Scaling functions for O(4) in three dimensions

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Monte Carlo simulation using a cluster algorithm is used to compute the scaling part of the free energy for a three-dimensional O(4) spin model. The results are relevant for the analysis of lattice studies of high temperature QCD. [S0556-2821(97)02301-1]

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I. INTRODUCTION

The high temperature phase transition for QCD with two flavors of light quarks is expected to be driven by chiral symmetry restoration, with an order parameter having O(4) symmetry in the continuum limit [1–3]. Thus, near the transition we expect the scaling properties of a three-dimensional O(4) spin model. For quark mass or temperature not too close to the transition, the system would be expected to behave like mean field theory. Recently Kocic and Kogut have suggested that mean field behavior might describe the system arbitrarily close to the critical point [4]. Finally, with Kogut-Susskind quarks on a nonzero lattice spacing, the exact chiral symmetry is only O(2), and it is possible that lattice simulations are better described by O(2) critical behavior. In addition to its intrinsic interest as an indicator of the physics of the transition, the form of the free energy near the critical point is important in extrapolating the QCD equation of state from the quark masses where lattice simulations are practical to the light quark masses of the real world [5,6].

Assuming a second order transition [7], we expect the singular behavior of thermodynamic observables near the transition to be universal, meaning that the symmetry group of the order parameter and the dimension of the system determine the critical exponents and the form of the singular part of the free energy, up to normalization of the scaling variables. (See, for example, [8].) The critical exponents for O(4) and O(2) are well known [9–11], but the form of the free energy, or the ''scaling function,'' is only poorly known. An ϵ expansion result is available [12], quoted in Ref. [2]. Similarly, Monte Carlo calculations of critical exponents have been used to study the critical behavior of high temperature QCD [13], but to date the full power of the scaling ansatz, namely, comparison with the universal scaling functions as well as critical exponents, has not been brought to bear.

Here we use Monte Carlo simulation to compute an approximate scaling function for O(4), to be used in comparing to Monte Carlo simulations of QCD.

For the O(N) spin model we use the partition function,

$$Z=\int [d\vec{s}]\exp\left(J\sum_{ij}\vec{s}_i\cdot\vec{s}_j+H\sum_i s_{0i}\right), \tag{1}$$

where ij are nearest neighbor pairs on a (hyper)cubic lattice in d dimensions and s_{0i} is the zero component of $\vec{s}_i$. Then the energy and magnetization are

$$\langle E\rangle=\frac{1}{dV}\frac{\partial\ln(Z)}{\partial J},\quad \langle M\rangle=\frac{1}{V}\frac{\partial\ln(Z)}{\partial H}. \tag{2}$$

In QCD, using the normalization where the plaquette ($\Box$) is three when all links are unity, the analogous equations are

$$\langle\Box\rangle=\frac{1}{2Vn_t}\frac{\partial\ln(Z)}{\partial 6/g^2},\quad \langle\overline{\psi\psi}\rangle=\frac{1}{Vn_t}\frac{\partial\ln(Z)}{\partial am_q}. \tag{3}$$

II. PARAMETRIZING THE SCALING FUNCTIONS

From invariance under a length rescaling by a factor b, the critical part of the free energy should have the property,

$$f_s(t,h)=b^{-d}f_s(b^{y_t}t,b^{y_h}h). \tag{4}$$

Here t and h are the scaling variables, with the critical point at $(t,h)=(0,0)$, and y_t and y_h are the corresponding critical exponents. Other exponents can be expressed in terms of y_t and y_h. Here $t=(T-T_c)/T_0$ and $h=H/H_0$ are conventionally normalized by requiring that $M(t=0,h)=h^{1/\delta}$ and $M(t<0,h=0)=(-t)^{\beta}$. The free energy also has a nonsingular part.

The scaling ansatz, Eq. (4), implies that the magnetization near the critical point is determined by a universal scaling function, conventionally written as

$$\frac{M}{h^{1/\delta}}=f(t/h^{1/\beta\delta})=f(x). \tag{5}$$

The normalization conditions on t and h then require that $f(0)=1$ and $f(x)\to(-x)^{\beta}$ as $x\to-\infty$.

