Effective potential, critical point scaling, and the renormalization group

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The desirability of evaluating the effective potential in field theories near a phase transition has been recognized in a number of different areas. We show that recent Monte Carlo simulations for the probability distribution for the order parameter in an equilibrium Ising system, when combined with low-order renormalization group results for an ordinary ϕ^4 system, can be used to extract the effective potential. All scaling features are included in the process. [S1063-651X(98)08709-1]

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I. INTRODUCTION

In the realm of statistical physics, as well as in quantum field theory, the need for non-perturbative approaches to study the vicinity of a phase transition has long been appreciated. Results of recent simulations [1–4] show that the form of the effective potential for a variety of systems can be determined using Monte Carlo methods. Such methods have also been applied to the study of the electroweak phase transition [5]. Additional continuum limit work has recently been performed on a $\lambda\phi^4$ theory in three dimensions [6]. Extracting the effective potential provides one with an additional window onto the equilibrium—and possibly the dynamical—behavior of a system near and at its critical point.

Binder [7] and more recently Tsypin [1] and Chen and Dohm [8] utilized Monte Carlo and binning techniques to generate probability distributions of the order parameter of an $O(1)$ (Ising-like) system in the vicinity of its critical point. In Tsypin's work data were generated at a single temperature, and over a range of symmetry-breaking fields in order to explore the full scaling domain. Above the critical temperature the distribution was found to be consistent with a low-order polynomial form for the effective potential, which, as discussed below, is essentially the logarithm of the probability distribution. The results of simulations were most closely fit when the effective potential was terminated at the sixth order. The standard quartic Ginzburg-Landau form for the effective potential failed to produce an adequate fit for any choice of coefficients, and the addition of eighth- and higher-order terms did not materially improve the agreement between the fitting form and the results of simulations.

This remarkable set of results persists below the critical temperature [2]. Here, it was found that a sixth-order polynomial form for the effective potential leads to an outstanding match to the results of simulations. In this case the best-fit effective potential was found to contain a *negative* quartic term. An additional feature of Tsypin's fitting form is a prefactor, proportional to the square root of the second derivative of the effective potential.

It is reasonable to ask whether or not the data are consistent with a scaling form for the effective potential. In fact, the nature of the polynomial strongly suggests a form incorporating thermodynamic scaling with exponents appropriate to the Ising model. The rationale for this will be explored in more depth in subsequent sections.

It should be noted that the renormalization group has been utilized previously to generate order parameter distributions in the vicinity of the critical point [4,8,9]. The principal novelty in this paper is the attempt to produce a unified form for the order parameter distribution that fits data above, below, and at the critical point. It is found that the inclusion of the prefactor mentioned above leads to excellent agreement with data based on Monte Carlo simulations. The prefactor does not play an important role in the fitting of a scaling form to the order parameter distribution in the high- and low-temperature phases. However, this finite size correction is essential to the construction of a high-precision fit to data at the critical point.

Checks on the quality of the fit include comparisons of a universal ratio of moments of the distribution with values in the literature determined by a variety of alternative techniques, and comparison between our optimum fit value of the fourth-order coupling u with a variety of other determinations of that quantity. These checks are very encouraging. It appears that a scaling form based on renormalized mean-field theory (to be described below) agrees to a high degree of accuracy with published results. On this basis, one has confidence that an equation of state constructed in a similar manner from renormalized mean-field theory will accurately describe systems in the $O(1)$, or Ising model, universality class.

The remainder of this paper is laid out as follows. In the next section the effective potential is defined and a phenomenological scaling description is presented. In Sec. III a renormalization-group derivation of the scaling form is given, and in the following section the ''prefactor'' is discussed. In Sec. V finite size effects are addressed, while Sec. VI assesses the success of the scaling form of the effective potential as a fit to Tsypin's Monte Carlo simulations. Section VII is devoted to concluding remarks. An Appendix contains a discussion of the effect of the prefactor on an important universal quantity.

II. SCALING CONSIDERATIONS

We imagine a scalar (Ising-like) system described by order parameter ϕ and ordering field h in equilibrium at temperature T. If the system is described by Hamiltonian $H(\phi)$ the constrained (reduced) free energy, $F(T,h;M)$, is given by

$$Z=\exp[-F(t,h;M)]=\int D\phi\,\delta(M-I(\phi))\exp[-H(\phi)/T], \tag{2.1}$$

where $I(\phi)\equiv\Omega^{-1}\int\phi d^dx$ is the average order in configuration $\{\phi\}$, Ω represents the volume of the system, and d is the dimensionality. The quantity M is also proportional to the infinite wavelength contribution to the spatial Fourier decomposition of $\phi(\vec{r})$. The effective potential $\mathcal{H}$ may be defined as

