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Non-Equilibrium Relaxation of Fluctuations and Its Application to Critical Phenomena

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The non-equilibrium relaxation method is an efficient numerical technique to analyze phase transition and critical phenomena. Recent development and its applications are reviewed. Relaxations of fluctuations provide various kinds of critical exponents accurately. It is applied to estimate prisice values of β, γ, ν and z for the three-dimensional ferromagnetic (FM) Ising model. The non-universal behavior of the FM transition in the $\pm J$ Ising model is discussed.

KEYWORDS: non-equilibrium relaxation, critical phenomena, Monte Carlo simulation, $\pm J$ Ising model, universality

§1. Introduction

The analysis of non-equilibrium relaxation process is shown to be useful to investigate the phase diagram and the critical phenomena.[1–13] It is called the non-equilibrium relaxation (NER) method. It was firstly applied to estimate the critical point and the dynamic critical exponent quite accurately for the ferromagnetic (FM) transitions. The relaxation process is simulated from the all-up state and the total magnetization $m(t)$ is measured. The statistical average is taken from independent Monte Carlo runs. Since simulation steps for equilibration are not necessary in non-equilibrium process, one can treat large systems in which the equilibrium simulation is difficult to perform.

The NER method now becomes one standard strategy to study the phase transition and critical phenomena. It is applied to study on the dynamical universality (weak universality),[5] spin-glass problems,[6–9] XY models[10,11] and quantum transitions.[12,13] Recently, the method is extended to estimate various exponents using quantities of fluctuations (the susceptibility, the specific heat and so on).[14,15] The critical exponents can be determined by asymptotic powers of such quantities or their combinations. The estimation is simple and quite accurate, and can be applied to wide variety of critical phenomena.

In this article, we review the recent progress on the NER method, especially focus on the NER analysis of fluctuations. The organization of this paper is as follows. In the next section, the basic idea of the NER method is described for the FM case. In section 3, the analysis of fluctuations is introduced, and the NER analysis of fluctuations is applied to the FM Ising model in three dimensions to check the efficiency and accuracy. In section 4, the universality of the FM transition in the $\pm J$ Ising model in three dimensions is studied. The non-universal behavior of the FM critical phenomena in this random system is discussed. The last section is devoted to some remarks.

§2. Non-Equilibrium Relaxation Method

The NER analysis is simple and efficient for conventional critical phenomena. In the FM case, one may simulate the relaxation process from the all-up state, and measure the magnetization $m(t)$ at time t. The relaxation of $m(t)$ shows a power-law decay

$$m(t) \sim t^{-\lambda_m} \tag{2.1}$$

asymptotically only at the critical point, while it decays exponentially in time to zero in the paramagnetic (PM) phase, and to a positive spontaneous-magnetization value in the FM phase. One of two ordering states has been selected by choosing one of the completely ordered states as the initial non-equilibrium state. The phase simulated is distinguished by examining this asymptotic behavior of $m(t)$.

If one assumes the dynamic scaling form,[17,18]

$$m(t,\varepsilon,L) = L^{-\beta/\nu} g(L^{1/\nu}\varepsilon, L^{-z}t), \tag{2.2}$$

for the non-equilibrium process, where L is the linear size of the system and $\varepsilon \equiv |T-T_c|/T_c$, the asymptotic power is related to conventional static and dynamic critical exponents as

$$\lambda_m = \frac{\beta}{z\nu}. \tag{2.3}$$

To distinguish the phase precisely from the data calculated, it is convenient practically to define the local exponent $\lambda_m(t)$ of the relaxation function by the logarithmic derivative of $m(t)$, *i.e.*

$$\lambda_m(t) \equiv -\frac{\mathrm{d}\log m(t)}{\mathrm{d}\log t}. \tag{2.4}$$

It approaches to λ_m asymptotically ($t \to \infty$) at the critical temperature T_c, while it approaches to 0 and ∞ in FM and PM phases, respectively. The finite-time correction for $\lambda_m(t)$ is the same order as the correction in $m(t)$, for example, if one assumes

$$m(t) = t^{-\lambda_m}(a_m + o(1/t)) \tag{2.5}$$

at the critical temperature,

$$\lambda(t) = \lambda + o(1/t) \tag{2.6}$$

is satisfied. At the critical point, the correction term $o(1/t)$ would be the order of $1/t^{\omega_m}$ ($\omega_m > 0$). Therefore, one can determine the critical point as the point where $\lambda_m(t)$ changes its behavior in $1/t = 0$ limit. The error bar is estimated directly by asymptotic behaviors indicating out of criticality; the upper bound of T_c is the lowest temperature indicating $\lambda_m(t) \to \infty$, and the lower bound of T_c is the highest temperature indicating $\lambda_m(t) \to 0$. Such an estimation of error bar will be much reliable as compared with those obtained by conventional scaling-plot analyses.

