Orissa Journal of Physics
ISSN 0974-8202

Vol. 23, No.1
February 2016
pp. 123-129

Microscopic Theoretical study of the Interplay of Ferromagnetism and Charge Ordering in CMR Systems through Conductance Spectra

S. PANDA , P. SAHOO [2] and G.C. ROUT[3]

[1]Trident Academy of Technology, F2/A, Chandaka Industrial Estate, Bhubaneswar-751024, Odisha, India.Email: saswatip7@gmail.com

[2]S. S. College, Talpatia, Jharasuguda, Odisha, India.

[3]Condensed Matter Physics Group, Physics Enclave, Plot No.- 664/4825, Lane-4 A,Shree Vihar, Patia , Bhubaneswar- 751031, Odisha, India. Emai:gcr@iopb.res.in. Mob: 09937981694.

Received : *13.12.2015* ; *Accepted : 21.01.2016*

Abstract. Here we address the role of Kubo-Ohata type double exchange (DE) interaction on the interplay of ferromagnetism (FM) and charge density wave (CDW) interactions in the CMR manganite systems. The CDW ordering is associated with the e_g electrons of the conduction band, while the ferromagnetism is associated with the localized t_{2g} electrons of the core states of the manganese ion. The ferromagnetic magnetization and CDW gap parameters are calculated using Zubarev's Green's function technique and then solved self-consistently and numerically. We study the effect of DE coupling on the interplay of magnetism and CDW interactions and interpret the experimentally observed temperature dependent gap parameters as well as the tunneling conductance spectra by varying the physical parameters of the system.

Keywords. Manganites, charge density wave systems, electron density of states

PACS Nos. 75.47.Lx, 71.45.Lr, 73.20.Fz

1. Introduction

The perovskite colossal magnetoresistive (CMR) manganites are drawing the attention of physicists because of the rich phase diagram consisting of various magnetic and electrical phases and their potential applications in data storage devices and sensors [1,2]. The parent compound $LaMnO_3$ is an antiferromagnetic insulator (AFMI), but on doping it gives rise to a ferromagnetic metallic (FMM) phase below the ferromagnetic transition temperature (T_c) and a paramagnetic insulating (PMI) phase above (T_c). The ferromagnetism in manganites arises due to the double-exchange (DE) interaction. Millis *et al* have reported that besides

DE, other mechanisms like Jahn Teller (JT) distortion and charge/orbital ordering (CO/OO) are required to explain the CMR property. Understanding of transport properties of manganites requires understanding of the electronic density of states (DOS) near the Fermi level (E_F=0) as the conductivity is directly proportional to the electron density of states of the system. Thus low conductivity implies depletion of DOS at E_F. Experimentally depletion of DOS near E_F of different manganite systems has been studied with the help of scanning tunneling spectroscopy measurements [3, 4] and photoemission spectroscopy studies [5]. Here we describe the CMR manganite system by a model Hamiltonian considering the CDW interaction as the extra mechanism along with DE mechanism to explain the cause of large resistivity near T_c. The CMR property is explained through the study of electron density of states near the Fermi level

2. Formalism and Calculation of Gap Equations

In the present model calculation, we consider the kinetic energies of itinerant conduction electrons and localized t_{2g} core electrons in presence of external magnetic field. Due to Hund's coupling there exists ferromagnetic (FM) order in the localized core states. This magnetism is described by Heisenberg type spin-spin interaction. In order to associate the core level magnetism to the itinerant electron system, we consider Kubo-Ohata type double exchange interaction [6] among the spins of e_g and t_{2g} electrons. In order to take into account of the CMR effect, we incorporate here charge order (CO) effect through charge density wave (CDW) interaction in the $e_g$electron band. The spin interactions are considered within Hartree-Fock type mean-field approximation giving rise to mean-field FM magnetization $M^d$of the core electrons and the induced $e_g$electron magnetization $\mathrm{M^c}$. Based upon our earlier report [7,8] we write the mean Hamiltonian as