In computing the energy and pressure of QCD, we require the plaquette, analogous to the energy in the spin model, extrapolated to zero quark mass, which is analogous to zero magnetic field. The magnetization (or $\overline{\psi\psi}$ in QCD) is

$$\frac{1}{V}\frac{\partial\ln(Z)}{\partial H}=\frac{1}{VH_0}\frac{\partial\ln(Z)}{\partial h},$$

while the energy (or plaquette in QCD) is

$$\frac{1}{V}\frac{\partial\ln(Z)}{\partial T}=\frac{1}{VT_0}\frac{\partial\ln(Z)}{\partial t}.$$

Since the energy and magnetization are derivatives of the free energy with respect to t and h, respectively, information

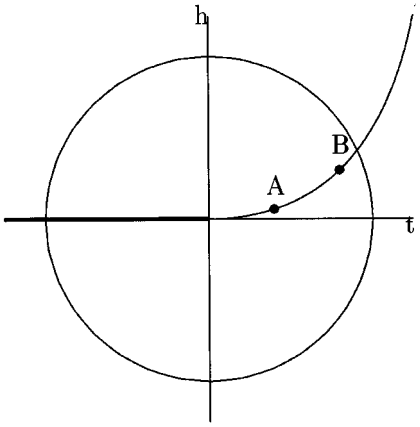

FIG. 1. A length rescaling by a factor of b is accomplished by changing the couplings (t,h) at point A to $(b^{y_t}t,b^{y_h}h)$ at point B by moving along the renormalization group trajectory (curved line). The trajectories may be labeled by their intersections with the unit circle, so specifying the free energy on the unit circle, together with the scaling ansatz which tells how the free energy changes along a trajectory, specifies the free energy everywhere. The discontinuity in the order parameter at $t<0$ and $h=0$ (heavy line) implies that the derivative of the free energy is discontinuous there.

about one quantity constrains the other. In particular, the behavior of $\psi\psi$ in QCD can help in extrapolating the plaquette to zero or small quark mass. (It is important to enforce consistency of the plaquette and $\psi\psi$ in computing the equation of state. Using a plaquette and $\psi\psi$ which are not derivatives of the same free energy could lead to inconsistent thermodynamics.) Because our analysis requires that we handle the energy and magnetization on the same footing, in addition to Eq. (5), we develop a formulation of the scaling ansatz which treats the magnetization and energy equally.

The scaling ansatz, Eq. (4), tells us that if we specify the singular free energy on any circle in the t,h plane, we have specified it for all t,h. (See Fig. 1.) In particular, if $g(\theta)$ is the scaling free energy on the unit circle in the t,h plane, then the rescaling factor b which takes t,h to the unit circle is determined by

$$(b^{y_t}t)^2+(b^{y_h}h)^2=1. \tag{6}$$

For y_t and y_h positive this clearly has a unique solution for $b>0$ given t and h. Although in general this cannot be solved analytically for b, it is straightforward to do differentiations implicitly and solve the equation numerically. Then the singular free energy (actually $-1\times$ temperature $\times$ free energy per volume) is

$$\frac{1}{V}\ln[Z_s(t,h)]=b(t,h)^{-d}g(\theta(t,h)), \tag{7}$$

where $\theta(t,h)=\arctan^{-1}(b^{y_h}h/b^{y_t}t)$, and $g(\theta)$ is a universal function.

Equivalently, the relation between t,h and b,θ can be expressed as

$$b^{y_h}h=\sin(\theta),\quad b^{y_t}t=\cos(\theta). \tag{8}$$

After some differentiations, the magnetization and energy can be expressed in terms of $g(\theta)$:

$$M=\frac{1}{H_0}\left(\frac{-d}{b^{d+1}}\frac{\partial b}{\partial h}g(\theta)+b^{-d}g'(\theta)\frac{\partial\theta}{\partial h}\right), \tag{9}$$

$$E=\frac{1}{dT_0}\left(\frac{-d}{b^{d+1}}\frac{\partial b}{\partial t}g(\theta)+b^{-d}g'(\theta)\frac{\partial\theta}{\partial t}\right), \tag{10}$$

where

$$\left.\frac{\partial b}{\partial h}\right|_t=\frac{-hb^{2y_h}}{y_tt^2b^{2y_t-1}+y_hh^2b^{2y_h-1}}=\frac{-\sin(\theta)b^{y_h+1}}{y_t\cos^2(\theta)+y_h\sin^2(\theta)},$$

$$\left.\frac{\partial b}{\partial t}\right|_h=\frac{-tb^{2y_t}}{y_tt^2b^{2y_t-1}+y_hh^2b^{2y_h-1}}=\frac{-\cos(\theta)b^{y_t+1}}{y_t\cos^2(\theta)+y_h\sin^2(\theta)},$$

$$\left.\frac{\partial\theta}{\partial h}\right|_t=tb^{y_t+y_h}+ht\frac{\partial b}{\partial h}(y_h-y_t)b^{y_h+y_t-1}=\frac{y_tb^{y_h}\cos(\theta)}{y_t\cos^2(\theta)+y_h\sin^2(\theta)},$$

$$\left.\frac{\partial\theta}{\partial t}\right|_h=-hb^{y_t+y_h}+ht\frac{\partial b}{\partial t}(y_h-y_t)b^{y_h+y_t-1}=\frac{-y_hb^{y_t}\sin(\theta)}{y_t\cos^2(\theta)+y_h\sin^2(\theta)}. \tag{11}$$

Physical insight into the form of $g(\theta)$ comes from considering special cases.

