MAGNETIC AND TRANSPORT PROPERTIES OF (La,Sr)MnO$_3$

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Magnetic and transport properties of the perovskite-type 3$d$ transition-metal oxide (La,Sr)MnO$_3$ are theoretically studied using the double-exchange model in infinite dimension. Magnetoresistance properties as well as the magnetic transition temperatures are in good agreement with the experimental data.

Keywords: colossal magnetoresistance, double-exchange model, (La,Sr)MnO$_3$

§1. INTRODUCTION

After the discovery of the high-$T_c$ superconducting oxides, many strongly correlated 3$d$ electron systems have been reinvestigated. Recently, perovskite-type manganese oxides (R,A)MnO$_3$ have been studied extensively. The above group of materials exhibit colossal magnetoresistance (MR) at the carrier doped region, which is interesting not only from the standpoint of strongly correlated systems but also from application. Under appropriate hole doping, the system becomes a ferromagnet which is explained by a double-exchange mechanism [1, 2].

Transport properties for filling-controlled single crystals of La$_{1-x}$Sr$_x$MnO$_3$ have been investigated systematically [3, 4]. It has been made clear that the resistivity is controlled by the magnetization of the system. In either case of applying external magnetic field or lowering the temperature below the Curie point, the resistivity behaves universally as a function of induced or spontaneous magnetization. In the small magnetization region, the universal scaling function is given by $\rho(M)/\rho(0) = 1 - C(M/M_{\text{sat}})^2$, where $\rho(M)$ is the resistivity and $\rho(0)$ is its zero-field value. Here $M$ is the magnetization while $M_{\text{sat}}$ is its saturated value. This experimental fact shows that the magnetism and the transport properties are strongly correlated. The experimental data also show that the coefficient is $C \approx 4$ at $x \approx 0.175$, and the value of $C$ decreases as the hole concentration $x$ is increased.

In this paper, we investigate the mechanism of the colossal MR responses in this family of manganese oxides.

§2. MODEL AND RESULTS

In this paper, we study the double-exchange model (or the Kondo lattice model with ferromagnetic spin couplings) as a microscopic model for manganese oxides. We assume that the 3$d$ electrons in $t_{2g}$ orbitals form localized spins while electrons in $e_g$ orbitals form itinerant band. Localized spins and band electrons are strongly coupled with Hund’s interaction. The Hamiltonian is described as

$$\mathcal{H} = -t \sum_{<ij>,\sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) - J \sum_i \vec{\sigma}_i \cdot \vec{m}_i, \quad (1)$$

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where \( \vec{m}_i = (m_{ix}, m_{iy}, m_{iz}) \) is the classical spin with normalization \(|\vec{m}|^2 = 1\). In the infinite-dimensional limit \( D \to \infty \), Green’s function as well as magnetic transition temperatures and conductivity are obtained exactly \([5]\). We consider the Bethe lattice so that the density of states (DOS) is semicircular with the bandwidth \( W \). The action of the system has the form

\[
S(\tilde{G}_0, \vec{m}) = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \Psi^*(\tau_1) \tilde{G}_{0}^{-1}(\tau_1 - \tau_2) \Psi(\tau_2) \\
- J \int_0^\beta d\tau \vec{m} \cdot \Psi^*(\tau) \vec{\sigma} \Psi(\tau),
\]

(2)

where \( \Psi \) and \( \Psi^* \) are the Grassmann variables and \(|\vec{m}| = 1\). Green’s function \( \tilde{G}_0 \) is the Weiss field which contains the information about the electron transfer and the interaction.

Figure 1 shows the Curie temperature \( T_c \) as a function of doping concentration \( x \), together with the experimental data of \( \text{La}_{1-x}\text{Sr}_x\text{MnO}_3 \) \([4]\). Here we assume \( W = 1\text{eV} \) as a unit of energy, and the experimental data are also scaled by \( W \). Increase of \( T_c \) is observed as the hole concentration \( x \) is increased due to the increase of the kinetic energy. For the set of parameters \( W \simeq 1\text{eV} \) and \( J/W \simeq 4 \), we see that the Curie temperatures of \( \text{La}_{1-x}\text{Sr}_x\text{MnO}_3 \) at \( 0.1 \lesssim x \lesssim 0.2 \) are well reproduced by the above simplified model \([6]\).

