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Static and Dynamic Finite-Size Scaling Theory Based on the Renormalization Group Approach

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Fisher's static finite-size scaling law is derived on the basis of the renormalization group theory and it is extended to dynamic critical phenomena in a finite system. This dynamic finite-size scaling law yields a cross-over effect with respect to the size and time-region. This effect is useful in analyzing computer simulations and also in studying the scaling property of the Kondo effect near the absolute zero temperature.

§ 1. Introduction

It is well-known that a phase transition occurs in the thermodynamic limit, namely for an infinite volume limit. However, real systems are of finite size, although this effect can be practically neglected in most cases. In particular, this effect of finite size is very important in discussing films and surfaces,[1] and also in analyzing the Monte Carlo simulations,[2),3] because they are always limited to small systems due to the restricted machine-time.

Fisher[1] proposed a finite-size scaling law for this effect. This insists that the free energy of an $L\times L\times L$ lattice should take the following scaling form:

$$F(L,T)\cong L^{-\psi}\mathscr{F}(L^{\theta}\varepsilon)=\xi^{-d}f(L/\xi);\ \theta=\nu^{-1}, \tag{1·1}$$

for large N and small ε, where

$$\psi=(2-\alpha)/\nu \quad \text{and} \quad \varepsilon=|1-T/T_c(\infty)| \tag{1·2}$$

with the ordinary notations of critical exponents α, ν, etc., and with the infinite lattice transition temperature $T_c(\infty)$. Here, ξ denotes the correlation length for the infinite system: $\xi\propto\varepsilon^{-\nu}$.

This finite-size scaling law is also very useful in discussing[4] the scaling property of the Kondo effect on the basis of classical representations[5] through the generalized Trotter formula.[6]

The purpose of this paper is to derive[7] Fisher's finite-size scaling law using the renormalization group approach,[8),9] and to extend[7] this to *dynamic* critical phenomena for a finite size. From this finite-size scaling law both in static and dynamic critical phenomena, we discuss the cross-over effect with respect to the size, reduced temperature and time in these finite systems.

In § 2, a derivation of Fisher's static finite-size scaling law is given on the basis of the renormalization group theory. In § 3, a dynamic finite-size scaling law is derived by extending the previous generating function formalism[10] to finite but large systems. The cross-over effect in dynamics is also discussed. Summary and discussion are given in § 4.

§ 2. Derivation of Fisher's static finite-size scaling law

In this section, we consider two types of static finite systems.

a) *Type A: an $L\times L\times L$ lattice*

One of our keypoints to treat a finite but large system is to introduce the following generating function:

$$\Phi(\varepsilon, k_0, h)=\frac{1}{\Omega}\log\int\prod_{k_0\leq k<1,\, k=0}\exp(hM-\mathcal{H}), \tag{2·1}$$

for an $L\times L\times L$ finite system, where $\varepsilon=(T-T_c(\infty))/T_c(\infty)$, Ω is the volume of the system, M the total magnetization (we consider here magnetic systems for simplicity), and $\mathcal{H}$ is the Hamiltonian of the system divided by k_BT. The parameter k_0 is put to be equal to

$$k_0=L^{-1}. \tag{2·2}$$

This choice of the parameter k_0 is essential in our treatment, because we study here the finite system of size L, and long-wave modes with wave length larger than L are irrelevant to our present problem except $k=0$. Thus, the system-size L comes into our scheme through the *long wave-length cutoff parameter* k_0. Then, our strategy is to apply the ordinary renormalization transformation[8),9)] to (2·1). Only one new aspect of our theory is that the number n of renormalization steps in the present problem is restricted to the region $k_0b^n<b^{-1}$ for the scale transformation $k\to bk$, so that the outer region $b^{-1}<k<1$ may always exist in each renormalization step. Thus, the following renormalization recursion formula has a meaning only asymptotically, namely for a very large but finite number of steps when k_0 is very small (i.e., L is very large).

