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Theoretical Model Study of Magnetoresistance in CDW Ordered CMR Manganites

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Abstract: We report here a microscopic model study for colossal magnetoresistive manganite (CMR) systems. We consider an interplay between the ferromagnetic (FM) and charge ordered (CO) states of the manganite systems in a Kubo-Ohata type double exchange (DE) model. The model Hamiltonian is solved using Zubarev's Green's function technique. The temperature dependent FM and CO order parameters are calculated and computed numerically. We have also calculated and studied the temperature dependent electrical resistivity of the manganite system. The temperature dependence of magnetoresistivity is discussed.

Keywords: Colossal magneto-resistance; charge ordering; electrical resistivity

1. Introduction

The perovskite type doped rare-earth manganites of general formula $R_{1-x}A_xMnO_3$ (R: trivalent rare-earth ion, A: divalent alkaline-earth ion, x: doping concentration) are attracting the attention of materials scientists due to the presence of the highly desired colossal magnetoresistive (CMR) property [1]. The CMR property makes manganites a suitable material for spintronic devices. These materials exhibit a wide range of electronic, magnetic and structural correlations as a function of temperature. It goes from a metallic (M) to insulating (I) state at the ferromagnetic (FM) to paramagnetic (PM) phase transition temperature, T_c. Among the structural phases the charge-ordered (CO) and Jahn-Teller (JT) states are prominent. Spin ordering (FM state) in manganites arises due to the hopping of itinerant e_g electrons involving the double exchange (DE)

mechanism. Considering only the DE mechanism, stabilization of FM metallic state throughout the temperature range could be explained. But from electron diffraction experiment of $La_{1-x}Ca_xMnO_3$ [2], a CO state is observed below Curie temperature within the FM state. This CO-FM state opens up a band gap and hence the system goes to an insulating phase. The interaction between FM and CO state is assumed to be the cause of the observed CMR effect in manganites. But till now, there is no evidence to explain the MI transition interrelation with CO-FM phase transition, as observed in experiments. In this communication, we report the MI phase transition near the Curie temperature through the study of temperature dependent electrical resistivity.

2. Formalism

The model Hamiltonian for the manganite system consists of Kubo-Ohata [3] type DE interaction, Heisenberg type ferromagnetic spin-spin interaction among the neighboring core spins and charge density wave (CDW) interaction in conduction band electrons due to the presence of charge ordering. The DE interaction and core-electron spin-spin interaction are treated within mean-field approximation using Ising model. This is explained earlier in our publication [4]. The total electron mean-field Hamiltonian for the Manganite system considered is written as

$$H_{el} = \sum_{k,\sigma}\left(\varepsilon(k) - \mu - B\sigma + \frac{1}{2}JM^d\sigma\right)c^{\dagger}_{k,\sigma}c_{k,\sigma} + \Delta_c\sum_{k,\sigma}c^{\dagger}_{k+Q,\sigma}\,c_{k,\sigma} + \sum_{k,\sigma}\left(\varepsilon_{\mathrm{d}} - \mathrm{B}\sigma + \frac{\left(\mathrm{JM^c} + \mathrm{J_H M^d}\right)}{2}\sigma\right)d^{\dagger}_{k,\sigma}d_{k,\sigma} \qquad (1)$$

where $\varepsilon(k)$, μ, B, J, J_H are the $e_g$electron band energy, chemical potential, external magnetic field energy, FM-DE coupling and Heisenberg coupling respectively. The magnetic spin $\sigma = +1$ for up spin and $\sigma = -1$ for down spin electron. Δ_c is the CDW gap and Q is the CDW nesting wave vector. The position of core level with respect to Fermi level is represented by ε_{d}. The detailed calculation of the model Hamiltonian and calculation of temperature dependent FM and CO gap is given in our earlier paper [4]. In order to calculate electrical resistivity, we consider the phonon coupling to the conduction electron and free phonon Hamiltonian. The electron-phonon interaction is $H_{ep} = \sum_{k,q,\sigma} f(q)c^{\dagger}_{k+q,\sigma}\,c_{k,\sigma}\mathrm{A_q}$ and free phonon interaction is $H_{\mathrm{ph}} = \sum_{\mathrm{q}}\omega_{\mathrm{q}}b^{\dagger}_{q}\,b_q$, where $f(q)$, ω_{q} are the electron phonon coupling constant and free phonon frequency of wave vector q respectively. The total Hamiltonian is $H = H_{el} +$

$H_{ep} + H_{\rm ph}$. The temperature and magnetic field dependent electrical resistivity is calculated from the Drude-Lorentz formula $(T, B) = \frac{m}{ne^2\tau}$, where m, e, n, τ are respectively the mass, charge, concentration and relaxation time of conduction electron. The temperature and magnetic field dependent electron relaxation time is calculated from the imaginary part of the electron self-energy. Calculation of electron self-energy for this Hamiltonian is discussed in detail [5]. In order to do numerical computation all the physical parameters are made dimensionless by scaling with respect to the conduction band width $W \simeq 1eV$. The scaled parameters are: the DE coupling $g = J/W$, the CDW coupling $g1 = V_0 N(0)/W$, the Heisenberg coupling in t_{2g} band $g2 = J_H/W$,the reduced temperature $t = k_B T/W$, the reduced CDW gap parameter $z = \Delta_c/W$, the spectral width $\eta = \frac{\gamma}{W}$, the reduced resistivity $\rho = \rho(T)/\rho(0)$.

