PHYSICAL REVIEW LETTERS

VOLUME 70 | 22 MARCH 1993 | NUMBER 12

Application of Finite Size Scaling to Monte Carlo Simulations

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(Received 28 September 1992)

A new application of finite size scaling to Monte Carlo simulations is introduced. Using this technique, critical behavior can be investigated at temperatures arbitrarily close to the critical point without large lattice sizes. Applying this method to the two-dimensional standard O(3) model it is shown that for the correlation length asymptotic scaling holds for $\beta \geq 2.25$; the magnetic susceptibility converges to the asymptotic scaling very slowly. In the scaling region, it is observed that the specific heat decreases with β, which implies no singular behavior of the specific heat for this model.

PACS numbers: 02.70.−c, 12.38.Gc, 64.60.−i

Monte Carlo simulations have been widely used for the studies of critical phenomena. The main idea behind these methods is to measure the thermodynamic values of a certain physical quantity in the scaling region and then to fit the data to a certain scaling function. The crucial difficulty here is that, without an exact solution of the model, the scaling region cannot be determined precisely; in other words, it is impossible to predict at what range of the temperature the data can be ideally fitted to an appropriate scaling function. To avoid this ambiguity, measurements must be done arbitrarily close to the critical point. The cost is that the size of the lattice must be extremely large to obtain proper thermodynamic data. The series expansion method has the same difficulty: it is impossible to decide how many expansion terms are needed for the proper determination of critical behavior. Because of this difficulty, often, the less singular terms are included in the leading scaling function in order to fit the data obtained at temperatures not sufficiently close to the critical point. However, this procedure usually makes the fittings highly unstable.

To overcome such difficulties, various methods such as finite size scaling (FSS) and the Monte Carlo renormalization group (MCRG) method have been developed. However, it turns out that the standard usage of these methods still requires large lattice sizes [1].

Our technique is based on the observation that finite size effects of any thermodynamic quantities on a finite lattice of linear size L depend only on L/ξ_∞, where ξ_∞ is the bulk (thermodynamic) correlation length. More precisely, for a typical thermodynamic quantity P,

$$\frac{P_L(t)}{P_\infty(t)} = f_P(x(t)), \quad x(t) \equiv \frac{L}{\xi_\infty(t)}, \tag{1}$$

where t, P_L, P_∞, and f_P are the reduced temperature $(T-T_c)/T_c$, the value of P on a lattice of linear size L, the thermodynamic value of P, and a function depending on P, respectively.

Equation (1) was initially suggested by Brézin [2], and using the analyticity property of $P_L(t)$ it was shown [3] that if P has a power critical behavior, $P_\infty(t) \sim t^{-\rho}$ with $\rho > 0$, from Eq. (1),

$$P_L(t) = L^{\rho/\nu}(p_0 + p_1 L^{1/\nu} t + p_2 L^{2/\nu} t^2 + \cdots) \tag{2}$$

follows for small values of t, where $p_0, p_1, \ldots$ are constants depending on P. It is obvious that Eq. (2) implies the usual FSS at $t=0$, $P_L(t=0) \sim L^{\rho/\nu}$, and that it implies $T_c(L) - T_c \sim 1/L^{1/\nu}$, considering Eq. (2) up to the second order of t [$T_c(L)$ is the *fictitious* critical point on the finite lattice at which $P_L(t)$ has its maximum value]. So far we have shown that Eq. (1) is consistent with the results of FSS in the absence of the magnetic field, and we stress that various analytical methods[4] have proved that FSS is exact for $D < 4$, suggesting that Eq. (1) is also exact for $D < 4$.

The relation (1) is significant in that, by fixing $x(t)$ as a constant, obtaining $P_L(t)$ is sufficient for the determination of the critical behavior of P_∞. In order for the $x(\beta)$—β is the inverse temperature—to be fixed, estimates of β_c and ν are needed in advance. However, once they are given it can be easily checked whether the estimates are correct or not using Eq. (1): if the values of ν are underestimated or β_c are overestimated compared to the exact values, $\xi_L(\beta)/\xi_\infty(\beta)$ will increase as β grows up to β_c, and vice versa. For the exact values of ν and β_c, $\xi_L(\beta)/\xi_\infty(\beta)$ will remain constant, and other critical exponents can be determined from measurements at small lattices since these values are proportional to their thermodynamic values.