Following Wilson[8)] and Hubbard,[11)] we consider a sequence of Hamiltonians, each of the form

$$\mathcal{H}_l=\sum_{n=1}^{\infty}\Omega^{1-n}\sum_{k_0\leq k_1,k_2,\cdots k_{2n}<1}{}' u_{2n,l}(k_1,\cdots,k_{2n})\sigma_{lk_1}\cdots\sigma_{lk_{2n}} \tag{2·3}$$

with long wave-length cutoff k_0, where σ_{lk} are the Fourier components of the spin variable $s_l(x)$. Here, $\sum'$ denotes to include the sum over uniform modes $k_1=0,\cdots$, or $k_{2n}=0$. Corresponding to each $\mathcal{H}_l$, we consider the generating function Φ_l defined by (2·1) with $\mathcal{H}_l$ for the Hamiltonian $\mathcal{H}$. The sequences of $\mathcal{H}_l$ are generated by the well-known procedure[8),9)] with the simple long wave-length cutoff in the sequences of the Hamiltonians. At each step, we rescale the variables according to

$$k \to k' = bk\,, \quad L \to L' = b^{-1}L \quad \text{and} \quad \sigma_{l,k} \to \sigma_{l+1,bk} = b^{-1+\eta/2}\sigma_{l,k}\,. \tag{2·4}$$

Here, the critical exponent η is determined in the ordinary method from the recursion relation[8),9)] between $\mathcal{H}_l$ and $\mathcal{H}_{l+1}$.

With these preparations, we study the recursion relation between Φ_l and Φ_{l+1}. As in Hubbard's arguments,[11)] (2·1) has only an additional term $h\Omega^{1/2}\sigma_{l,0}$ (where $\sigma_{l,0}$ is $\sigma_{l,k}$ at $k=0$). Therefore, the renormalization procedure in the region $b^{-1}<k<1$ for the Hamiltonian $\mathcal{H}_l$ with the above additional Zeeman term yields a recursion relation similar to the infinite case. If we rescale the new variable h as

$$h_l \to h_{l+1} = b^x h_l\,;\; x = \tfrac{1}{2}d + 1 - \tfrac{1}{2}\eta\,, \tag{2·5}$$

then we obtain the following recursion relation:

$$\Phi_l(h, \varepsilon, k_0) = b^{-d}\Phi_{l+1}(h, \varepsilon, k_0) + f_l(\varepsilon)\,, \tag{2·6}$$

where $f_l(\varepsilon)$ is a certain function[8)] of $u_{2n,l}$, and

$$\Phi_{l+1}(h, \varepsilon, k_0) = \Phi_l(hb^x, \varepsilon b^y, bk_0)\,, \tag{2·7}$$

where $y=1/\nu$. Thus, we arrive at the following recursion relation:

$$\Phi_l(h, \varepsilon, k_0) = b^{-d}\Phi_l(hb^x, \varepsilon b^y, bk_0) + f_l(\varepsilon)\,. \tag{2·8}$$

Differentiating (2·8) with respect to h, we obtain the functional equation of the magnetization

$$m_l(h, \varepsilon, k_0) = b^{x-d} m_l(hb^x, \varepsilon b^y, bk_0)\,. \tag{2·9}$$

The general solution of this recursion relation is given by

$$m(h, \varepsilon, k_0) = k_0^{\beta y} m(h\varepsilon^{-\beta\delta}, \varepsilon k_0^{-y})\,, \tag{2·10}$$

where

$$y = \frac{1}{\nu}\,, \quad \delta = \frac{x}{d-x} = \frac{d+2-\eta}{d-2+\eta}\,, \quad \beta = \frac{x}{y\delta} = \frac{\gamma}{\delta - 1}\,. \tag{2·11}$$

