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The specific heat behavior of the Kondo lattice model in manganese oxides

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Materials that present the phenomenon of "colossal" magnetoresistance are currently under much experimental investigation due to their potential technological applications. Typical compounds that have this phenomenon are ferromagnetic (FM) metallic oxides of the form $R_{1-x}A_xMnO_3$ (where R = La, Pr, Nd; A = Sr, Ca, Ba, Pb). In this paper we investigate the specific heat behavior of these manganese oxides by Monte Carlo simulations on the ferromagnetic Kondo lattice model. We present the dependence of specific heat for square and simple cubic lattices with temperature for different electron densities and Kondo lattice model parameters

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1. Introduction

Manganese oxides such as $La_{1-x}Ca_xMnO_3$ have been attracting a great attention since the discovery of colossal magneto resistance (CMR)[1,2].

These materials crystallize in the perovskite – type lattice structure where the crystal field breaks the symmetry of the atomic wave function of the manganese d-electrons. Due to a strong Hund coupling, the spins of the t_{2g} electrons are aligned, forming a localized core spin with S=3/2. The electron configuration of the Mn^{3+} ions is $t_{2g}^3\ e_g^1$, whereas for Mn^{4+} ions the e_g electron is missing. Due to a hybridization of the e_g wave function with the oxygen 2p orbitals, the e_g electrons are itinerant and can move from an Mn^{3+} ion to a neighboring Mn^{4+} via a bridging O^{2-}.

The electronic degrees of freedom are generally treated by a Kondo lattice model which, in the strong Hund coupling limit, is referred to as the double – exchange (DE) model, a term introduced by Zener[3]. In this paper we will concentrate on the thermodynamic properties of itinerant e_g electrons interacting with the local t_{2g} core spins. We neglect the degeneracy of the e_g orbitals. The degrees of freedom of the e_g electrons are described by a single – orbital Kondo lattice model. The t_{2g} spins $\vec{S}_i$ are treated classically, witch is equivalent to the limit $S \to \infty$[4].

In this paper, we study the specific heat of the Kondo lattice model, described by the Hamiltonian:

$$H = -\sum_{\langle ij\rangle\alpha} t_{ij} c_{i\alpha}^{+} c_{j\alpha} - J \sum_{i,\alpha,\beta} c_{i\alpha}^{+} \vec{\sigma}_{\alpha\beta} c_{i\beta} \vec{S}_i - \mu \sum_{i\alpha} n_{i\alpha} \quad (1)$$

The first term describes a single band of conduction electrons, the "Kondo coupling" term represents an exchange interaction between conduction electrons and the localized S=3/2 spins, and the final term allows for variable conduction electron density via a chemical potential. In the above Hamiltonian, t_{ij} represents the hopping matrix, $c_{i\alpha}^{+}$ and $c_{i\alpha}$ are the creation and annihilation operators, respectively, J is the Hund's coupling, $\vec{\sigma}_{\alpha\beta}$ represents the Pauli matrices, $\vec{S}_i$ is the 3/2 localized spins, μ depicts the chemical potential and $n_{i\alpha}$ is the density operator at site i, with spin α . For the hopping matrix, in this work, we will use $t_{ij} = t\cos\theta_{ij}/2$, where θ_{ij} is the angle between the semiclassical localized spins.

The Kondo lattice model combines two competing physical effects. In the strong coupling limit, the conduction electrons will form local singlets (J< 0) or triplets (J> 0) with the localized spin at each site.

In either case these will be a gap to spin excitation and spin correlation will be short ranged. On the other hand, at weak coupling, the conduction electrons can induce the RKKY interaction between localized spins, leading to magnetic order.

In the present paper we focus on finite temperature thermodynamic properties. We mention on a few previous studies of the kind: Shibata[5] have studied the 1D antiferromagnetic model via a finite – temperature DMRG approach, Haule[6] have treated the 2D case via a numerical finite temperature Lanczos method. Röder[7] considered the ferromagnetic model in the limit $J \to \infty$, on the simple cubic lattice, via a high temperature expansion.

