Journal of Statistical Physics, Vol. 41, Nos. 3/4, 1985

Finite-Size Scaling and the Renormalization Group

Joseph Rudnick,[1] **Hong Guo,**[2] **and David Jasnow**[2]

Received May 7, 1985

Renormalization group calculations in $d=4$ and $d=4-\varepsilon$ are performed for a system of finite size. A form of mean-field theory is used which yields a rounded transition for a finite system, and this allows a sensible expansion in fluctuations. A combination of Ewald and Poisson sum techniques is used to produce explicit numerical results for the specific heat in $d=4$ which, with the setting of two nonuniversal metrical factors and the fourth-order coupling constant may be compared with simulations. The numerical visibility of logarithmic corrections is investigated. The universal scaling function for the specific heat to relative $O(\varepsilon)$ is also evaluated numerically.

KEY WORDS: Finite size; scaling; critical phenomena; logarithmic corrections.

1. INTRODUCTION

Monte Carlo methods seem destined to play an increasingly prominent role in the study of equilibrium and nonequilibrium problems in statistical physics. This is due in large measure to the greater availability of powerful, high-speed computers and to the ongoing development of special purpose processors. Even with the best computing systems, however, simulations are still restricted essentially to microscopic systems. Studies of phase transitions are thus made problematical; the thermodynamic singularities that are the hallmark of a phase transition occur only in the infinite system limit. The central task in the interpretation of Monte Carlo data, when one is studying phase transitions, is to extrapolate to the thermodynamic limit from results for relatively small systems.

[1] Department of Physics, U.C.L.A., Los Angeles, California 90049.
[2] Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260.

0022-4715/85/1100-0353$04.50/0

The most widely used method of extrapolation to large size is based on phenomenological finite-size scaling.[1] In its traditional and simplest form a thermodynamic function, denoted generically by A, which is a function of reduced temperature $t=(T-T_c)/T_c$ and (linear) system size L, is assumed to take the asymptotic form.

$$A(t, L) \sim t^{\tau} X(t^{\nu} L) \tag{1.1}$$

where τ is the bulk critical exponent associated with the particular function A, and ν is the standard correlation length exponent. Such a form is expected to hold in the domain $L \gg a$, $\xi \sim t^{-\nu} \gg a$, where a is the microscopic length or lattice spacing. In general the function $X(x)$ is expected to have a singularity as $x \to 0$ which causes the function A to behave smoothly as $t \to 0$ for fixed L. On the other hand $X(x \to \infty)$ approaches a constant yielding the proper singular behavior in t for an infinite system.

To extract, say, the critical exponent τ (or more precisely τ/ν) from a Monte Carlo simulation one typically might evaluate $A(t=0, L)$, assuming the bulk critical temperature is known or can be estimated. Then one extrapolates it according to $A(t=0, L) \sim L^{-\tau/\nu}$, which comes from the limiting form $X(x) \sim x^{-\tau/\nu}$ as $x \to 0$. Many successful evaluations of the usual critical exponents[2] along with such less well-studied exponents as that for the surface tension[3] have been accomplished using this approach.

Recently, Brézin[4] has shown that the form (1.1) appears within the field theoretic renormalization group structure. Brézin also performed calculations on the isotropic N-vector model in the spherical model ($N \to \infty$) limit. Other spherical model calculations have also been carried out by Fisher and Barber,[5] Singh and Pathria,[6] and Rudnick.[7]

Special subtleties appear in $d \geqslant 4$ because of the breakdown of hyperscaling, and some aspects of this behavior may be seen within the context of spherical models. In the upper critical dimension $d_c = 4$ one expects logarithmic corrections to mean-field-like critical singularities. Such corrections have remained experimentally elusive (for example, in tricritical behavior in $d_c = 3$), and it is reasonable to ask whether simulations, with proper guidance as to the detailed size dependences to be expected, can be used to extract logarithms. At present no explicit calculations of scaling functions for Ising-like systems (or more generally for finite N) have been caried out.

We thus feel it instructive to carry out an explicit finite-system calculation in $d=4$ to see what subtleties simulators may have to deal with to achieve a proper extrapolation. A proper renormalization group calculation in $d=4$ is presumably asymptotically exact in the case of the Ising model and, in principle, may be compared to a standard Ising simulation with the adjustment of two nonuniversal amplitudes and the fourth-order coupling constant. As will be seen graphically below, without knowledge of the true infinite system (second-order transition) behavior, one might easily conclude from simulations that the ordering transition is first-order or, perhaps, that there is no transition at all. Using the results of this calculation one can also attempt to determine whether logarithmic behavior is visible in the finite-size region.

A fundamental objection to the application of field theoretical techniques—and the epsilon expansion in particular—to the study of finite systems has been raised by Brézin.[4] He has noted that strict mean field theory, the asymptotically correct description of the $d=4$ critical point and the theory about which one expands in $4-\varepsilon$ dimensions, predicts a sharp phase transition in *all dimensions* for *infinite* as well as *finite* systems. Such a prediction for a finite system is clearly pathological since all singularities are rounded. We have managed to overcome this objection by using a variant of mean field theory[7] that rounds properly when the system is finite. We find that hyperscaling breaks down when $d \geqslant 4$ as it does in the thermodynamic limit, but there are otherwise no difficulties in principle or practice in our approach.

The outline of this paper is as follows. In Section 2 we present a version of man-field theory for a finite system, while in Section 3 we evaluate a one-loop graph for such a system. A combination of Ewald and Poisson sum methods is required for good convergence. In Section 4 the proper renormalization group calculation is performed, while in Section 5 numerical evaluations and plots are presented. Calculations for $d=4-\varepsilon$ are presented in Section 6 and concluding remarks and summary appear in Section 7. Some further details are included in an Appendix.