By noting that $k_0 = L^{-1}$, we obtain

$$\begin{aligned} m(h, \varepsilon, L) &= L^{-\beta/\nu} m(h\varepsilon^{-\beta\delta}, \varepsilon L^{1/\nu}) \\ &\equiv L^{-\phi} m(h\varepsilon^{-\beta\delta}, \varepsilon L^{\theta})\,. \end{aligned} \tag{2·12}$$

Therefore, we have

$$\phi = \beta/\nu \quad \text{and} \quad \theta = 1/\nu\,. \tag{2·13}$$

Similarly, the free energy is obtained as

$$F(h, \varepsilon, L) = L^{-d}\mathcal{F}(h\varepsilon^{-\beta\delta}, \varepsilon L^{\theta})\,. \tag{2·14}$$

Thus, the exponent ψ defined in (1·1) is given by

$$\psi = d = (2-\alpha)/\nu\,. \tag{2·15}$$

This gives the derivation of Fisher's finite-size scaling law.

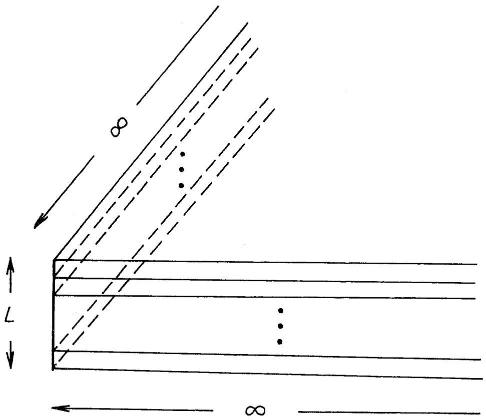

Fig. 1. An $\infty\times\infty\times L$ lattice.

b) *Type B: an* $\infty\times\infty\times L$ *lattice*

As in Fig. 1, we consider another type of lattice with a finite thickness L. In this situation, the reduced critical temperature ε defined by

$$\dot{\varepsilon}=(T-T_c(L))/T_c(\infty) \tag{2·16}$$

is more convenient, because there exists a phase transition even for a finite L in an ordinary one-component system. Now, we consider the following generating function:

$$\Phi_l(h,\varepsilon,k_0)=\frac{1}{\Omega}\log\int\prod_{\substack{0\leq k_x,k_y\leq 1\\ k_0\leq k_z\leq 1,k_z=0}}d\sigma_{l,k}\exp(-\mathcal{H}_l+hM). \tag{2·17}$$

Quite similarly to the case of Type A, we have the following recursion relation:

$$\Phi_l(h,\dot{\varepsilon},k_0)=b^{-d}\Phi_{l+1}(h,\dot{\varepsilon},k_0)+\hat{f}_l(\dot{\varepsilon}), \tag{2·18}$$

where

$$\Phi_{l+1}(h,\dot{\varepsilon},k_0)=\Phi_l(hb^x,\dot{\varepsilon}b^y,k_0b). \tag{2·19}$$

Therefore, we get

$$\Phi_l(h,\dot{\varepsilon},k_0)=b^{-d}\Phi_l(hb^x,\dot{\varepsilon}b^y,k_0b)+\hat{f}_l(\dot{\varepsilon}). \tag{2·20}$$

This yields the functional equation of the magnetization

$$m_l(h,\dot{\varepsilon},k_0)=b^{x-d}m_l(hb^x,\dot{\varepsilon}b^y,k_0b), \tag{2·21}$$

and the solution is given by

$$m(h,\dot{\varepsilon},L)=L^{-\beta/\nu}m(h\dot{\varepsilon}^{-\beta\delta},\dot{\varepsilon}L^{1/\nu}). \tag{2·22}$$

The susceptibility is given by the scaling form

$$\chi(\dot{\varepsilon},L)=L^{-\beta/\nu}\dot{\varepsilon}^{-\beta\delta}\chi(\dot{\varepsilon}L^{1/\nu}). \tag{2·23}$$

