PHYSICAL REVIEW
LETTERS

VOLUME 69 9 NOVEMBER 1992 NUMBER 19

Histogram Monte Carlo Renormalization Group Method for Phase Transition Models without Critical Slowing Down

Chin-Kun Hu
Department of Physics, Harvard University, Cambridge, Massachusetts 02138
and Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 11529, Republic of China
(Received 6 April 1992)

Based on the subgraph expansions for phase transition models, we present a histogram Monte Carlo method to calculate the free energy and other physical quantities for such models as continuous functions of the system parameter. The method does not have any critical slowing down. We then use physical quantities thus obtained in a percolation renormalization group method to calculate critical point, critical exponents, and thermodynamic order parameter. Our method gives quite accurate results and may be applied to many phase transition models.

PACS numbers: 05.50.+q, 75.10.-b

The Monte Carlo (MC) simulation [1] and the renormalization group (RG) [2] are popular tools in studying phase transitions and critical phenomena. In 1976, Ma [3] proposed a Monte Carlo renormalization group (MCRG) to combine the advantages of the MC and the RG methods. Ma's MCRG suffers from the critical slowing down. For example, in the MCRG studies of the Ising model on the simple cubic lattice with linear dimension $L = 64$ by Pawley *et al.* [4], 15 h of calculation were done in a distributed array processor of International Computer Limited to equilibrate the system near the critical point and independent configurations are obtained typically in the order of every 2.5×10^5 sweeps [4]. In this Letter, we propose a histogram Monte Carlo renormalization group method [5] for phase transition models, which does not have any critical slowing down. The method is easy to implement, makes efficient usage of simulation data, gives quite accurate global and critical results, may be applied to many phase transition models, and has many potential applications. It is closely related to the connection between percolation and phase transition models [6–15] and recent efforts to improve MC simulations [16–18].

Based on the subgraph expansion of Ising-type models in external fields, Hu has shown that phase transitions of many Ising-type models can be described as geometric percolation transitions [6, 9–11]. In particular Hu has shown that phase transitions of the q-state Potts model (QPM) are percolation transitions of a q-state bond-correlated percolation model (QBCPM) [9], in which subgraphs G' of $b(G')$ occupied bonds and $n(G')$ clusters will appear with the probability weight

$$\pi(G', p, q) = p^{b(G')}(1-p)^{E-b(G')}q^{n(G')}, \tag{1}$$

where $p = 1 - \exp(-K) = 1 - \exp(-\beta J)$ with J being the nearest-neighbor ferromagnetic coupling constant and $\beta = (k_B T)^{-1}$. The spontaneous magnetization M and the magnetic susceptibility χ of the QPM are related to the percolation probability P and the mean cluster size S of the QBCPM, respectively [9]. Based on the connection between the QPM and the QBCPM, Hu and Chen [12] have formulated a percolation renormalization group method (PRGM) and Swendsen and Wang [17] have proposed a cluster Monte Carlo simulation method. The PRGM may be used to calculate the free energy, the critical point, the critical exponent, and the spontaneous magnetization of the QPM. The systems simulated by cluster algorithms may reach equilibrium much more quickly than the traditional MC simulation method; however, the critical slowing down is not completely eliminated [19]. Recently, Ferrenberg and Swendsen proposed a new MC technique for studying phase transitions [18]. The method makes very efficient usage of the data from MC simulations. For optimizing the analysis of data from

multiple MC simulations over a wide range of parameter values, one should solve a set of coupled nonlinear equations [18], which is not a trivial problem.

The histogram Monte Carlo simulation method (HMCSM) proposed below may be realized easily to calculate the free energy and other quantities over a wide range of parameter values. It does not have any critical slowing down. The basic data thus obtained may be used in the PRGM [12] to obtain the critical point, critical exponents, and the order parameter. In the following, we present our method for the QPM and the QBCPM [9]. The extension to other systems and the potential applications of the method are discussed at the end of this paper.

