Magnetoresistance of the Double-Exchange Model in Infinite Dimension

Nobuo FURUKAWA

Institute for Solid State Physics,
University of Tokyo, Roppongi 7-22-1,
Minato-ku, Tokyo 106

Abstract

Double-exchange model in infinite dimension is studied as the strong Hund’s coupling limit \( J \to \infty \) of the Kondo lattice model. Several quantities such as Green’s function and the d.c. conductivity are calculated in analytical forms. Magnetoresistance in lightly doped \( \text{La}_{1-x}\text{Sr}_x\text{MnO}_3 \) is reproduced very well.

KEYWORDS: Transition-metal oxide, transport properties, giant magnetoresistance, double-exchange model, infinite dimensions
Physics of the strongly correlated electron systems is one of the most challenging fields in the material science. Especially, after the discovery of the high-$T_c$ superconducting oxides, many related compounds of 3$d$ transition-metal oxides have been revisited in an extensive way. One of such materials is the manganese oxides with the perovskite-type structure $R_{1-x}A_xMnO_3$, where $R$ and $A$ denote trivalent rare-earth ions and divalent alkaline-earth ions, respectively. The most eminent feature in this family of materials is the giant magnetoresistance (MR) with negative sign. In the experiment of $La_{1-x}Sr_xMnO_3$, the negative MR value is scaled at the small magnetization region as

$$\frac{\rho(0) - \rho(M_{\text{tot}})}{\rho(0)} = C_{\text{exp}} \left( \frac{M_{\text{tot}}}{M_s} \right)^2,$$

where the coefficient $C_{\text{exp}}$ is nearly temperature-independent. Here, $M_{\text{tot}}$ and $M_s = 4\mu_B$ are the total magnetization and the nominal saturation magnetization, respectively, and $\rho$ is the resistivity.

From the theoretical point of view, the author has calculated the Kondo lattice model with Hund’s ferromagnetic coupling in the infinite-dimensional limit $D = \infty$ and the infinite high-spin limit $S = \infty$. Results with respect to MR as well as optical conductivity and magnetic transition temperature are in good agreement with experimental data of $La_{1-x}Sr_xMnO_3$. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{ij,\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - J \sum_i \vec{\sigma}_i \cdot \vec{m}_i,$$

where $\vec{m}_i = (m_i^x, m_i^y, m_i^z)$ and $|\vec{m}|^2 = 1$. Here, itinerant fermions and localized spins represent electrons in $e_g$ orbitals and $t_{2g}$ orbitals of Mn ions, respectively. Fermion concentration in $La_{1-x}Sr_xMnO_3$ is nominally considered to be $n = 1 - x$. From the recent band calculation, the bandwidth of the itinerant electron is estimated to be $W \sim 1\text{eV}$. Since Hund’s coupling is considered to be larger than the bandwidth, the system is regarded to be in the strong coupling region. In the limit $J/W = \infty$, the model is identical to the double-exchange model.

Although the experimental results have been well explained by the above model at finite $J/W$, it is still worthwhile to examine the properties at $J/W \to \infty$: As we will show below, several quantities such as Green’s functions and d.c. conductivity are calculated analytically in a simple form, which helps us to obtain physical intuition on properties of the model in the strong coupling region. Analytical expressions are also convenient for
the data analysis in experimental and numerical researches. In this paper, we study the double-exchange model in $D = \infty$ as the strong coupling limit $J/W \to \infty$ of the Kondo lattice model with $S = \infty$.

Infinite-dimensional system is investigated using the effective single-site approach. Green’s function is obtained exactly as

$$ G = \left\langle \left( G_0^{-1} + J \vec{m} \vec{\sigma} \right)^{-1} \right\rangle, \quad (3) $$

where the thermal average $\langle \cdots \rangle$ is taken with respect to the orientation of the local spin $\vec{m}$. Self-energy is given by $\Sigma = G_0^{-1} - G^{-1}$. The Weiss field $G_0$ should be determined self-consistently from

$$ G_0^{-1} = G_{\text{loc}}^{-1} + \Sigma, \quad (4) $$

$$ G_{\text{loc}} = \int d\varepsilon N_0(\varepsilon) [i\omega_n - (\varepsilon - \mu) - \Sigma]^{-1}. \quad (5) $$

Here we consider the case of the Lorentzian density of states with the bandwidth $W$, $N_0(\varepsilon) = \frac{1}{\pi} \cdot \frac{W}{(\varepsilon^2 + W^2)}$.

At $J \gg W$, the spectral weight splits into two sub-bands at $\omega \sim \pm J$. Since we restrict ourselves to the hole doped case $n < 1$, we may treat the lower sub-band only. Therefore, we describe the chemical potential as $\mu = -J + \delta \mu$ where $\delta \mu = O(W)$. From the self-consistency equation, $G_0$ is given by

$$ G_0(\omega + i\eta) = (\Omega - J + iW)^{-1}. \quad (6) $$

Here, $\Omega \equiv \omega + \delta \mu = O(W)$ is the energy which is measured from the center of the lower sub-band $-J$.