In Fig. 1, a typical plot of the local exponent is shown for the pure FM Ising model in three dimensions. Simulations are performed on the simple-cubics lattice with sizes up to $127 \times 127 \times 128$. In the following, inverse temperature $K = \beta J$ is often used. At each temperature, we choose several hundreds to thousands independent Monte Carlo runs for averaging. Further, $m(t)$ is averaged over all sites for each time step. It is clearly observed in this figure that the curves for $K \leq 0.221658$ turn up when $1/t$ goes to zero — indicating the PM phase in this region — and the curves for $K \geq 0.221661$ turn down — indicating the FM phase. This means that the critical point exists in $0.221658 < K < 0.221661$. Consequently, the transition temperature is estimated as $K_c = 0.2216595(15)$ or $T_c = 4.511424(30)$. The extrapolated value of $\lambda_m(t)$ is estimated as $\lambda_m = 0.248(1)$.

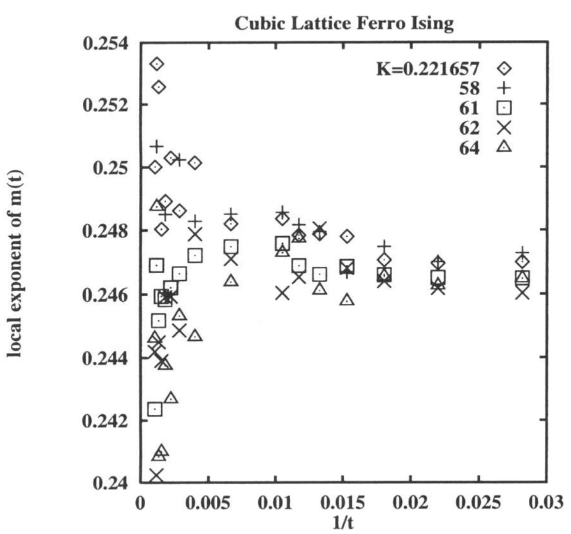

Fig. 1. Typical plot of the local exponent as a function of $1/t$ for the pure FM Ising model in three dimensions. The corresponding inverse temperatures K are indicated in the figure. For $K \geq 0.221661$, bending down behavior appears for $1/t \to 0$ indicating the FM ordering. For $K \leq 0.221658$ bending up behavior appears indicating the PM phase.

In general, the correlation length $\xi(t)$ is growing in the non-equilibrium process from zero at the initial state up to the equilibrium value $\xi_{\rm eq}(T)$. In the region far from the criticality where $\xi_{\rm eq}(T) < L$ holds, $\xi(t) < L$ is always satisfied and the non-equilibrium process is recognized as that in the thermodynamic limit. In the critical region where $\xi_{\rm eq}(T) > L$, the characteristic time defined by $\xi(\tau_L) \sim L$ exists. The finite-size effect is observed in $t > \tau_L$. The analysis of non-equilibrium relaxation mentioned above should be made only up to the time much smaller than this τ_L. Since simulation steps for equilibration are not necessary, one can treat large systems for which the equilibrium simulation is unreachable. In such systems, τ_L is large enough to analyze the asymptotic behavior in the thermodynamic limit sufficiently from the non-equilibrium relaxation in $t < \tau_L$.

§3. Relaxation of Fluctuations

It is confirmed that, in the non-equilibrium relaxation from the all-up state, not only the magnetization but also quantities of fluctuations defined by

$$\chi(t)/N \equiv \langle m(t)^2 \rangle - \langle m(t) \rangle^2, \tag{3.1}$$

$$m'(t)/N \equiv \langle m(t)e(t) \rangle - \langle m(t) \rangle \langle e(t) \rangle, \tag{3.2}$$

$$C(t)/N \equiv \langle e(t)^2 \rangle - \langle e(t) \rangle^2, \tag{3.3}$$

show a power-law behavior at the critical point,[14,15] where $e(t)$ is the per-site energy and N is the number of sites. Note that $\langle m(t) \rangle$ in the PM phase is non-zero in general because the initial state may have a non-zero value. The magnetization $m(t)$ decays in time, while fluctuations $\chi(t)$, $m'(t)$ and $C(t)$ diverge. This means they have positive powers. The above fluctuations approach to equilibrium quantities asymptotically; they are proportional to the susceptibility, the temperature derivative of the spontaneous magnetization $\dfrac{\partial m}{\partial T}$ and the specific heat, respectively