2. Numerical algorithm

The grand canonical partition function of the present model with chemical potential can be denoted by:

$$Z = Tr_S Tr_c e^{-\beta(H-\mu N)} \quad (2)$$

where Tr_S and Tr_c represent traces over the localized spin configuration and the conduction electron degree of freedom at inverse temperature β, respectively, and $N = \sum_i c_i^+ c_i$ is the operator for the total number of e_g electrons. Here the conduction electron density $\langle n \rangle = \langle N \rangle / L^d$ is determined by adjusting chemical potential μ. Thus the resulting partition function becomes:

$$Z = \prod_i^{L^d} \left(\int_0^{\pi} d\theta_i \sin\theta_i \int_0^{2\pi} d\phi_i \right) \prod_{\alpha=1}^{L^d} \left(1 + e^{-\beta(\varepsilon_\alpha - \mu)} \right) \quad (3)$$

Now, we can apply a Monte Carlo integration procedure for the summation over the configuration angles $\{\theta_i, \phi_i\}$ of localized spins using a standard Metropolis algorithm[8].

The simulations are done in N^d – square or simple cubic lattice with periodic boundary conditions (d been the dimension of the lattice). Although the localized spins are considered classical, the kinetic energy of the conduction electrons is calculated by diagonalizing the DE Hamiltonian because we consider it as a quantum quantity. The standard Metropolis algorithm was used in the MC simulations. The sites to be considered for a change in the spin orientation are randomly chosen. Once a site is selected for a spin reorientation, the angle associated with an attempted change of the spin is chosen at random from within a specified range[9]. Then the energy change, ΔE associated with the attempted update, is calculated. If the quantity $\exp(-\Delta E / KT)$ is smaller than a random number between 0 and 1, the change is allowed, otherwise, it is rejected. Typically, 2000-3000 MC steps per spin are used for equilibration and 3000-5000 steps for spin are used for calculating averages. In the simulation we calculate the average of the internal energy density for d dimension of the lattice:

$$E = \frac{\langle H \rangle}{N^d} \quad (4)$$

where ⟨⟩ denotes statistical average and N is the number of sites. We can calculate the specific heat by fitting the MC energy results and than express **c** by derivative of the energy:

$$c = \frac{dE}{dT} \quad (5)$$

or by computation both $\langle H^2 \rangle$ and $\langle H^2 \rangle$. Adopting the second version, we obtain in this strain, the specific heat of the lattice, given by:

$$c = \frac{1}{N^d KT^2} \left(\langle H^2 \rangle - \langle H^2 \rangle \right) \quad (6)$$

3. Results for square lattice

In this section we present the numerical results for specific heat for square lattice at half filling and we display the specific heat behavior for various t / J ratios (fig. 1). We observe a single peak structure at small values of t / J and a two – peak behavior at large t / J. The high temperature peak becomes broadened and less prominent, in the larger t / J limit, and is due to conduction electrons whereas the low temperature peak arises from the fluctuating local spins.

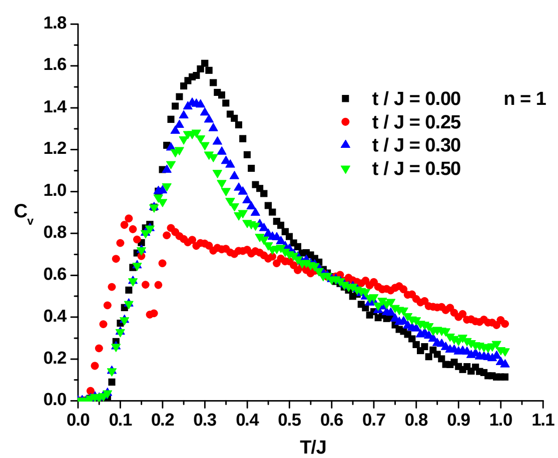

*Fig. 1. The specific heat **c** versus T / J at half filling (n = 1) for different t / J ratios.*

In the next paragraph we present the numerical results for the dependence of the specific heat on doping for square lattice. In Fig. 2 we show the specific heat for different electron densities. The specific heat decrease with decreasing n confirms that, at the high T specific heat is due to conduction electrons.