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

In the first term of the Hamiltonian, $\varepsilon(k)$, μ, B, J are the $e_g$electron band energy, chemical potential, external magnetic field and FM-DE coupling (J>0) respectively. The second term represents the CDW interaction due to charge ordering in the manganite system with CO gap $\Delta_c = -\mathrm{V_0}\sum_{k,\sigma} < c^{\dagger}_{k+Q,\sigma}\,c_{k,\sigma} >$

and nesting vector Q. The third term describes core electron hopping interaction including the mean-field magnetic parameters. The other parameters are the position of core level ε_d and Heisenberg coupling J_H and $\sigma = \pm 1$ for up and down spins. Z-component of the longitudinal core magnetization and induced $e_g$electron magnetization are defined as $M^d = -\left(n_\uparrow^d - n_\downarrow^d\right)$ and $M^c = -(n_\uparrow^c - n_\downarrow^c)$. The $t_{2g}$and $e_g$electron occupancies n_σ^d and n_σ^c are written as $n_\sigma^d = \sum_{k,\sigma} < d_{k,\sigma}^\dagger \, d_{k,\sigma} >$ and $n_\sigma^c = \sum_{k,\sigma} < c_{k,\sigma}^\dagger \, c_{k,\sigma} >$. Before studying the interplay of CO gap and FM magnetization, we have scaled the physical parameters by conduction electron bandwidth W=1eV for the manganite systems. 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 $\eta = \gamma/W$. Finally the electron density of states (DOS) is computed.

3. Results and discussion

The temperature dependent charge ordering energy E_{CO}= 2z and the ferromagnetic energy of core electron, E_{md}=g2xM^d are solved numerically and self-consistently by using the expressions of z and M^d. For a given set of coupling parameters, the plots are shown in figure 1.a showing the CO transition temperature t_{CO}=0.0155 (T_{CO}≃155K) and Curie temperature t_c=0.018 (T_c≃180K) corresponding to the conduction bandwidth W=1eV≃10000K. These temperature dependent energies exhibit mean-field behavior. This nearly describes different transition temperatures of manganites i.e. T_{CO} =150K and T_C =183K for $La_{7/8}Sr_{1/8}MnO_3$ [10] and T_c=187K, T_{CO}=150K in $La_{1-x}Sr_xMnO_3$ (x=0.125) [11]. Due to DE, the FM order is induced in the e_g electrons in the conduction band. The induced magnetic energy (E_{mc} = g x M^c) sharply increases near t_c to a maximum value and suddenly decreases towards lower temperatures and becomes zero at very low temperatures (see inset of figure 1.a). Since the same e_g electrons are associated with both charge and magnetic orderings, the electrons strongly related with CO at lower temperatures do not contribute to the FM orderings at lower temperatures. Hence FM ordering is completely suppressed at lower temperatures due to the robust charge ordering of e_g electrons. This type of temperature dependence of E_{mc} is observed experimentally for the charge ordered manganite systems [12].

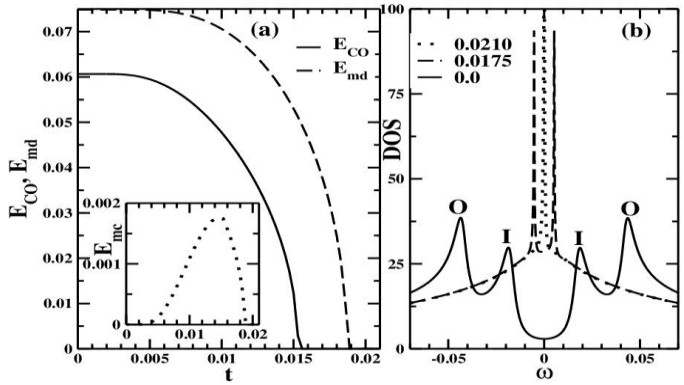

Fig. 1 (a) The temperature (t) dependent self-consistency plot of CO gap energy (E_{CO}), longitudinal component of core t_{2g} electron magnetization gap energy E_{md} and induced magnetization gap energy in $e_g$band electron E_{mc} (inset) for fixed values of g=0.025, g1=0.06, g2=0.075. (b) The plot of energy (ω) dependent $e_g$electron DOS for η=0.003 at different temperatures t=0.021, 0.0175, 0 and other physical parameters remainins same as in figure 1.a.