Assuming the dynamic finite-size scaling hypothesis,[17,18] the free-energy-like generating function f has scaling form

$$f(\epsilon, h, t) = t^{-d/z} \bar{f}(\epsilon \cdot t^{y_\epsilon/z}, h \cdot t^{y_h/z}) \tag{3.4}$$

in the scaling region, where h denotes the symmetry breaking field which is conjugate to the order parameter. The exponents y_ϵ and y_h are $1/\nu$ and $d - \beta/\nu$, respectively, and d denotes the spatial dimensionality. The NER exponents of fluctuations are given by derivation of this scaling form and they are

$$\chi(t) \sim t^{d/z - 2\beta/z\nu}, \tag{3.5}$$

$$m'(t) \sim t^{(1-\beta)/z\nu}, \tag{3.6}$$

$$C(t) \sim t^{\alpha/z\nu}. \tag{3.7}$$

It is convenient to use the following functions of NER fluctuations:

$$f_{mm}(t) = N \left[\frac{\langle m(t)^2 \rangle}{\langle m(t) \rangle^2} - 1 \right], \tag{3.8}$$

$$f_{me}(t) = N \left[\frac{\langle m(t)e(t) \rangle}{\langle m(t) \rangle \langle e(t) \rangle} - 1 \right], \tag{3.9}$$

$$f_{ee}(t) = N \left[\frac{\langle e(t)^2 \rangle}{\langle e(t) \rangle^2} - 1 \right], \tag{3.10}$$

which are introduced and used also in Ref. (14-15). Asymptotic growth exponents at the critical points of these NER functions are denoted by λ_{mm}, λ_{me} and λ_{ee}, respectively, and they are

$$\lambda_{mm} = \frac{d}{z}, \tag{3.11}$$

$$\lambda_{me} = \frac{1}{z\nu}, \tag{3.12}$$

$$\lambda_{ee} = \frac{\alpha}{z\nu}. \tag{3.13}$$

Similarly to the magnetization, we denote the local exponents of these functions as $\lambda_{mm}(t)$, $\lambda_{me}(t)$ and $\lambda_{ee}(t)$. The conventional critical exponents are obtained asymptotically by combinations of these local exponents:

$$\alpha(t) \equiv \frac{\lambda_{ee}(t)}{\lambda_{me}(t)} \quad \to \alpha, \tag{3.14}$$

$$\beta(t) \equiv \frac{\lambda_{m}(t)}{\lambda_{me}(t)} \quad \to \beta, \tag{3.15}$$

$$\nu(t) \equiv \frac{1}{d}\frac{\lambda_{mm}(t)}{\lambda_{me}(t)} \quad \to \nu, \tag{3.16}$$

$$z(t) \equiv \frac{d}{\lambda_{mm}(t)} \quad \to z. \tag{3.17}$$

So the study on the relaxation of fluctuations at the critical point provides the estimates for various exponents.[15]

We apply the above method to the FM Ising model in three dimensions, and check the validity, the efficiency and the accuracy of it. Calculations are performed on the simple-cubics lattice at the critical temperature obtained by the previous section with sizes up to $127 \times 127 \times 128$. At each temperature, we choose about 10^6 independent Monte Carlo runs for averaging. The results are shown in Figs. 2-5. Those for two different sizes are plotted. It is seen that the size dependency is almost negligible in the present accuracy. If one assumes that the asymptotic form of local exponents is analytic to $1/t$, the critical exponents are obtained by simple extrapolations. It is obtained that $z = 2.06(1)$, $\nu = 0.630(5)$ and $\beta = 0.320(3)$. Note that the data of α does not converge enough to the the expected value (~ 0.11) in the present observation time. This would be due to the smallness of the exponent providing the slow convergence in time.[16] Although the problem of the asymptotic form remains unsolved, our present estimations are consistent with those obtained so far.

