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Nonequilibrium relaxation method – An alternative simulation strategy

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Abstract. One well-established simulation strategy to study the thermal phases and transitions of a given microscopic model system is the so-called equilibrium method, in which one first realizes the equilibrium ensemble of a finite system and then extrapolates the results to infinite system. This equilibrium method traces over the standard theory of the thermal statistical mechanics, and over the idea of the thermodynamic limit. Recently, an alternative simulation strategy has been developed, which analyzes the nonequilibrium relaxation (NER) process. It is called the *NER method*. NER method has some advantages over the equilibrium method. The NER method provides a simpler analyzing procedure. This implies less systematic error which is inevitable in the simulation and provides efficient resource usage. The NER method easily treats not only the thermodynamic limit but also other limits, for example, non-Gibbsian nonequilibrium steady states. So the NER method is also relevant for new fields of the statistical physics. Application of the NER method have been expanding to various problems: from basic first- and second-order transitions to advanced and exotic phases like chiral, KT spin-glass and quantum phases. These studies have provided, not only better estimations of transition point and exponents, but also qualitative developments. For example, the universality class of a random system, the nature of the two-dimensional melting and the scaling behavior of spin-glass aging phenomena have been clarified.

Keywords. Nonequlibrium relaxation; phase transition; exponents, Kosterlitz–Thouless transition; chiral transition; two-dimensional melting; first-order transition; spin-glass system; random system; computer simulation; computer emulation.

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1. Introduction

Nonequilibrium relaxation (NER), which is a relaxation process from a nonequilibrium initial state, has turned out to be useful to study the equilibrium phase diagram and transitions. The relaxation process, even if it is from a nonequilibrium state, knows about its destination (that is, its equilibrium state), and the nature and the behavior of the equilibrium state can be studied by using the NER process. The methods by which one can study the equilibrium state in NER process are

called the *NER methods*. It is remarkable that the NER method often provides a simpler and more efficient simulation strategy than the standard equilibrium simulation strategy.

Studies of the NER process have a long history, at least as long as that of studies of relaxation behavior. Among them, Suzuki's dynamical finite-size scaling hypothesis [1,2], which includes both equilibrium and nonequilibrium relaxations, gives a good starting point to the NER method. After this hypothesis, simulational studies of NER process appeared [3–8], mainly observing the dynamical Monte Carlo renormalization in NER, and it was discovered that exponent values can be estimated with good accuracy just by using very early stages of the NER process [8]. This feature was applied first to estimate the values of the dynamical exponent of the Ising ferromagnet [9–14], whose values had not been settled for many decades, and we reached reliable estimates by using the estimation method of the NER process [13]. With this method, dynamical weak universality was verified [15].

Another motivation to study the NER process came from the scaling hypothesis of the initial relaxation process of NER, which is often called the short-time dynamics [16,17]. It should be noted that the studies using this idea of short-time dynamics and its universality have also been developed [18–22]. But the real short-time dynamics does not seem to be a suitable tool to establish a new simulation strategy, and these studies have been coming from the same direction as the present NER strategy [23–27].

The purpose of this article is to give a concise review of the idea of the NER method and some of its applications. In the following sections, NER results for various kinds of phases and transitions are given briefly. The last section is for discussions and a perspective of NER in statistical physics.

2. Basic second-order transition

Let us consider a ferromagnetic transition as an example of a basic second-order transition. The phase diagram and transition temperature are estimated by using the magnetization NER function denoted by $f_{\rm m}(t)$. A completely ordered state is most useful for this purpose as at the initial state at $t = 0$, the magnetization is taken as unity and therefore $f_{\rm m}(0) = 1$. This $f_{\rm m}(t)$ decays to zero or to a positive spontaneous magnetization value denoted by $m_{\rm s}$ in the paramagnetic (PM) or ferromagnetic (FM) phases, respectively. The relaxation is exponential [27a]. At the transition point, it shows a power-law decay and the asymptotic decay exponent is $\beta/\nu z$, where β, ν and z denote the exponents of magnetization, correlation length and dynamics, respectively [1,2]. In short,

$$f_{\rm m}(t) \sim \begin{cases} a{\rm e}^{-t/\tau} & {\rm PM} \\ at^{-\beta/\nu z} & \text{critical point} \\ m_{\rm s} + a{\rm e}^{-t/\tau} & {\rm FM} \end{cases}, \tag{1}$$

where a and τ are constants depending on the temperature.

