Non-equilibrium Relaxation Study of Ferromagnetic Transition in Double-Exchange Systems

Yukitoshi Motome and Nobuo Furukawa

Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-0006
1Department of Physics, Aoyama Gakuin University, Setagaya, Tokyo 157-8572

(Received )

Ferromagnetic transition in double-exchange systems is studied by non-equilibrium relaxation technique combined with Monte Carlo calculations. Critical temperature and critical exponents are estimated from relaxation of the magnetic moment. The results are consistent with the previous Monte Carlo results in thermal equilibrium. The exponents estimated by these independent techniques suggest that the universal class of this transition is the same as that of short-range interaction models but is different from the mean-field one.

KEYWORDS: double-exchange system, ferromagnetic transition, non-equilibrium relaxation, Monte Carlo, polynomial expansion, colossal-magnetoresistance manganites

Since the proposal by Zener, the double-exchange (DE) mechanism has been studied to explain ferromagnetic transition in doped manganites which show the colossal magnetoresistance. The ferromagnetism itself is well explained by the DE mechanism; at low temperatures, itinerant electrons which interact with localized spins through the strong Hund’s-rule coupling favor parallel configuration of localized spin in order to gain the kinetic energy. The colossal magnetoresistance is understood by this mechanism also, at least, qualitatively.

However, in spite of the long history of theoretical studies, finite-temperature properties of the DE systems have not been fully understood thus far. At finite temperatures, especially near the ferromagnetic transition, fluctuations are quite large through the strong interplay between itinerant electrons and localized spins. This makes it difficult to describe the thermodynamics quantitatively. Approximational methods, for instance, the mean-field approximation, have been known to be insufficient because they neglect the fluctuation effects.

Recently, the thermodynamics of the DE systems has been studied intensively by the Monte Carlo (MC) method which fully includes large fluctuations. A new algorithm is developed by using the moment-expansion technique for the density of states to calculate MC weight efficiently and the computational speed is accelerated considerably by using parallel computers. This enables us to calculate large-size clusters and take account of the finite-size errors systematically by the finite-size scaling. The critical temperature $T_c$ and the critical exponents are estimated by applying the finite-size scaling analysis on the MC data.

The previous MC studies are for thermal equilibrium. Some initial MC steps (typically 1,000-10,000 steps) are discarded for thermal equilibration, and measurement of physical properties is performed by taking the thermal averages for the grand canonical ensemble using MC samples after the thermalization.

There is another powerful technique to investigate the critical properties by using the MC method, i.e., the non-equilibrium relaxation (NER) technique. In this technique, dependence on MC steps of the order parameter is studied in the non-equilibrium relaxation from an initial state which is chosen to be a symmetry-broken one. The order parameter decays exponentially above the critical temperature $T > T_c$. On the other hand, it approaches a constant for $T < T_c$. As a critical relaxation, a power decay is observed at $T = T_c$ whose exponent relates to the critical exponents.

One of the advantages of the NER technique is that one can study larger-size clusters than by the equilibrium technique since the relaxation is measured in the primary part of the MC samplings which are discarded as a thermalization process in the equilibrium method. The finite-size effect can be exponentially small and neglected in the relaxation if one calculates a sufficiently large-size cluster. The NER technique gives information on the critical temperature and the critical exponents, independently of the equilibrium MC method.

In this paper, we investigate the ferromagnetic transition in DE systems by the NER technique combined with the MC calculations. To our knowledge, this is the first application of the technique to critical phenomena in itinerant electron systems. The results are compared with those by the previous equilibrium technique.

We study the DE model where itinerant electrons couple to localized spins with Ising symmetry on square lattices. This is a minimum model which shows the ferromagnetic transition at finite temperatures by the DE mechanism. We consider the limit of strong Hund’s-rule coupling for simplicity. The Hamiltonian is written by

$$\mathcal{H} = - \sum_{<ij>} \frac{t}{2} (1 + S_i S_j) c_i^\dagger c_j, \quad (1)$$

where $c_i$, ($c_i^\dagger$) annihilates (creates) an electron at site $i$, and $S$ describes the localized Ising spin which takes $S = \pm 1$. The summation is taken for nearest-neighbor sites.
We apply the moment-expansion MC method. We take the same computational conditions as in ref. We study a square lattice of 24 × 24 sites which seems to be large enough to observe the critical relaxation. We will comment on the finite-size effect later. The relaxation is measured for typically 100-1000 different Markov sequences to estimate statistical errors. The energy unit is the half-bandwidth of noninteracting electrons; \( W = 4t \).