From the above procedures, it is clear that with a sufficiently small value of x, measurements can be done at temperatures as close to the critical point as desired while keeping the sizes of the lattice small, and at these temperatures the less singular corrections to the leading singularity can be safely ignored.

Consequently, besides the indirect justification through the FSS, for a model whose exact value of ν and β_c are known the validity of the relation (1) can be tested using numerical measurements. In the following, we present the numerics which confirm Eq. (1) for the 2D Ising model. From now on, for the bulk quantities the proportionality constants appearing in the scaling functions will be ignored for the sake of simplicity. For example, $\xi_\infty(\beta) = |\beta_c - \beta|^{-\nu}$, and $x(\beta) \equiv L/\xi_\infty(\beta)$. For the 2D Ising model, four arbitrarily small values of x $(10^{-1}, 10^{-2}, 2\times10^{-3}, \text{and } 2\times10^{-5})$ were tried, and for each x, ξ_L and χ_L were measured. Our measurements are summarized in Table I, and leave no doubt of the validity of (1).

Our technique can be applied to the 2D standard, nearest neighbor, O(3) model as well. It is well known that this model shares a couple of the important properties of the 4D QCD [5], such as asymptotic freedom and the existence of the instantons. Using perturbation theory for β sufficiently large, the universal scaling law [referred to as the asymptotic scaling (AS)] of correlation length and magnetic susceptibility were derived [5, 6]; namely,

$$\xi_\infty(\beta) = \frac{\exp(2\pi\beta)}{\beta}, \quad \chi_\infty(\beta) = \frac{\exp(4\pi\beta)}{\beta^4}, \tag{3}$$

where our convention of ignoring the proportionality constant is used.

Since the nonperturbative proof of AS is crucial to the validity of QCD, considerable amounts of numerical work to show AS have been conducted [7]. However, all the work up to β=2.05, where the corresponding ξ_∞ is nearly 300 in lattice units, failed to show AS [8]. Finally, using an improved MCRG, Hasenfratz and Niedermayer [9] reported agreement with AS for the mass gap (i.e., the inverse of the correlation length) at $\beta = 2.26$. On the other hand, the validity of perturbative calculations in non-Abelian theories was questioned, and Patrascioiu and Seiler [10] suspect that a new phase transition may take place in these models. An argument based on the renormalization group recursion formula also appeared [11], supporting Patrascioiu and Seiler.

At β=2.26, the value of ξ_∞ is at least of the order of 10^3, which makes the computer time needed to obtain the proper thermodynamic data prohibitive; consequently, our method is ideally suited to this model. We have simulated the standard 2D O(3) model for the vari-

TABLE I. The result of the 2D Ising model for the various x values. As shown below for $\beta > 0.4369$, $\chi_\infty \sim t^{-7/4}$ and $\xi_\infty \sim t^{-1}$ become exact within the characteristic statistical errors (0.3%) of our numerical tests. For both ξ_L and χ_L, it is clearly shown that they are proportional to their thermodynamic values.

x	β	L	ξ_L	ξ_L/ξ_∞	χ_L	χ_L/χ_∞
10^{-1}	0.4323534610	18	9.38(6)	0.782(5)E-01	76.0(2)	0.175(0)E-01
	0.4369830900	27	21.00(9)	0.778(3)E-01	312.2(8)	0.174(0)E-01
	0.4391483320	65	50.58(22)	0.778(3)E-01	1453(4)	0.174(0)E-01
10^{-2}	0.4401312380	18	16.07(5)	0.893(3)E-02	169.6(3)	0.341(1)E-03
	0.4402867935	25	22.25(6)	0.890(2)E-02	301.4(4)	0.341(0)E-03
	0.4403742935	32	28.67(9)	0.894(3)E-02	465.3(7)	0.342(1)E-03
	0.4404867935	50	44.57(13)	0.891(3)E-02	1015.3(17)	0.342(1)E-03
	0.4405569234	77	68.50(22)	0.890(3)E-02	2160.0(98)	0.341(2)E-03
2×10^{-3}	0.4405201268	12	10.94(5)	0.182(1)E-02	84.3(2)	0.206(0)E-04
	0.4406242935	32	28.96(10)	0.181(1)E-02	469.1(3)	0.206(0)E-04
	0.4406467935	50	45.34(15)	0.181(1)E-02	1025.4(31)	0.207(1)E-04
	0.4406590157	72	65.02(26)	0.181(1)E-02	1939.0(95)	0.206(1)E-04
2×10^{-5}	0.440685126844	12	10.91(6)	0.182(1)E-04	84.1(2)	0.650(1)E-08
	0.440686052769	27	24.47(12)	0.181(1)E-04	348.8(7)	0.652(1)E-08
	0.440686485817	65	59.08(32)	0.182(1)E-04	1620(4)	0.651(2)E-08