One of the most remarkable features of NER methods is that the estimation of the NER function of infinite-size system is rather easily done even at the critical

point. This is because the size dependence of $f_{\rm m}(t)$ at a fixed t is exponential [12,13].

The phases are identified by observing the $t \to \infty$ behavior of the local exponent $\lambda_{\rm m}(t)$ defined by

$$\lambda_{\rm m}(t) = -\frac{{\rm d}\log f_{\rm m}(t)}{{\rm d}\log t}. \tag{2}$$

From eq. (1), this local exponent behaves like

$$\lambda_{\rm m}(t) \sim \begin{cases} t/\tau & \text{PM}, \\ -\beta/\nu z & \text{critical point}, \\ (t/\tau m_{\rm s}){\rm e}^{-t/\tau} & \text{FM}. \end{cases} \tag{3}$$

A convenient way to distinguish these behaviors is to plot the local exponent vs. $1/t$ and observe the behavior near $1/t = 0$, where it grows in PM and decays in FM [28–30]. One example of such a local exponent plot is given in figure 1. The system is the ferromagnetic Ising model on a cubic lattice whose interaction energy is defined by $E = -J\sum_{\langle i,j\rangle} s_i s_j$ ($s_i = \pm 1$, $J > 0$), where the summation $\langle i, j\rangle$ runs over the nearest-neighbor site pairs. In long time limit ($1/t \to 0$), the growth of the local exponent value is observed for $K \leq 0.2216542$, where K denotes the inverse temperature βJ, which implies that the system is in paramagnetic phase

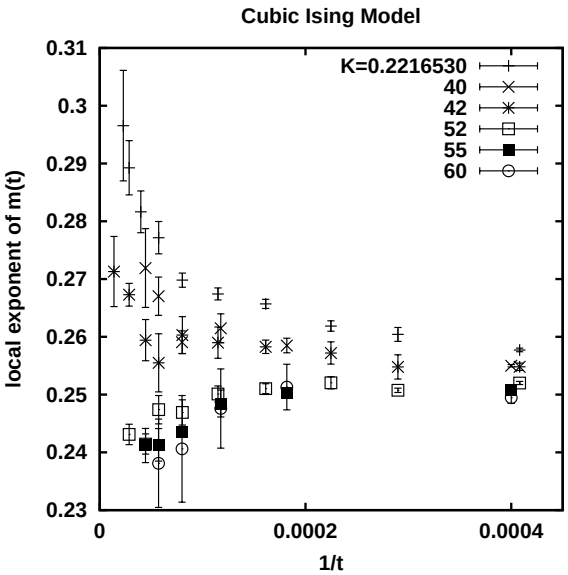

Figure 1. Estimated values of the local exponent $\lambda_{\rm m}(t)$ of a cubic Ising ferromagnet are shown for several values of inverse temperature K near the transition point.

in this inverse temperature range and decay is observed for $K \geq 0.2216552$ where the system is ferromagnetic. Therefore the transition point is estimated to be $K_{\rm c} = 0.2216547(5)$. This simulation was executed on the Earth Simulator [31]. The largest lattice was $6648 \times 6648 \times 6656$ using 512 nodes of the Earth Simulator. Simulation performance was 26.5 TUPS ($= 26.5 \times 10^{12}$ updates per second) only for configuration updates with two-sublattice single-spin dynamics using the Metropolis-type transition probabilities [32–35], and 20.4 TUPS for configuration updates with a magnetization calculation. The maximum simulation time is 100,000 Monte Carlo sweeps.