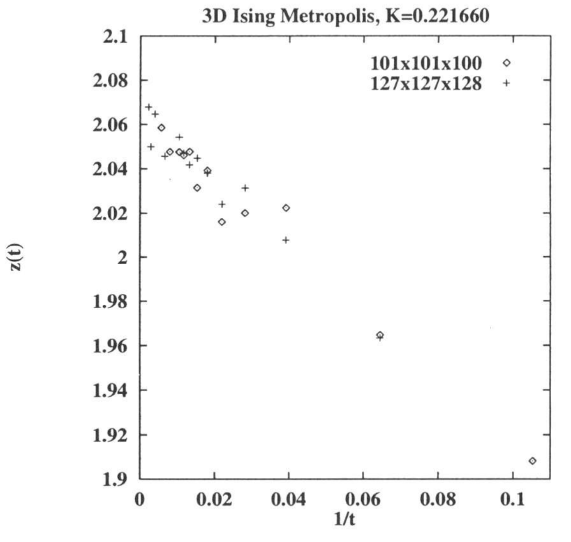

Fig. 2. Local exponent of the dynamic critical exponent as a function of $1/t$ for the $3D$ pure FM Ising model.

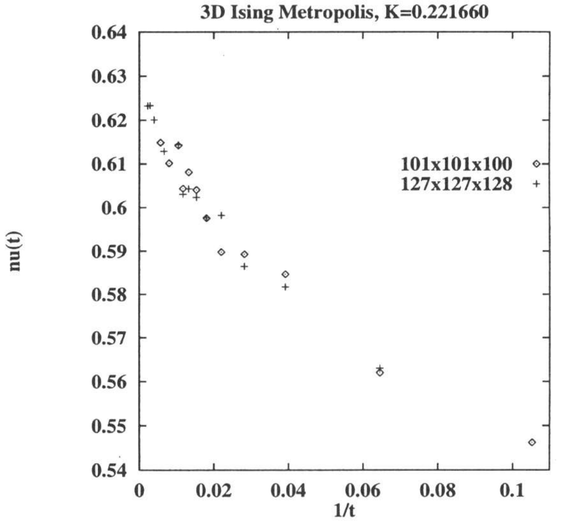

Fig. 3. Local exponent of ν as a function of $1/t$ for the $3D$ pure FM Ising model.

§4. Application to the FM Transition in the $\pm J$ Ising Model

The model we study is the $\pm J$ Ising model on the simple-cubic lattice:

$$\mathcal{H} = -\sum_{<i,j>} J_{ij} S_i S_j, \tag{4.1}$$

where the summation runs over all nearest neighbor sites on the simple-cubic lattices. The quenched coupling constant takes $J (> 0)$ with probability p, or $-J$ with probability $(1 - p)$.

The behavior of this model along so-called the Nishimori-line,[19)]

$$2K = \log \frac{p}{1-p}, \tag{4.2}$$

is well-studied. The multi-critical point (MCP) where the PM, the FM and the spin glass (SG) phases merge is considered to be located on this line. The specific heat does not diverge on this line, providing $\alpha \leq 0$. It was suggested by Monte Carlo renormalization study[20] that the static exponents along the boundary of FM transition are not much different from those of the pure system – universality – except the MCP, and so do the ratio of them $(\beta/\nu, \gamma/\nu)$ – weak universality – including the MCP. The series expansion study[21] concluded that $\nu = 0.85(8)$ and

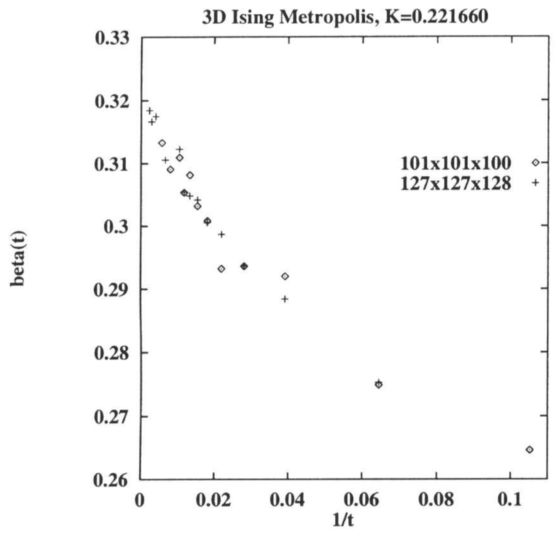

Fig. 4. Local exponent of β as a function of $1/t$ for the $3D$ pure FM Ising model.

