TRANSPORT PROPERTIES IN A SIMPLIFIED DOUBLE-EXCHANGE MODEL

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Transport properties of the manganites by the double-exchange mechanism are considered. The system is modeled by a simplified double-exchange model, i.e. the Hund coupling of the itinerant electron spins and local spins is simplified to the Ising-type one. The transport quantities such as the electronic resistivity, the thermal conductivity, and the thermal power are calculated by using the dynamical mean-field theory. The transport quantities obtained qualitatively reproduce the ones observed in the manganites. The results suggest that the simplified double exchange model underlies the key properties of the manganites.

Keywords: Strongly correlated electron systems; magnetism; intermediate valence.

1. Introduction

The interesting phenomena in the family of doped manganese oxides \( T_{1-x}D_x\text{MnO}_3 \) have been recently renewed.\(^1\)–\(^4\) As doping \( x \) and temperature \( T \) are varied, these manganites show a rich variety of phases.\(^1\)–\(^4\) Particularly interesting is the doping region \( 0.1 < x < 0.3 \), where the compounds undergo a transition from either insulating or very high resistance metallic, paramagnetic (PM) phase at high temperatures to a ferromagnetic (FM) phase at low temperatures. Near the transition point, the resistivity of the compounds changes by orders of magnitude. The application of a strong magnetic field substantially reduces this effect, thus giving rise to a very large negative magnetoresistance.\(^1\)–\(^4\) Although the physical mechanism which is responsible for the behavior has recently been the subject of much discussion and controversy,\(^1\)–\(^4\) the double-exchange (DE) mechanism\(^5\)–\(^6\) still provides a well-established starting point.\(^1\)–\(^4\) The DE model was proposed by Zener\(^5\) who considered the explicit movement of electrons from the \( \text{Mn}^{3+} \) ion to \( \text{Mn}^{4+} \) ion. There are two simultaneous motions involving electrons moving from the oxygen atom to the \( \text{Mn}^{4+} \) ions and other electrons from the \( \text{Mn}^{3+} \) to the oxygen atom. In the DE process the motion of the itinerant electron favors the ferromagnetic ordering of the local spins and, vice versa, the presence of ferromagnetic order facilitates the motion of the itinerant electron. Hence, only the \( z \)-component part of
the Hund interaction between the local spins and the itinerant electron spin plays an essential role in the DE. In this paper we study the transport properties by a simplified DE (SDE) model where only the $z$-component part of the Hund interaction is incorporated. The SDE model has been studied by several authors. However, the question on whether the SDE model could reproduce qualitatively the transport properties of the manganites is still open. In this paper the transport quantities such as the electronic resistivity, the thermal conductivity and the thermal power are calculated by using the dynamical mean-field theory (DMFT). The DMFT has been extensively used for investigating strongly correlated electron systems. It is based on the fact that the self-energy depends only on the frequency in the infinite-dimension limit. Using the DMFT these transport quantities can be expressed by the spectral function. We find that the SDE model captures the main features of the transport properties of the manganites. These results indicate that the DE process in the manganites can be studied by the SDE model which is much simpler than the full version of the DE model and hence simplifies calculations very much. This provides a starting point to the various variations of the DE mechanism such as randomness, charge or orbital ordering.

The paper is organized as follows. In Sec. 2 we present the SDE model and the background for calculating the resistivity, the thermal conductivity and the thermal power. In Sec. 3 we provide the application DMFT for the SDE model. Numerical result and discussions are presented in Sec. 4. Finally, Sec. 5 concludes the paper.

