. Kido, and N. Furukawa, J. Phys. Soc. Jpn. **63**, 3931 (1994).

[4] S. Jin, T. H. Tiefel, M. McCormack, R. A. Fastnacht, R. Ramesh, and L. H. Chen, Science **264**, 413 (1994).

[5] C. Zener, Phys. Rev. **82**, 403 (1951).

[6] P. W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).

[7] P. G. de Gennes, Phys. Rev. **118**, 141 (1960).

[8] K. Kubo and N. Ohata, J. Phys. Soc. Jpn. **33**, 21 (1972).

[9] N. Furukawa, J. Phys. Soc. Jpn. **63**, 3214 (1994).

[10] P. G. de Gennes and J. Friedel, J. Phys. Chem. Solids **4**, 71 (1958).

[11] M. E. Fisher and J. S. Langer, Phys. Rev. Lett. **20**, 665 (1968).

[12] A. J. Millis, P. B. Littlewood, and B. I. Shraiman, Phys. Rev. Lett. **74**, 5144 (1995).

[13] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).

[14] S. K. Sarker, J. Phys.: Condens. Matter **8**, L515 (1996).

[15] D. P. Arovas and F. Guinea, Phys. Rev. B **58**, 9150 (1998).

[16] M. J. Calderón and L. Brey, Phys. Rev. B **58**, 3286 (1998).

[17] S. Sarker, C. Jayaprakash, H. R. Krishnamurthy, and M. Ma, Phys. Rev. B **40**, 5028 (1989).

[18] H. Mori, Prog. Theor. Phys. **34**, 399 (1965).

[19] W. Götze and P. Wölfle, Phys. Rev. B **6**, 1226 (1972).

[20] M. J. Calderón, J. A. Vergés, and L. Brey, Phys. Rev. B **59**, 4170 (1999).