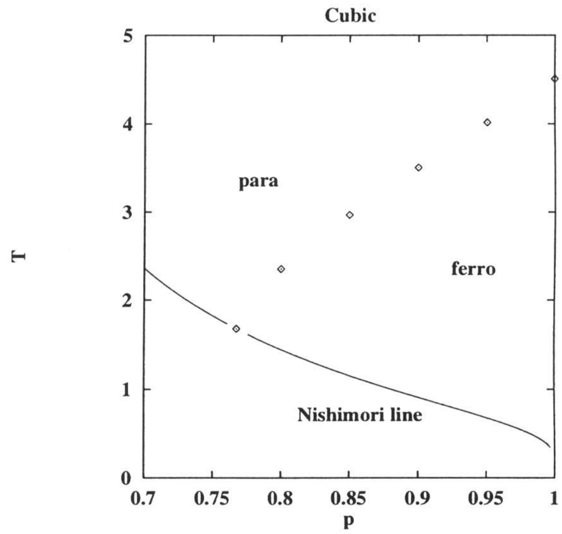

Fig. 6. FM transition points for the 3D $\pm J$ Ising model is plotted in the $p-T$ plane. The solid curve shows the Nishimori-line.[8)]

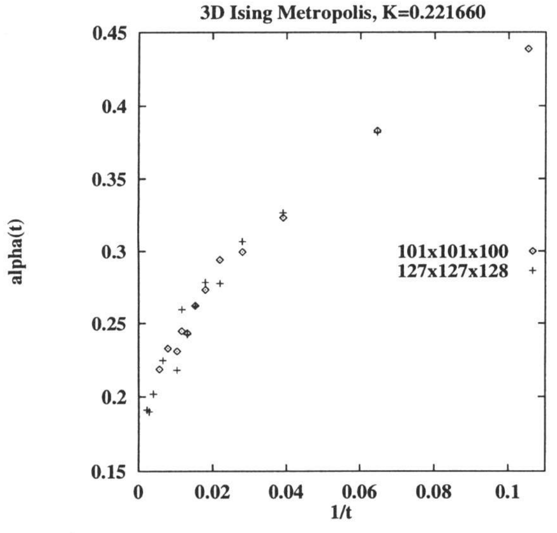

Fig. 5. Local exponent of α as a function of $1/t$ for the $3D$ pure FM Ising model.

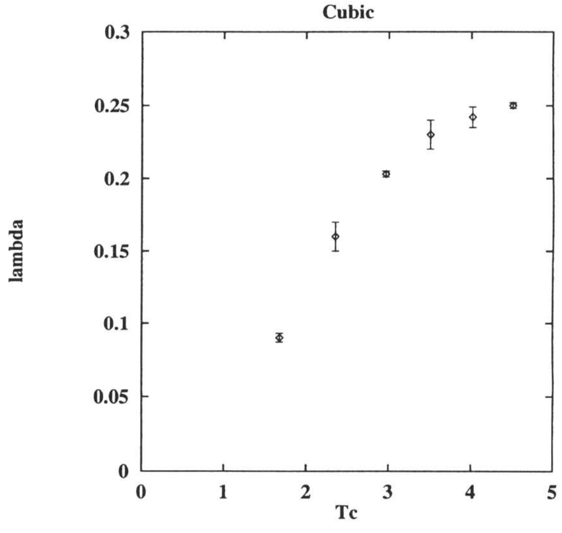

Fig. 7. The values of non-equilibrium exponent for the 3D $\pm J$ Ising model are plotted as a function of the transition temperature.[8)]

$\gamma = 1.80(15)$ at the MCP belong to a different universality class from that at the pure FM case ($\nu = 0.630$ and $\gamma = 1.24$). Recently, Hukushima[22)] investigated the phenomenological Monte Carlo renormalization group based on numerically calculated domain-wall free energies in the $p-T$ plane. His result suggests the existence of so-called the random fixed point around $p = 0.9$ (it is not sure to be located just on the $p-T$ plane). This means that a single universality class would hold along the FM phase boundary in $p_{\rm mc} < p < 1$, and at least three universality classes exist for FM transitions; the pure case, the random fixed point and the MCP.

