Critical Exponents for the Ferromagnetism in Colossal Magnetoresistance Manganites

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Abstract  Critical phenomena of ferromagnetic transition in colossal magnetoresistance manganites are theoretically studied. Concerning the critical exponents for this transition, there still remains controversy among experimental results. In order to clarify intrinsic physics of the manganites through a comparison with theoretical prediction, we investigate the critical phenomena of double-exchange models by using finite-size scaling analysis on unbiased numerical results. As a result, we show that the critical exponents of the ferromagnetic transition of the three-dimensional double-exchange model is consistent with those of the Heisenberg model, but are distinct from the mean-field one.

1 Introduction

Ferromagnetic transition in doped manganese oxides has revived interests since rediscovery of colossal magnetoresistance phenomena. [1,2] Recent refinement of experimental technique and improvement of sample quality make it possible to discuss critical phenomena of this transition in detail. Particularly, for the purpose of capturing intrinsic physics in these materials and promoting a better understanding of the colossal magnetoresistance phenomena, the critical exponents and the universality class have been investigated by various experimental methods. However, the estimates of the exponents are scattered and have not converged yet. For instance, the neutron scattering gives Heisenberg-like universality class, [3,4] and some d.c. and r.f. magnetization measurements give mean-field-like one. [5,6] It is strongly desired to solve this controversy.

The purpose of this work is to shed light on this problem from a theoretical viewpoint. We study the universality class of the ferromagnetic transition due to double-exchange (DE) mechanism, which is believed to be a major driving force to cause the metallic ferromagnetism in doped manganites. We compare the results with experimental data, and discuss the origin of the experimental controversy.

The DE mechanism itself was proposed more than half-century before, [7] and has been studied intensively. Nevertheless, the thermodynamics has not been fully understood thus far. Large spin fluctuations and the strong interplay between charge and spin degrees of freedom make it difficult to describe finite-temperature properties quantitatively, especially near the critical point of the ferromagnetic transition. In order to give a quantitative description of the critical phenomena, it is indispensable to take account of the large fluctuations. Approximational methods like the mean-field approximation are known to fail. [8]

As one of promising candidates to study this problem, in this paper, we employ a numerical calculation which includes the fluctuations properly and is free from uncontrolled approximations. Recent development of algorithm and computational environment enables us to perform large-scale unbiased calculations and to describe the finite-temperature properties in the thermodynamic limit. We analyze the numerical results which are obtained by a newly developed Monte Carlo (MC) method in the next section. In Sec. 3, we discuss the results and compare them with experimental results. Section 4 is devoted to summary.

2 Numerical Results

We develop and employ a new MC algorithm, which is called the moment-expansion MC method. [8,9] By using the moment expansion of the density of states which is efficiently performed on parallel computers, this new method reduces the computational time remarkably compared to the conventional MC technique.

We study DE models with a single conduction band (which stands for Mn eg bands) which couples to localized spins (in Mn t2g localized levels). The Hamiltonian
Fig. 1 Temperature dependence of the magnetization in the thermodynamic limit. The curve in the figure is the least-squares-fit to \( m \propto (T_c - T)^\beta \) with the Heisenberg exponent \( \beta = 0.365 \). The inset shows the system-size extrapolation of the spin structure factor.

is given by

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_i^\dagger c_j \sigma - J_H \sum_i \sigma_i \cdot S_i,
\]

(1)

where the first term describes the electron transfer between nearest-neighbor sites, and the second one is for the Hund’s-rule coupling \( (J_H > 0) \) between the conduction electron spin \( \sigma \) and the localized spin \( S \). For simplicity, hereafter, we consider the strong coupling limit, \( J_H \to \infty \), and the classical localized spin, \( |S| \to \infty \). The following calculations are done at quarter-filling.

First, we study a three-dimensional DE model with Heisenberg spin symmetry, which is realistic for comparison with experiments. We analyze the MC data by assuming the universality class of Heisenberg models with short-range interactions. Figure 1 shows the temperature dependence of the magnetization in the thermodynamic limit. The data are obtained by system-size extrapolation of the spin structure factor as shown in the inset. The magnetization data scale well with the fitting \( m \propto (T_c - T)^\beta \) with the Heisenberg exponent \( \beta = 0.365 \).

Next, in order to perform more intensive and precise MC samplings in large-size systems, we study a simplified model of eq. (1), that is, a two-dimensional DE model with Ising spin symmetry. The localized spins are Ising variables which take \( S = \pm 1 \). The model is much simplified, however, it still include the essence of the DE mechanism, that is, the kinetics of electrons is strongly correlated with spin degrees of freedom and energetically favors ferromagnetism. We analyze the MC data on spin structure factor by finite-size scaling analysis as in Fig. 2. Figure 2 shows the finite-size scaling plot for the spin structure factor in the three-dimensional model. Critical exponents in the Heisenberg universality class are assumed.

