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The Role of Charge Ordering in the Electron Specific heat of CMR Manganites

J K KAR[1] , S PANDA[2†] and G C ROUT[3]

[1]*Biju Patnaik University of Technology. Chhend, Rourkela-769015, Odisha, India.*
[2]*Dept.of Physics, Trident Academy of Technology, Chandaka Industrial Estate, Bhubaneswar-751024, India.*
[3]*Condensed Matter Physics Group, Physics Enclave, Plot No-664/4825, Lane 4A, Shree Vihar, Bhubaneswar-751031, India. Email:gcr@iopb.res.in,Mob:09937981694*
[†]*Corresponding author. Email Id: saswatip7@ gmail.com*

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Abstract: We consider here a tight binding model Hamiltonian which consists of the kinetic energy terms of conduction and core t_{2g} band electrons. The Kubo-Ohata type double exchange interaction is considered among the onsite spins of e_g and t_{2g} band electrons. The transverse antiferromagnetic spin fluctuations in XY plane of t_{2g} band arises due to Heisenberg type spin - spin interactions in the core band. The double exchange interaction induces antiferromagnetism in the XY plane of e_g band. As an extra mechanism we consider here the charge ordering interaction in the e_g band. The model Hamiltonian is solved using Zubarev's Green's function technique and the temperature dependent electron specific heat is calculated. The effect of charge ordering on the electron specific heat is studied.

Keywords: CMR, Charge orderings, Antiferromagnetism

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1. Introduction

$R_{1-x}A_xMnO_3$ (R- trivalent rare earth ion, A- divalent alkaline earth ion and x-doping concentration) type perovskite manganites have been subjected to intense research due to the existence of colossal magnetoresistance (CMR) property [1]. The CMR effect along with the presence of fully spin polarized conduction bands [2] makes these materials suitable candidates for spintronic devices. It has been widely accepted that the metal-insulator phase transition just near the magnetic phase transition temperature is responsible for CMR effect [3]. These strongly correlated systems exhibit complex charge, orbital and spin ordered states which arise due to the interplay of structural, electronic and magnetic degrees of freedom. In the MnO_6 octahedra of manganites the 3d orbitals of Mn ion splits

into the low lying t_{2g} triplets and high lying e_g doublets, in the presence of crystal field. Due to strong Hund's rule the spin - up channel of t_{2g} orbitals are fully occupied and spin - up channel of e_g band are partially filled. The spin - down channels are fully empty for all 3d bands. Upon hole doping the e_g band becomes fully empty. The presence of Mn^{3+} and Mn^{4+} ions in the doped manganites gives rise to a charge ordered (CO) state. The competition between the insulating CO state and the spin ordered (SO) state along with the double exchange (DE) mechanism may explain the physics of manganites successfully. In the present communication we will study the interplay of CO and SO parameters and its effect on the temperature dependent specific heat.

2. Formalism

The model Hamiltonian is written as

$$H = \sum_{k,\sigma}(\varepsilon_k - \mu - B\sigma)c^{+}_{k,\sigma}c_{k,\sigma} + \Delta_c \sum_{k,\sigma} c^{+}_{k,\sigma}c_{k+Q,\sigma}$$
$$- J\sum_i s^c_i \cdot S^d_i - J_\beta(i,j)\sum_{i,j} S^d_i \cdot S^d_j + \sum_{k,\sigma}(\varepsilon_d - B\sigma)d^{+}_{k,\sigma}d_{k,\sigma}$$

Here nearest neighbour (NN) and next nearest neighbour (NNN) interactions are considered for the band dispersion ε_k of e_g electrons and Heisenberg interaction coupling $J_\beta(i,j)$. We have $\varepsilon_k = -2t_1(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y$ and $J_H(q) = J_H(k-k') = J_1(\cos k_x + \cos k_y) + 2J_2 \cos k_x \cos k_y$. Here t_1 and t_2 are respectively the NN and NNN e_g electron hoppings and J_1 and J_2 are respectively the NN and NNN Heisenberg couplings. The creation (annihilation) operators for e_g and t_{2g} electrons are represented by $c^{+}_{k,\sigma}(c_{k,\sigma})$ and $d^{+}_{k,\sigma}(d_{k,\sigma})$ respectively. The terms μ, B (= $\mu_B g_L B_{ext}$) and σ represent chemical potential, external magnetic field energy and spin. The second term represents the CO interaction with CO order parameter Δ_c and nesting vector Q. Third and fourth terms represent the Kubo-Ohata type DE [4] and Heisenberg interactions respectively with DE coupling J. $\mathbf{s^c_i}$ and $\mathbf{S^d_i}$ are the spin operators of conduction and core electrons respectively. In the last term ε_d represents the position of core level with respect to Fermi level ($\varepsilon_F = 0$). The model Hamiltonian is solved using Zubarev's Green's function technique [5] and the coupled Green's functions for e_g and t_{2g} band electrons are calculated. From these Green's functions the transverse antiferromagnetic (AFM) spin fluctuation in e_g and t_{2g} band and the CO gap are calculated [6]. Further the temperature dependent specific heat is calculated from the free energy [6]. All the physical parameters are made dimensionless with respect to NN hopping integral t_1. The dimensionless parameters are CO