2. MEAN-FIELD THEORY FOR A FINITE SYSTEM

We begin, as usual, with a Landau–Ginzburg–Wilson description of the system in which case the Hamiltonian divided by $k_B T$ is taken to be

$$H=\int_{\Omega} d^d x \left[\frac{1}{2}(\nabla s)^2+\frac{1}{2} r s^2+\frac{1}{4!} u s^4-h s\right] \tag{2.1}$$

where the spatial integration is over a system of linear extent L in each of its d dimensions. Other shapes may also be considered and generalization to an N-component order parameter is straightforward. As usual, the parameter $r \propto T-T_0$, where T_0 is a reference temperature. The statistical mechanics of the system follow from the partition function

$$Z=\int Ds\, e^{-H} \tag{2.2}$$

The system is confined to a finite box with periodic boundary conditions. One writes $s = m + \sigma$, where it is understood that $m = \text{const}$, and σ contains no $k = 0$ part. Then

$$H = L^d \left(\frac{1}{2} rm^2 + \frac{1}{4!} um^4 - hm \right) + \int_\Omega d^dx \left[\frac{1}{2} (\nabla\sigma)^2 + \frac{1}{2} \left(r + \frac{um^2}{2} \right) \sigma^2 + \frac{um\sigma^3}{6} + \frac{1}{4!} u\sigma^4 \right] \tag{2.3}$$

The additional term involving $\int d^dx\sigma$ vanishes since σ has no $k = 0$ part. Hence the partition function (2.2) may be written

$$Z = \int dm\, e^{-H_{mf}(m)}\, e^{-\Gamma_1(m)} \tag{2.4}$$

where

$$\exp \Gamma_1(m) \equiv \int d\sigma\, e^{-H(\sigma;m)} \tag{2.5}$$

with $H(\sigma; m)$ the σ-dependent part of (2.3), and $H_{mf}(m)$ is the (mean-field) first term of that equation. $\Gamma_1(m)$ will be evaluated as usual via a diagram expansion; since there is no $k = 0$ term, the expansion will take the form

$$\Gamma_1(m) = \frac{1}{2} \sum_{\mathbf{k} \neq 0} \ln(k^2 + r + um^2/2) + \cdots \tag{2.6}$$

where the dots represent terms higher order in u. We shall return to this term below. The terms in $\Gamma_1(m)$ are at least $O(u^0)$, whereas the mean field part gives terms of order u^{-1}.

Neglecting fluctuctions completely one has the mean-field contribution to the free energy (in zero field)

$$\ln Z_{mf} = \ln \left\{ \int dm \exp[-L^d(rm^2/2 + um^4/4!)] \right\} \tag{2.7}$$

from which the entropy and spcific heat follow by differentiation with respect to r. Notice that even at $r = 0$ moments of m, i.e., $\langle m^{2j} \rangle$, are perfectly finite for finite L so long as $u > 0$ (which we, of course, assume). Within mean field theory the moments have the scaling form

$$\begin{aligned} \langle m^{2j} \rangle &\equiv Z_{mf}^{-1} \int dm\, m^{2j} \exp[-H_{mf}(m)] \\ &= (uL^d)^{-j/2} D_j(rL^{d/2}/u^{1/2}) \end{aligned} \tag{2.8}$$

The heat capacity then has the form

$$C = L^{-4} \frac{\partial^2 \ln Z_{mf}}{\partial r^2} = \frac{1}{4} [\langle m^4 \rangle - \langle m^2 \rangle^2] \tag{2.9}$$

The functions D_j are perfectly well behaved through zero argument; from (2.7) it is seen (from steepest descent arguments) that a singularity can develop in the limit of infinite L. In Fig. 1 we display the specific heat C/L^d as a function of "temperature" r for various values of L. Notice the sharpening up and the appearence of a discontinuous jump as $L \to \infty$. It is true, however, that such a discontinuity will appear for all $d > 0$, which is a well-known defect of mean-field theories. In our calculation in $d = 4$ moments of the form (2.8) will play a central role.

We turn now to evaluation of a basic fluctuation integral in $d = 4$.

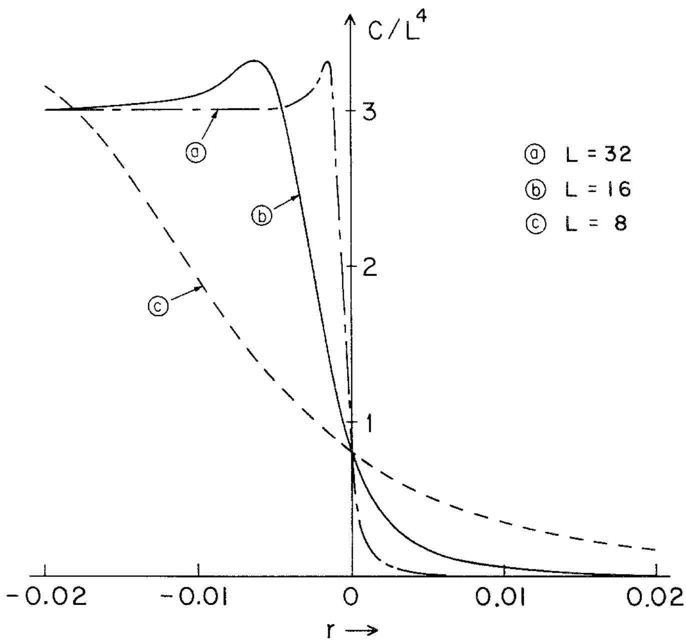

Fig. 1. Specific heat as a function of reduced temperature from mean-field calculation for various system sizes, L. The coupling constant u has been set to unity.