The electron density of states (DOS) is directly proportional to the imaginary part of the e_g electron Green's function. The DOS is described by the relation $-2\pi \sum_{k,\sigma} Im\, G(k, \omega + i\eta, \sigma)$, where $G(k, \omega + i\eta, \sigma)$ is the e_g electron Green's function with η as the spectral width. The DOS describes the tunneling conductance spectra measured by scanning tunneling microscopy (STM) and photo-electron spectroscopy. The DOS is shown in figure 1.b for different temperatures. In absence of charge and magnetic orderings, the DOS is plotted in high temperature paramagnetic phase at $t=0.021>t_c$, as shown by a sharp peak at the Fermi level, ω=0 (shown by dotted lines). In pure FM phase at temperature $t_{CO}<t=0.0175<t_c$, the single peak in DOS splits into two sharp peaks with lower spectral height due to FM ordering in the system separated by a induced magnetic gap energy, $E_i = g \times M^d \simeq 0.0105$. Even though the DOS shows U-shaped magnetic gap at Fermi level, the electron DOS is not zero but a finite value near Fermi level. At still lower temperatures, at t=0 in the mixed phases of CO and FM, the DOS shows a flat two gap structure with inner gap I-I and outer gap O-O with gap edge positions appearing respectively at energies $\omega_I = \pm\left(\frac{1}{2} g M^d - z\right)$and $\omega_O = \pm\left(\frac{1}{2} g M^d + z\right)$. Due to the presence of strong insulating CO at lower temperatures, the DOS is suppressed considerably leading to this type of flat peaks. Even though the parabolic inner gap is well defined, there exists small but finite electron DOS near Fermi level. This type of parabolic gap structure with finite DOS near Fermi level is observed by STM measurements for $La_{0.7}Ca_{0.3}MnO_3$ [3] and $La_{0.7}Pb_{0.3}MnO_3$ [4] systems. However they could not observe the sharp multiple peaks in the conductance spectra due to lack of high resolution STM measurements.

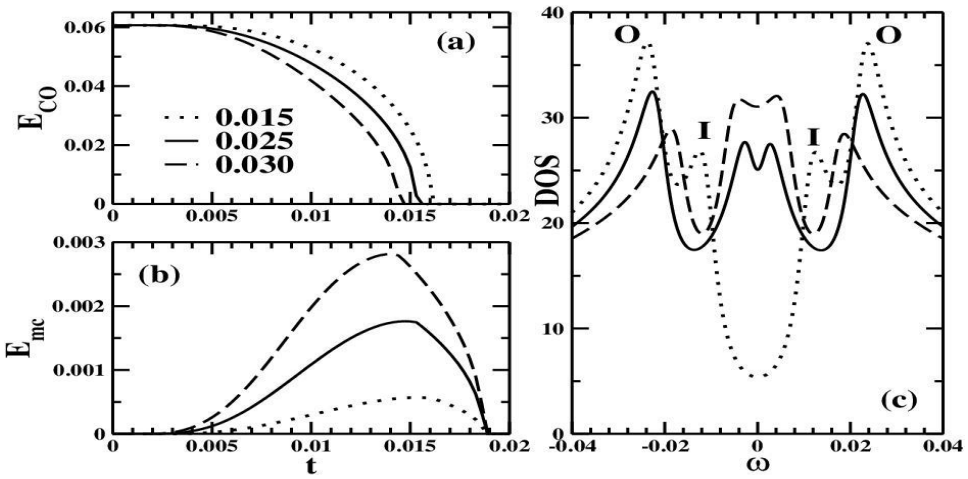

Fig. 2.(a) The self-consistency plot of t vs. E_{CO}, for different values of g=0.01, 0.02 and 0.03 and other parameters being same as in figure 1.a. (b) The self-consistency plot of t vs. E_{mc}, for different values of g=0.01, 0.02 and 0.03 and other parameters being same as in figure 1.a. (c) The plot of $\boldsymbol{e_g}$electron DOS for same physical parameters as in figure 1.a but different values of g=0.01, 0.02 and 0.03 and η=0.003.