Values of exponents are conveniently estimated by observing the NER of the fluctuations in physical quantities [36–38] defined by

$$f_{mm}(t) = L^d \left[\frac{\langle m(t)^2 \rangle}{\langle m(t) \rangle^2} - 1 \right], \quad f_{me}(t) = L^d \left[\frac{\langle m(t) e(t) \rangle}{\langle m(t) \rangle \langle e(t) \rangle} - 1 \right] \tag{4}$$

and

$$f_{ee}(t) = L^d \left[\frac{\langle e(t)^2 \rangle}{\langle e(t) \rangle^2} - 1 \right], \tag{5}$$

where $m(t)$ and $e(t)$ denote the values of the order parameter and the energy at time t. We call them the NER functions of fluctuations for simplicity, although they are diverging in time. At the critical point, these quantities are expected to show asymptotically,

$$f_{mm}(t) \sim t^{\lambda_{mm}}, \quad f_{me}(t) \sim t^{\lambda_{me}} \quad \text{and} \quad f_{ee}(t) \sim t^{\lambda_{ee}}, \tag{6}$$

where λ_{mm}, λ_{me} and λ_{ee} denote their divergence exponents, and they are expected to be related with the standard exponents as

$$z(t) = \frac{d}{\lambda_{mm}(t)}, \quad \nu(t) = \frac{\lambda_{mm}(t)}{d \cdot \lambda_{me}(t)}, \quad \beta(t) = \frac{\lambda_m(t)}{\lambda_{me}(t)}$$

and

$$\alpha(t) = \frac{\lambda_{ee}(t)}{\lambda_{me}(t)}, \tag{7}$$

where α denotes the specific heat exponent. So the analysis of local exponents, or the logarithmic derivatives, gives estimations of exponents, for example, those of cubic Ising ferromagnet are estimated to be $z = 2.055(10)$, $\nu = 0.635(5)$, $\beta = 0.325(5)$ and $\alpha = 0.14(2)$ [37].

It should be remarked here that the infinite-size limit of the fluctuation NER functions is not taken easily. So the system size should be selected more carefully than in the case of the magnetization NER function.

This estimation method of the transition point has been applied to various systems: the ferromagnetic transitions of Heisenberg, XY and generalized clock-type models in two- and three-dimensional lattices [38], $\pm J$ model [28,39–44] for which random ferromagnetic universality was confirmed [43,44], and the chiral transition [45].

3. Other transitions

NER methods for phases and transitions other than basic ferromagnetic transition have also been established. Some examples of such methods for other typical transitions are introduced briefly in the following:

3.1 *First-order transitions*

A first-order transition is studied by analyzing the behavior of NER functions from two different initial configurations: disordered and ordered. Outside the hysteresis region, they relax to the same values. In the hysteresis region, they relax to different values [38,46]. With this method, a first-order transition is clearly identified even if it is the so-called weak-first-order transition. The transition point is estimated using the NER functions from mixed initial configuration, that is, half of the system is in the disordered state and the other half is in the ordered state [46].

3.2 *Kosterlitz–Thouless transition*

NER characteristics of the Kosterlitz–Thouless (KT) transition is the essential-singular behavior of the time-scale, $\tau(\varepsilon)$, where ε denotes the difference of a control parameter from the KT transition point from the disordered phase, and the NER function $f(t)$ of the quantity affected by the KT transition has the scaling property

$$f(t) = t^{-\lambda}\bar{f}(t \cdot \exp[-a/\sqrt{\varepsilon}]), \tag{8}$$

where a and λ are constants. A scaling analysis of the NER function based on eq. (8) is useful to identify the KT transition [47–50]. With this method, XY and clock-type models [47–50], and melting of hard-disk systems [51–54] have been studied.