Now we calculate the MR curve. Conductivity is calculated from the Kubo formula. Since vertex corrections vanish in infinite dimension \([7]\), we have

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

(3)
where constant $\sigma_0$ gives the unit of conductivity and $f$ is the Fermi distribution function. The spectral weight $A_{\sigma}(\epsilon, \omega)$ is defined by

$$A_{\sigma}(\epsilon, \omega) = -\frac{1}{\pi} \text{Im} \left( \frac{1}{\omega - (\epsilon - \mu) - \Sigma_{\sigma}(\omega + i\eta)} \right).$$

The resistivity $\rho = 1/\sigma_{dc}$ and the magnetization $M$ is calculated as a function of temperature and the external magnetic field.

In Fig. 2, we show $\rho(M)/\rho(0)$ at $x = 0.175$ as a function of magnetization for the cases of applying the external magnetic field $H$ and changing temperature $T$ below the Curie temperature. Here we take $J/W = 4$. We then make a comparison with the experimental data of La$_{1-x}$Sr$_x$MnO$_3$ at $x = 0.175$ [4]. In Fig. 2, we also plot the resistivity at $T = 294K$ as a function of induced magnetization normalized by its zero-field value. Temperature dependence of the resistivity below $T_c$ with an appropriate normalization is also shown as a function of spontaneous magnetization. The experimental result for La$_{1-x}$Sr$_x$MnO$_3$ is well reproduced in a quantitative way. We see that the magnetization is the essential thermodynamical variable that determines the MR response.

The MR curve is obtained analytically if we consider the case of Lorentzian DOS with $J \to \infty$ [3]. Using the Kubo formula, we obtain

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

where

$$B = \frac{\cos 2\pi x}{2 - \cos 2\pi x}.$$
The result at $x = 0.175$ is in good agreement with the experimental data of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ at $x = 0.175$. At $M \ll 1$, we have

$$\frac{\rho(M)}{\rho(0)} = 1 - \frac{8 - \cos 2\pi x}{2 - \cos 2\pi x}M^2.$$  \hspace{1cm} (7)

We see that $C$ monotonically decreases as $x$ is increased.

\section*{§3. DISCUSSION}

Thus we see that the double-exchange model reproduces the universal curve of MR observed in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$. The mechanism of the MR as well as the metallic ferromagnetism are well understood from this minimal model. We still have to emphasize here that the double-exchange model is merely an effective model where many kind of degrees of freedom are reduced. In manganese oxides, we have to deal with electrons in Mn $3d\,t_{2g}$, $e_g$ and O $2p$ orbitals. We obtain the double-exchange model as a consequence of neglecting high-energy excitations as well as renormalizing Coulomb interactions and lattice effects. Therefore, we should always regard the model as the renormalized model with parameters $t = t_{\text{eff}}$ and $J = J_{\text{eff}}$ in eq. (1). Or, in a strict sense, we should consider the action of the double-exchange model in eq. (2) with renormalized Green’s function $G_{\text{eff}}$ and the coupling strength $J_{\text{eff}}$.

In the strong coupling limit $J \to \infty$, the only relevant parameter for the MR curve in the normalized form $\rho(M)/\rho(0)$ is the carrier number $x$. Therefore, as long as the MR curve is concerned, the double-exchange model is the relevant model, since it does not depend on other microscopic parameters. Of course, such renormalization is only valid in a certain range of parameters which flow to the double-exchange fixed point. Study of such renormalization flow is important in order to specify what region of A site atom combination in the family of manganese oxides does the MR response reproduced by the above simplified double-exchange model.

There are still many thermodynamical quantities that can not be explained by the double-exchange model alone. One example is the absolute value of the resistivity which should depend on microscopic parameters. It is also affected by the renormalization of the quasi-particle weight $z$. In such cases, thermodynamical quantities strongly depend on interactions such as lattice effects that are irrelevant to the universality of the model. Recently, the double-exchange model which also takes into account the effect of dynamic Jahn-Teller distortion is studied using the infinite-dimensional approach [9]. The result explains the temperature dependence of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ in the region of both above and below the Curie point. Above the Curie point, the increase of the resistivity is explained by the effect of Jahn-Teller distortion while below $T_c$ the decrease of the resistivity is mainly due to the double-exchange mechanism.

The above result may be interpreted as the consequence of the renormalization of Green’s function $\tilde{G}_{\text{eff}}$ by the thermodynamical fluctuation of Jahn-Teller field together with the double-exchange mechanism. Therefore, from the point of view of controlling the MR response, it is very important to study the renormalization effects from Coulomb repulsions and lattice distortions. Especially, the lattice effects appear in the energy scale of room temperature. Further study on the lattice effects as well as Coulomb interactions are necessary to understand the complex phenomena observed in manganese oxides.
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