3. ONE-LOOP TERM

An essential ingredient of the finite-size calculation is the evaluation of the term

$$I(r)=\sum_{\mathbf{k}\neq 0}\frac{1}{r+k^2} \tag{3.1}$$

from which one may obtain the lowest-order fluctuation term in the free energy by integration, namely,

$$\sum_{\mathbf{k}\neq 0}\ln\frac{k^2+T}{k^2}=\int_0^T dr\, I(r) \tag{3.2}$$

In (3.1) and (3.2) the wave vectors are appropriate to periodic boundary conditions,

$$\mathbf{k}(\mathbf{n})=\frac{2\pi}{L}\mathbf{n},\qquad n_i=0,\ \pm 1,\ \pm 2,... \tag{3.3}$$

for $i=1, 2,..., d=4$. Then $I(r)$ may be written

$$I(r)=\sum_{\mathbf{k}\neq 0}\left[\int_0^B d\alpha\, e^{-\alpha(r+k^2)}+\int_B^\infty d\alpha\, e^{-\alpha(r+k^2)}\right] \tag{3.4}$$

where we shall let $B=c(L/2\pi)^2$ and choose the arbitrary constant c for good convergence. (The choice $c=\pi$ will finally be made.) In the first term of (3.4) Poisson summation techniques are used below. But for the second term we have

$$\begin{aligned} I_2&=\frac{cL^2}{(2\pi)^2}\sum_{\mathbf{n}\neq 0}\int_1^\infty dx\, e^{-rc(L/2\pi)^2x}\, e^{-cn^2x}\\ &=\frac{cL^2}{(2\pi)^2}\int_1^\infty dx\, e^{-rc(L/2\pi)^2x}[X^4(cx)-1] \end{aligned} \tag{3.5}$$

where

$$X(y)\equiv\sum_{n=-\infty}^{\infty} e^{-yn^2} \tag{3.6}$$

Now consider the first term I_1 of (3.4) and use the Poisson formula[8]

$$\sum_{\mathbf{n}} f[\mathbf{k}(\mathbf{n})]=(L/2\pi)^4\sum_{\mathbf{m}=-\infty}^{\infty}\int d^4k\, f(\mathbf{k})\, e^{i\mathbf{m}\cdot\mathbf{k}L} \tag{3.7}$$

to find

$$I_1 = -\frac{1}{r}\left[1 - e^{-rc(L/2\pi)^2}\right] + \frac{\pi^2}{c}\left(\frac{L}{2\pi}\right)^2 \int_1^\infty dx\, e^{-rc(L/2\pi)^2 x^{-1}} \left[X^4\left(\frac{\pi^2 x}{c}\right) - 1\right] + \left(\frac{L}{2\pi}\right)^4 \int d^4k \frac{1 - e^{-c(L/2\pi)^2(r+k^2)}}{r+k^2} \tag{3.8}$$

Combining I_1 and I_2 one has

$$\begin{aligned}\sum_{\mathbf{k}\neq 0} \frac{1}{r+k^2} = {} & \left(\frac{L}{2\pi}\right)^4 \int \frac{d^4k}{r+k^2} + c\left(\frac{L}{2\pi}\right)^2 \int_1^\infty dx\, e^{-rc(L/2\pi)^2 x}\left[X^4(cx) - 1\right] \\ & + \frac{\pi^2}{c}\left(\frac{L}{2\pi}\right)^2 \int_1^\infty dx\, e^{-rc(L/2\pi)^2 x^{-1}} \left[X^4\left(\frac{\pi^2 x}{c}\right) - 1\right] \\ & + \pi^2 \left(\frac{L}{2\pi}\right)^4 r\, e^{-rc(L/2\pi)^2} \int_0^\infty \frac{e^{-x}\, dx}{x + rc(L/2\pi)^2} \\ & - \frac{\pi^2}{c}\left(\frac{L}{2\pi}\right)^2 e^{-rc(L/2\pi)^2} + \frac{1}{r}\left(e^{-rc(L/2\pi)^2} - 1\right)\end{aligned} \tag{3.9}$$

The first term is immediately recognizable as the bulk contribution. All the other terms are finite-size corrections in which $r \to 0$ may be taken. Clearly from the structure of (3.9) only usual bulk counterterms are required to remove the high momentum cutoff to infinity. This feature has previously been noted by Brézin.[4] Note also that formally the finite-size terms come in at $O(u^0)$.

Straightforward manipulations are required for effecting the r integration as in (3.2). The results may be expressed in terms of the exponential integral[9]

$$E_1(z) = \int_z^\infty dx \frac{e^{-x}}{x} \tag{3.10}$$

The most direct expression is valid for the case

$$T \equiv r + \frac{1}{2} u m^2 > 0 \tag{3.11}$$

although from (2.4) one would apparently need negative values. For r somewhat negative, but $r + (2\pi/L)^2 > 0$, an alternate representation can be constructed. It turns out to be sufficient to consider the case $T > 0$ (see below), in which case (choosing $c = \pi$)

$$\frac{1}{2L^4}\sum_{\mathbf{k}\neq 0}\ln\frac{k^2+T}{k^2}=\frac{1}{2}\int\frac{d^4k}{(2\pi)^4}\ln\frac{k^2+T}{k^2}$$
$$+\frac{1}{2L^4}\int_1^\infty\frac{1}{x}(1-e^{-\omega x})[X^4(\pi x)-1]\,dx+\frac{1}{64\pi^2}T^2E_1(\omega)$$
$$+\frac{1}{2L^4}\int_1^\infty x(1-e^{-\omega x^{-1}})[X^4(\pi x)-1]\,dx-\frac{1}{4L^4}(1-e^{-\omega})$$
$$-\left(\frac{\omega}{4L^4}\right)e^{-\omega}-\frac{1}{2L^4}(E_1(\omega)-\ln(\omega)+\gamma) \tag{3.12}$$

where $\gamma = 0.57721$ is Euler's constant and, for convenience, $\omega = L^2T/4\pi$. Notice the function X, defined in (3.6), has an argument at least equal to π in (3.12) and is rapidly convergent. Likewise E_1 has an accurate polynomial approximant; hence the representation (3.12) is free of numerical or convergence difficulties. It forms the core of the full renormalization group calculation to which we now turn.