First, for $t>0$ and h small,

$$M=\frac{1}{H_0}g'(0)t^{d/y_t}t^{-y_h/y_t},\quad E=\frac{g(0)}{T_0y_t}t^{d/y_t-1}. \tag{12}$$

Since M must vanish here, we require $g'(0)=0$. In fact, we expect the free energy to be an even function of h, with a cusp at $h=0$ and $t<0$ due to the discontinuity of M on this line. One more differentiation of the energy will give the specific heat $C\approx t^{d/y_t-2}=t^{-\alpha}$. We also find that the susceptibility is

$$\chi=\frac{1}{H_0^2}\left(\frac{dg(0)}{y_t}+g''(0)\right)t^{(d-2y_h)/y_t}. \tag{13}$$

For $t<0$ and h small and positive,

$$M=\frac{-1}{H_0}g'(\pi)(-t)^{(d-y_h)/y_t}\approx(-t)^{\beta},$$

$$E=\frac{-g(\pi)}{T_0y_t}(-t)^{d/y_t-1}. \tag{14}$$

For $t=0$ and $h>0$,

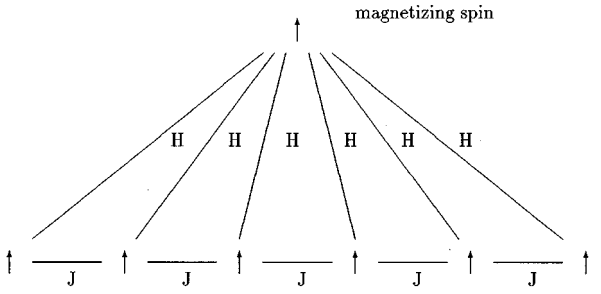

FIG. 2. Cluster updating with a magnetic field. A single ''magnetizing spin'' is coupled to every spin in the lattice by a bond with strength H.

$$M=\frac{d}{H_0 y_h}g(\pi/2)h^{d/y_h-1},$$

$$E=\frac{-1}{dT_0}g'(\pi/2)h^{(d-y_t)/y_h}. \tag{15}$$

From these expressions we get the following intuition about the scaling free energy $g(\theta)$: (1) $g(0)$ controls the singular part of the energy for $T>T_c$; (2) $g(\pi)$ controls the singular part of the energy for $T<T_c$; (3) $g'(\pi/2)$ controls the energy for $t=0$, $h\neq 0$; (4) $\lim_{\theta\uparrow\pi}g'(\theta)=-\lim_{\theta\downarrow-\pi}g'(\theta)$ controls the expectation value of M for $T<T_c$; (5) $g(\pi/2)$ controls M for $t=0$ and $h\neq 0$.

Here it is convenient to choose T_0 and H_0 so that $H_0M(t=0,h)=h^{1/\delta}$ and $H_0M(t<0,h=0)=(-t)^{\beta}$. The normalization conditions on t and h then require that $g(\pi/2)=y_h/d$ and $g'(\pi)=-1$. When it is necessary to distinguish, we will call H_0 for the ''$f(x)$'' and ''$g(\theta)$'' forms H_f and H_g, respectively. Similarly we distinguish T_f and T_g. They are related by $H_f=H_g^{\delta+1}$ and $T_f=T_gH_g^{1/\beta}$.

III. SIMULATIONS

Monte Carlo simulations were run on 16^3, 24^3, 32^3, 40^3, 48^3, and 64^3 lattices using a multiple cluster updating algorithm [14].

To use a cluster updating algorithm with a nonzero magnetic field, just imagine that in addition to the regular bonds with strength J connecting neighboring spins, each spin is connected to a fake ''magnetizing spin'' by a bond of strength H, as illustrated in Fig. 2. Then break both ''J bonds'' and ''H bonds'' and update clusters according to the usual cluster algorithm [14]. The ''magnetizing spin'' is a member of a cluster, and is reflected just like any other spin. When evaluating the magnetization of the lattice, we take the components of the lattice spins in the current direction of the magnetizing spin.

