Universality Class of Ferromagnetic Transition in Three-Dimensional Double-Exchange System - O(N) Monte Carlo Study -

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Curie temperature and exponents are studied for the three-dimensional double-exchange model. Applying the O(N) Monte Carlo algorithm, we perform systematic finite-size scaling analyses on the data up to 20³ sites. The obtained values of the critical exponents are consistent with those of the Heisenberg universality class, and clearly distinct from the mean-field values.

KEYWORDS: double-exchange system, ferromagnetic transition, universality class, Monte Carlo, O(N) method, colossal-magneto resistance manganites

Rediscovery of colossal magneto resistance (CMR) phenomena has revived much interests in manganese oxides.¹,² As sample quality and experimental precision are improved, many experiments have been done to examine critical properties of the ferromagnetic transition in these compounds. Critical properties, especially critical exponents which assign the universality class of the transition, are highly important to understand the nature of the transition as well as basic physics of the CMR phenomena. Estimates of critical exponents, however, are scattered between different experimental results and widely range from the Heisenberg-like ones to the mean-field-like ones.³ There still remains experimental controversy on this issue.

Theoretical estimates of critical exponents in the double-exchange (DE) model, which is considered to be a relevant model in these compounds,⁴ would help to reconcile this experimental controversy. However, it is difficult to clarify critical properties of this transition because the system is a strongly-correlated electron system; itinerant electrons interact with localized spins through a strong Hund’s-rule coupling whose magnitude is much larger than the bandwidth of electrons. Near the temperature transition, spin fluctuations are critically enhanced due to the interplay between itinerant electrons and localized spins. A sophisticated tool is necessary to handle this many-body problem.

Numerical calculation which includes all the correlation effects is one of the most promising tools for this problem. Monte Carlo (MC) method has been applied for studying the critical properties of this system.⁵ However, most of the MC studies suffered from finite-size effects since they were limited to small-size systems due to the rapid increase of the computational cost as the system size increases. Systematic analysis on the finite-size effect is indispensable to examine the critical properties of this transition in detail.

The authors studied this problem by developing a MC algorithm, which is called the polynomial expansion Monte Carlo (PEMC) method.⁶ In this method, the computational cost has reduced to \( O(N^3) \) from \( O(N^4) \) in the conventional MC method⁷ (\( N \) is the system size), and the finite-size scaling was applied to results up to 8³ sites. The problem was also studied by Alonso et al.⁸ They applied the hybrid MC algorithm in which the computational cost is proportional to \( O(N^2) \) (they claim it can be reduced to \( O(N) \) empirically), and estimated the critical exponent from the data up to 12³ sites. In both studies, the estimates of the exponents are consistent with those in the universality class of the Heisenberg model with short-range interactions. They are, however, not enough to estimate the values precisely and to show a clear deviation from the mean-field values. Further study supported by an improvement in the algorithm is strongly desired for this purpose.

We study the ferromagnetic transition in model (1) by using an improved PEMC method. In this method, we introduce effective truncations for the vector-matrix product and the trace operation, which reduce the computational cost for one MC update to \( O(N) \). Readers are referred to Ref. 9 for the details of this algorithm. This technique enables us to study up to 20³ sites within a reasonable time on parallel computers. We choose periodic boundary conditions and have typically run 4000 MC samplings for measurements after thermalization with 1000 MC steps. The doping concentration is fixed at...
quarter filling, namely, 0.5 electron per site on average. The energy unit is the half-bandwidth of noninteracting case, $W = 6t = 1$.

Figure 1 shows the temperature dependence of the magnetization $m = |S(k = 0)/N|^{1/2}$. Here $S(k)$ is the spin structure factor which is defined as $S(k) = \sum_{ij} (S_i \cdot S_j) \exp(ik \cdot r_{ij})/N$, where the bracket denotes the thermal average for the grand canonical ensemble. The magnetization data are the thermodynamic-limit values which are estimated by the system-size extrapolation of $S(0)/N$ as shown in the inset. We fit the magnetization data by assuming the scaling relation $m \propto (T - T_c)^\beta$ (the gray curve in the figure) to estimate the value of $T_c$ and the critical exponent $\beta$. The fit gives $T_c = 0.0226(2)$ and $\beta = 0.36(1)$. (Errors in the last digit are shown in parentheses.) The estimate of $\beta$ is consistent with the Heisenberg one $\beta = 0.365$ and definitely distinct from the mean-field one $\beta = 0.5$.

We also examine the finite-size scaling plot for $S(0)$ to determine the critical exponents. The scaling form is given by $S(0)L^{n-2} = f(\varepsilon L^{1/\nu})$ which is derived based on the hyperscaling hypothesis. Here $\varepsilon = (T - T_c)/T_c$, $L = N^{1/3}$ and $f$ is the scaling function. We plot $S(0)L^{-2}$ as a function of $\varepsilon L^{1/\nu}$, and optimize the values of $(T_c, \eta, \nu)$ so that all the MC data for different $L$ and $T$ converge to a single curve.10) Figure 2 shows the optimized fit. This fit gives the estimates as $T_c = 0.0222(+5, -3)$, $\nu = 0.60(+13, -10)$ and $\eta = 0.07(+34, -7)$. By using the relation $\beta = \nu(1+\eta)/2$ with the obtained distribution of $\nu$ and $\eta$, we obtain the estimate $\beta = 0.32(+10, -6)$. Both estimates of $T_c$ and $\beta$ are consistent with the estimates in Fig. 1. We confirmed that the mean-field exponents $\nu = 1/2$ and $\eta = 0$ do not give a satisfactory convergence in the scaling fit.

These results indicate that the ferromagnetic transition in the DE model (1) belongs to the universality class of the Heisenberg spin system with short-range interactions rather than to that of the mean-field solution. This suggests that the critical exponents in the Heisenberg universality class should be observed in manganites when the DE mechanism plays a key role in the transition as widely believed. Other additional elements which are not included in the simple model (1), such as the electron-lattice coupling, may not affect the universality class because the fluctuations through the additional degrees of freedom will make correlations more short-ranged.

To summarize, we have investigated the critical exponents in the ferromagnetic transition in the three-dimensional double-exchange model by using the improved Monte Carlo method. The finite-size scaling analysis up to $20^3$ sites indicates that the transition belongs to the universality class of the Heisenberg spin system with short-range interaction and is distinct from the mean-field one. In manganese oxides, we expect this Heisenberg universality class to be observed if the double-exchange mechanism plays a major role in the transition. Our results give a theoretical background to reconcile the experimental controversy on the estimates of the critical exponents.

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Fig. 2. The best-fit result of the finite-size scaling plot for the Monte Carlo data.