2. Transport Coefficients in the SDE Model

The physically relevant electrons in the manganites are those from the Mn 3$d$ levels, which are split by the cubic crystal field into triply degenerate $t_{2g}$ levels and higher-energy doubly degenerate $e_g$ levels. Electrons from the $e_g$ levels are able to hop between the Mn sites forming a conduction band, while those from the $t_{2g}$ levels are localized. The itinerant electrons and the local spins are coupled by the Hund interaction. The Hamiltonian we study is described as follows:

$$ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i, \sigma} c_{i\sigma}^\dagger c_{i\sigma} - J \sum_i S_i^z \hat{s}_i^z, \quad (1) $$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the creation (annihilation) operator for an itinerant electron at site $i$ with spin $\sigma$. The first term in the Hamiltonian equation (1) represents the hopping between the nearest neighbor sites. $t$ is the hopping integral and is scaled with the spatial dimension $d$ in the limit $d \to \infty$ as $^9 t = t^*/2\sqrt{d}$. In the following we will take $t^* = 1$ as the unit of energy. In the limit $d \to \infty$, the bare density of states of the itinerant electrons becomes $\rho(\varepsilon) = \exp(-\varepsilon^2)\sqrt{\pi}$ for a hypercubic lattice. $\mu$ is the chemical potential which controls the doping of the itinerant electrons. The last term in the Hamiltonian equation (1) is the Hund coupling between the itinerant electron spin $s_i^z$ and local spin $S_i^z$. Here, only the $z$ component (Ising interaction) is concerned. This simplification does not allow any
spin flip processes which can be important at low temperature where spin-wave excitations may govern the thermal dynamics of the system. However, as we have noticed, in the DE processes the spins of the itinerant electron and the local electron favored to parallel each other, hence, the Ising part of the Hund interaction plays a dominant role. The DMFT calculations for the DE model with classical local spins show that the simplification of the Hund coupling does not change the self energy of the single particle Green function.\(^{10}\) Moreover, within the DE model the DMFT results of quantum local spins does not show significant differences from the ones of classical local spins.\(^{11}\) Thus one expects that within the DMFT the simplification of the Hund interaction does not result in serious backwardness. With the simplified Hund coupling the ferromagnetic state along \(z\)-axis will be naturally favorable for decreasing the free energy at low temperature. Meanwhile, the spin of itinerant electron has the ferromagnetic type coupling with the local spin so that the ground state will be spin polarized resulting in the half metal if the coupling \(J\) becomes large. The half-metal nature of the ground state is expected to be exhibited in the transport properties, as we will show later. In this paper we will consider the local spins with their actual value \(S = \frac{3}{2}\) of \(t_{2g}\) level.

The transport quantities are calculated within the Kubo–Greenwood formalism.\(^{12}\) Within this formalism the DC-conductivity \(\sigma\), the thermal power \(S\) and the thermal conductivity \(\kappa\) can be expressed with the relevant correlation functions of the current operators. We have\(^{12}\)

\[
\sigma = \frac{e^2 T}{L^{11}},
\]

\[
S = \frac{1}{eT} L^{12},
\]

\[
\kappa = L^{22} - \frac{(L^{12})^2}{L^{11}},
\]

where coefficients \(L^{11}, L^{22}\) are determined from the analytic continuation of the relevant current–current correlation function at zero frequency, i.e.

\[
L^{ij} = \lim_{\nu \to 0} T \text{Im} \frac{\tilde{L}^{ij}(\nu)}{\nu}.
\]

Here \(\tilde{L}^{ij}(\nu)\) is the current–current correlation functions

\[
\tilde{L}^{11}(i\nu_n) = \int_0^\beta d\tau e^{i\nu_n \tau} \langle T_\tau j(\tau) j(0) \rangle, 
\]

\[
\tilde{L}^{12}(i\nu_n) = \int_0^\beta d\tau e^{i\nu_n \tau} \langle T_\tau j(\tau) j_Q(0) \rangle, 
\]

\[
\tilde{L}^{22}(i\nu_n) = \int_0^\beta d\tau e^{i\nu_n \tau} \langle T_\tau j_Q(\tau) j_Q(0) \rangle, 
\]

where \(j\) and \(j_Q\) are the particle-current operator and the heat-current operator, respectively. The particle-current operator is defined by taking commutator of the
Hamiltonian with the polarization operator $\sum_i \mathbf{R}_i n_i$. After some algebraic calculations we obtain:

$$j = \sum_q v_q c^\dagger_{q\sigma} c_{q\sigma},$$

(9)