A proper KT analysis often requires large systems, but it is hard with equilibrium methods. With the NER method, behavior of infinite system is easily estimated, and that is why the NER method succeeded to analyze various KT transitions.

3.3 *Spin-glass phase*

The spin-glass (SG) transitions and phases are characterized by the NER behavior of the so-called clone-correlation function $Q(t, t_{\rm w})$. For the Ising spin-glass model, it is the spin-overlap of two replicas, that is,

$$Q(t, t_{\rm w}) = \frac{1}{N}\sum_i \langle s_i(t) \cdot s'_i(t)\rangle, \tag{9}$$

where $s_i(t)$ and $s'_i(t)$ denote the values of Ising spins taking values $+1$ or -1 at time t after the replica is duplicated after a waiting time $t_{\rm w}$ from a random initial configuration. Each replica after duplication evolves independently.

The SG transition point is characterized by the scaling relation,

$$Q(t, t_{\rm w}) = t_{\rm w}^{-\lambda_q} \bar{Q}(t/t_{\rm w}). \tag{10}$$

In the SG phase, $Q(t,\ t_{\rm w})$ shows the so-called aging like behavior and this is an important characteristic of the SG phase [55].

The SG system was extensively studied by T Nakamura with the NER method: chiral-glass possibility in the three-dimensional Heisenberg SG [56] and weak universality [57] have been explored.

4. Discussion and perspective

The NER method is reviewed briefly in this article, mainly concentrating on how to estimate the phase and transition by using computer simulation. It should be remarked here that the NER strategy often saves not only the computer time but also human time, because infinite system extrapolation of the NER function is often easier than the infinite time extrapolation of the ensemble average even at the critical point, especially for a system with a large dynamical exponent. Although the algorithmic complexity of the NER method and the equilibrium method to reach the same accuracy is usually the same and the difference comes from the overall coefficients, and the simpler procedure suffers less bias and less systematic error.

Not only the computational efficiency, but also the interesting features of the NER process have been clarified: For example, NER Rushbrooke's inequality [58], gauge symmetric relation between the NER function of magnetization and the equilibrium relaxation function of the spin-glass order parameter [39], and so on.

Applications to quantum system [59–63], axial next-nearest-neighbor Ising model [64] and magneto-dielectric phase transition [65] have also been developed.

Statistical mechanics is the theory connecting the microscopic equations of motions to the macroscopic equilibrium state. The standard theory, that is, the Boltzmann–Gibbs (BG) statistical mechanics is regarded as the theory which takes the long-time limit first and then takes the infinite-size limit. After the first long-time limit, the system is considered to reach the equilibrium state of a finite system. Then the second infinite-size limit, or the thermodynamics limit, the thermodynamic behavior appears.

The NER method does not insist on this limiting order. Let us observe this aspect in case of the NER method for the basic second-order transition we have seen in the second section, for simplicity. These two limiting procedures of $t \to \infty$ and $N \to \infty$ are exchanged: take the infinite-size limit first, then the long-time limit is studied. These relations are summarized schematically in figure 2. One question arises: *are they commutable?* If the answer is *yes*, we can safely use the NER method. Actually, they will be commutable for thermal system with short-range interaction from initial states whose energy corresponds to the disordered phase [65a]. If the answer is *no*, we should use the NER method instead of the BG theory at least for the macroscopic behavior because the macroscopic behavior is the dynamical behavior of an (almost) infinitely large system. Such examples are observed in the system with long-range interaction, for example, gravitational and charged systems, and densely coupled oscillator systems [66].