In the HMCSM for the QBCPM on a lattice G of N sites and E nearest-neighbor bonds, the bond random percolation process is used to generate subgraphs G' of G using a sequence of bond probabilities of increasing magnitudes: $0 \le p_1 < p_2 < p_3 \cdots < p_w \le 1$. For each p_j, $1 \le j \le w$, we generate N_R different subgraphs G' of G. The total number of occupied bonds in G', $b(G')$, may be calculated easily. The multiple labeling technique [20] is applied to G' to calculate the total number of clusters in G', $n(G')$, and the total number of sites in percolating clusters, $N^*(G')$, which is 0 for nonpercolating subgraphs. The data obtained from wN_R different G' are then used to construct three matrices with elements $N_p(b,n)$, $N_f(b,n)$, and $N_{pp}(b,n)$, with $0 \le b \le E$ and $1 \le n \le N$. Here $N_p(b,n)$ is the total number of generated percolating subgraphs with b occupied bonds and n clusters, $N_f(b,n)$ is the total number of generated nonpercolating subgraphs with b occupied bonds and n clusters, and $N_{pp}(b,n)$ is the sum of $N^*(G')$ over percolating subgraphs with b occupied bonds and n clusters. In the large number of simulations, we expect that the total number of percolating subgraphs with b occupied bonds and n clusters, $N_{tp}(b,n)$, and the total number of nonpercolating subgraphs with b occupied bonds and n clusters, $N_{tf}(b,n)$, should be proportional to $N_p(b,n)$ and $N_f(b,n)$ with the same proportionality constant $C(b)$, which may be determined from the following equation:

$$C(b)\sum_{n=1}^{N}[N_p(b,n)+N_f(b,n)] = \sum_{n=1}^{N}[N_{tp}(b,n)+N_{tf}(b,n)] = C_b^E. \tag{2}$$

Now we define $I(p,q,b,n)$ by the equation: $I(p,q,b,n) = (e^K-1)^b q^n = e^{KE}p^b(1-p)^{E-b}q^n$. The sum of $I(p,q,b,n)$ over all possible percolating subgraphs G'_p gives $R(G,p,q)$; the sum of $I(p,q,b,n)$ over all possible nonpercolating subgraphs gives $Q(G,p,q)$. In the HMCSM, $R(G,p,q)$, $Q(G,p,q)$, and the percolation probability $P(G,p,q)$ may be calculated from the following equations:

$$R(G,p,q) = \sum_{b=0}^{E} I(p,q,b,n)C_b^E \times \frac{\sum_{n=1}^{N} N_p(b,n)q^n}{\sum_{n=1}^{N}[N_p(b,n)+N_f(b,n)]}, \tag{3}$$

$$Q(G,p,q) = \sum_{b=0}^{E} I(p,q,b,n)C_b^E \times \frac{\sum_{n=1}^{N} N_f(b,n)q^n}{\sum_{n=1}^{N}[N_p(b,n)+N_f(b,n)]}, \tag{4}$$

$$P(G,p,q) = \frac{1}{Z_N}\sum_{b=0}^{E} I(p,q,b,n)C_b^E \times \frac{\sum_{n=1}^{N} N_{pp}(b,n)q^n}{\sum_{n=1}^{N}[N_p(b,n)+N_f(b,n)]}. \tag{5}$$

The sum of $R(G,p,q)$ and $Q(G,p,q)$ gives the partition function $Z_N(G,p,q)$, from which we may calculate the energy $f(G,p,q)$:

$$f(G,p,q) = \ln Z_N(G,p,q)/N = F_e(G,p,q) + Kz/2, \tag{6}$$

where $F_e(G,p,q)$ is the difference between $f(G,p,q)$ and $Kz/2$ with z being the coordination number of the lattice. It approaches $\ln q$ as $p \to 0$ and approaches 0 as $p \to 1$ and $N \to \infty$. It is more convenient to plot F_e as a function of p than to plot f, so we will plot F_e instead of f below. The internal energy U and the specific heat C_h may be obtained from the derivatives of the free energy,

$$U(G,p,q) = -\frac{\partial}{\partial\beta} f(G,p,q), \qquad C_h = \frac{\partial}{\partial T}U(G,p,q). \tag{7}$$

The existence probability $E_p(G,p,q)$ is defined to be the ratio of $R(G,p,q)$ and $Z(G,p,q)$. It should be noted that F_e, U, C_h, E_p, and P presented above are continuous functions of p. This is quite different from the results obtained by traditional MC simulation methods [1]. We have calculated F_e, U, C_h, E_p, and P for the QPM on lattices of different linear dimensions L. Typical calculated results for the square (sq) lattice are shown in Figs. 1(a),1(b), where the exact results of Ferdinand and Fisher [21] are shown by dashed lines for comparison. Figure 1(a) shows that our F_e, U, and C_h are consistent with the exact results [21] to a high degree of accuracy. Thus our method gives a very nice account of global properties of the spin model.