The NER method is applied also to the SG model.[6–9)] The MCP is located finely with the estimations of the non-equilibrium and equilibrium relaxation exponent using the aging relation[23,24)] which connects the non-equilibrium relaxation to the equilibrium relaxation on the Nishimori-line. These studies show that the NER is useful to analyze the FM transition even in disordered systems in which randomness and frustration make it difficult to analyze thermodynamic behaviors. The MCP was estimated as $p_{\rm mc} = 0.7673(3)$ for the simple-cubic lattice.[7)] The FM phase boundary and corresponding dynamic critical exponent $\lambda_m = \beta/z\nu$ were obtained as in Figs. 6 and 7.[8)] It was confirmed that $\beta/z\nu$ is non-universal and varies from the pure case to the MCP. What is the origin of this non-universal behavior? If it is due to the dynamical effect, only the exponent z is non-universal which is not contradict with the existence of the random fixed point.

In the following, we estimate z, ν and β using the NER of fluctuations to discuss the origin of non-universal behavior of $\beta/z\nu$. Calculations are carried out for several points on the phase boundary appeared in Fig. 6 with the size of $101 \times 101 \times 102$. At each point, we choose 5×10^5 to 1.5×10^6 independent Monte Carlo runs for averaging. The local exponents defined by eqs. (3.15)-(3.17) are plotted in Figs. 8-10. It is seen that, for each exponent, the extrapolated value to $1/t \to 0$ varies with p in the present accuracy. This means the non-universal behavior for z, β and ν. The estimated exponents at the MCP, $\nu = 0.85(5)$ and $0.40(3)$, are consistent with those obtained by the series expansion,[21] if we use the hyperscaling relation, $2\beta+\gamma = d\nu$. It is also consistent with the non-divergence of the specific heat, since $\alpha = 2 - d\nu = -0.55(15)$. We also plot the combination $\beta(t)/\nu(t)$ in Fig. 11. As compared with other plots, the extrapolated value seems to be universal for $p_{\rm mc} < p \leq 1$, and that for the MCP is different from that. This means the weak universality holds for $p_{\rm mc} < p \leq 1$, and the MCP belongs to a different class.

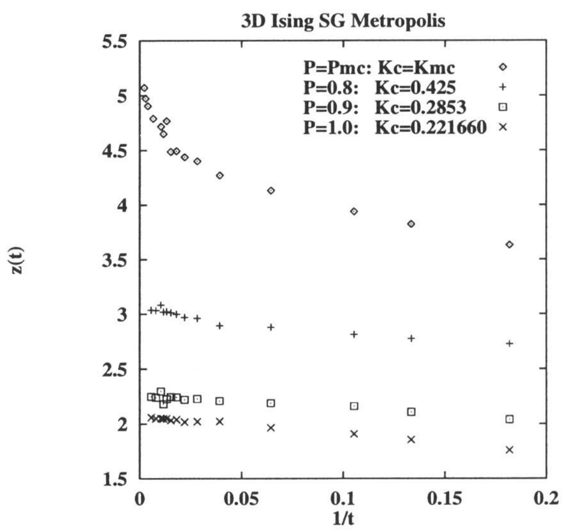

Fig. 8. Local exponent $z(t)$ defined by eq. (3.17) at $p = 1.0, 0.9, 0.8$ and $p_{\rm mc}$ for the 3D $\pm J$ Ising model. The extrapolated value for $1/t \to 0$ is the critical exponent.

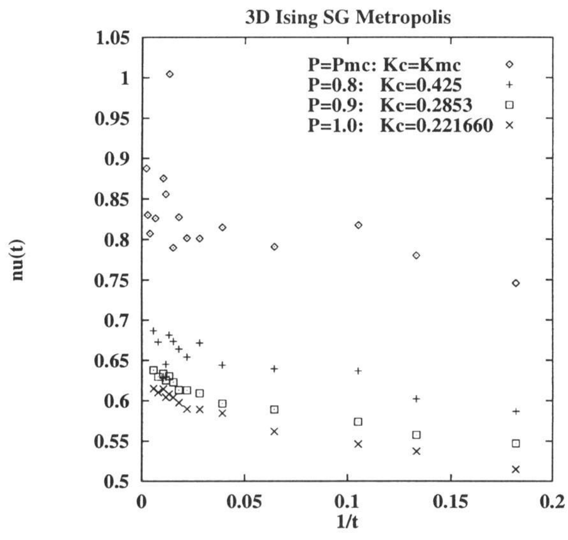

Fig. 9. Local exponent $\nu(t)$ defined by eq. (3.16).