4. RENORMALIZATION GROUP APPROACH

Standard bulk counterterms are sufficient to renormalize the theory.[10] They are introduced into (2.1) in which case the full (renormalized) exponential, $L^{-4}(H_{\text{mf}} + \Gamma_1)$, becomes

$$\Gamma_R(t, m, u, \kappa, L) = \Gamma_{\text{bare}}(r, m, u, \Lambda, L) - \Gamma_{\text{bare}}\big|_{\substack{t=0\\m=0}}$$
$$-\,t\left.\frac{\partial\Gamma_{\text{bare}}}{\partial t}\right|_{\substack{t=0\\m=0}}-\frac{1}{2}t^2\left.\frac{\partial^2\Gamma_{\text{bare}}}{\partial t^2}\right|_{\substack{t=\kappa^2\\m=0}} \tag{4.1}$$

where, as usual, the following replacements are made in the unrenormalized or bare quantities r, m, u on the right-hand side:

$$\begin{aligned} r &\to Z_{\phi^2}t+\delta t\\ u &\to \kappa^{\varepsilon}Z_u u\\ m &\to Z_\phi^{1/2}m \end{aligned} \tag{4.2}$$

and from now on t, u, m, etc. all refer to renormalized quantities. As usual, $\varepsilon = 4 - d$. The three additive renormalizations are the same as for the bulk system, and Γ_{bare} is calculated diagrammatically from (2.1), the leading contributions being the mean field part $H_{mf}(m)$ and the loop in (2.6). All momentum integrals may be regularized with a hard cutoff Λ which is eventually removed to infinity, and κ in (4.1) introduces the basic (inverse) length scale into the renormalized theory. Then acting with $\kappa d/d\kappa$ on (4.1) and introducing $S_d = [2^{d-1}\pi^{d/2}\Gamma(d/2)]^{-1}$ as the surface of a unit sphere in d dimensions, one finds the inhomogeneous RG equation,

$$\left\{\kappa\frac{\partial}{\partial\kappa} + W(u)\frac{\partial}{\partial u} - \frac{1}{2}\eta(u)m\frac{\partial}{\partial m} + [-2+\gamma_{\phi^2}(u)]t\frac{\partial}{\partial t}\right\}\Gamma_R$$
$$= -\frac{S_d}{8\nu}\left(1-\frac{\varepsilon}{2}+\frac{5}{4}S_d u\right)t^2\kappa^{-(4-d)} \tag{4.3}$$

which is solved in the usual fashion.[3] Note that the inhomogeneous term is appropriate to two loops, which is necessary in getting all $O(\varepsilon^0)$ contributions to the free energy. One finds in $d=4$

$$\Gamma_R = \Gamma_R(\rho^2 t(\rho), m(\rho), u(\rho), \kappa\rho, L)$$
$$+ \frac{S_d}{8\nu}\int_\rho^1 \frac{dx}{x}\left[1-\frac{\varepsilon}{2}+\frac{5}{4}S_d u(x)\right]t^2(x)(\kappa x)^{-(4-d)} \tag{4.4}$$

where the last term is the trajectory term and formally is $O(u^{-1})$. The flow equations are, as usual,[10]

$$\rho\frac{dt(\rho)}{d\rho} = [-2+\gamma_{\phi^2}(u(\rho))]\,t(\rho)$$
$$\rho\frac{du(\rho)}{d\rho} = W(u(\rho)) \tag{4.5}$$
$$\rho\frac{dm(\rho)}{d\rho} = -\frac{1}{2}\eta(u(\rho))\,m(\rho)$$

with, in $d=4$,

$$W(u) = \tfrac{3}{2}S_d u^2, \qquad \gamma_{\phi^2}(u) = \tfrac{1}{2}S_d u, \qquad \eta(u) = \tfrac{1}{24}S_d u^2$$

Generalization to an N-component system is straightforward. Solutions of the flow equations yield

$$u(\rho) = \frac{u}{1-(3/2)S_d u \ln\rho}$$
$$t(\rho) = \frac{t}{[1-(3|2)\,S_d u\ln\rho]^{1/3}} \tag{4.6}$$
$$m(\rho) = m\exp\{1/72[u-u(\rho)]\}$$

[3] For future reference, the form of general d has been written.

which may be substituted into (4.4) to give a complete representation of the finite-size free energy. The partition function (2.4) becomes

$$Z = \int_{-\infty}^{\infty} dm\, e^{-L^4 \Gamma_R} \tag{4.7}$$

For evaluation of the free energy a choice of $\rho = \rho^*$ will be required. This will be discussed below.

At lowest order, often refered to as renormalized man field theory (Rmf), and which yields the free energy correctly to leading logarithms, one neglects loop contributions to Γ_R but retains the trajectory term in (4.4). Hence at this order, which formally keeps terms $O(u^{-1})$,

$$\Gamma_{\mathrm{Rmf}}(t, m, u; \kappa, L) = \frac{1}{2}\rho^{*2} t(\rho^*)\, m^2(\rho^*) + \frac{1}{4!} u(\rho^*)\, m^4(\rho^*) + \frac{t^2}{16\pi^2 u}\left[1 - \left(1 - \frac{3}{2} S_d u \ln \rho^*\right)^{1/3}\right] \tag{4.8}$$

The specific heat follows from (4.8) according to

$$\frac{C}{L^4} \equiv L^{-4} \frac{\partial^2}{\partial t^2} \ln Z_{\mathrm{Rmf}} = L^4 \left\langle \left(\frac{\partial \Gamma_{\mathrm{Rmf}}}{\partial t}\right)^2 \right\rangle - L^4 \left\langle \frac{\partial \Gamma_{\mathrm{Rmf}}}{\partial t} \right\rangle^2 - \left\langle \frac{\partial^2 \Gamma_{\mathrm{Rmf}}}{\partial t^2} \right\rangle \tag{4.9}$$

where averages are evaluated according to the probability distribution in (2.7) with

$$r \to \rho^{*2} t(\rho^*), \qquad u \to u(\rho^*) \tag{4.10}$$

(Henceforth all averages are considered to be taken by such procedure.) Note that in (4.9) only *explicit* temperature derivatives are taken; the implicit t dependence of ρ^* is ignored. The results are formally independent of ρ^* and taking derivatives of ρ^* formally yields higher-order contributions.[11] Note also that all averages entering (4.9), namely, $\langle m^4(\rho^*)\rangle$ and $\langle m^2(\rho^*)\rangle$ depend on the combination $wv^{-1/2}$ where $w = L^2 \rho^{*2} t(\rho^*)$ and $v = u(\rho^*)$. These same variables enter the loop corrections. A more explicit evaluation of (4.9) is provided in the Appendix.