3. Results and Discussion

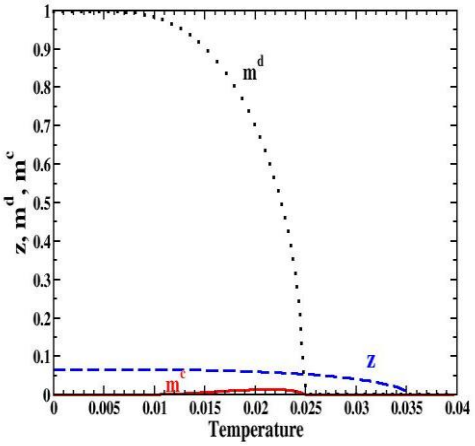

Fig. 1. Self-consistency plots of temperature dependent z, m^d and m^c for fixed values of g=0.025, g1=0.1035, g2=0.0995.

Figure 1. shows the temperature dependent self-consistency graphs for FM gap m^d in core band, m^c in conduction band and CO order parameter z in conduction band. The magnified plot of m^c is shown in figure 2. The graphs are plotted for a set of fixed coupling constants g=0.025, g1=0.1035 and g2=0.0995, so that the FM transition temperature $t_c \simeq 0.025$ ($T_c \simeq 250K$) and CO transition temperature $t_{co} \simeq 0.035$ ($T_{co} \simeq 350K$) as observed in experiments [6]. Both m^d and z exhibit mean-field like behavior, whereas m^c increases as the temperature is lowered down below t_c and attains a maximum value for $t \simeq 0.022$. On further decreasing the temperature m^c is suppressed and disappears at $t \simeq 0.01$. The disappearance

of m^c is due to the presence of strong charge ordering at lower temperature regions which makes the e_g electrons localized. A metal-insulator phase transition takes place at the magnetic transition temperature t_c. Below t_c in the FM-CO coexistence region the phase is metallic and above t_c in the pure CO state the phase is insulating.

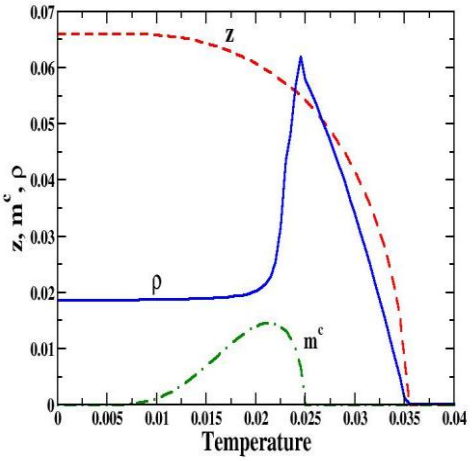

Fig. 2. Temperature dependent resistivity graph and self-consistency plots of temperature dependent z and m^c.

Figure 2 shows the temperature dependent electrical resistivity, ρ (blue solid line) along with temperature dependent z (red dashed line) and m^c (green dash-dot line). From the resistivity graph it is observed that the resistivity is small at lower temperatures, $t< t_c$ and it remains nearly independent of temperature exhibiting metallic character. As the temperature approaches t_c, suddenly ρ increases to a large value showing a peak like structure for $t_c < t< t_{co}$ in the pure CO phase. This high value of ρ signifies the insulating behavior of manganites. As the temperature $t \geq t_{co}$, in the paramagnetic phase, resistivity vanishes. Similar temperature dependent resistivity is observed in experiments for $La_{1-x}Ca_xMnO_3$ system [7]. On application of external magnetic field the resistivity peak is suppressed considerably exhibiting CMR property (not shown in figure). A similar high resistivity peak is observed in the Jahn-Teller distorted insulating phase of manganite systems [8].

4. Conclusion

We have studied the phase change in CMR manganite systems through a microscopic model study, considering an usual Kubo-Ohata type DE model with charge ordering as an extra-mechanism. From the temperature dependent resistivity it is observed that the ferromagnetic phase of the model CMR

manganite system exhibits metallic character, whereas the pure CO state is associated with an insulating character.

References

[1] M B Salamon and M Jaime, *Rev. Mod. Phys.* **73**, 583 (2001)

[2] J C Loudon, N D Mathur, and P A Midgley, *Nature* **420**, 797 (2002)

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

[4] G C Rout, S Panda and S N Behera, *Physica B* **404**, 4273 (2009)

[5] S Panda, P K Purohit, G C Rout, *Adv. Sci. Lett.* **20**, 643 (2014)

[6] Y Tomioka, A Asamitsu, Y Moritomo, H Kuwahara, and Y Tokura, *Phys. Rev. Lett.* **74**, 5108 (1995)

[7] M Roy, J F Mitchell, A P Ramirez and P Schiffer, *Phys. Rev. B* **58**, 5185(1998)

[8] G C Rout, S Panda and S N Behera, *J. Phys.: Condens. Matter* **23,** 396001 (2011)