On the other hand, the magnetization of the three-dimensional lattice ($L=\infty$) takes the following scaling form:

$$m_\infty(h,\varepsilon)=h\varepsilon^{-\gamma}m(h\varepsilon^{-\beta\delta}), \tag{2·24}$$

where

$$\varepsilon=(T-T_c(\infty))/T_c(\infty). \tag{2·25}$$

In particular, the susceptibility takes the form

$$\chi_\infty(\varepsilon)\propto\varepsilon^{-\gamma}. \tag{2·26}$$

The limit of (2·23) for a large L should approach the singularity (2·26). Therefore, the function $\chi(x)$ takes the following asymptotic form:

$$\chi(x) \sim Ax^{\beta} \quad \text{for} \quad x \to \infty \tag{2·27}$$

and

$$\chi(x) \sim Bx^{\beta\delta - \gamma} \quad \text{for} \quad x \to +0\,, \tag{2·28}$$

as was already discussed by Fisher.[1] Here, γ denotes the susceptibility exponent in two dimensions. Thus, the cross-over effect occurs between the three-dimensional critical behavior and two-dimensional one around the cross-over temperature

$$\dot{\varepsilon}^{\times} \cong L^{-1/\nu}\,. \tag{2·29}$$

This is one of typical cross-over effects[12)~16)] in critical phenomena.

§ 3. Dynamic finite-size scaling law—Cross-over effect in dynamics

The arguments in § 2 can be easily extended to dynamic critical phenomena, if we confine our arguments into the following simple stochastic (or TDGL) model without conservation:

$$\frac{\partial}{\partial t} P_l(\{\sigma_{lq}\}, t) = \Gamma_l P_l(\{\sigma_{lq}\}, t)\,, \tag{3·1}$$

where

$$\Gamma_l = \int \prod_{k_0 \leq q \leq 1,\, q=0} d\sigma_{lq} \frac{\partial}{\partial \sigma_{lq}} \left(\frac{\partial \mathcal{H}_l}{\partial \sigma_{l,-q}} + \frac{\partial}{\partial \sigma_{l,-q}} \right) \tag{3·2}$$

with the cutoff parameter k_0, which corresponds to the finiteness of the system. Now, we consider the following two types of finite systems corresponding to the static case discussed in § 2:

a) *Type A: an $L \times L \times L$ (or $L \times L$) lattice*

It is convenient to introduce the following generating function in non-equilibrium systems:[10)]

$$\Phi_l(\lambda, h, \varepsilon, k_0, t) = \frac{1}{\Omega} \log \int \prod_{k_0 \leq k \leq 1,\, k=0} d\sigma_{l,k}\, e^{\lambda M} e^{t\Gamma_l} e^{hM - \mathcal{H}_l} \tag{3·3}$$

with $k_0 = L^{-1}$. The recursion relation for Γ_l has been given in various kinds of formulations.[17),18)] At each step of renormalization, we rescale the variables according to

$$k \to k' = bk\,, \quad \sigma_{l,k} \to \sigma_{l+1,bk} = b^{-1+\eta/2} \sigma_{l,k} \quad \text{and} \quad t \to t' = b^{-z} t\,, \tag{3·4}$$

where the dynamic critical exponent z is determined[17),18)] from the requirement that

$$t\Gamma_l = t'\Gamma_{l+1} = \text{invariant}\,. \tag{3·5}$$

In quite the same way as in § 2, we obtain the following recursion relation of the generating function Φ_l:

$$\Phi_l(\lambda, h, \varepsilon, k_0, t) = b^{-d}\Phi_l(\lambda b^x, hb^x, \varepsilon b^y, k_0 b, tb^{-z}). \tag{3·6}$$

Differentiating (3·6) with respect to λ, and then putting $\lambda=0$, we get

$$m_l(h, \varepsilon, k_0, t) \equiv \left(\frac{\partial}{\partial\lambda}\Phi_l\right)_{\lambda=0} = b^{x-d} m_l(hb^x, \varepsilon b^y, k_0 b, tb^{-z}). \tag{3·7}$$

The general solution of this equation is given in the following scaling form:

$$m(h, \varepsilon, L, t) = L^{-\beta/\nu} f(h\varepsilon^{-\beta\delta}, \varepsilon L^{1/\nu}, tL^{-z}). \tag{3·8}$$

This is reduced to (2·12), if the time-dependence of (3·8) is neglected, as it should be. This is the dynamic finite-size scaling law.