TABLE II. The result of the 2D O(3) model. For $1.151 \leq \beta \leq 1.395$, ξ_L/ξ_∞ is decreasing, which indicates that correlation length scales slower than AS in this range of β; it is the case for the magnetic susceptibility also. In the intermediate range of β, they scale faster than AS. For $2.23 \leq \beta$, it is clearly seen that correlation length converges to AS, while the magnetic susceptibility seems to converge to AS much more slowly than the correlation length. Note that the specific heat per link (C_v) in this range of β, which is proportional to its thermodynamic value, is decreasing.

x	β	L	ξ_L	ξ_L/ξ_∞	χ_L	χ_L/χ_∞	C_v
10^{-2}	1.1507712900	12	2.70(1)	0.225(0)E-02	16.7(0)	0.153(0)E-04	0.658(2)
	1.3182253200	30	4.88(2)	0.163(1)E-02	44.3(1)	0.855(2)E-05	0.780(6)
	1.3952986700	46	6.71(3)	0.146(1)E-02	75.8(3)	0.698(2)E-05	0.819(7)
10^{-3}	1.6057803200	15	8.18(2)	0.546(1)E-03	82.1(1)	0.940(1)E-06	0.747(6)
	1.7907457800	43	23.57(4)	0.548(1)E-03	524.7(4)	0.910(1)E-06	0.696(4)
	1.8922447700	77	42.66(16)	0.554(2)E-03	1501.6(15)	0.907(1)E-06	0.663(4)
2×10^{-5}	2.2463085984	30	23.42(4)	0.390(1)E-04	432.(2)	0.605(0)E-08	0.604(6)
	2.3810679912	66	51.61(8)	0.391(1)E-04	1846.(2)	0.601(1)E-08	0.592(7)
	2.5090853592	128	109.64(27)	0.392(1)E-04	7441(16)	0.597(1)E-08	0.582(8)
	2.6284991888	283	222.05(57)	0.392(1)E-04	27574(68)	0.595(1)E-08	0.574(6)
2×10^{-6}	2.7069989050	18	17.07(3)	0.190(0)E-05	201.9(1)	0.183(0)E-10	0.571(4)
	2.7932937450	30	28.49(5)	0.190(0)E-05	524.6(2)	0.182(0)E-10	0.570(2)
	2.9183470800	63	59.84(6)	0.190(0)E-05	2110.9(1)	0.181(0)E-10	0.566(3)

ous ranges of β (see Table II) employing the one-cluster-type Monte Carlo algorithm [12]. The correlation length was measured based on the second moment calculation [13]. That is,

$$\xi_L = \frac{L}{2\pi}\sqrt{\chi/\chi' - 1}\,, \tag{4}$$

where

$$\chi' = \frac{1}{L^2}\left|\sum_{x,y}\vec{s}(x,y)e^{2\pi x/L}\right|^2 . \tag{5}$$

The numerics for $\beta \geq 2.25$ show that for the correlation length AS becomes exact, while magnetic susceptibility converges to AS much slower than the correlation length. It thus appears that the existence of a new phase transition is unlikely. One very unusual and interesting scaling behavior is also observed: the specific heat decreases as the β_c is approached in this scaling region, meaning that the specific heat is nonsingular for all the values of β for this model.

Repeating the same procedure, it is shown that for $1.151 \leq \beta \leq 1.395$, both the correlation length and the magnetic susceptibility scale slower than AS, whereas in the intermediate range, $1.606 \leq \beta \leq 1.892$, they scale faster than AS. Hence, the existence of the crossover is obvious, which is consistent with the previous numerical results [7].