Suppose we already carry out histogram MC simulations on lattices G_1 and G_2 of linear dimensions L_1 and

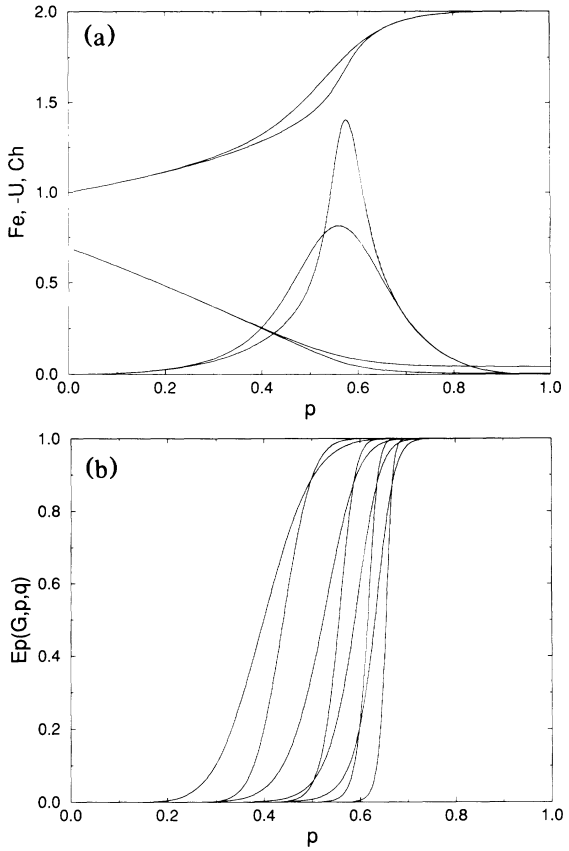

FIG. 1. Calculated results for the q-state Potts model (QPM) on the sq lattices with $L = 4$, 6, and 12, $N_R = 10^5$ for $L = 4$ and $N_R = 2 \times 10^5$ for $L = 6$ and 12, and $w = 459$ for every case. (a) The free energy F_e, the internal energy $-U$, and the specific heat C_h for the Ising model as a function of p. We set $k_B = J = 1$. As a function of p, F_e is decreasing, $-U$ is increasing, and C_h has a maximum. The upper curves of F_e and U are for $L = 4$; the lower curves are for $L = 12$. Near $p = 0.58$ the curves for C_h from bottom to top are for $L = 4$ and 12, respectively. Our results and the exact results of Ferdinand and Fisher [21] are shown by solid and dashed lines, respectively. The invisibility of the dashed line means that our results and exact results are consistent. (b) The existence probability E_p as a function of p. The curves which intersect at a point near $E_p = 0.8$ come from the same q value. The intersections from left to right are for $q = 1$, 2, 3, and 4, respectively. Below the intersections, the curve at the left is for $L = 6$ and the curve at the right is for $L = 12$.