Magnetic field in the $z$ direction is applied to the localized spins in the paramagnetic phase, and the induced magnetization is expressed as $M = \langle m_z \rangle$. From eqs. (3) and (6), Green's function is given by

$$ G_\sigma(\omega + i\eta) = \frac{(\Omega - J + iW) - J M \sigma}{(\Omega - J + iW)^2 - J^2} $$

$$ = \frac{1 + M \sigma}{2} \frac{1}{\Omega + iW} + O(1/J). \quad (7) $$

At $J/W \to \infty$, the spectral weight is calculated as

$$ A_\sigma(\omega) = -\text{Im} \frac{G_\sigma(\omega + i\eta)/\pi}{1 + M \sigma \cdot \frac{1}{\pi \Omega^2 + W^2}}. \quad (8) $$
We see that the center of the spectral weight is indeed shifted to $-J$. The amplitude of $A_\sigma$ is proportional to the population of the local spin parallel to $\sigma$, which indicates that the electronic states that are anti-parallel to the local spin are projected out.

The self-energy is calculated from eqs. (6) and (7) as

$$\Sigma_\sigma(\omega + i\eta) = -J - \frac{1 - M\sigma}{1 + M\sigma}(\Omega + iW). \quad (9)$$

Then, eq. (9) gives $\Re \Sigma \sim -J$, so the shift in $\mu$ is self-consistently justified again. We also see $\Im \Sigma = -W$ at $M = 0$, which means that the quasi-particle excitation is very incoherent; the lifetime of a quasi-particle is comparable with the length of time that an electron transfers site to site. In the strong coupling region, quasi-particles loose their coherence in a macroscopic scale due to the inelastic scattering by thermally fluctuating spins. The divergence of $\Im \Sigma_\sigma$ is observed at $M\sigma \to -1$, in accordance with the diminishment of $A_\sigma$, since the propagation of the quasi-particle with spin anti-parallel to the magnetization is energetically forbidden at $\omega \sim -J$.

Now, we calculate the MR value. At finite $J/W$, the MR value has been obtained from the Kubo formula as

$$\frac{\rho(0) - \rho(M)}{\rho(0)} = CM^2 \quad (10)$$

at small magnetization regime, where $C$ is a function of $x$ and $J/W$. We have $C = 1$ at $J \ll W$, and $C$ increases as $J/W$ is increased. Here we study the limit $J/W \to \infty$.

Conductivity in infinite dimension is calculated from the formula

$$\sigma_{dc} = \sigma_0 W^2 \sum_\sigma \int N_0(\epsilon) d\epsilon \int d\omega \left( -\frac{\partial f}{\partial \omega} \right) A_\sigma^2(\epsilon, \omega), \quad (11)$$

$$A_\sigma(\epsilon, \omega) = -\frac{1}{\pi} \frac{\text{Im} \Omega}{\omega - (\epsilon - \mu) - \Sigma_\sigma(\omega + i\eta)}, \quad (12)$$

where $f$ is the Fermi distribution function. The constant $\sigma_0$ gives the unit of conductivity. Hereafter we restrict ourselves to the low temperature regime $T \ll W$. From eqs. (9), (11) and (12), we have

$$\sigma_{dc}(M) = \sigma_{dc}(0) \times r(M), \quad (13)$$

$$r(M) = \frac{1 + 3(1 + B)M^2 + BM^4}{1 - M^2}, \quad (14)$$
where $\sigma_{dc}(0)$ and $B$ are functions of the hole concentration $x$,

$$
\frac{\sigma_{dc}(0)}{\sigma_0} = \left(\frac{1 - \cos 2\pi x}{2\pi}\right) \times \left(\frac{2 - \cos 2\pi x}{4\pi}\right),
$$

(15)

$$
B = \frac{\cos 2\pi x}{2 - \cos 2\pi x}. \quad (16)
$$

Here we have used the relation $\delta\mu/W = \cot \pi x$ derived from eq. (8) at $T \ll W$. From eqs. (13) and (14), we have

$$
\frac{\rho(0) - \rho(M)}{\rho(0)} = \frac{(4 + 3B)M^2 + BM^4}{1 + (3 + 3B)M^2 + BM^4}, \quad (17)
$$

so that

$$
C = \frac{8 - \cos 2\pi x}{2 - \cos 2\pi x}. \quad (18)
$$

We see that $C$ monotonically decreases as $x$ is increased; the maximum is $C = 7$ at $x \to 0$ and the minimum is $C = 3$ at $x = 0.5$.