The choice of ρ^* must be made for detailed evaluations. The choice we have made is to determine ρ^* from

$$\rho^{*2} t(\rho^*) + \frac{1}{2} u(\rho^*) \langle m^2(\rho^*)\rangle + \frac{1}{L^2} = (\kappa\rho^*)^2$$

where, as noted, $\langle m^2(\rho^*)\rangle$ is determined as follows from (2.7) with $r \to \rho^{*2} t(\rho^*)$ and $u \to u(\rho^*)$. The choice has the following interpretation. The quantity $\rho^{*2} t(\rho^*) + 1/2u(\rho^*)\, m^2(\rho^*)$ has the interpretation of the "mass" appearing in the renormalized Hamiltonian. If the temperature $t \sim T - T_c$ is such that the bulk correlation length ξ is *large* compared to the system size L, renormalization must end when the effective block spin size $[\sim (\kappa\rho^*)^{-1}]$ is on the order of L. This is the strongly finite-size regime and $\rho^* \approx (\kappa L)^{-1}$. On the other hand if L is *much larger* than the bulk correlation length, renormalization transformations are continued until the block spin size is on the order of ξ. This corresponds to $\rho^{*2} t(\rho^*) + 1/2u(\rho^*)\, m^2(\rho^*) = (\rho^* \kappa)^2$, the usual bulk-system determination of ρ^*. Equation (4.13) interpolates between these regimes. To find $\rho^*(t, L)$ we must numerically solve (4.11). This must be done iteratively since ρ^* is required for $\langle m^2(\rho^*)\rangle$. The starting choice $\langle m^2(\rho^*)\rangle = -6\rho^{*2} t(\rho^*)/u(\rho^*)$ allows convergence after a small number of iterations. Numerical results will be displayed in the next section.

Loop corrections may now be handled, in fact, iteratively. Formally one must insert the renormalized Γ_1 which is given in the Appendix into (4.7). However, order-by-order one may make the following expansion:

$$Z = \int_{-\infty}^{\infty} dm \exp[-L^4(\Gamma_{\mathrm{Rmf}} + \Gamma_{R,1})]$$

$$= \int_{-\infty}^{\infty} dm \exp\{-L^4[\Gamma_{\mathrm{Rmf}}(m^2(\rho)) + \Gamma_{R,1}(\langle m^2(\rho)\rangle) + \Delta]\} \quad (4.12)$$

where

$$\Delta \equiv \Gamma_{R,1}(m^2(\rho)) - \Gamma_{R,1}(\langle m^2(\rho)\rangle)$$

and averages are computed with respect to the (renormalized) mean field theory. It is to be understood that $\rho = \rho^*$ has been chosen in what follows. Then

$$Z = \exp\{-L^4 \Gamma_{R,1}(\langle m^2(\rho)\rangle)\} \cdot Z_{\mathrm{Rmf}} \cdot \langle \exp\{-L^4\Delta\}\rangle$$

which is expanded in terms of cumulants, so that

$$\ln Z = \ln Z_{\mathrm{Rmf}} - L^4 \Gamma_{R,1}[\langle m^2 \rho)\rangle] + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \langle (L^4\Delta)^n\rangle_c \quad (4.13)$$

where $\langle \cdots \rangle_c$ are cumulant averages. Recall that we are searching for terms of order u^0 in the specific heat [leading terms being $O(u^{-1})$]. Temperature differentiation promotes terms so some care must be taken. It is easy to verify using scaling relations like (2.8) that

$$\langle L^4 \Delta \rangle_c = L^4 \sum_{p=1}^{\infty} a_p \langle (m^2(\rho) - \langle m^2(\rho) \rangle)^p \rangle$$
$$\simeq L^4 a_2 (\langle m^4(\rho) \rangle - \langle m^2(\rho) \rangle^2) \tag{4.14}$$

where of course the coefficients a_p arise from the expansion of $\Gamma_{R,1}(m^2(\rho))$ about $\Gamma_{R,1}(\langle m^2(\rho) \rangle)$. The same reasoning allows the replacement

$$\langle (L^4 \Delta)^2 \rangle_c \simeq (L^4 a_1)^2 [\langle m^4(\rho) \rangle - \langle m^2(\rho) \rangle^2] \tag{4.15}$$

all other cumulants yield contributions beyond the (one-loop) order of the calculation.

Substitution of (4.14) and (4.15) into (4.13) yields the free energy consistently so that the specific heat is correctly given to $O(u^0)$. The only two expansion coefficients which enter are

$$a_1 \equiv \left. \frac{\partial \Gamma_{R,1}}{\partial m^2(\rho)} \right|_{m^2(\rho) = \langle m^2(\rho) \rangle}$$
$$a_2 \equiv \left. \frac{1}{2} \frac{\partial^2 \Gamma_{R,1}}{\partial (m^2(\rho))^2} \right|_{m^2(\rho) = \langle m^2(\rho) \rangle} \tag{4.16}$$

and $\Gamma_{R,1}(m^2(\rho))$ may be found in the Appendix. The specific heat follows from $d^2 \ln Z/dt^2$ keeping ultimately terms $O(u^0)$.