where the velocity $v_q = \nabla_q \epsilon(q)$, and $\epsilon(q)$ is the dispersion of the noninteracting electrons. The heat current $j_Q$ can be determined by the energy current $j_E$ and the particle current $j$ through the equation $j_Q = j_E - \mu j$. The energy-current is defined by taking the commutator of the Hamiltonian with the energy polarization operator $P_i R_i h_i (where H = \sum_i h_i)$. We obtain:

$$j_Q = \sum_{q\sigma} v_q [\epsilon(q) - \mu] c^\dagger_{q\sigma} c_{q\sigma} - \frac{1}{2} \sum_{q,q'\sigma} J\sigma S(q - q') (v_{q'} + v_q) c^\dagger_{q\sigma} c_{q\sigma},$$

(10)

where $S(q - q') = \frac{i}{\hbar} \sum_i S_i^z e^{-i(q-q') R_i}$. Substituting $j$ and $j_Q$ from Eqs. (9) and (10) into Eqs. (6), (7) and (8), the transport coefficients are able to be calculated within the DMFT$^{13,14}$:

$$L^{11} = T \sum_{\sigma} \int d\rho(\epsilon) \int d\omega \left(-\frac{\partial f(\omega)}{\partial \epsilon}\right) A_{\sigma}^2(\epsilon, \omega),$$

(11)

$$L^{12} = T \sum_{\sigma} \int d\rho(\epsilon) \int d\omega \left(-\frac{\partial f(\omega)}{\partial \epsilon}\right) A_{\sigma}^2(\epsilon, \omega) \omega,$$

(12)

$$L^{22} = T \sum_{\sigma} \int d\rho(\epsilon) \int d\omega \left(-\frac{\partial f(\omega)}{\partial \epsilon}\right) A_{\sigma}^2(\epsilon, \omega) \omega^2,$$

(13)

where $f(\omega) = 1/(\exp(\omega/T) + 1)$ is the Fermi–Dirac distribution function and $A_{\sigma}(\epsilon, \omega) = -\text{Im} G_{\sigma}(\epsilon, \omega)/\pi$ is the spectral function of the Green function $G_{\sigma}(\epsilon, \omega)$ of the itinerant electrons. In deriving formulas (11)–(13) the vertex corrections to the current–current correlation functions have been neglected. It has been shown that the vertex corrections vanish in the limit $d \to \infty$.$^{14}$ In such the way the transport coefficients are fully determined by the single-particle spectral function.

3. Application the DMFT for the SDE Model

We solve the SDE model (1) by the DMFT.$^9$ The DMFT is based on the infinite dimension limit. In the infinite dimension limit the self-energy is pure local and does not depend on momentum. The Green function of the itinerant electrons with spin $\sigma$ satisfies the Dyson equation:

$$G_{\sigma}(k, \omega) = \frac{1}{\omega - \epsilon(k) + \mu - \Sigma_{\sigma}(\omega)},$$

(14)

where $\epsilon(k) = -2t \sum_\alpha \cos(k_\alpha)$ is the dispersion of the free itinerant electrons on a hypercubic lattice, and $\Sigma_{\sigma}(\omega)$ is the self-energy which depends only on frequency.
The self-energy is determined by solving an effective single-site problem. The action of this effective problem is

\[ S_{\text{eff}} = - \int d\tau \int d\tau' \sum_{\sigma} c_\sigma^\dagger(\tau) G_\sigma^{-1}(\tau - \tau') c_\sigma(\tau') + J \int d\tau S^z \sum_{\sigma} \sigma c_\sigma^\dagger(\tau) c_\sigma(\tau), \]

where \( G_\sigma(\tau - \tau') \) is the Green function of an effective medium. It plays as the bare Green function of the effective problem. The local Green function also satisfies the Dyson equation:

\[ G_\sigma^{-1}(\omega) = G_\sigma^{-1}(\omega) - \Sigma_\sigma(\omega). \]