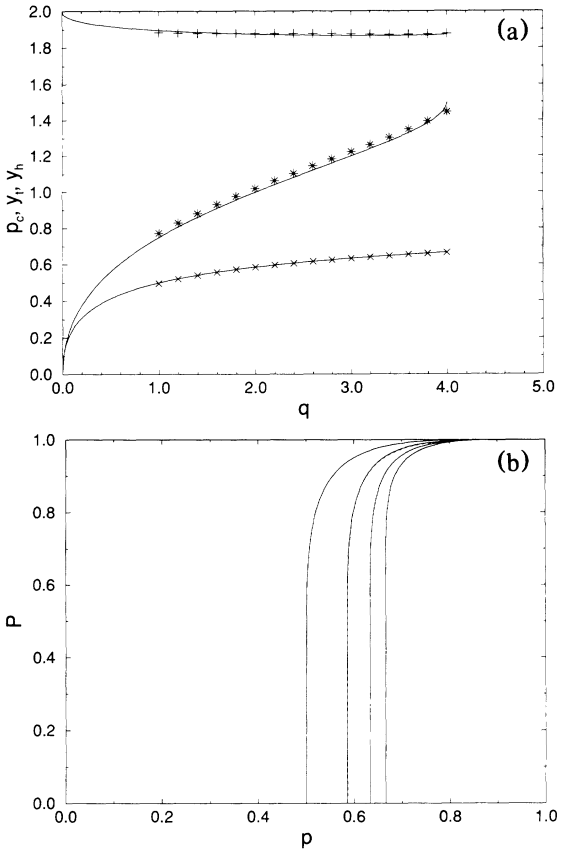

FIG. 2. HMCRG approach to the QPM on the sq lattice with $L_1 = 16$, $N_R = 6 \times 10^5$, w=369, and $L_2 = 8$, $N_R = 12 \times 10^5$, $w = 369$. (a) The critical point p_c ($\times$), the thermal scaling power y_t ($*$), and the field scaling power y_h ($+$) as a function of q. The solid curves from bottom to top represent exact solutions for p_c, y_t, and y_h, respectively. (b) The percolation probability P as a function of p. The solid curves from left to right are for $q = 1$, 2, 3, and 4, respectively, they represent our results. The dashed line represents Yang's exact solution [24]. For $q = 1$ alone, we use $N_R = 10^5$ for $L_1 = 20$, $N_R = 5 \times 10^5$ for $L_2 = 10$, and $w = 459$ for both cases.

L_2, respectively, where $L_1 > L_2$. The percolation RG transformation from lattice G_1 to lattice G_2 is given by [12]

$$E_p(G_2, p', q) = E_p(G_1, p, q), \tag{8}$$

which gives the renormalized bond probability p' as a function of p. The fixed point of Eq. (8) gives the critical point p_c. The thermal scaling power y_t and the field scaling power y_h, which is equal to the fractal dimension D of the percolating cluster at p_c [15, 22], may be obtained from the equations

$$\frac{1}{\nu} = y_t = \frac{(\ln \frac{\partial p'}{\partial p})_{p_c}}{\ln \frac{L_1}{L_2}}, \quad y_h = D = \frac{\ln \frac{P(G_1', p_c) L_1^d}{P(G_2', p_c) L_2^d}}{\ln \frac{L_1}{L_2}}. \tag{9}$$

Using Eqs. (8) and (9) with $L_1 = 16$ and $L_2 = 8$, we have calculated p_c, y_t, and y_h for the sq lattice. The results are shown in Fig. 2(a), where the exact solutions [23] are also shown by solid lines for comparison. Figure 2(a) shows that our method gives quite accurate results. Using the method of Ref. [12], we iterated Eq. (8) to obtain the percolation probability, i.e., the spontaneous magnetization, for the QPM on the sq lattice in the thermodynamic limit. The results are shown by solid lines

in Fig. 2(b), where the exact result of Yang [24] for the Ising model is shown by a dashed line for comparison. The agreement of our result with Yang's exact solution [24] is excellent. In all calculations, we impose a periodic boundary condition on the lattice.

Since we use the random percolation process to carry out the simulation, which contains no dynamics at all, there is no critical slowing down. This is better than traditional MC method [1] and Swendsen-Wang algorithms [17]. Equations (3)–(5) suggest that very large values of q and n will make the factor q^n overflow. Fortunately, most interesting critical phenomena appear in small values of q, i.e., $q \leq 4$, and to get accurate results one need not use very large lattices as may be seen from Fig. 2. In the present paper, we used a Sun workstation to carry out numerical calculations; it has only 32 bits per word.

The method presented above is for any lattice and space dimensions. It is almost impossible to obtain an exact order parameter for three-dimensional systems. However, using faster computers with 64 bits a word and some data reduction technique, we may expect to calculate order parameters for three-dimensional systems as good as that of Fig. 2(b), i.e., almost indistinquishable from the exact solution. This capability of our method is very interesting and important when we try to compare theoretical calculations with experimental data.

Our method may be extended to other Ising-type models, e.g., the Ising model with multispin interactions including the Baxter model as a special case, the dilute Potts model including the BEG model as a special case, the antiferromagnetic Potts model, etc., based on their subgraph expansions [6, 10, 11, 25], to hard-core particle models based on Hu and Mak's definition of clusters [5, 13], and to quantum systems based on Suzuki-Trotter decomposition [26]. The idea of the method can also be of value in lattice gauge theory. Since our method may determine accurate free energy and other physical quantities for finite systems in a simple way, it is useful for finite-size scaling analysis near the critical point [27] and critical spin component q_c [28], and for determining zeros of the partition function [29] and the order of phase transitions [30].

In summary, we have proposed a histogram Monte Carlo renormalization group method, which may be implemented easily, yet gives pretty accurate global and critical results and has many potential applications.

The author thanks Dr. H. Flyvbjerg, Dr. B. Hu, Dr. H. Muller-Krumbhaar, Dr. J.-S. Wang, and C.-K. Peng for useful comments or a critical reading of the paper. This work was supported by the National Science Council of the Republic of China (Taiwan) under Contract No. NSC 81-0208-M001-55 and by the NSF of U.S.A. through Grant No. DMR 91-15491 and through the Harvard University Materials Research Laboratory.

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