Next, we discuss the cross-over effect in this dynamic critical phenomena. For the infinite system ($L=\infty$), we should have

$$m_\infty(h, \varepsilon, t) = \varepsilon^\beta m_\infty(h\varepsilon^{-\beta\delta}, t\varepsilon^{\nu z}). \tag{3·9}$$

This is nothing but the time-dependent nonlinear equation of state.[10] From this, we can discuss the nonlinear critical slowing down.[10),19)~21)] By comparing (3·8) with (3·9), we arrive at the following conclusions of the cross-over phenomena:
(i) For $L^{1/\nu} \gg 1$ (i.e., $\varepsilon \gg \varepsilon^\times$; $\varepsilon^\times \sim L^{-1/\nu}$) and $tL^{-z} \ll 1$ (i.e., $t \ll t^\times$; $t^\times \sim L^z$), the three-dimensional bulk critical phenomena are observed.
(ii) For $\varepsilon \ll \varepsilon^\times$ or $t \gg t^\times$, no sharp singularity but only rounded anomaly will be observed.

This cross-over phenomenon is very important in analyzing computer simulations or experimental data on small systems, as is shown in Fig. 2. Namely, one has to be very careful about the long-time tail which reflects the finite-size effect. The cross-over time $t^\times$ becomes larger and larger, proportionally to L^z, as the system size L increases. Finally, the whole region comes into the bulk one in the limit $L\to\infty$.

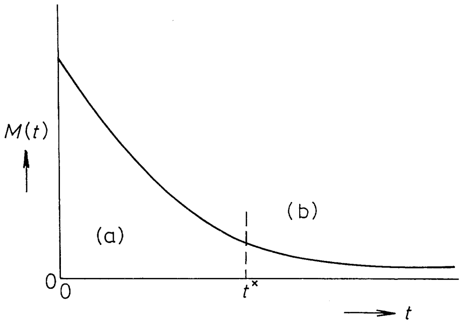

Fig. 2. Cross-over effect in critical dynamics: (a) bulk region ($t<t^\times$) and (b) finite-size region ($t>t^\times$), where $t^\times$ is the cross-over time: $t^\times \sim L^z$.

b) *Type B*: *an* $\infty\times\infty\times L$ *lattice*

Next, we consider a lattice of Type B as is shown in Fig. 1. We introduce here the following generating function:

$$\Phi_l(\lambda, h, \dot{\varepsilon}, k_0, t) = \frac{1}{\Omega} \log \int \prod_{\substack{0 \leq k_x, k_y \leq 1 \\ k_0 \leq k_z \leq 1, k_z = 0}} d\sigma_{l,k} e^{\lambda M} e^{t\Gamma_l} e^{hM - \mathcal{H}_l}, \tag{3·10}$$

with long wave-length cutoff k_0 only in the z-direction, where $\dot{\varepsilon}$ is defined by (2·16). By making the scale transformation (3·4) at each step as in a), we obtain the following recursion relation:

$$\Phi_l(\lambda, h, \dot{\varepsilon}, k_0, t) = b^{-d} \Phi_l(\lambda b^x, hb^x, \dot{\varepsilon} b^y, k_0 b, tb^{-z}) + f_l(\dot{\varepsilon}, t). \tag{3·11}$$

This yields the following scaled equation of state:

$$m(h, \dot{\varepsilon}, L, t) = L^{-\beta/\nu} g(h\dot{\varepsilon}^{-\beta\delta}, \dot{\varepsilon} L^{1/\nu}, tL^{-z}). \tag{3·12}$$