The local Green function \( G_\sigma(\omega) \) of the effective single-site problem is solely determined by the partition function. It can be calculated by the equation:

\[ G_\sigma(i\omega_n) = \frac{\delta \ln Z_{\text{eff}}}{\delta G_\sigma^{-1}(i\omega_n)}, \]

where \( Z_{\text{eff}} \) is the partition function, and \( \omega_n = (2n + 1)\pi T \) is the Matsubara frequency. The self-consistent condition of the DMFT requires the local Green function \( G_\sigma(\omega) \) obtained within the effective problem must coincide with the local Green function of the original lattice, i.e.

\[ G_\sigma(\omega) = \frac{1}{N} \sum_k G_\sigma(k, \omega) = \int d\rho(\epsilon) \frac{1}{\omega - \epsilon + \mu - \Sigma_\sigma(\omega)}. \]

Eqs. (16)–(18) form the self-consistent equations for determining the self-energy, and hence, also the Green function of the original lattice. Within the effective single-site problem, the partition function becomes

\[ Z_{\text{eff}} = \text{Tr} \int Dc_\sigma^\dagger Dc_\sigma e^{-S_{\text{eff}}}, \]

where the trace is taken over \( S^z \). This partition function can be calculated exactly. It is similar to DMFT solving the Falicov–Kimball model. Indeed, within the action (15) the dynamics of the local spins is independent, and hence, we can take the trace over \( S^z \) independently. We obtain

\[ Z_{\text{eff}} = 4 \sum_m \exp \left\{ \sum_{n\sigma} \ln(G_\sigma^{-1}(i\omega_n) - J\sigma m) - \ln[i\omega_n] e^{i\omega_n0^+} \right\} \]

where \( m = -3/2, -1/2, \ldots, 3/2 \) is the projection of the local spin \( S^z \) on \( z \) axis. Using Eq. (16) we obtain the local Green function on real axis after taking analytical continuation:

\[ G_\sigma(\omega) = \sum_m \frac{w_m}{G_\sigma^{-1} - J\sigma m}, \]

where

\[ w_m = \frac{1}{Z_{\text{eff}}} \exp \left\{ -\beta \int d\omega f(\omega) \frac{1}{\pi} \text{Im} \sum_\sigma \ln[G_\sigma^{-1}(\omega) - J\sigma m] \right\}. \]
Equation (21) is similar to the one with the classical local spin. It can be considered as a generalized formula of the local Green function for any value of the local spins. Equations (16), (18) and (21) form complete self-consistent equations of the DMFT.

4. Numerical Results
In this section we present the solution of the self-consistent DMFT Eqs. (16), (18) and (21). The self-energy and the Green function are obtained by iterations. The algorithm for determining the Green function is as follows.

(i) Begin with an initial self-energy for each spin (for example $\Sigma_\uparrow = 0.5$ and $\Sigma_\downarrow = 0.0$).
(ii) Then Eq. (18) is used to find the local Green function.
(iii) Substituting $\Sigma_\sigma$ in (i) and $G_\sigma$ were calculated in (ii) to Eq. (16) we calculate $G_\sigma$.
(iv) Putting $G_\sigma$ into Eq. (21) we find $G_\sigma$.
(v) From these $G_\sigma$ and $G_\sigma$ were determined in (iii) and together with Eq. (16) a new self energy $\Sigma_\sigma$ is obtained.

Thereafter go back to Step (ii) and repeat the iteration until convergence is reached. In all our calculations, the relative error for the Green function of less than $10^{-7}$ is used to stop the iteration loop. With the obtained Green function we calculate the electronic resistivity, the thermal conductivity and thermal power by Eqs. (11)–(13).