couplings $g = V_0N(0) / t_1$, the DE coupling $g_1 = J / t_1$, the NN Heisenberg coupling in t_{2g} band $g_{1k} = J_1 / t_1$, the NNN Heisenberg coupling in t_{2g} band $g_{2k} = J_2 / t_1$ and the reduced temperature $t = k_BT / t_1$.

3. Results and Discussion

The interplay of CO gap (z) and antiferromagnetic (AFM) SO gap ($< s^c >$) is shown in fig.1(a) by varying the CO coupling (g). The temperature dependent CO gap exhibits mean-field like behaviour. The temperature dependent AFM - SO gap ($< S^d >$) decreases nearly linearly with increase of temperature then decreases

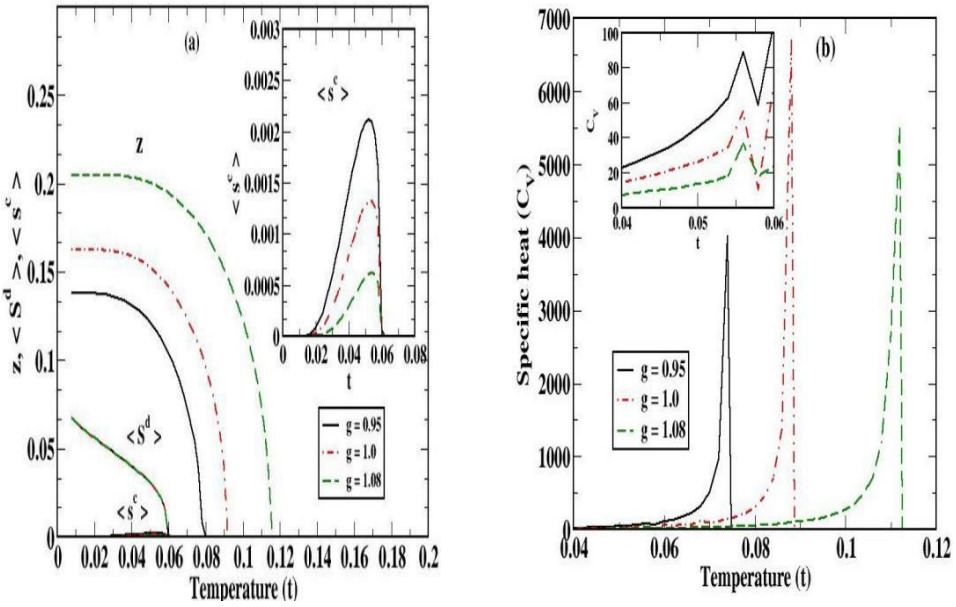

Figure 1.(a) The temperature dependent self-consistency graphs of CO gap (z), transverse spin fluctuation ($< S^d >$) in t_{2g} band and induced transverse spin fluctuation $< s^c >$ in e_g band for fixed values of $g_1 = 0.3$, $g_{1k} = 6.72$, $g_{2k} = 0.25$, $t_2 = 0.075$ and for different values of g = 0.95, 1.0, 1.08. **Inset**: the magnified temperature dependent self-consistency graph of $< s^c >$. **(b)** The temperature dependent specific heat for different parameters as given in (a). **Inset**: the magnified temperature dependent specific heat at lower temperatures.