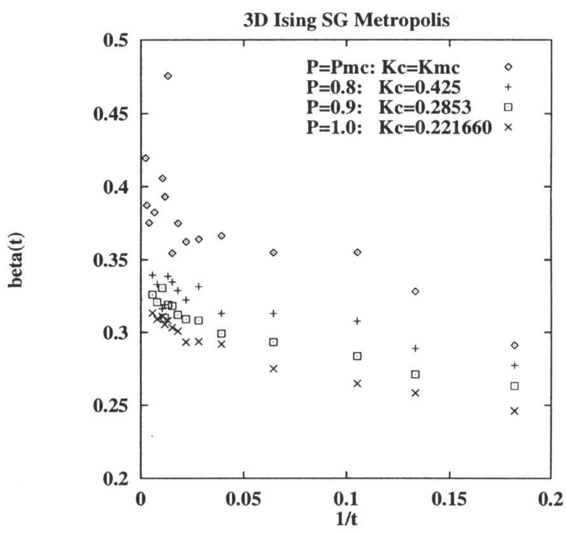

Fig. 10. Local exponent $\beta(t)$ defined by eq. (3.15).

§5. Remarks

The applications of the non-equilibrium relaxation (NER) to the phase transition and critical phenomena are reviewed. The phase and the critical point are efficiently studied by observing the NER function of the order-parameter, and critical exponents are estimated from the NER functions of fluctuations.[15] First, it is applied to the pure FM Ising model in three dimensions, and confirmed the accuracy.

Next, it is applied to the $\pm J$ Ising model in three dimensions to investigate the universality of FM critical phenomena. It is confirmed that the estimated critical exponents at the multi-critical point (MCP) are consistent with results by the gauge theory[19] and the series expansion.[21] The universality does not hold along the FM phase boundary, while the weak universality holds except at the MCP. The origin of non-universal behavior for $\lambda_m = \beta/z\nu$ comes from the dynamic critical exponent z. These result is partly consistent with that of the Monte Carlo renormalization study[20] for the case of the weak universality. It is not observed three different classes provided by the random fixed point suggested by the phenomenological Monte Carlo renormalization study.[22]

It is noted that the asymptotic form of local exponents is not apparent, while we assume the analyticity of them to $1/t$, and estimate the critical exponents by sim-

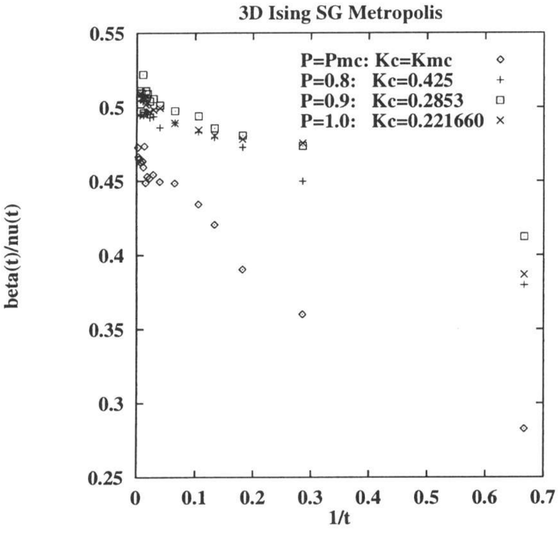

Fig. 11. Local exponent $\beta(t)/\nu(t)$.

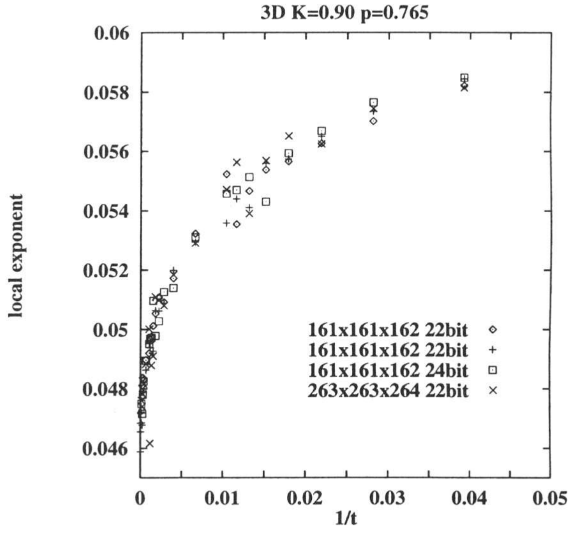

Fig. 12. The local exponent of $m(t)$ at $p = 0.765$ and $K = 0.9$ for the 3D $\pm J$ Ising model. The FM ordering is indicated.

ple extrapolations to $1/t \to 0$. If this is not true, values of the extrapolation would vary as time steps increases. Further investigation is necessary to clarify it.