$$Z=\exp(-\mathcal{H}), \tag{2.2}$$

which identifies it with the constrained free energy [10]. According to standard scaling notions, when the linear extent L of the system is sufficiently great, the free energy $F(t,h)$ of an $O(1)$ system will have the ''generalized homogeneous'' form

$$L^d|t|^{d\nu}G\left(h|t|^{-\Delta},\frac{t}{|t|}\right), \tag{2.3}$$

where the exponent Δ is equal to $\nu(d+2-\eta)/2$, d is the system's spatial dimensionality, and the standard exponents ν and η are given below. The parameter t is the reduced temperature, $t=(T-T_c)/T_c$, where T_c is the critical temperature, and the ordering, or symmetry-breaking, field h has been introduced above. This scaling form, which arises from an integration over the order parameter M in the constrained partition function, is consistent with the following more general expression for the effective potential:

$$\mathcal{H}(t,h,M)=L^d|M|^{2d/(d-2+\eta)}\times\mathcal{F}(t|M|^{-2/\nu(d-2+\eta)},h|M|^{-(d+2-\eta)/(d-2+\eta)}). \tag{2.4}$$

The exponents ν and η appear in the (unconstrained) two-point correlation function $C(\vec{r}-\vec{r}',t,h)$, which, in the scaling regime, has the form

$$C(\vec{R},t,h)=|\vec{R}|^{-(d-2+\eta)}\mathcal{C}(|\vec{R}|t^{\nu},ht^{-\nu(d+2-\eta)/2}). \tag{2.5}$$

All thermodynamic exponents follow from the two correlation function exponents, ν and η, given the standard scaling and hyperscaling relations [11]. When the spatial dimensionality is $d=3$, the critical exponents are [12]

$$\nu=0.63\pm0.002, \tag{2.6}$$

$$\eta=0.037\pm0.001. \tag{2.7}$$

An immediate consequence of expression (2.4) is that the effective potential at bulk criticality ($t=h=0$) has the form

$$\mathcal{H}_{\text{critical}}\propto L^d|M|^{2d/(d-2+\eta)}=L^d|M|^{\approx 5.8}. \tag{2.8}$$

Now, imagine that the reduced temperature is quite small. The equilibrium correlation length, which can be expressed as $\xi(t,M)$, will under these circumstances appear to be controlled by the finite value of the order parameter M. Further it will appear to diverge as the M is reduced, until being cut off, for example, by the small but finite value of t. Likewise, for appropriate values of the order parameter (that is, if the order parameter controls the decay of correlations) the effective potential will behave in much the same way as it does at the critical point. In view of Eq. (2.8) a naive expectation would be that an attempt to approximate the effective potential by a polynomial in M would yield something not too different from M^6. Interestingly, this is precisely the result of Tsypin's unbiased attempt to fit his simulation data to a polynomial effective potential: A *fourth-order*, Ginzburg-Landau form *fails* to adequately represent the data, while the coefficients of terms *beyond sixth order* are so small as to cast doubt on their appearance in the true effective potential. This result holds both above and below the critical temperature—that is, whether the system is in the disordered or the ordered state.

Now, the form (2.4) is expected to apply only when the order parameter M lies at—or close to—the value which minimizes the free energy at fixed t,h. In particular, there are known difficulties in applying the above scaling form (2.4) to the case of a system in the coexistence region, which impinge directly on the scaling regime. The equilibrium state within the coexistence regime ($T<0$, $h=0$) will generally involve one or more interfacial regions separating two homogeneous thermodynamic phases of arbitrary volume fraction. Because of this, the scaling form, which is hypothesized for a *single* homogeneous phase, does not necessarily do an adequate job of describing the behavior of a system in which two different phases coexist. On the other hand, a scaling form ought to predict with great accuracy the dependence of thermodynamic functions on temperature and ordering field as these fields approach the coexistence line, that is, at the phase boundary for two-phase coexistence.

There is one more consequence of scaling that is worthy of note. The scaling form in Eq. (2.4) together with correlation function scaling implies the following form for the free energy [13,14]:

$$\mathcal{H}=\hat{\mathcal{G}}(M\xi^{(d-2+\eta)/2},h\xi^{(d+2-\eta)/2},t\xi^{1/\nu},L\xi^{-1})=\hat{G}\left(M|t|^{-\nu(d-2+\eta)/2},h|t|^{-\nu(d+2-\eta)/2},L|t|^{\nu},\frac{t}{|t|}\right). \tag{2.9}$$

In the first line of Eq. (2.9) the quantity ξ is the *bulk* correlation length at $h=0$.

