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Dynamical Rushbrooke's inequality for nonequilibrium relaxation process

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Abstract

An inequality for dynamic critical exponents is proved for relaxation processes of arbitrary magnetic systems. This is a dynamical extension of Rushbrooke's inequality. It can be applied to any continuous-transition systems with various dynamics. The relation is demonstrated on the result of nonequilibrium relaxation analysis of fluctuations applied to the three-dimensional ferromagnetic Ising model.

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1. Introduction

Several decades ago, Rushbrooke proved an inequality for critical exponents in Ising systems using a thermodynamic identity [1],

$$\alpha + 2\beta + \gamma \geqslant 2. \tag{1.1}$$

It is general and extended to a wide variety of physical systems. This is called Rushbrooke's inequality. It is consistent with the scaling relation

$$\alpha + 2\beta + \gamma = 2 \tag{1.2}$$

which is derived from the scaling hypothesis for the free energy density,

$$f(\varepsilon, H) = L^{(-2+\alpha)/\nu} g(L^{1/\nu}\varepsilon, L^{y} H) \tag{1.3}$$

where $\varepsilon \equiv (T - T_c)/T_c$ is the reduced temperature and H is the external field. While equation (1.2) is not rigorous, together with the exact inequality (1.1) it has been playing an important role in statistical physics of phase transitions.

The nonequilibrium relaxation (NER) method is an efficient numerical technique for analysing equilibrium phase transitions [2–5]. One observes a relaxation of order parameter in thermalization process from a completely ordered state. It indicates the critical point when it shows a power-law decay instead of the exponential decay or a decay to a spontaneous ordering corresponding to the paramagnetic (PM) and ferromagnetic (FM) phases, respectively. The relaxation power λ_m is relating to conventional critical exponents including the dynamic exponent z as

$$\lambda_m = \frac{\beta}{z\nu}. \tag{1.4}$$

If one observes relaxations of other quantities relating to fluctuations such as susceptibility, specific heat and so on, each exponent can be evaluated individually [3–5]. The method is based on the dynamic scaling hypothesis [6], in which the observation time t plays the role of a scaling field like the system size L in the finite size scaling analysis. This analysis has been used successfully to study various problems including frustrated and/or random systems [7–9]. In the NER analysis, the equilibration step is not necessary. Simulation is made only up to steps when the asymptotic behaviour indicates the equilibrium state. This advantage becomes more effective for slow-relaxation systems.

Although, the NER approach for the estimations of critical exponents is successful in many systems, only phenomenological arguments support it theoretically. Thus, exact theories concerning this field are desirable to check the validity of the method. In the present paper, first we recall that the inequality used in Rushbrooke's proof is equivalent to Schwartz's inequality. In section 3, we extend it to the dynamical quantities, and derive a dynamical version of Rushbrooke's inequality for the relaxation exponents appeared in the NER analysis. The inequality is demonstrated for an NER simulation on the three-dimensional FM Ising model in section 4. Using this simulation, we discuss the difference of convergence speeds to asymptotic behaviour among NER functions. The last section is devoted to remarks.

2. Rushbrooke's inequality

Let us recall the original proof by Rushbrooke [1]. We treat arbitrary spin systems under the external field H. The starting point is the thermodynamic identity,

$$C_H - C_m = T\left(\frac{\partial m}{\partial T}\right)_H^2 \bigg/ \left(\frac{\partial m}{\partial H}\right)_T \tag{2.1}$$

where m is the per-site magnetization and C_H and C_m denote the specific heat under constant H and constant m, respectively. It is derived from the exact differential of entropy with respect to the temperature and the external field,

$$\mathrm{d}S = \left(\frac{\partial S}{\partial T}\right)_H \mathrm{d}T + \left(\frac{\partial S}{\partial H}\right)_T \mathrm{d}H. \tag{2.2}$$

Since the specific heat is non-negative, equation (2.1) yields the inequality

$$C_H\left(\frac{\partial m}{\partial H}\right)_T \geqslant T\left(\frac{\partial m}{\partial T}\right)_H^2. \tag{2.3}$$

If the system undergoes a continuous phase transition at a definite transition temperature T_c and the spontaneous ordering (magnetization) appears below it, one can consider static critical exponents defined by

$$C_H \sim (-\varepsilon)^{-\alpha} \tag{2.4a}$$

$$\left(\frac{\partial m}{\partial T}\right)_H \sim (-\varepsilon)^{\beta-1} \tag{2.4b}$$

$$\left(\frac{\partial m}{\partial H}\right)_T \sim (-\varepsilon)^{-\gamma}. \tag{2.4c}$$

Then, equation (2.3) reveals Rushbrooke's inequality (1.1).

