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Effect of randomness on magnetics and thermodynamics properties in double-exchange model

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In this paper we study the impurity effect on magnetic and thermodynamic properties in double-exchange systems using the Monte Carlo calculation. We find the effect of randomness on ferromagnetic transitions and on the specific heat for finite-size clusters. We observe that the transition temperature decreases with the strength of the randomness by diminution of the coherence of the itinerant electrons.

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1. Introduction

The theoretical model of manganites materials based on double-exchange (DE) interaction, was given in 1951 by Zener [1]. The discovery of colossal magneto resistance in those materials brought a revival of the interest in this model. Colossal magneto resistive (CMR) manganites are a class of materials under study for future spinotronics applications such as nonvolatile magnetic computer memory (MRA). CMR manganites are important to spinotronics for two reasons: First, the exhibit an extremely large drop in electrical resistance when a magnetic filed is applied and second, for some cases CMR materials conduct electricity via electrons of only one spin (half – metallic ferromagnetism). Phase competition and randomness play a key role in the colossal magnetoresistance (CMR) phenomena in manganese oxides [2]. The former phase competition between the ferromagnetic metal (FM) and the charge-ordered insulator (CO) leads to large fluctuations near the multicritical point [3]. The latter randomness suppresses the transition temperatures above which CMR is much enhanced [4]. Theoretically, except for a phenomenological argument [5], this multicritical phenomenon has not been fully investigated thus far.

To explain the magneto conductive properties of these manganites, in which the manganese is present in at least two different valence states (Mn^{3+} and Mn^{4+}), Zener proposed the mechanism of double exchange. The $Mn\ 3d$ levels are split into two subsets t_{2g} (threefold degenerate) and (twofold degenerate). The t_{2g} electrons lower in energy, are more delocalized capable of hopping from site to site provided that the t_{2g} spines on adjacent manganese atoms are parallel. According to DE, the alignment of adjacent localized t_{2g} spins in manganese atoms rules the dynamics of itinerant e_g carriers, which hop prom one atom to the next to yield electrical conductivity. If adjacent t_{2g} spins are parallel (the ferromagnetic state), conduction is favored, if they are randomly aligned (the paramagnetic high – temperature state), conductivity drops dramatically.

2. The model

The DE model is shown to give a quantitative description of the ferromagnetic transition [6], in the typical material $La_{1-x}Ca_xMnO_3$ near $x = 0.3$. We use the Hamiltonian given by:

$$H = H_{Kondo} + H_{imp} \tag{1}$$

$$H_{Kondo} = -t\sum_{\langle i,j\rangle\sigma}\left(c^{+}_{i\sigma}c_{j\sigma} + hc\right) - J_H\sum_{i}\vec{\sigma}_i\vec{S}_i \tag{2}$$

$$H_{imp} = \sum_{i\sigma}\varepsilon_i c^{+}_{i\sigma}c_{i\sigma} \tag{3}$$

where, in equation (2), the first term denotes the nearest neighbor hopping on the cubic lattice and the second term is for the Hund's coupling. The Hamiltonian (3) denotes the on-site randomness which modifies the one body potential energies energy on each site. The potential ε_i takes $\pm W_{imp}/2$ in equal probability in each site. We apply the Monte Carlo (MC) [7] method to the above Hamiltonian and we try to give out the influence of the impurities on the transition temperature if this manganites and also the behavior of the specific heat for these materials.

For simplicity in the following we consider for the Hund's coupling the limit $J_H \to \infty$ and for the localized spin $|S| \to \infty$. We use for the next numeric approaches an energy unit $W=4t=1$ which is the half band – width for the pure system. The temperature dependence of the magnetization for finite size cluster is a monotonic function and has an inflection point which we adopt as the characteristic temperature T^*. Thus, T^* for a finite – size cluster is expected to give a good approximation for the Curie temperature [8]. In this mode we can study the approximately estimated transition temperature as a function of the strength of the randomness. We also give off the numerical results about the influence of impurity on specific heat in the present model.

We have achieved a computational calculation of the specific heat by Monte Carlo (MC) simulations [9] to the above described model. For a given configuration of disorder, we have typically run 1000 MC samplings for measurements after 1000 MC steps for thermalization. We can calculate the specific heat by fitting the MC energy results and than expressing c by the derivative of the internal energy density:

$$c = \frac{dE}{dT} \tag{4}$$

$$\text{where} \quad E = \frac{\langle H\rangle}{N} \tag{5}$$

But, for the numerical computing, we adopt to evaluate the specific heat by the expression:

$$c = \frac{1}{NKT^2}\left(\langle H^2\rangle - \langle H^2\rangle\right) \tag{6}$$

3. Results and discussion

Now we investigate the randomness effect on the ferromagnetic transition in the DE model. Fig. 1 shows the magnetization curve for the system size of 4x4x4 sites when we change the value of W_{imp}.

The decrease of magnetization with the increase of the disorder strength W_{imp} indicates that the ferromagnetism is suppressed by the randomness. The decrease is the most significant near the critical temperature T_C, where the fluctuations are dominant and the coherence of the itinerant electrons becomes very sensitive to the randomness.