III. RENORMALIZATION-GROUP BASED FORM FOR THE EFFECTIVE POTENTIAL

The general form in Eq. (2.4) restricts, but does not specify, the detailed dependence of the effective potential $\mathcal{H}$ on t and h. Other considerations are required for an explicit evaluation. One candidate form is based on the renormaliza-

tion group, particularly the field-theoretical expansion in $\epsilon = 4-d$, where, as above, d is the spatial dimensionality of the system. We consider a standard ϕ^4 Hamiltonian

$$\frac{-H}{T} = \int \left(\frac{1}{2}[(\vec{\nabla}\phi)^2 + r\phi^2] + u\phi^4 - h\phi \right) d^d x. \quad (3.1)$$

At lowest nontrivial order in ϵ, the effective potential has the form [15,16]

$$\mathcal{H}(M,t,h) = e^{-\ell^* d}\left[\frac{1}{2} t e^{(1/\nu)\ell^*} M^2 e^{(d-2+\eta)\ell^*} + \frac{u}{4} M^4 e^{2(d-2+\eta)\ell^*} - hMe^{\ell^* d} \right]. \quad (3.2)$$

This approximate effective potential is at the level of a *renormalized* Ginzburg-Landau free energy, and hence is equivalent to ''renormalized mean-field theory.'' That is to say, the constrained free energy, as approximated by Eq. (3.2), has the same general form as mean-field theory, except for the coefficients of M, M^2, and M^4. The mean-field coefficients, which depend on the temperature and magnetic field in a relatively simple way, are replaced by coefficients with more complicated (and as it turns out, implicit) dependence on the physical fields t and h. These new coefficients give rise to a free energy that exhibits the full scaling properties displayed in Eq. (2.4). The form (3.2) results from a renormalization-group (RG) calculation, carried out to lowest order in a loop expansion. A higher-order calculation produces contributions to the effective potential explicitly at all orders in the quantity M. The renormalization of coefficients, indeed the full effect of the renormalization-group trajectories, resides in the quantity e^{ℓ^*} which plays the role of the ''block spin'' size. This key quantity may be determined via [15]

$$te^{(1/\nu)\ell^*} + 3uM^2 e^{(d-2+\eta)\ell^*} = 1. \quad (3.3)$$

The effective potential described by Eq. (3.2) along with Eq. (3.3) is fully consistent with the scaling hypotheses embodied in Eq. (2.4). It is completely determined once the coupling constant u has been set, along with ''metrical'' factors associated with the scales of h and t.

On a technical level, the quantity ℓ^* indicates where integration of the renormalization-group flow equations is stopped. Physically it is the value of the block spin parameter at which the evaluation of the partition function via differential recursion relations is ''matched'' to perturbation theory with a renormalized effective Hamiltonian [15]. This matching occurs when the correlation length in the effective Hamiltonian is of order unity (i.e., the integration proceeds until the renormalized Hamiltonian is noncritical). As this is an intermediate step in the calculation, the precise value of ℓ^* ought to have no effect on the ultimate determination of the statistical mechanical properties of the system. (This is analogous to choice of renormalization point.) In fact, this independence can be demonstrated order by order in the relevant expansion parameter (e.g., $\epsilon = 4-d$). In practice, one can establish optimal choices for ℓ^*. The combination of Eqs. (3.2) and (3.3) produces an effective potential that is fully consistent with scaling hypotheses and with lowest order (in ϵ) calculations of the equation of state [16].

The inclusion of higher-order, loop expansion contributions leads to modifications of the effective potential, so, on the face of it, there is no reason to expect that Eq. (3.2) will be exact. However, given that it is entirely consistent with critical point scaling, that it embodies the full RG trajectories, and that it represents the leading-order contribution in a systematic renormalization-group expansion for the free energy, it seems at least a plausible ''zeroth-order'' candidate for the critical effective potential. This optimism is bolstered by other situations in which ''renormalized mean-field theory'' provides surprisingly good numerical results when applied in three dimensions [17].

IV. THE PREFACTOR

In this section we discuss the prefactor introduced by Binder and Landau [18] and used by Tsypin in fitting Ising simulations [1,2]. A variety of arguments have been advanced for the existence of this term. Here we introduce additional justification for the prefactor.