The form of the scaling can be explicitly discussed at this point. At renormalized mean field level one finds directly that

$$\ln Z(t, u; \kappa, L) = \bar{F}[w, v] \qquad [w = L^2 \rho^2 t(\rho), v = u(\rho)] \tag{4.17}$$

where $\bar{F}$ is a dimensionless function. (A smooth background term of the form $L^4 t^2/u$ and additional background constants which can be removed by normalization have been omitted.) There is further simplification here since $\bar{F}(w, v)$ takes the form

$$\bar{F}_{\text{Rmf}}(w, v) = f(z = wv^{-1/2})$$
$$= z^2 + \ln \int_{-\infty}^{\infty} dy \exp \left\{ - \left(\frac{1}{2} zy^2 + \frac{1}{4!} y^4 \right) \right\} \tag{4.18}$$

This form contains the *leading* logarithms in $d = 4$.

More generally

$$\ln Z(t, u; \kappa, L) = F \left[\frac{t(\rho)}{\kappa^2}, u(\rho), \rho \kappa L \right] \tag{4.19}$$

which form reproduces (4.17). This is a general statement of finite size scaling; the loop correction discussed above takes this form. Such scaling forms have been discussed by Brézin.[4] In usual cases in which $u(\rho) \to u^* \neq 0$ as $\rho \to 0$ one may show that a relationship like (4.19) produces the intuitive sort of finite-size scaling discussed in the Introduction.

Because of the marginality of u in $d=4$, $u(\rho)$ iterates slowly to zero as $\rho \to 0$ as indicated in (4.6). This will yield additional L dependence and explicit dependence on the coupling constant u.

5. NUMERICAL RESULTS

It is instructive to plot numerical results for the specific heat which is given in the Appendix (A2). First, however, we return to the pure mean-field theory discussed in Section 2. The results have been shown in Fig. 1. Note in particular that for larger sizes the specific heat maximum does not change significantly; the curve merely sharpens up.

The situation with respect to renormalized mean field theory is shown in Fig. 2. Recall that the central ingredient is given in (4.8). A more explicit

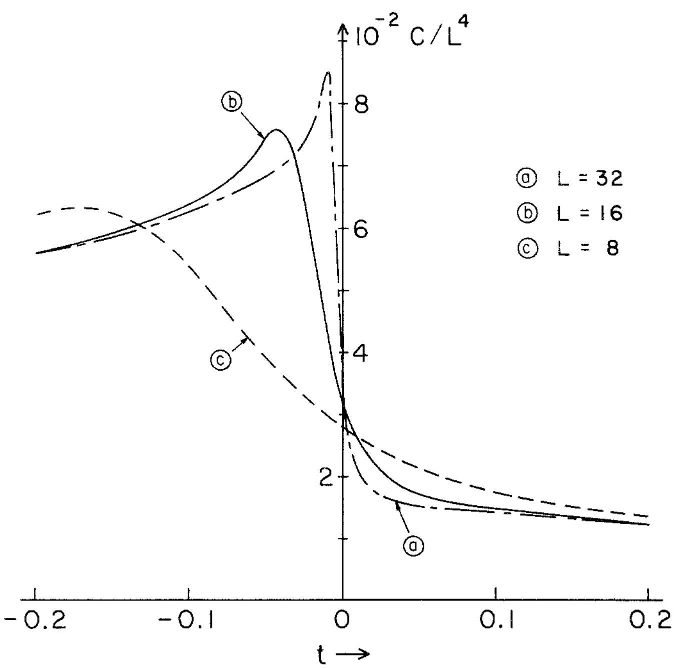

Fig. 2. Specific heat from renormalized mean-field theory at $d=4$ for various system sizes L. The characteristic inverse length κ and uS_4 have been set to unity.

form is shown in (A.2) where renormalized mean field theory contains all terms without $\Gamma_{R,1}$. It is easy to show that $C(t=0)$ diverges as $(\ln \kappa L)^{1/3}$ as $L \to \infty$ although such slow dependence is barely visible in the plots. One may also demonstrate that the specific heat peak diverges with the same L dependence. By direct computation for the infinite system, the per unit volume specific heat diverges as $C \sim |\ln |t|/\kappa^2|^{1/3}$, so that the mechanism for the divergence is that the values at the peak and at $t=0$ diverge together.

It is interesting to consider numerically $C(t_{\max})/L^4$, i.e., the peak height, vs. system size, since this is what a simulator might do to look for logarithmic corrections. At present simulations involving 10^6 Ising spins are possible, and a signature of the logarithm may be possible to detect if sufficient precision in a narrow temperature range can be maintained. However even with less precision it might to be possible to detect the increase in peak height itself as a sign of logarithmic corrections. The ability to make definitive statements is restricted because the strength of the logarithmic corrections depends crucially on the strength of the coupling constant u. If u were reduced, the peak structure would remain

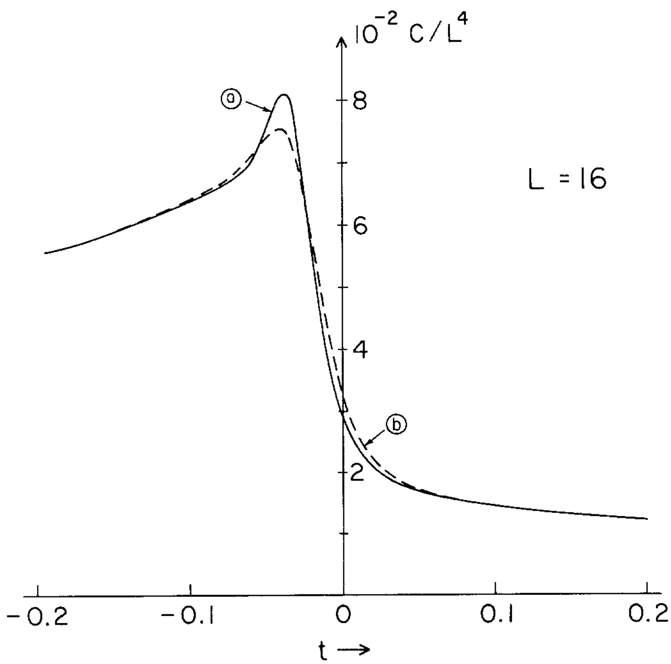

Fig. 3. Specific heat at $d=4$, $L=16$, showing (b) the renormalized mean-field theory and (a) the result including the loop correction. The characteristic inverse length κ and the coupling constant uS_4 have been set to unity.