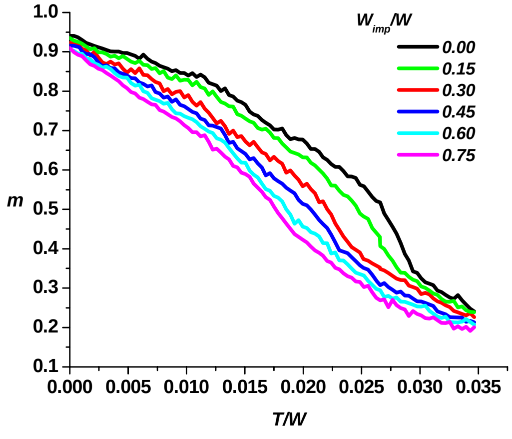

Fig. 1. Temperature dependence of the magnetization for different value of W_{imp}

In our MC study, the spatial distribution of the randomness as well as its effect on the coherence of electrons is included properly. In Fig. 2 we present the transition temperature as a function of the strength of the randomness. We observe the decrement of the critical temperature with the strength of the randomness. For the large values of the W_{imp}/W ratio, the decrease is quite linear, while for the small W_{imp}/W ratio, the abatement of the critical temperature does not present the linear behavior.

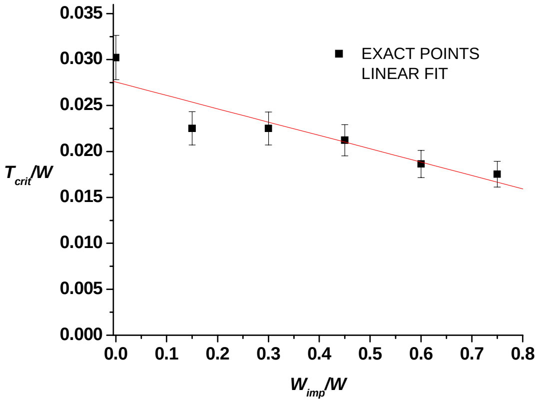

Fig. 2. The transition temperature versus the strength of the randomness

In the next we investigate the influence of the impurities on the specific heat in DE model. We plot in Fig. 3 the specific heat as a function of temperature for different strength of the randomness. The randomness suppresses the ferromagnetism of the DE origin by reducing the coherence of the electron motion. The results indicate that the suppression is significant in the critical region, where the fluctuations are dominant.

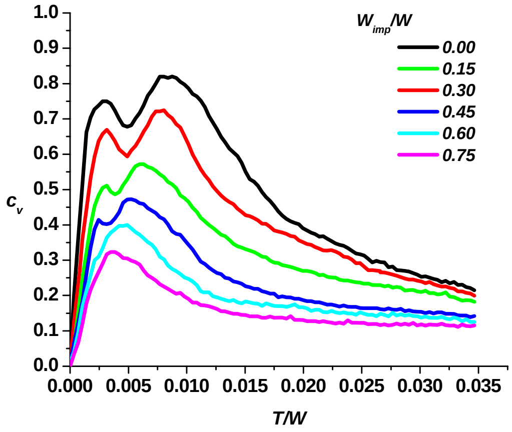

Fig. 3 The specific heat versus T/W for different W_{imp}/W ratio in t/J→0 limit.

This decrease of the electron coherence affects also the specific heat by reducing it with the randomness increment. The specific heat plot versus T/W, at different

W_{imp}/W ratio in $t / J \rightarrow 0$ limit, show off that the peak is shifting for low T/W values with the randomness increment. Thus we point out that the randomness effect on the thermodynamics properties is significant.

4. Conclusions

We have investigated the randomness effect on the ferromagnetic transition in the DE model, by showing the magnetization curve for the system size of 4x4x4 sites when we change the value of W_{imp}. The decrease of magnetization with the increase of the disorder strength W_{imp} indicates that the ferromagnetism is suppressed by the randomness. The decrease is the most significant near the critical temperature T_C, where the fluctuations are dominant and the coherence of the itinerant electrons becomes very sensitive to the randomness. We have presented the transition temperature as a function of the strength of the randomness. We observe the decrement of the critical temperature with the strength of the randomness. For the large values of the W_{imp}/W ratio, the decrease is quite linear, while for the small W_{imp}/W ratio, the abatement of the critical temperature does not present the linear behavior. Also, we have investigated the influence of the impurities on the specific heat in DE model, by plotting the specific heat as a function of temperature for different strength of the randomness. The randomness suppresses the ferromagnetism of the DE origin by reducing the coherence of the electron motion. The results indicate that the suppression is significant in the critical region, where the fluctuations are dominant. This decrease of the electron coherence affects also the specific heat by reducing it with the randomness increment. The specific heat plot versus T/W, at different W_{imp}/W ratio in $t / J \rightarrow 0$ limit, show off that the peak is shifting for low T/W values with the randomness increment. Thus we point out that the randomness effect on the thermodynamics properties is significant, particularly in the critical region.

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