Suppose we allow spatial variations of the order parameter around the globally constrained value M in the form $M + \sigma(\vec{k})$. Note that $\langle \sigma(\vec{k}) \rangle = 0$. Neglecting terms of greater than quadratic order in the $\sigma(\vec{k})$'s, the dependence of the effective Hamiltonian on the $\sigma(\vec{k})$'s at Gaussian order will be

$$\frac{H_{\rm Gauss}[\sigma(\vec{k})]}{T} = \sum_{k\neq 0} \left[\frac{1}{2} \left| \vec{\nabla}\sigma(\vec{k}) \right|^2 + \frac{1}{2} \mathcal{H}'' \sigma(\vec{k})\sigma(-\vec{k}) \right]. \quad (4.1)$$

The term $\mathcal{H}''$ is the second derivative with respect to the order parameter M of the effective potential $\mathcal{H}$ at renormalized mean-field level discussed above. As noted, the sum excludes the $\vec{k} = \vec{0}$ mode of the order parameter fluctuations. Integration over the $\sigma(\vec{k})$'s yields the following ''Gaussian'' correction to the effective potential:

$$\sum_{k\neq 0} \frac{1}{2} \ln\left(\frac{\mathcal{H}'' + k^2}{2\pi} \right) \to \frac{\Omega}{(2\pi)^d} \int d^d k \, \frac{1}{2} \ln\left(\frac{\mathcal{H}'' + k^2}{2\pi} \right) - \frac{1}{2} \ln\left(\frac{\mathcal{H}''}{2\pi} \right). \quad (4.2)$$

As above, Ω is the spatial volume of the system. The last term on the right hand side of Eq. (4.2) is the leading-order difference between the sum on the left hand side and its asymptotic limit as the integral on the right. This term can be thought of as a finite size correction to the extensive result in the limit, $\Omega \to \infty$. A general feature of the prefactor that will prove to be of some use shortly is its connection with the renormalized mean-field susceptibility, χ. It is straightforward to verify that the second derivative of the effective potential with respect to the order parameter is inversely related to the susceptibility, i.e.,

$$\mathcal{H}''(M) = \frac{1}{\chi(M)}. \quad (4.3)$$

When the effective potential displays the effects of critical fluctuations, the derivation above acquires modifications, specifically the inclusion of counterterms in a full renormalization-group treatment. Most of the steps leading to this finite size correction are as displayed above. The final result preserves the relationship between the prefactor and the isothermal susceptibility implied by the above equation. Specifically, the new prefactor has the form

$$\sqrt{\frac{\mathcal{H}''}{2\pi}}=\frac{1}{\sqrt{2\pi\chi}}. \tag{4.4}$$

At the level of renormalized mean-field theory, one can write for the susceptibility

$$\chi=e^{(2-\eta)\ell^*}=e^{\gamma\ell^*/\nu}, \tag{4.5}$$

where γ is the critical exponent for the isothermal susceptibility ($\chi\propto|t|^{-\gamma}$). As noted previously, the quantity ℓ^* is determined by Eq. (3.3).

There is a more general argument for the existence of the prefactor. This argument is based on the ''infinitesimal'' momentum shell version of the renormalization group used in the calculation of the partition function of the Ginzburg-Landau-Wilson model [20]. In this approach, modes at the surface of a shrinking Brillouin zone are integrated out. The contributions to the free energy have a Gaussian-like form. The key contribution to the net free energy is

$$\frac{1}{2}\sum_k \ln[\Sigma_k+k^2]. \tag{4.6}$$

In expression (4.6), the self-energy term Σ_k contains the effects of fluctuations whose wave vectors exceed k in magnitude. If the uniform mode is singled out, the sum in Eq. (4.6) is carried out over all nonzero k's. The one term that does not contribute to the free energy is, thus, equal to

$$\frac{1}{2}\ln[\Sigma_0]. \tag{4.7}$$

In this term the restriction on the momenta of the fluctuations contributing to Σ_0 no longer differentiates the quantity from the standard self-energy, Σ. Standard arguments suffice to establish the connection between the the susceptibility and the self-energy. If the $k=0$ term is added to the sum in Eq. (4.6), we end up with a sum over *all* k that constitutes the leading-order bulk contribution to the effective potential. It is then necessary to perform a subtraction leading to a term in the exponent of the form $\frac{1}{2}\ln[\Sigma_0]=\ln\sqrt{\chi_T}$. That the ''subtracted'' term appears in the exponent with a positive sign reflects the fact that the partition function is the exponential of minus the free energy.

V. FINITE SIZE EFFECTS

There are other finite size effects. For example, there is a limit on the maximum possible size of a block spin in the renormalization procedure. This limit appears as a modification of Eq. (3.3). A limit on the block spin size, and hence the quantity ℓ^*, is enforced if Eq. (3.3) is modified so as to ensure that the size of the block spin does not exceed the dimensions of the system. The new requirement on ℓ^* is

$$te^{(1/\nu)\ell^*}+3uM^2e^{(d-2+\eta)\ell^*}+\left(\frac{c}{L}\right)^2e^{2\ell^*}=1. \tag{5.1}$$

The additional term in Eq. (5.1) takes into account the fact that the size of a block spin should not exceed the physical dimensions of the system of interest. This new term leads naturally to the incorporation of finite size scaling effects into the the statistical properties of the system of interest [19]. The quantity c is a number of order unity. In principle, the results of a calculation will not depend on the specific value of c, as the value of ℓ^* is a detail of the renormalization-group procedure, which has no effect on the final result [15]. In practice, the results that follow from the use of Eq. (5.1) depend sensitively on the choice of the parameter c. In the work reported here, this quantity thus acquires the status of a fitting *metrical* parameter connecting the lattice size in the Ising simulations to the length parameter L in the renormalization-group approach.