Results for the magnetization of the O(4) model are plotted in Fig. 3. Results from the largest lattice size run at each point are shown. The remaining finite size effects are about the same size as the statistical error bars. Then, in Fig. 4 the results for $h=0.002$, 0.005, 0.01, and 0.02 are plotted in the form in Eq. (5). Here we used the values for the critical coupling and exponents from Kanaya and Kaya [9].

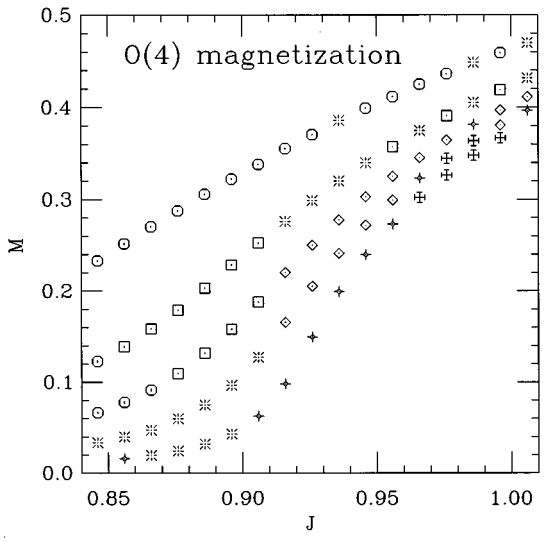

FIG. 3. Magnetization in the O(4) model for $h=0.002$, 0.005, 0.01, 0.02 and 0.05. Octagons are for $L=16$, squares for $L=24$, bursts for $L=32$, diamonds for $L=40$, decorated diamonds for $L=48$ and decorated plusses for $L=64$.

Then we fit the magnetization results to find an approximate scaling function $g(\theta)$ for the free energy in the form in Eq. (7). A simple parametrization of $g(\theta)$ which satisfies the normalization conditions on $g(\pi/2)$ and $g'(\pi)$ is

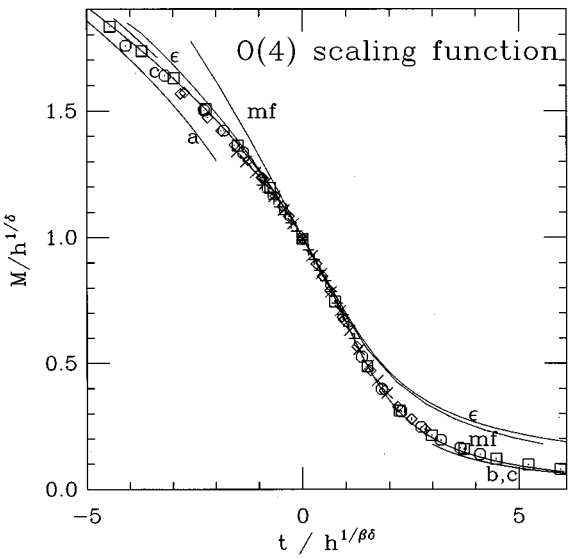

FIG. 4. O(4) magnetization for $h=0.002$, 0.005, and 0.01 plotted as a scaling function in the conventional form. I use the results of Kanaya and Kaya [9] for the critical coupling and critical exponents. In this plot the points for $h=0.05$ are plotted with plus σ, those for 0.02, with crosses, 0.01 with diamonds, 0.005 with octagons, and 0.002 with squares. Also shown are the asymptotic forms $f(x)\approx(-x)^{\beta}$ as $x\to-\infty$ (a) and $f(x)\approx Cx^{-\gamma}$ as $s\to\infty$ (b). A four-parameter fit to the scaling function from the ''$g(\theta)$'' form is shown with a solid line (c), running through the entire graph. The mean field scaling function, and the second order ϵ expansion scaling function [12] are shown, labeled ''ϵ'' and ''mf.'' Finally, the short line segment in the upper left corner is a result of Wallace and Zia [15], quoted in the Appendix of Ref. [2], incorporating the correct behavior of the susceptibility near the critical line.