It is noted that equation (2.3) is nothing but Schwartz's inequality. Let us denote the equilibrium correlation function for quantities A and B,

$$X(A,B) \equiv \langle AB\rangle - \langle A\rangle\langle B\rangle \tag{2.5}$$

where $\langle\cdots\rangle$ represents the thermal equilibrium average. Since the positivity $X(A,A) \geqslant 0$ holds for any A, Schwartz's inequality is derived,

$$X(A,A)\,X(B,B) \geqslant X(A,B)^2. \tag{2.6}$$

Setting $A = m$ and $B = e$, where e is the per-site energy, one obtains an inequality

$$[\langle m^2\rangle - \langle m\rangle^2][\langle e^2\rangle - \langle e\rangle^2] \geqslant [\langle me\rangle - \langle m\rangle\langle e\rangle]^2 \tag{2.7}$$

which is equivalent to equation (2.3).

3. Dynamical Rushbrooke's inequality

We consider a nonequilibrium process starting from a fixed state, in which the dynamical average at time t is denoted by $\langle\cdots\rangle_t$. The correlation function in this dynamical process is defined by

$$X_t(A,B) \equiv \langle AB\rangle_t - \langle A\rangle_t\langle B\rangle_t. \tag{3.1}$$

Since the positivity $X_t(A,A) \geqslant 0$ is satisfied for any A and any t, Schwartz's inequality,

$$X_t(A,A)\,X_t(B,B) \geqslant X_t(A,B)^2 \tag{3.2}$$

holds. Setting $A = m$ and $B = e$, one obtains an inequality

$$\left[\langle m^2\rangle_t - \langle m\rangle_t^2\right]\left[\langle e^2\rangle_t - \langle e\rangle_t^2\right] \geqslant [\langle me\rangle_t - \langle m\rangle_t\langle e\rangle_t]^2 \tag{3.3}$$

for every t. This is a dynamical extension of the inequalities (2.3) or (2.7).

While equation (3.3) is valid for any dynamical process, it is interesting to apply it to the process starting from a completely ordered state—the all-aligned state in the FM case—at time $t = 0$. Note that the magnetization $\langle m\rangle_t$ is non-zero in $t > 0$ since the spin-flop symmetry has broken at the initial state. In the NER analysis of fluctuations [3–5], the following dynamical functions are useful to estimate critical exponents,

$$f_{mm}(t) \equiv N\left(\frac{\langle m^2\rangle_t}{\langle m\rangle_t^2} - 1\right) \tag{3.4a}$$

$$f_{me}(t) \equiv N\left(\frac{\langle me\rangle_t}{\langle m\rangle_t\langle e\rangle_t} - 1\right) \tag{3.4b}$$

$$f_{ee}(t) \equiv N\left(\frac{\langle e^2\rangle_t}{\langle e\rangle_t^2} - 1\right). \tag{3.4c}$$

At the critical point, they are supposed to be diverging with t according to power laws as

$$f_{mm}(t) \sim t^{\lambda_{mm}} \tag{3.5a}$$

$$f_{me}(t) \sim t^{\lambda_{me}} \tag{3.5b}$$

$$f_{ee}(t) \sim t^{\lambda_{ee}}. \tag{3.5c}$$

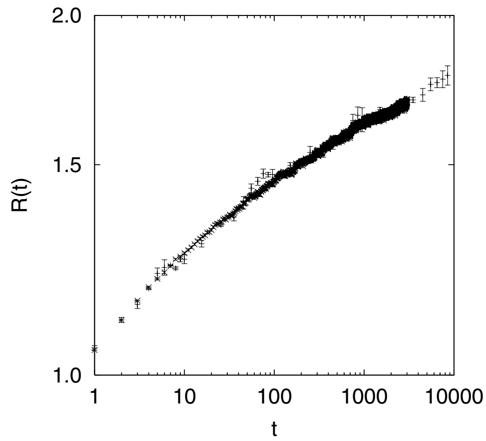

Figure 1. Calculated $R(t)$ for the FM Ising model in three dimensions. Double-log scale is used.