VI. COMPARISON WITH DATA

The effective potential (3.2) is now compared to the results of the Ising model simulations performed by Tsypin [1–3]. Four data sets from Tsypin's simulations are fit, one in the ordered phase ($\beta_o=0.2227$), one in the disordered ($\beta_d=0.220\,55$), and two at the critical temperature $T=T_c$ ($\beta_c=0.221\,65$). The data in the disordered phase are gathered in a Monte Carlo investigation of the order parameter distribution of a system of 58^3 Ising spins. In the case of the ordered phase, the simulations were performed on a system of 74^3 spins, while lattices of 16^3 and 32^3 were used for the simulations at criticality. The data are fit with the renormalized mean-field approximation Eq. (3.2) including the prefactor. The fitting procedure includes the use of the restriction on ℓ^* obtained by solving the transcendental equation, (5.1). The overall normalization is set such that the area under our curve matches that of Tsypin's histograms.

Our fitting procedure utilizes a grid-search minimization of the $\tilde{\chi}^2(\vec{\alpha})$ merit function.

$$\tilde{\chi}^2(\vec{\alpha})=\frac{1}{D}\sum_i \frac{[y(x_i;\vec{\alpha})-d_i]^2}{\sigma_i^2}. \tag{6.1}$$

The parameters $\{\alpha_j\}$ for the zeroth-order fit are t, u, and c that appear in Eqs. (3.2) and (5.1). Technically, this expression is the *reduced* $\tilde{\chi}^2$ since we divide by the number of degrees of freedom, D. D is the number of data bins less the number of free parameters. The errors σ_i were assumed to be of Gaussian order; i.e., $\sigma_i^2=y(x_i;\vec{\alpha})$.

As an initial effort to minimize $\tilde{\chi}^2$, a *blind fit* is performed across all the histograms of a given data set (e.g., in the disordered phase the seven histograms corresponding to the seven different values of the external field h). See Table I. In this blind fit each bin of each histogram is treated with the same weight. This procedure certainly leads to an unbiased minimization of $\tilde{\chi}^2$, but further fine tuning is required as explained below.

TABLE I. The values of fitted parameters t, u, and c obtained from the blind fits for four different data sets. D is the number of degrees of freedom less free parameters. The stated errors are 68% confidence limits; i.e., one standard deviation. Note that the χ^2 here is not reduced.

	$T=T_c$	$T=T_c$	$T>T_c$	$T<T_c$
L	16	32	58	74
t	0[a]	0	$0.00355^{+0.00055}_{-0.00045}$	$-0.00428^{+0.00048}_{-0.00112}$
u	$0.225^{+0.005}_{-0.007}$	$0.218^{+0.005}_{-0.005}$	$0.230^{+0.004}_{-0.004}$	$0.232^{+0.006}_{-0.003}$
c	$0.439^{+0.04}_{-0.03}$	$0.459^{+0.03}_{-0.03}$	$1.94^{+1.86\,b}_{-1.94}$	$1.83^{+2.17}_{-1.83}$
χ^2	376	141	1570	1230
D	126	126	534	442

[a]The reduced temperature is *fixed* at zero for the $T=T_c$ data sets.

[b]Due to the extremely weak dependence of the free energy on the variable c in the $T\neq T_c$ phases there is a large range of values within the 68% confidence limit.

It is important to note the similarity between the values of u in both temperature regimes. In zeroth-order approximation we find $u_d=0.230$ and $u_o=0.232$ for the disordered and ordered phases, respectively. This is quite significant in that Landau-Ginzburg theory dictates that the fourth-order coupling be the same everywhere. Also note that the value of t that best fits the data from the critical simulations is indeed zero, as expected. We do observe one anomaly in the best-fit values of the reduced temperature in the ordered and disordered phases, however. Namely, if we compare the ratio of the temperatures we obtain

$$\frac{t_d}{-t_o}=0.829$$

while from Tsypin's simulation we have

$$\frac{t_d}{-t_o}=-\frac{\beta_d-\beta_c}{\beta_o-\beta_c}=1.05.$$

This is unfortunate as we expect this ratio to be the same in the simulations and our fit even though the temperatures themselves need not be.