In this work, no special efforts were made to locate the exact point from which AS become exact, or at which the crossover occurs. However, detailed numerical results will be available soon. Currently, I am applying this technique to the investigation of the critical behaviors of the 2D ferromagnetic Ising model where one of the two different and positive values of the coupling constants is realized randomly from link to link. A crucial question regarding this system is whether the critical index such as γ and ν changes from those values of the pure (uniformly coupled) system or multiplicative logarithmic correction to the critical behaviors of the pure system exists. It is a notoriously difficult task to distinguish numerically a power critical behavior with a small change in the critical exponent from a logarithmic correction, and vice versa, because the clear difference between the two can be visible only at the points extremely close to the critical point. Since this system is self-dual with certain realizations of the randomness this technique can be easily applied to test the logarithmic correction; current preliminary data seem to show that the correlation length of this system scales according to the multiplicative logarithmic correction that was predicted by a renormalization group equation technique [14]. The details along with the results of different realizations of the randomness will be published elsewhere.

I am grateful to Doug Toussaint for his help in making the O(3) code, to Adrian Patrascioiu for bringing the asymptotic scaling problem to my attention, and to Robert Thews for his hospitality. The numerical computations were made on the CONVEX C240 and IBM 3090 300E at the University of Arizona, and this work was supported in part by the Department of Energy (Grant No. DE-FG02-85ER40213).

[1] See for example, M.N. Barber, R.B. Pearson, D. Toussaint, and J.L. Richardson, Phys. Rev. B **32**, 1720 (1985); C.F. Baillie, R. Gupta, K.A. Hawick, and G.S. Pawley, Report No. LA-UR-91-2853; A.M. Ferrenderg and D.P. Landau, Phys. Rev. B **44**, 5081 (1991).

[2] E. Brézin, J. Phys. (Paris) **43**, 15 (1982).
[3] J.K. Kim, "Finite Size Scaling for Critical Behaviors with Multiplicative Logarithmic Corrections," University of Arizona, 1992 (to be published).
[4] M.P. Nightingale, Physica (Amsterdam) **83A**, 561 (1976); B. Derrida, J. Phys. A **14**, L5 (1981); H. Blöte, M. Nightingale, and B. Derrida, J. Phys. A **14**, L45 (1981); C.J. Hamer and M.N. Barber, J. Phys. A **14**, 241 (1981); E. Brézin and J. Zinn-Justin, Nucl. Phys. **B257** **[FS14]**, 867 (1985).
[5] A.M. Polyakov, Phys. Lett. **59B**, 79 (1975); E. Brézin and J. Zinn-Justin, Phys. Rev. B **14**, 3110 (1976).
[6] M. Falcioni and A. Treves, Phys. Lett. **159B**, 140 (1985); Nucl. Phys. **B265**, 671 (1986).
[7] S.H. Shenker and J. Tobochnik, Phys. Rev. B **22**, 4462 (1980); B. Berg and M. Lücher, Nucl. Phys. **B190** **[FS3]**, 412 (1981); G. Fox, R. Gupta, O. Martin, and S. Otto, Nucl. Phys. **B205** **[FS5]**, 188 (1982); R. Fukugita and Y. Oyanagi, Phys. Lett. **123B**, 71 (1983); B. Berg, S. Meyer, and I. Montvay, Nucl. Phys. **B235** **[FS11]**, 149 (1984); A. Hasenfratz and A. Margaritis, Phys. Lett. **148B**, 129 (1984); M. Lücher and P. Weiss, Nucl. Phys. **B300**, 325 (1988); P. Bonnier and M. Hontebeyrie, Phys. Lett. B **226**, 361 (1989); U. Wolff, Phys. Lett. B **222**, 473 (1989); Nucl. Phys. **B334**, 581 (1990).
[8] J. Apostolakis, C.F. Baille, and G.C. Fox, Phys. Rev. D **43**, 2687 (1991).
[9] P. Hasenfratz and F. Niedermayer, Nucl. Phys. **B337**, 233 (1990).
[10] A. Patrascioiu, Phys. Rev. Lett. **54**, 2292 (1985); **56**, 1023 (1986); **58**, 2285 (1987); E. Seiler, I.O. Stamatescu, A. Patrascioiu, and V. Linke, Nucl. Phys. **B305** **[FS23]**, 623 (1988).
[11] K. Ito, Phys. Rev. Lett. **64**, 2839 (1990).
[12] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989); Phys. Lett. B **228**, 379 (1989).
[13] F. Cooper, B. Freedman, and D. Preston, Nucl. Phys. **B210**, 210 (1982).
[14] B.N. Shalaev, Fiz. Tverd. Tela (Leningrad) **26**, 3002 (1984) [Sov. Phys. Solid State **26**, 1811 (1984)].