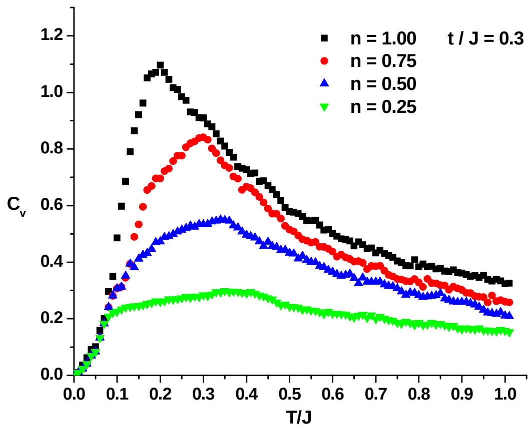

Fig. 2. The specific heat C_v versus T / J for different electron densities.

4. Results for simple cubic lattice

In this paragraph we show the specific heat behavior for various t / J ratios for simple cubic lattice. In fig. 3 we show the specific heat versus T / J at half filling for t / J = 0, 0.25, 0.3, 0.5.

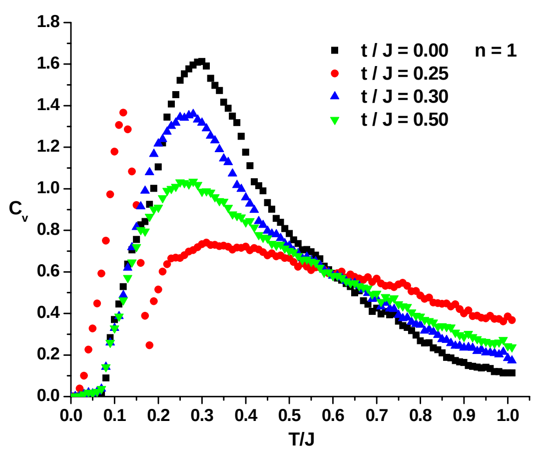

Fig. 3. The specific heat versus T / J for different t / J ratios at half filling.

We observe that at small t / J the specific heat has a single peak appearance where as at large t / J values the specific heat has double peak behavior.

Below, we present the specific heat versus T / J for different doping (Fig. 4).

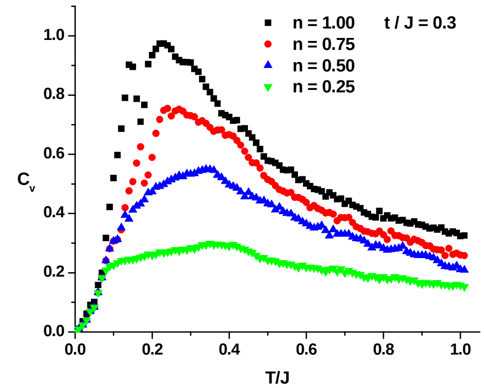

Fig. 4. The specific heat C_v versus T / J for different electron densities.

At small electron densities the specific heat manifests a simple peak behavior and for large electron densities we observe the two-peak pictures of the specific heat.

The particular aspect of the specific heat is very suggestive in terms of magnetic transitions, because it is reading about the potential magnetic phase transitions with temperature increment or with Hund's coupling variation.

5. Conlusions

In this paper we have used the Kondo lattice model to find out the behavior of the specific heat.

In this order, we have analyzed the dependence of specific heat on the t / J ratio by the ferromagnetic Kondo model for square and simple cubic lattices. For this type of lattices we have studied the influence of the electronic density on the specific heat by Monte Carlo simulations applied on ferromagnetic Kondo Model.

We also have analyzed the influence of t / J ratios on specific heat. We have observed that at small t / J ratios the specific heat present a one peak behavior whereas at high t / J ratios the specific heat have a two peak picture, the high temperature peak arising from the conduction electrons and the low temperature peak from the fluctuating localized spins.

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