An additional comment needs to be made for the fitting of the ordered phase data. Notice that in the $h=0$ histogram we have removed the data lying to the left of the peak. Attempts to fit the data in that regime did not produce satisfactory results. We attribute this failure to the fact that a single renormalized Ginzburg-Landau form [such as Eq. (3.2)] is inappropriate to the region of two-phase coexistence.

TABLE II. The values of fitted parameters t, u, and c after constraining to fit all temperature regimes simultaneously.

	$T=T_c$	$T>T_c$	$T<T_c$
L	16, 32[a]	58	74
t	0[b]	$0.00399^{+0.0003}_{-0.0006}$	$-0.00383^{+0.0002}_{-0.0004}$
u	$0.228^{+0.004}_{-0.009}$	$0.228^{+0.008}_{-0.005}$	$0.228^{+0.006}_{-0.003}$
c	$0.432^{+0.10}_{-0.05}$	$0.432^{+2.5}_{-0.432}$	$0.432^{+2.5}_{-0.432}$
χ^2	2240	3050	3080
D	254	534	442

[a]We fit both $L=16$ and $L=32$ data sets simultaneously.

[b]The reduced temperature is fixed at zero.

One expects that the scaling form for the free energy (combined with the prefactor) should provide a reasonable approximation to the free energy in *all* temperature regimes using a single value of u and c. To this end, we search for a set of parameters that minimize the χ^2 for all data sets. The most effective strategy for accomplishing this task is to first determine a range of parameters u and c that fit the $t=0$ data. These bounds are then used for a three-parameter fit in the $t>0$ and $t<0$ phases which yields final values of t, u, and c. It should be noted that a significant amount of ''tweaking'' of the parameters is necessary in addition to the blind minimization of the χ^2. These values are tabulated in Table II and the resulting probability densities are plotted against Tsypin's data in the three temperature regimes. The plots are displayed in Figs. 1–3. It is interesting to note that the ratio of temperatures discussed above is now

$$\frac{t_d}{-t_o}=1.04,$$

which is within 1% of Tsypin's value.

To further evaluate our scaling form we also calculate the universal quantity [21,7]

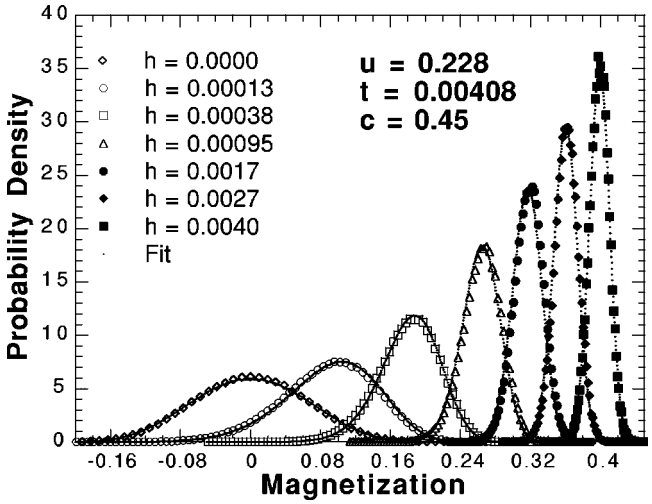

FIG. 1. The order parameter distribution in the disordered phase, as obtained by Tsypin [1] (data points) and the results of the best constrained fit based on the effective Hamiltonian embodied in Eqs. (3.2) and (5.1).

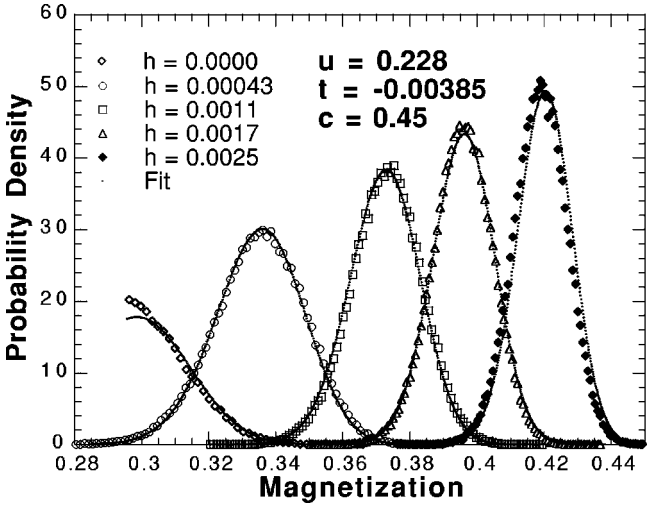

FIG. 2. The order parameter distribution in the ordered phase, as obtained by Tsypin [1] (data points) and the results of the best constrained fit based on the effective Hamiltonian embodied in Eqs. (3.2) and (5.1).

$$\Gamma_4=\frac{\langle M^4\rangle}{(\langle M^2\rangle)^2}-3. \tag{6.2}$$

The values of Γ_4 from our calculations compared to other sources are tabulated in Table III.