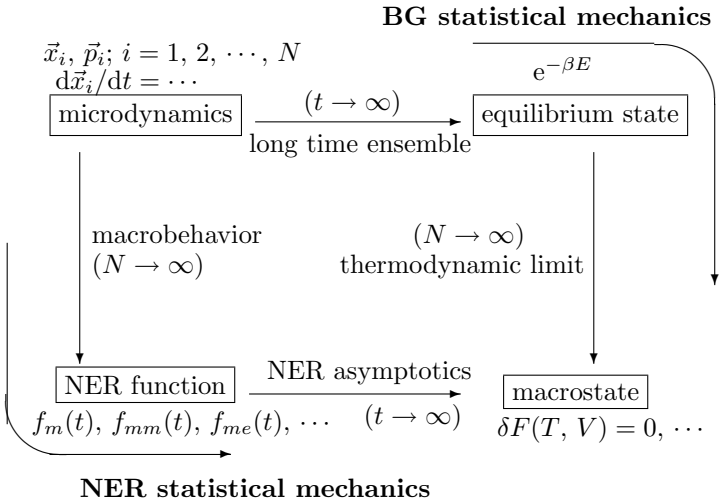

Figure 2. Schematic representation of the relation between the Boltzmann–Gibbs (BG) approach and the NER approach.

Furthermore, there are crucial differences between BG and NER approaches not only in the limiting orders, but also in the theoretical interpretations of macroscopic behaviors. First of all, the nature of the correction to the macroscopic behavior is different. In BG, the finite-size correction appears in the equilibrium ensemble of the finite system. In NER, finite-time corrections exist in the NER functions. Both corrections become relevant near the critical point.

Secondly, in BG, macroscopic phases are interpreted as stable fixed points of renormalization transformation for the degrees of freedom in the system, and renormalization flows go into these points. In NER, they are converging points and flow of local exponents of their long-time asymptotic behavior. In general, the renormalization fixed points and flow are infinite dimensional and rather abstract. But the local exponent converging points and flows are in two dimensions (time and local exponent) concrete object. This will be an advantage of the NER approach because this interpretation of phase and transition is easier than that of BG.

There are numerous distinctions, and just one more is described here: phase transition phenomena are interpreted as spontaneous symmetry breaking in BG, and they are initial state dependence in NER. If a transition is a simple symmetry breaking like ferromagnets, initial state dependence also shows the same symmetry breaking. There are transitions whose symmetry are not obvious, for example, glass transitions. Even for such systems, NER approach can control the transition by studying the initial state dependence.

Those differences are summarized in table 1.

The development of computing statistical physics has been continuing for half a century. Its growing speed is ten times more degrees of freedom at every four years, and this will continue for the time being. Assuming that this speed-up continues, one simulational work can treat more than the Avogadro number degrees of freedom totally till the middle of this century [45,67]. We saw the simulation result of the

Table 1. Comparison between the NER and the BG.

	Boltzmann–Gibbs	NER
State	$\mathrm{e}^{-\beta\mathcal{H}}$	$\mathrm{e}^{-t\mathcal{L}} \cdot \rho(t=0)$
From microdynamics	$t \to \infty$	$L \to \infty$
From macrostate	Finite size correction	Finite time correction
Phase	Renormalization flow	Local exponent flow
Transition	Spontaneous symmetry breaking	Initial state dependence

cubic Ising model larger than 6000^3 in the second section, and this size corresponds to more than a few micrometer cubes in the real magnetic crystal. The simulation is now reaching macroscale beyond mesoscale, where nonequilibrium dynamical behavior like magnetic domain is crucial. The computational statistical physics is now diving into the nonequilibrium phenomena beyond the local equilibrium fragment. The computer *simulation* may be becoming the computer *emulation*, which is the theoretical virtual reality emulating the real physical phenomena. In these situations, a simple, reliable and computer-oriented analysis method is very important and the NER method will so far be the simplest simluation strategy to study the thermal property of macroscopic materials. Furthermore, the NER method observes macroscopic dynamical behavior, the same quantities as the ones we get experimentally. So the NER method will naturally link the equilibrium theory to nonequilibrium statistical mechanics.

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