approximately the same, but the overall magnitude of the specific heat would increase. This would make such logarithmic effects more difficult to observe in an hypothetical simulation of a system characterized by a small fourth-order coupling. Additional numerical and analytic results suggest that the position of the maximum $t_{\max}$ goes to zero with size rather rapidly, i.e., $|t_{\max}| \sim [L^2 \ln^{1/6}(\kappa L)]^{-1}$.

In Fig. 3, the effect of the loop correction to renormalized mean field theory is shown. As might be expected, the specific heat peak is enhanced and sharpened.

6. RESULTS IN $4-\epsilon$ DIMENSIONS

The analysis presented above may be carried over directly to $d=4-\varepsilon$ dimensions. In the preceding sections we have concentrated on $d=4$ because an asymptotically correct finite size calculation is possible. Here one may calculate order-by-order in ε in analogy with ordinary bulk phenomena. Note, however, that since the finite-size corrections are $O(1)$, a consistent calculation must include bulk contributions to the trajectory integral to two-loop order. This gives $O(1)$ bulk contributions correctly.

One must solve the renormalization group flow equations (4.5) in which case now one finds

$$\begin{aligned} u(\rho) &= \frac{u\rho^{-\varepsilon}}{Q(\rho)}, \qquad Q(\rho) = 1 + \frac{3}{2}\frac{u}{\varepsilon}(\rho^{-\varepsilon} - 1) \\ t(\rho) &= tQ(\rho)^{-1/3} \\ m(\rho) &= m \exp\{1/72[u - u(\rho)]\} \end{aligned} \tag{6.1}$$

consistent to one-loop order. The expressions for $u(\rho)$, $t(\rho)$, and $m(\rho)$ reduce to those of (4.6) when $\varepsilon \to 0$. Hence the renormalized mean-field contribution (including the trajectory integral) is

$$\begin{aligned} \Gamma_{\mathrm{Rmf}} = {} & \frac{1}{2}\rho^{*2} t(\rho^*)\, m^2(\rho^*) + \frac{1}{4!}(\kappa\rho)^{\varepsilon}\, u(\rho^*)\, m^4(\rho^*) \\ & - \frac{t^2\kappa^{-\varepsilon}}{32\pi^2}\int_{\rho^*}^{1} \frac{dx}{x^{1+\varepsilon}}[Q(x)]^{-2/3} \end{aligned} \tag{6.2}$$

which goes over to the four-dimensional result (4.8) as $\varepsilon \to 0$. Since the loop integral may actually be calculated in $d=4$ consistent to one loop order, the one-loop part $\Gamma_{R,1}$ properly goes to the previous result as $\varepsilon \to 0$.

On the other hand for $\varepsilon > 0$ one may set $u = u^*$ and observe that $m(\rho) \approx m$ to this order. Then

$$L^d \Gamma_R(t, m, u, \kappa, L) = L^d \Gamma_{\text{Rmf}} + L^d [\Gamma_{R,1}]_{d=4-\varepsilon} \tag{6.3}$$

where the product $L^d[\Gamma_{R,1}]_{d=4-\varepsilon}$ is identical to $L^4[\Gamma_{R,1}]_{d=4}$, where $[\Gamma_{R,1}]_{d=4}$ is given in (A1), except that the *bulk* term

$$\frac{1}{64\pi^2} L^4 T^2(\rho) \left[\ln \frac{L^2 T(\rho)}{(\kappa \rho L)^2} + \frac{1}{2} \right] - \frac{1}{4} S_d \rho^4 L^4 t^2(\rho)$$

is divided by $(\kappa \rho L)^\varepsilon$. With these modifications it is clear that the free energy takes the form (within additive constant)

$$\ln Z = \ln \int dm \exp\{ -L^d \Gamma_R \} = L^d [\text{T.I.}] + \ln \int dx\, e^{-A} \tag{6.4}$$

where A depends only on the combination $L^2 \rho^{*2} t(\rho^*) + \frac{1}{2} u^* x^2$, and T.I. is the trajectory term of (6.2). The final free energy depends only on the combination $L^2 \rho^{*2} t(\rho^*)$. To see the scaling form one sets $\kappa \rho^* L = 1$ so that $L^2 \rho^{*2} t(\rho^*) = (\rho^*)^{2-1/\nu} L^2 t = (t/\kappa^2)(\kappa L)^{1/\nu}$. Hence the full free energy $F = \ln Z$ is a function of this variable and

$$\begin{aligned} L^{-d} \ln Z &= L^{-d} F[(t/\kappa^2)(\kappa L)^{1/\nu}] \\ &= \kappa^d (t/\kappa^2)^{d\nu} \tilde{F}[(t/\kappa^2)(\kappa L)^{1/\nu}] \end{aligned}$$

Differentiation twice with respect to temperature yields the heat capacity. Further details are provided in the Appendix.