As a final check on our results, we compare our best-fit value of the renormalized coupling constant u with results obtained by other methods. A variety of techniques have been utilized to determine this universal quantity, including the ϵ expansion [23], high-order loop expansions in three dimensions [24–26], Monte Carlo simulations, and high-temperature series [27]. Recently reported values of the renormalized fourth-order coupling constant range from 0.233 [25] to 0.236 [24]. This is to be compared with our optimum global fit $u=0.228$; see Table II. Given that no attempt was made to match previously determined values of the renormalized fourth-order coupling in our fitting procedure, the quality of agreement can be described as, at the very least, encouraging.

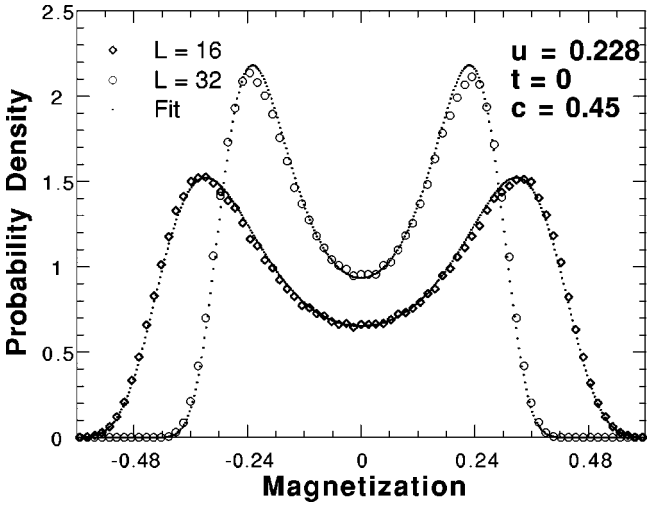

FIG. 3. The order parameter distribution of the system at $t=0$, as obtained by Tsypin [3] and the results of the fit using Eqs. (3.2) and (5.1). We include both the 16^3 and 32^3 systems on the plot.

TABLE III. The value of the universal quantity Γ_4 calculated for $d=3$ Ising systems at $t=0$ from various sources.

Source	L	Γ_4
Independent fit	16	-1.4218
Independent fit	32	-1.4082
Constrained fit[a]	16,32	-1.4267
	Simulations	
Tsypin [3]	16	$-1.424(3)$
Tsypin [3]	32	$-1.410(3)$
Barber *et al.* [22]	16	$-1.4239(6)$
Barber *et al.* [22]	32	$-1.4095(18)$

[a]Here we calculate Γ_4 using the parameters $u=0.228$ and $c=0.432$.

VII. CONCLUDING REMARKS

We arrive at the conclusion that a low-order scaling form provides an excellent fit to the order parameter distribution both quite near the three-dimensional Ising model critical point and exactly at criticality. Our approximant, while at the lowest nontrivial order in the interdimensional ϵ expansion, nonetheless includes full renormalization-group flows for the relevant variables and thus has critical point (hyper) scaling built in. The scaling result is that at criticality $\mathcal{H}\sim|M|^{2d/(d-2+\eta)}$, where $2d/(d-2+\eta)\sim 5.8$ is in close agreement with Tsypin's [2,1] polynomial fit. That this ought to be so follows from straightforward scaling arguments.

The fitting parameters used were the nonuniversal metrical factors for the reduced temperature t, the fourth-order coupling constant u, and the parameter c, which controls the effects of finite size on the determination of the quantity $\mathscr{l}^*$ through the relationship Eq. (5.1). This is certainly fewer than allowed; the ϕ^4 model and the Ising model are presumably in the same universality class, but are not identical. We also took the coupling u to be constant. However, there is no reason to believe that the Ising model at criticality is at its fixed point for coupling constants. Hence, corrections to scaling should certainly be allowed, which in practice would mean the renormalization-group flow for the fourth-order coupling $u(\mathscr{l})$ could be included. We have chosen not to do so in order to minimize the number of free parameters.

The prefactor used by Binder [18] and Tsypin [1,2] is discussed in Sec. IV within the setting of a renormalization-group calculation. While this prefactor has only limited effect on the quality of fits in the high- and low-temperature phases, it plays a crucial role at the critical point. This issue is discussed in more depth in the Appendix, where the influence of the prefactor on the universal ratio Γ_4 is also explored.

The fact that a low-order-in-ϵ expression for the renormalized free energy of the Ising system reproduces simulation data to such a high degree of accuracy has encouraging implications with respect to the derivation of an equation of state applicable to an $O(1)$ system in the immediate vicinity

of a critical point. In addition, there is every reason to be hopeful that low-order corrections to the zero loop expression utilized in this work will allow for an even higher-precision fit to data.