Assuming the dynamic scaling hypothesis, one obtains the relations of the above dynamical exponents with conventional ones

$$\lambda_{mm} = \frac{\gamma}{z\nu} + \frac{2\beta}{z\nu} = \frac{d}{z} \tag{3.6a}$$

$$\lambda_{me} = \frac{1}{z\nu} \tag{3.6b}$$

$$\lambda_{ee} = \frac{\alpha}{z\nu}. \tag{3.6c}$$

Together with the exponent for magnetization (1.4), one can evaluate each exponent individually.

Using equation (3.3), one obtains an inequality for NER functions,

$$R(t) \equiv \frac{f_{mm}(t) f_{ee}(t)}{f_{me}(t)^2} \geqslant 1 \tag{3.7}$$

which is the dynamical extension of equation (2.3) in this NER process. Assuming the power-law divergence (3.5), one obtains the dynamical Rushbrooke's inequality,

$$\lambda_{mm} + \lambda_{ee} \geqslant 2\lambda_{me}. \tag{3.8}$$

If one assumes the dynamic scaling hypothesis and equations (3.6), the inequality (3.8) becomes identical with the original Rushbrooke's one (1.1).

4. Numerical simulation

It is valuable to see the behaviour of $R(t)$ defined in equation (3.7) in an NER analysis of fluctuations. This provides the validity of numerical calculations as well as the details of asymptotic behaviour of NER functions in equation (3.5). In figure 1, we plot $R(t)$ for the FM Ising model on the simple cubic lattice at the transition temperature $T_c = 4.511\,5258$ ($K_c = 0.221\,6545$) obtained previously by the NER method [4, 5, 10]. The Metropolis Monte Carlo simulations are performed on the $381^2 * 380$ lattice with skew boundary condition up to 10^4 MCS. About 10^4 samples are used for averaging. It is shown that $R(t)$ is always greater than unity, which is consistent with equation (3.7).

In the plot in figure 1, the slope of the curve which indicates the power of relaxation seems non-zero and positive up to the observed MCS. If this remains true in the asymptotic regime, $\lambda_{mm} + \lambda_{ee} - 2\lambda_{me}$ has a non-zero value. Because of equations (3.6), it reveals the breaking of scaling relation (1.2). However, we consider another explanation for this observation. In [4], the FM Ising model on the cubic lattice was analysed and we obtained the result: $z = 2.055(10)$, $\nu = 0.625(5)$, $\beta = 0.325(5)$ and $\alpha = 0.14(2)$. The calculations of fluctuations were made on a 150×150 cubic lattice with skew boundary condition at the estimated T_c up to 5000 MCS. About 10^6 samples were used for averaging. As pointed out in that paper, the estimated values of z, ν and β are almost consistent with those obtained so far, while that of α is a little larger. It is natural to consider that the observation time is still short, and the asymptotic regime has not been reached. In fact, the curve shows a little convexity in figure 1, which indicates that the power would be decreasing in a longer time regime. Since only the estimated α gives a remarkable deviation, the convergence speed to the asymptotic regime, which is related to the corrections to scaling, is different among NER functions. It is expected that the convergence speed of the function $f_{ee}(t)$ is much slower than those of others.

5. Remarks

We derive an inequality (3.8) for dynamic critical exponents appearing in the NER analysis of fluctuations. This is a dynamical extension of Rushbrooke's inequality (1.1). The basic inequality (3.7) is demonstrated on the result of nonequilibrium relaxation analysis of fluctuations applied to the three-dimensional ferromagnetic Ising model. It is discussed that the convergence speeds to asymptotic behaviour are different among NER functions. That of the energy fluctuation $f_{ee}(t)$ is much slower than the others. At present, we have no idea how to explain this phenomenon. Further investigations would be necessary in the future.

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