The figure 2.a and 2.b show the effect of DE coupling (g) on the temperature dependent CO gap energy E_{CO} and induced FM gap energy E_{mc} respectively. For g=0.015 the E_{CO} shows mean-field behavior with CO transition temperature t_{CO}=0.01625, but the induced E_{mc} is completely suppressed at low temperatures, then increases to a maximum value and then decreases to zero at Curie temperature t_c=0.018. With increase of DE coupling the t_{CO} is suppressed accompanied by the suppression of the CO ordering energy. On the other hand, the magnetization energy is enhanced with increase of DE coupling with its Curie temperature remaining unchanged. There exists a strong interplay between CO and FM ordering just below the Curie temperature. The colossal magnetoresistance (CMR) effect is observed in manganites just below the Curie temperature. Therefore it is conjectured that the CO may play a vital role to explain the CMR effect in manganites as observed experimentally [13]. Earlier Rout *et al* have predicted that the strong JT effect plays a dominant role in the formation of CMR effect in manganite systems [14, 15]. Figure 2.c shows the effect of DE coupling on the DOS of the system. The multiple peaks with two gap structure in DOS change with increase of DE coupling. With increase of g both the inner and outer gap edges I-I and O-O shift towards the Fermi level (ω=0). Simultaneously the peak heights of the outer edges are suppressed, while the peak heights of the inner edges are enhanced displaying the conservation of electron DOS. As a result the inner gap becomes flat. For lower DE coupling

g=0.015, the inner gap is very deep exhibiting the characteristic of insulating gap due to strong CO states with less electronic DOS at Fermi level. For higher DE coupling g=0.030, the CO state is suppressed, but the magnetic ordering dominates in the DOS, so that the DOS displays large value near Fermi level displaying itinerant character of the FM metallic state of the manganite system. This type of finite DOS near the Fermi level has been predicted by Lin *et al* by their calculations taking polaron effect in the manganite system [16].

4. Conclusions

We consider here the interplay of charge and ferromagnetic orderings in the manganite systems employing the DE coupling. Due to the presence of strong charge ordering, the FM order is suppressed considerably at lower temperatures. The DE coupling suppresses the CO and enhances the FM ordering in the manganites just below the Curie temperature. This explains the CMR effect observed experimentally just below Curie temperature. The effect of temperature and DE coupling on the electron DOS is discussed exhibiting the strong interplay of these two orders.

References

[1] V B Shenoy, C N R Rao, Phil. Trans. R. Soc. A **366**, 63 (2008)

[2] P K Siwach, H K Singh, O N Srivastava, *J. Phys.: Condens. Matter* **20,** 273201 (2008)

[3] J Y Wei, N -C Yeh, R P Vasquez, A Gupta, J. Appl. Phys. **83**, 7366 (1998)

[4] A Biswas, S Elizabeth, A K Raychaudhuri, H L Bhat, Phys. Rev. B **59**, 5368 (1999)

[5] M K Dalai, B R Sekhar, D Biswas, S Thakur, T-C Chiang, D Samal, C Martin, K Maiti, Phys. Rev. B **89,** 245131 (2014)

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

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

[8] G C Rout, S Panda, J. Physics: Condensed Matter **21** 416001 (2009)

[9] R Klingeler, J Geck, S Arumugam, N Tristan, P Reutler, B Büchner, L Pinsard-Gaudart, A Revcolevschi, Phys. Rev. B **73**, 214432 (2006)

[10] S Uhlenbruck, R Teipen, R Klingeler, B Büchner, O Friedt, M Hücker, H Kierspel, T Niemöller, L Pinsard, A Revcolevschi, R Gross, Phys. Rev. Lett. **82**, 185 (1999)

[12] H Kuwahara, Y Tomioka, A Asamitsu, Y Moritomo, Y Tokura, Science **270,** 961 (1995)

[13] C N R Rao and B Raveau (eds) Colossal Magnetoresistance, Charge Ordering and Related Properties of Manganese Oxides (Singapore: World Scientific) (1998)

[14] G C Rout, N Parhi, S N Behera, Physica B **404**, 2315 (2009)

[15] G C Rout, S Panda and S N Behera, J. Physics: Condensed Matter **23**, 396001 (2011)

[16] C Lin, A J Millis, Phys. Rev. B **79**, 205109 (2009)