Let us now make a comparison between the above result and the experimental data in La$_{1-x}$Sr$_x$MnO$_3$. In this case, we should scale the magnetization with $M_{tot}/M_s$. Since $3d$ electrons in La$_{1-x}$Sr$_x$MnO$_3$ form localized $S = 3/2$ spins and mobile electrons, we have $M_{tot} = \frac{3}{2}M + M_e$ and $M_s = 2$. Here, $M_e \equiv \frac{1}{2} \langle n^+ \rangle - \langle n^- \rangle = \frac{1}{2}(1 - x)M$ is the magnetization of itinerant electrons in the limit $J/W \to \infty$. In Fig. 1, $\rho(M_{tot})/\rho(0)$ at $x = 0.175$ is shown as a function of $M_{tot}/M_s$. The experimental data at $x = 0.175$ and $T = 294K$ is taken from ref. 1. The result at $J/W \to \infty$ shows excellent agreement with the experimental data of La$_{1-x}$Sr$_x$MnO$_3$ at $M_{tot}/M_s < 0.2$. It should be noted that no adjustable parameter is used here.

In Fig. 1, the result at $J/W = 4$ and $x = 0.175$ is also shown. Here, $\sigma_{dc}$ and $M_e$ are obtained numerically. We see that at $J/W = 4$, the MR value is already in the strong coupling limit. Therefore, together with the previous study, we see that in the whole range of $J/W$ the MR value is expressed as in eq. (10) at $M \ll 1$.

The experimental data show that the coefficient in eq. (1) is $C_{exp} \approx 1$ at the heavily doped metallic system. As the hole concentration is decreased, the value of $C_{exp}$ increases. In the vicinity of the metal-insulator transition $x \sim 0.15$, it approaches the maximum value $C_{exp} \approx 4$. Enhancement of $C_{exp}$ gives stronger responses to the magnetic field in the resistivity, which is an important feature for applications. In La$_{1-x}$Sr$_x$MnO$_3$ at $x = 0.175$, the MR value seems to be already in the strong coupling limit. Therefore, further increase
in $C_{\text{exp}}$ can not be expected in this material by increasing the value of $J/W$ in a chemical way. The present result shows that $C$ is upper-bounded; at maximum, the increase of $C$ is slightly less than one order of magnitude. From the point of view of making sensitive MR devices, it should be better to make attempts in other directions than increasing the value of $C_{\text{exp}}$.

In order to obtain the MR value quantitatively, it is necessary to calculate the magnetization dependence of Green’s functions in a proper way. At present, it seems that the infinite-dimensional approach is the most powerful and successful method to investigate the properties of lightly doped La$_{1-x}$Sr$_x$MnO$_3$ in the weakly magnetized incoherent-metal state, since it can handle thermal fluctuations in a proper way. Nevertheless, we see the discrepancy between the theoretical result and the experimental data as the magnetization is increased. Due to the decrease in the magnitude of the thermal fluctuation of spins, quasi-particle excitation recovers its coherence. Then, in this region, spatial correlations should also play important roles. Further study seems to be necessary to explain the MR value in the whole region of $M$.

Recently, Millis et al.\cite{Millis} have studied the resistivity of the double-exchange model, emphasizing the role of the nearest-neighbor correlation of local spins. They have obtained the increase of the resistivity as the magnetic moment is increased, which not only fails to explain the experimental results but also is against the physical intuition. The discrepancy seems to be mainly due to the total neglect of the thermal fluctuation of local spins and its effect to the self-energies, which should not be justified near the paramagnetic region. In contrast to their conclusion, it seems to be clear that the double-exchange model do explain the MR of the lightly doped La$_{1-x}$Sr$_x$MnO$_3$.

To summarize, double-exchange model in infinite dimension with the Lorentzian density of states is studied as the strong coupling limit of the Kondo lattice model. Exact Green’s function is obtained analytically. Resistivity as a function of magnetization is expressed in a simple form. The MR values in La$_{1-x}$Sr$_x$MnO$_3$ are well reproduced without any adjusting parameters.

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Fig. 1: Total magnetization dependence of the resistivity $\rho(M_{tot})/\rho(0)$ at $x = 0.175$. The solid (dotted) curve show the theoretical result at $J/W = \infty$ ($J/W = 4$). The dots in the figure shows the experimental data.
References

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

[2] A. Urushibara, Y. Morimoto, T. Arima, A. Asamitsu, G. Kido and Y. Tokura: preprint.

[3] N. Furukawa: J. Phys. Soc. Jpn. 63 (1994) 3214.

[4] N. Furukawa: in Proc. 17th Taniguchi International Conference, edited by A. Fujimori and Y. Tokura (Springer Verlag, Berlin, 1995).

[5] N. Furukawa: preprint, SISSA:cond-mat/9505009.

[6] N. Hamada: private communication.

[7] K. Kubo and N. Ohata: J. Phys. Soc. Jpn. 33 (1972) 21.

[8] C. Zener: Phys. Rev. 82 (1951) 403.

[9] A. J. Millis, P. B. Littlewood and B. I. Shraiman: preprint, SISSA:cond-mat/9501034.