rapidly just below the Neel temperature (t_N), and vanishes at t_N showing a magnetic phase transition. Similar first order phase transition in $< S^d >$ is observed by Okamoto et. al. [7]. The induced $< s^c >$ has the same t_N as that of $< S^d >$. As the temperature decreases from t_N, the $< s^c >$ increases and attains a maximum value and then decreases with further decrease in temperature. At very low temperatures in the presence of robust CO gap, $< s^c >$ vanishes. As the CO

coupling (g) increases from 0.95 to 1.08, z increases throughout the temperature range, so also t_{CO} increases from 0.08 (T_{CO}≈ 0.08X2500 = 200K) to 0.115 (T_{CO}≈ 287.5K), whereas the $< s^c >$ is suppressed considerably without any change of t_N. This exhibits a strong interplay between the charge and spin degrees of freedom in manganites. The temperature dependent electron specific heat (C_V) is shown in Figure 1(b) for different values of g. For a constant value of g, the C_V shows two peaks, a sharp peak near t_{CO} and a small peak at t_N. Similar two peak structure in specific heat is observed experimentally for $La_{0.25}Ca_{0.75}MnO_3$ and $Pr_{0.8}Na_{0.2}MnO_3$ systems [8, 9] and microscopic model studies [6, 10]. With increase of g, the peak at t_{CO} shifts towards higher temperatures and the spectral weight increases, whereas the height of the peak near t_N increases without any lateral shifting.

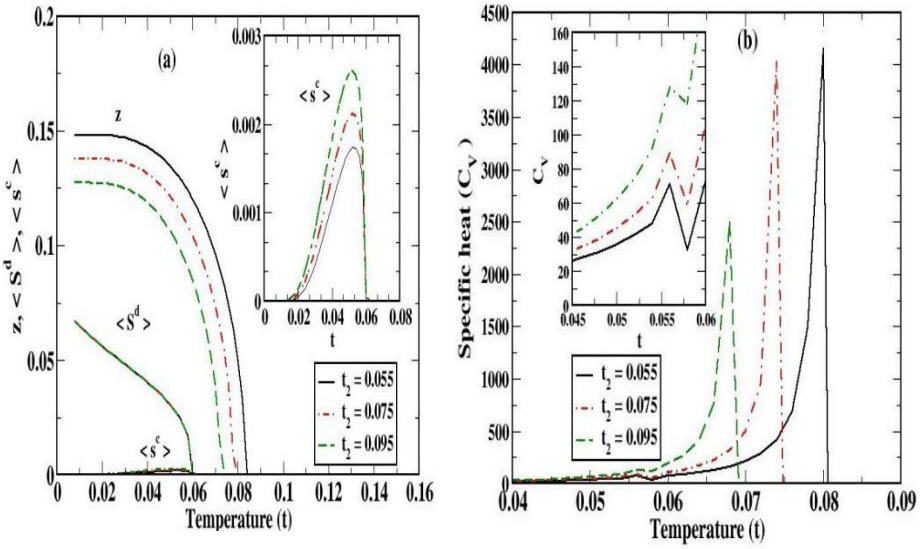

Figure 2.(a) The temperature dependent self-consistency graphs of z, $< S^d >$ and $< s^c >$ for fixed values of g_1 = 0.3, g_{1k} = 6.72, g_{2k} = 0.25, t_2 = 0.075 and for different values of t_2 = 0.055, 0.075, 0.095. **Inset**: the magnified temperature dependent self-consistency graph of $< s^c >$. **(b)**The temperature dependent specific heat for different parameters as given in (a). **Inset:** the magnified temperature dependent specific heat at lower temperatures.

The effect of second nearest neighbour hopping integral (t_2) on the interplay of z and $< s^c >$, and temperature dependent specific heat is shown in fig. 2(a) and (b) respectively. As the value of t_2 increases from 0.055 to 0.095, the CO gap as well as t_{CO} decrease and correspondingly $< s^c >$ increases without any variation in t_N. This is because increase of t_2 increases the itinerancy of e_g electrons and the charge ordering gap which is a phenomenon due to localization of charges decreases. As t_2 is associated with e_g electrons, no variation is observed in the SO

gap, $< S^d >$ of t_{2g} band. The peaks at t_{CO} observed in the temperature dependent specific heat (fig. 2b) are suppressed and shift towards lower temperatures with increase of $t_{2,}$ whereas the peak near t_N shifts up without lateral shifting.

In conclusion we say that there is a strong interaction between the spin and electronic degrees of freedom in the CMR manganite systems.

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