Fig. 2 Finite-size scaling plot for the spin structure factor in the three-dimensional model. Critical exponents in the Heisenberg universality class are assumed.

Fig. 3 Finite-size scaling plot of the spin structure factor in the two-dimensional model. Critical exponents of Ising universality class are assumed.

where \( L \) is the linear dimension of the finite-size clusters, \( f \) is the universal scaling function and \( \varepsilon = (T - T_c)/T_c \). In Fig. 2, we assume the Heisenberg exponents, \( \nu = 0.705 \) and \( \eta = 0.034 \). The MC data for different \( L \) and \( T \) appear to follow a universal function. We have tried the mean-field exponents \( \beta = \nu = 0.5 \) and \( \eta = 0 \) also, and we confirm that the Heisenberg exponents give better scaling fits than the mean-field ones.
models with short-range interactions. The estimates of the exponents are distinct from the mean-field ones. These results are discussed and compared with experimental results in the next section.

3 Discussion

The DE interaction has a distinguishable property compared to ordinary exchange interactions in spin systems. Effective ferromagnetic interaction is induced by the kinetics of electrons which favor extended states with ferromagnetic spin background to gain the kinetic energy. If we integrate out the electron degrees of freedom to describe the action as a function of spin configurations, it is necessary to introduce effective long-range two-spin interactions as well as multiple-spin interactions which depend on sizes and shapes of ferromagnetic domain structure. The range of the interaction is determined to minimize the total free energy for charge and spin degrees of freedom. As the system approaches the critical point, the magnetic domain structure fluctuates strongly. Thus, it is highly nontrivial how the DE interaction is renormalized, whether it is renormalized to a short-range one, or the long-range and the multiple-spin interactions become relevant to cause the mean-field-like transition through suppression of fluctuations.

The results in the previous section indicate that the universality class of the ferromagnetic transition in the DE model is consistent with that of models with short-range interactions. It is distinct from the mean-field universality class. Thus, we conclude that the DE interaction does not become effectively long-range, but is renormalized to be short-range near the critical point.

As mentioned in Sec. 3, experimental estimates of the critical exponents are widely scattered including the Heisenberg-like (short-range) and the mean-field-like (long-range) ones. Our numerical results indicate that the short-range Heisenberg universality class should be observed in real materials when the ferromagnetic transition is ascribed to the DE mechanism as a major origin.

In order to solve the experimental controversy, the following points should be considered carefully. The first point is sample quality. For precise estimates of the critical exponents, it is crucial to determine the critical temperature $T_c$ precisely. Sharpness of the transition as well as the value of $T_c$ depends strongly on homogeneity of samples. The second point is the range of the critical region. The exponents may depend on the region where they are estimated, particularly when different interactions compete with each other. Generally, it is difficult to determine true critical region, but the dependence of the exponents on the critical range should be tested. The third point is that, in real materials, there may be other elements which are neglected in the simple DE model (1), for instance, orbital degrees of freedom, Coulomb repulsion between conduction electrons, and electron-phonon coupling.

We comment on the final point. We believe that these additional elements neglected in model (1) do not alter the short-range universality class of the ferromagnetic transition because they will not suppress the fluctuations. The spin fluctuations may become more strong through these additional channels. At the same time, the electrons become more incoherent by these additional elements. This makes the effective magnetic interaction more short-range since the incoherence shortens the range of the effective electron transfer. These considerations support our conclusion that the short-range Heisenberg universality class will be found in experiments if the transition is purely magnetic.

4 Summary

We have investigated the critical phenomena of the ferromagnetic transition by the double-exchange mechanism in order to discuss the experimental controversy on the estimates of the critical exponents. We have estimated the critical exponents by using the finite-size scaling analysis on the Monte Carlo data. The obtained exponents suggest that the universality class of the three-dimensional double-exchange model is the same as that of the Heisenberg models with short-range interactions. The double-exchange interaction is renormalized to be short-range when the system approaches the critical point. This theoretical result provides a useful reference to consider the experimental controversy. We have discussed possible origins of the discrepancy among experiments. Although our conclusion is favorably compared with the neutron scattering data, further experimental studies are desired to settle this controversy. A conclusive determination of the critical exponents and the universality class will help us to understand the intrinsic physics of doped manganites and of the colossal magnetoresistance phenomena.

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