In the simulation, single-spin flip dynamics with two-sublattice update are used. An independent-spin coding technique[25,26] and shuffling technique[27] are applied with Lewis-Payne-type pseudo-random number.[28,29] The simulations are performed on Fujitsu VPP500/40, each of whose 40 processors has 1.6GFLOPS peak performance, and the typical performance for simple-cubic lattice is 773 MUPS(million updates per second) per processor only for spin update, and it becomes 556 MUPS per processor for spin update and magnetization calculation at every step.

We finally comment on the shape of the phase boundary below the MCP. It is concluded exactly by the gauge theory[19] that the long-range FM ordering does not appear in $p < p_{\mathrm{mc}}$ at any temperature. This means that the boundary is vertical or reentrant. However, in our preliminary calculation with $p = 0.765 < p_{\mathrm{mc}} = 0.767$ and $K = 0.9 > K_{\mathrm{mc}} = 0.596$, the bending down behavior is observed (see Fig. 12). This indicates the FM phase there, which contradicts with the exact result. Two possibilities are considered. One is that the boundary of the FM long-range order is deviated from that of the FM spontaneous symmetry breaking. The NER analysis from the all-up state detects the latter case and the gauge theory restricts the former point. The other is the first order phase transition below the MCP, in which the NER analysis from the all-up state overestimates the FM phase; the observation is due to the hysteresis. The same phenomenon is observed in the XY gauge glass model in three dimensions.[30] Further investigation is necessary to conclude it.

Acknowledgements

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1) D. Stauffer: Physica A **186** (1992) 197.
2) G. A. Kohring and D. Stauffer: Intern. J. Mod. Phys. **C3** (1992) 1165.
3) N. Ito: Physica A **192** (1993) 604.
4) N. Ito: Physica A **196** (1993) 591.
5) F.-G. Wang and C.-K. Hu: Phys. Rev. **E56** (1997) 2310.
6) N. Ito, T. Matsuhisa and H. Kitatani: J. Phys. Soc. Jpn. **67** (1998) 1188.
7) Y. Ozeki and N. Ito: J. Phys. A bf 31 (1998) 5451.
8) N. Ito, Y. Ozeki and H. Kitatani: J. Phys. Soc. Jpn. **68** (1999) 803.
9) Y. Ozeki and N. Ito: submitted to Phys. Rev. B.
10) H. Luo, L. Schülke and B. Zheng: Phys. Rev. Lett. **81** (1998) 180.
11) Y. Ozeki and Ito N: in preparation.
12) Y. Nonomura: J. Phys. Soc. Jpn. **67** (1998) 5.
13) Y. Nonomura: J. Phys. **A31** (1998) 7939.
14) A. Jaster, J. Mainville, L. Schülke and B. Zheng: cond-mat/9808131.
15) N. Ito, K. Hukushima, K. Ogawa and Y. Ozeki: in preparation.
16) N. Ito and Y. Ozeki: to appear in Int. J. Mod. Phys. C.
17) M. Suzuki: Phys. Lett. **A58** (1976) 435.
18) M. Suzuki: Prog. Theor. Phys.**58** (1977) 1142.
19) H. Nishimori: Prog. Theor. Phys. **66** (1981) 1169.
20) Y. Ozeki and H. Nishimori: J. Phys. Soc. Jpn. **56** (1987) 1568.
21) R. R. P. Singh: Phys. Rev. Lett. **67** (1991) 899.
22) K. Hukushima: private communication.
23) Y. Ozeki: J. Phys A: Math. and Gen. **28** (1995) 3645.
24) Y. Ozeki, J. Phys C: Condensed Matter. **10** (1997) 11171.
25) C. Michael: Phys. Rev. **33** (1986) 7861.
26) N. Ito and Y. Kanada: Supercomputer **5** No. 3 (1988) 31.
27) N. Ito, M. Kikuchi and Y. Okabe: Intern. J. Mod. Phys. **C4** (1993) 569.
28) T. S. Lewis and W. H. Payne: J. ACM **20** (1973) 456.
29) N. Ito and Y. Kanada: Supercomputer **7** No. 1 (1990) 29.
30) K. Ogawa and Y. Ozeki: private communication.