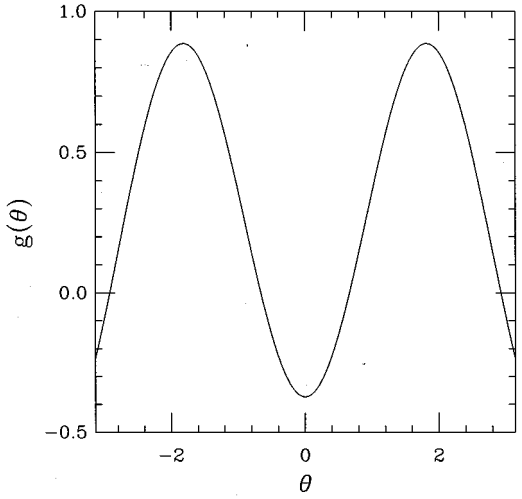

FIG. 5. Four-parameter fit to the scaling function $g(\theta)$ for the O(4) free energy.

$$g(\theta)=y_h/3+2[\cos(\theta/2)-\sqrt{1/2}]+a_0\cos(\theta)+a_1[\cos(3\theta/2)+3\cos(\theta/2)-2\sqrt{1/2}]+a_2[\cos(2\theta)+1]+a_3[\cos(5\theta/2)-5\cos(\theta/2)+6\sqrt{1/2}] \quad (16)$$

($d=3$ in this equation.)

In this fit I used the energy and magnetization for $0.89<J<0.99$ and $H=0.005$ and 0.002. The free energy also included an analytic part $f_A=C_{H2}h^2+C_{J1}t+C_{J2}t^2+C_{J3}t^3$. The resulting $g(\theta)$ is plotted in Fig. 5. T_g and H_g were 0.44 and 1.31, respectively. The magnetization corresponding to this free energy is also plotted in Fig. 6. In principle, the critical exponents y_t and y_h and the critical coupling are also parameters in this fit. However, to get these parameters to the same accuracy as has already been done by Kanaya and Kaya [9] or Butera and Comi [11] would require a careful correction for finite size effects, and care in using only data for small enough t and h that corrections to scaling are small. Therefore, the exponents and critical coupling were fixed to those found by Kanaya and Kaya. Because of the remaining finite size effects and corrections to scaling, the χ^2 of this fit was very bad (243 for 30 degrees of freedom). However, since the results are already many times more accurate than the QCD data with which we intend to compare, there is little incentive to make the necessary corrections. This scaling function was then converted to the ''$f(x)$'' form [by computing the resulting magnetization as a function of t for $h=0.002$ and plotting according to Eq. (5)], and plotted as a solid line in Fig. 4, where it can be seen to describe the magnetization quite well. [It is necessary to convert the normalization of t and h used in the ''$g(\theta)$'' form to the conventional normalizations for the ''$f(x)$'' form: $H_f=H_g^{\delta+1}$ and $T_f=T_gH_g^{1/\beta}$] In this figure I have also included the mean field form of the scaling function and the epsilon expansion form.

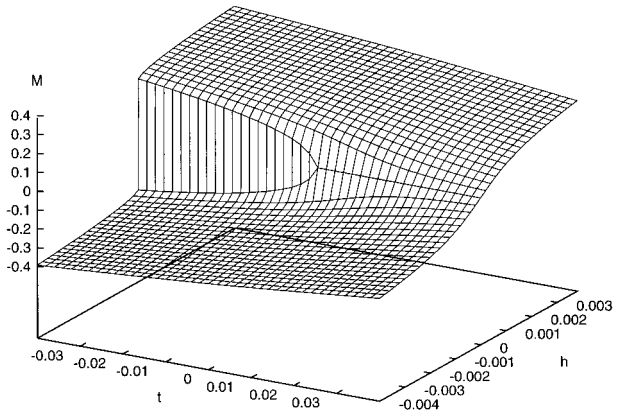

FIG. 6. The scaling part of the magnetization for O(4), corresponding to the scaling function in Fig. 5.

Figure 4 also shows the properly normalized asymptotic form for $f(x)$ as $x\to-\infty$, $x^{-\beta}$. It can be seen that the scaling function approaches this asymptotic form quite slowly. This is the region where long distance physics is dominated by Goldstone bosons. In particular, we expect that for $t<0$ and h small, the magnetization takes the form $M=M(t,0)+Ah^{1/2}$, so that the susceptibility diverges at $h=0$ for all $t<0$ [15]. The fitting function (16) should really be modified to support this behavior at $\theta=\pi$, but this problem seems to occur in a region beyond where these O(4) results, and the QCD results to which they will be compared, are taken.

The Monte Carlo scaling function and the ϵ expansion are in good agreement for $t<0$ because of the normalization condition on t, $M(t<0,h=0)=(-t)^{\beta}$. Had we chosen the equally sensible normalization condition $\chi=dM/dh=t^{-\gamma}$ for $t>0$ and $h=0$, we would have found agreement of the Monte Carlo and ϵ expansion for $t>0$ with a discrepancy for $t<0$.

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