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APPENDIX: EFFECT OF THE PREFACTOR ON Γ_4

The prefactor represents a finite size correction to the free energy. To see that this is so, it suffices to exponentiate the prefactor. The contribution of the prefactor to the free energy is nominally independent of the size of the system, while the leading-order terms scale as the system's volume. Clearly, in the thermodynamic limit, the prefactor is swamped by those terms. Nevertheless, the prefactor cannot be ignored, even as the volume approaches infinity. That this is so is evident when one plots out the order parameter distribution at the critical point. Given Eq. (2.4), neglect of the prefactor leads to an order parameter distribution at the critical point ($t=0$, $h=0$) that has the form

$$P(M)\propto e^{-AL^d|M|^{2d/(d-2+\eta)}}. \tag{A1}$$

Such a distribution does not manifest one important feature of the critical point order parameter distribution, and that is a depression in the neighborhood of $M=0$. The absence of this feature has an effect on the fit to data, and in addition, on the quantity Γ_4, defined in Eq. (6.2). As an indication of the importance of the prefactor on this universal ratio, we first calculate its value in the absence of this contribution. We make use of the general relationship

$$\begin{aligned}\int_0^\infty M^p e^{-AM^{2d/(d-2+\eta)}}dM &= A^{-(p+1)(d-2+\eta)/2d}\frac{d-2+\eta}{2d}\\ &\quad\times\int_0^\infty y^{(p+1)(d-2+\eta)/2d-1}e^{-y}dy\\ &= \frac{d-2+\eta}{2d}A^{-(p+1)/(d-2+\eta)/2d}\Gamma\left(\frac{(p+1)(d-2+\eta)}{2d}\right),\end{aligned} \tag{A2}$$

where the function Γ is the standard gamma function. The universal combination in Eq. (6.2) is, then, equal to

$$\frac{\Gamma(5(d-2+\eta)/2d)\Gamma(d-2+\eta/2d)}{\Gamma(3(d-2+\eta)/2d)}-3. \tag{A3}$$

When $d=3$ and $\eta=0.037$, one finds $\Gamma_4=-0.987\,593$. As a comparison, the unrenormalized Ginzburg-Landau theory predicts $\Gamma_4=-0.811\,56$. By contrast, numerical studies indicate $\Gamma_4\simeq-1.4$ [3,22]. While renormalization of the theory changes Γ_4 in the right direction, the full scaling form is inadequate to the challenge of reproducing the correct value of this quantity.

The defect in the above analysis lies in the fact that finite size effects have been ignored. These effects are crucial at the critical point, where the bulk correlation length is infinite. As it turns out, the most important finite size effect is the prefactor. The influence of the prefactor is dramatically highlighted when one ignores the finite size contribution to Eq. (5.1) for $\mathscr{l}^*$. If the coefficient c is set equal to zero, then one finds immediately

$$e^{\mathscr{l}^*}=(3uM^2)^{-1/(d-2+\eta)}. \tag{A4}$$

This means that the order parameter distribution is of the form

$$P(M)\propto M^{(2-\eta)/(d-2+\eta)}\exp[-\kappa M^{2d/(d-2+\eta)}]. \tag{A5}$$

The quantity κ in the above equation is a combination of the size of the system, L, and the fourth-order coupling constant u. This quantity scales out of the result for Γ_4 in the same way that the constant A divided out in the ratio in Eq. (A3). The result for Γ_4 following from Eq. (A5) is then

$$\Gamma_4=\frac{\Gamma([2-\eta+5(d-2+\eta)]/2d)\Gamma([2-\eta+(d-2+\eta)]/2d)}{\Gamma([2-\eta+3(d-2+\eta)]/2d)}-3. \tag{A6}$$

Inserting appropriate values for d and η into Eq. (A6), we obtain a $\Gamma_4=-1.691\,47$. In utilizing the prefactor as the *sole* finite size correction, we have overshot the proper value of Γ_4. Note, however, that the value obtained is *independent of system size*. Even though the prefactor is a finite size correction to the free energy, in the case of Γ_4 it is fully as important as the ''leading-order'' contributions to the order parameter distribution.

As for the distribution $P(M)$, it is immediately evident that the prefactor leads to a depression in the neighborhood of $M=0$. In fact, the order parameter distribution is forced to go to zero at $M=0$ by the prefactor in Eq. (A5). This is a more pronounced effect than is desired. The suppression of the order parameter distribution is reduced when finite size effects are restored to Eq. (5.1). It is the combination of these latter finite size effects and the finite size correction embodied in the prefactor that yields a proper order parameter distribution at the critical point and a value of Γ_4 that is in agreement with previous determinations of this quantity.

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