In Fig. 1 we present the temperature dependence of the resistivity for different electron doping $n$ and the Hund coupling constant $J$. Figure 1(a) shows the case of quarter filling ($n = 0.5$). The temperature dependence of the resistivity shows the metallic behavior ($d\rho/dT > 0$). The kink in the resistivity curve indicates the FM transition. Immediately below the transition temperature the resistivity declines with decreasing temperature due to the reduction of the magnetic contribution to electron scattering. Hence, the low temperature phase is the metallic FM. The change of the resistivity near the FM transition by an order of magnitude has been observed experimentally. Figure 1(b) shows the temperature dependence of the resistivity for half-filling ($n = 1$). In this case the system may exhibit the metallic ($d\rho/dT > 0$) or the “semiconductor” ($d\rho/dT < 0$) behavior depending on the temperature $T$ and the Hund coupling $J$. As in Fig. 1(a), the kink in the resistivity curve corresponds to the FM transition temperature. For $J = 2$, the resistivity curve shows the transition from the “semiconductor” paramagnetic to the metallic FM, while for $J = 4$ both phases below and upper the transition temperature exhibit semiconductor-like behavior. However, careful analysis of the density of states (DOS) shows that the low temperature phase (below the FM transition temperature) is never a semiconductor but a half metal as we have noticed. Indeed, in Fig. 2 we present the DOS for various doping $n$ and Hund coupling $J$. For low doping $n = 0.5$ the chemical potential always lies within the lower band, hence the
system exhibits the metallic behaviors. For half-filling \( n = 1 \) at high temperature (upper the FM transition temperature) the chemical potential lies in the gap, hence the system is either semiconductor or insulator. However, the Zeeman splitting due to the Hund coupling FM ground state of the SDE model show a perfect spin polarization, and the ground state is thus half metal. The half metal behavior has also been observed experimentally in the manganites.\textsuperscript{16,17} One also notices that at half-filling \((n = 1)\) (Fig. 2(b)) for weak and intermediate Hund coupling (for example, \( J = 2 \)) in the FM ground state the chemical potential lies within the overlap of the bands of two spin species, hence the resistivity exhibits the metallic behavior (Fig. 1(b)). For strong Hund coupling (for example, \( J = 4 \)) at half-filling \((n = 1)\) (Fig. 2(b)) the chemical potential lies neither in the band of spin-up nor spin-down, hence the resistivity exhibits the semiconductor-like behavior at low temperature (below the FM transition temperature), although the system is half metal. Moreover, at low temperature the DOS for spin-up and spin-down are clearly separated. This indicates that the FM state is stabilized at low temperature.

The behaviors of the DOS also reflect on other transport properties such as thermal conductivity and thermal power. In Fig. 3(1) we present the temperature dependence of the thermal conductivity \( \kappa(T) \) for various electron doping and Hund coupling. As \( T \to 0 \) the thermal conductivity tends towards zero. However, for \( n = 0.5 \) the thermal conductivity always decreases with lowering temperature, while for \( n = 1 \) the thermal conductivity peaks, and then tends to zero as \( T \to 0 \). In Fig. 3(2) we plot the temperature dependence of the thermal power \( S(T) \). As \( T \to 0, S(T) \to 0 \), this feature reflects the metallic behavior of the FM ground state.
Fig. 2. Density of states (DOS) of itinerant electron with spin-up and spin-down as a function of frequency at different temperatures \( T \) for (a) \( n = 0.5 \) and (b) \( n = 1.0 \).

Fig. 3. Temperature dependence of the thermal conductivity \( \kappa(T) \) (on the left (1)) and the thermal power \( S(T) \) (on the right (2)) for different electron fillings: (a) \( n = 0.5 \) and (b) \( n = 1.0 \).

It is consistent with the DOS behavior which we have already analyzed above. One notices that the present SDE model could not explain the change of sign of the thermal power which has been observed experimentally in manganites.\(^1\) However, the feature is neither explained by the DE model.\(^2,10\) Perhaps, the feature is beyond the DE mechanism.
5. Conclusions

In this paper, we have considered the transport properties in the SDE model by employing the DMFT. Although the manganites are too complicated to be described completely by this simple model, the obtained transport properties qualitatively reproduce the ones observed in the manganites. The results show that the present simplified model could capture main features of the full DE model. This suggests that the DE processes can be studied by the SDE model, and hence, calculations are simplified. The SDE model provides a good starting point towards complex variations of the DE mechanism such as randomness, charge or orbital ordering.

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