We calculate the relaxation of the magnetic moment per site from the perfectly polarized configuration of localized spins. Figure 1 shows the results. For \( T/W \gtrsim 0.059 \), the moment decays exponentially. This indicates that the system is in the paramagnetic state, i.e., \( T > T_c \). On the contrary, the data at \( T/W = 0.056 \) seem to approach a constant, which suggests the broken symmetry below \( T_c \). Power-decay behavior is observed between these temperatures. We estimate \( T_c/W = 0.0575 \pm 0.001 \). This result is consistent with the estimate by the equilibrium technique, \( T_c/W = 0.058 \pm 0.001 \).

The estimate of \( \lambda \) is examined to identify the universality class of this transition. The mean-field universality class gives the exponents as \( \beta = \nu = z = 1/2 \). The dynamical exponent \( z \) is obtained from the consideration that the MC update from \( n \) to \( n + 1 \)-th step at \( T = T_c \) is described by \( m_{n+1} = \tanh(m_n) \) in mean-field models. Thus, the exponent \( \lambda = 2 \) in the mean-field universality class. On the other hand, in the universality class of the Ising model with short-range interactions in two dimensions, the critical exponents are estimated as \( \beta = 1/8, \nu = 1/2 \); and \( z = 2.16 \). In this case, the exponent \( \lambda \) becomes 0.058. Our estimate \( \lambda = 0.14 \pm 0.1 \) is consistent with the universality class of the short-range Ising model, and is distinct from the mean-field one.

The present results are compared with the previous ones obtained by the equilibrium MC calculations. The previous estimates of the critical exponents were \( \beta = 0.09 \pm 0.08 \) and \( \nu = 0.9 \pm 0.3 \), which are consistent with those for the short-range Ising model but different from the mean-field ones. Therefore, the present result by the NER technique is consistent with those by the equilibrium technique. It is suggested that the universality class of the ferromagnetic transition in the DE system is the same as that of short-range interaction models with the same spin symmetry, but different from the mean-field one, from these independent techniques.

We comment on the finite-size effect in the present NER study briefly. One of the finite-size effects is an exponential decay due to an energy gap inherent in finite-size systems. This should decrease the temperature where the relaxation shows the power-decay behavior. Thus, the present estimate of \( T_c \) is considered to give a lower limit. The agreement between the present estimate and the previous one by the equilibrium technique indicates that the finite-size effect is negligibly small in the present precision of the data.

To summarize, we have investigated the ferromagnetic transition in the double-exchange systems by the non-equilibrium-relaxation Monte-Carlo method. To our knowledge, this is the first example of the application of this method to the phase transition in itinerant electron systems. From the relaxation of the magnetic moment, we have estimated the critical temperature and the critical exponents. The results are consistent with the previous ones which are obtained by the finite-size scaling analysis on the Monte-Carlo data in thermal equilibrium. The exponents estimated by these independent techniques indicate consistently that the universality class of this transition appears to be the same as that of short-range interaction models but is different from the mean-field one.

The authors thank H. Nakata for helpful support in developing parallel-processing systems. The computations have been performed mainly using the facilities in the AOYAMA+ project [http://www.phys.aoyama.ac.jp/~aoyama+] and in the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. This work is supported by "a Grant-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology".
[1] C. Zener: Phys. Rev. 82 (1951) 403.
[2] N. Furukawa: in Physics of Manganites, eds. T. Kaplan and S. Mahanti (Plenum Publishing, New York, 1999), and references therein.
[3] Y. Motome and N. Furukawa: J. Phys. Soc. Jpn. 68 (1999) 3853.
[4] Y. Motome and N. Furukawa: J. Phys. Soc. Jpn. 69 (2000) 3785.
[5] Y. Motome and N. Furukawa: J. Phys. Soc. Jpn. 70 (2001) No.6 in press.
[6] M. Kikuchi and Y. Okabe: J. Phys. Soc. Jpn. 55 (1986) 1359.
[7] D. Stauffer: Physica A 186 (1992) 197.
[8] G. A. Kohring and D. Stauffer: Int. J. Mod. Phys. C 3 (1992) 1165.
[9] N. Ito: Physica A 192 (1993) 604.
[10] B. Kaufmann and L. Onsager: Phys. Rev. 76 (1944) 1244.
[11] J. Stephenson: J. Math. Phys. 5 (1964) 1009.