This is the dynamic finite-size scaling law. From this expression, we can study the cross-over effect between the two-dimensional critical behavior and three-dimensional one. For the limit $L \to \infty$, we should have the bulk critical behavior

$$m_\infty(h, \varepsilon, t) = t^{-\psi} m(h\varepsilon^{-\beta\delta}, t\varepsilon^{\nu z}); \; \psi = \beta/\nu z. \tag{3·13}$$

For a finite L, (3·12) can be rewritten as

$$m(h, \dot{\varepsilon}, L, t) = t^{-\psi} m(h\dot{\varepsilon}^{-\beta\delta}, t\dot{\varepsilon}^{\nu z}, Lt^{-1/z}). \tag{3·14}$$

In particular, the critical magnetization at $\varepsilon = 0$ takes the following scaling form:

$$M(t) = t^{-\psi} m(Lt^{-1/z}) \quad \text{at} \quad \dot{\varepsilon} = 0. \tag{3·15}$$

On the other hand, the two-dimensional critical magnetization $M(t)$ should take the following asymptotic form:

$$M(t) \propto t^{-\dot{\psi}} \text{ for } t \to \infty \text{ and } L < \infty \; ; \; \dot{\psi} = \dot{\beta}/\dot{\nu}\dot{z}, \tag{3·16}$$

where $\dot{\beta}$, $\dot{\nu}$ and $\dot{z}$ denote the corresponding two-dimensional critical exponents. Then, from the condition that (3·15) should match with (3·16), we get

$$m(\xi) \approx M_0 \xi^{-z(\psi - \dot{\psi})} \quad \text{as} \quad \xi \to 0 \tag{3·17a}$$

and

$$m(\xi) \approx \text{constant} \quad \text{as} \quad \xi \to \infty. \tag{3·17b}$$

Thus, we arrive finally at

$$M(t) \approx M_0 L^{-z(\psi - \dot{\psi})} t^{-\dot{\psi}} \tag{3·18}$$

or

$$M(t) \approx M_0 L^{-z\psi} (t/L^z)^{-\dot{\psi}}. \tag{3·18'}$$

From this asymptotic expression of the relaxation function $M(t)$, we conclude the following dynamic *cross-over effect*:

(i) For $t > t^\times$, we get

$$M(t) \sim t^{-\dot{\psi}} \quad (d=2), \tag{3·19}$$

and

(ii) for $t \lesssim t^{\times}$, we have

$$M(t) \sim t^{-\phi} \quad (d=3), \tag{3·20}$$

where the *cross-over time* is given by

$$t^{\times} \sim L^{z}. \tag{3·21}$$

After the Fourier transformation, we obtain the following equivalent proposition: For $\omega < \omega^{\times}$, we get $M(\omega) \sim \omega^{\phi}(d=2)$, and for $\omega > \omega^{\times}$, we have $M(\omega) \sim \omega^{\phi}(d=3)$, where the *cross-over frequency* $\omega^{\times}$ is given by

$$\omega^{\times} \sim L^{-z} = k_0^{z}. \tag{3·22}$$

§ 4. Summary and discussion

In the present paper, a formal derivation of Fisher's static finite-size scaling law has been derived and it has been extended to dynamic critical phenomena in a finite system on the basis of the renormalization group theory. The cross-over effect in critical dynamics has been discussed in detail, with respect to the size and time.

As has been mentioned in § 1, this concept of finite-size scaling is useful in discussing[4] the global scaling property of the Kondo effect, which can be reduced to a classical system with a finite thickness in the $(d+1)$-th direction. For details, see Ref. 4).

In order to obtain the scaling functions in (2·12), (2·22), (3·8) and (3·12), explicit renormalization group calculations such as the ε-expansion[8),9)] will be necessary, and they will remain interesting problems in the future.

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