For the above discussion it is clear that a scaling form

$$\frac{\kappa^\varepsilon C}{L^d} = (\kappa^{-2} t)^{-\alpha} X[\kappa^{-2} t (\kappa L)^{1/\nu}] \tag{6.5}$$

holds for the specific heat. As such the function $X(y)$ is not itself universal; the limiting form $X(y \to 0)$ essentially yields the nonuniversal specific heat amplitude for the bulk system ($T > T_c$). Given an arbitrary overall amplitude the function $X(y)$ is then universal, and one may compare two differential systems in the same universality class. [Alternatively $\tilde{X}(y) = X(y)/X(\infty)$ is expected to be universal.] In Fig. 4 the approximate ($d = 3$) form for $X(y)$ is given by setting $\varepsilon = 1$ in the numerical evaluation of Eq. (A4).[4] The scaling function is evaluated by fixing κL and evaluating the

[4] The limiting values of function $X(y)$, as $y \to \pm\infty$, give the specific heat amplitudes of the bulk system. The amplitude ratio of the bulk system is

$$\frac{A^+}{A^-} = \frac{2^\alpha}{4} \frac{1 + (7/12)\varepsilon}{1 - (5/12)\varepsilon} = \frac{2^\alpha}{4} (1 + \varepsilon) + O(\varepsilon^2)$$

and our function $X(y)$ gives the value consistent with the first equality evaluated at $\varepsilon = 1$.

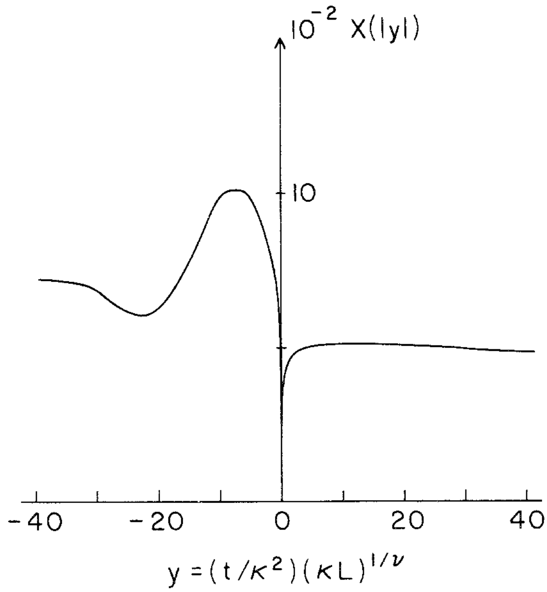

Fig. 4. The scaling function $X(|y|)$ at $d=4-\varepsilon$ evaluated at $\varepsilon=1$, where $y=(t/\kappa^2)(\kappa L)^{1/\nu}$. The two branches for $t \gtrless 0$ have been shown.

specific heat at values of t/κ^2. The argument y is extracted using $\nu = (1/2 + 1/12\varepsilon) \rightarrow 0.58$ at $\varepsilon = 1$. (Alternatively, one may use the appropriate values of ν and α for $d=3$ to obtain a "hybrid" estimate which may offer better agreement with other schemes.) To compare $X(y)$ with a simulation or experiment, in which one would plot

$$\frac{C}{L^d(\Delta T/T_c)^{-\alpha}} \text{ vs. } L^{1/\nu}\left(\frac{\Delta T}{T_c}\right)$$

one must allow for a rescaling of the magnitude X as well as the independent variable y. The latter rescaling allows for a nonuniversal "metrical" factor associated with the combination $tL^{1/\nu}$.

If $u \neq u^*$ ordinary corrections to scalling get mixed in with finite size corrections. Keeping $u \neq u^*$ allows one to consider the crossover from "Gaussian" to "Wilson–Fisher" fixed points and investigate circumstances in which the crossover is or is not completed before the thermodynamic functions are rounded. Experimentally one typically sees "nonclassical" exponents before the rounding regime is reached, but on small systems there may in principle be interference.

7. CONCLUDING REMARKS

The application of finite-size scaling ideas has become widespread since it has become appreciated that, for determining critical properties of systems which undergo second-order phase transitions, some sort of extrapolation with size is essential. Using ideas of finite-size scaling a simulator can infer behavior of the infinite system from "rounded" data. Brézin[4] has shown that the phenomenological form of finite-size scaling follows from renormalization group equations. The essential point is that counterterms for the infinite system suffice to renormalize the theory for finite L.

In this paper we have shown how to compute explicitly thermodynamic functions in the scaling regime $L/a \gg 1$, $ta^2 \ll 1$, where a represents the microscopic length scale of the system, say, the lattice spacing. The computation in $d=4$ is exact to leading logarithms and so provides a potentially useful benchmark for simulations. By adjusting two "metrical" factors, corresponding to a $T-T_c$ scale dilation or contraction and an amplitude for, say, the specific heat, along with the nonuniversal parameter u, the theoretical form discussed in the Appendix is expected to agree in the scaling regime with a simulation. (Of course only if the u which one obtains by such a fitting is small can one expect one-loop corrections to give a reasonable representation in a region about criticality.)

The calculation in $d=4$ also has the advantage of addressing the question of visibility of logarithmic corrections in a rounded regime. This information is carried in the increase of the peak height shown in Fig. 2. For the Ising case the increase is proportional to $\ln^{1/3}(L/a)$. Our numerical estimates indicate that if data in the range $L/a=8$ to $L/a=32$ (or 64) were available and if specific heat peaks were determined to $\pm 5\%$, then a case might be made for direct observation of the logarithmic corrections. (These statements assume a reasonable value of $uS_d \approx 1$.)

Below $d=4$ we cannot calculate the asymptotically correct result without working order by order in $\varepsilon = 4-d$. However, to one-loop order we have produced the finite-size scaling function for the specific heat. With the adjustment of two metrical factors (now $u \to u^*$ and need not be adjusted) it would be interesting to see how results at $\varepsilon = 1$ compare with Ising simulations in three dimensions.

After the completion of this work we learned that Brézin and Zinn-Justin[12] have recently shown that an ε expansion for finite-size systems can be constructed. Their scheme for expanding about mean-field theory in finite systems is essentially the same as ours.

ACKNOWLEDGMENTS

The authors are grateful to the National Science Foundation for partial support of this work. For D. J. and J. R., respectively, the support has been through the Division of Materials Research under grant Nos. DMR-83-02326 and DMR81-15542. Part of this work was done while D. J. was a visitor at the Institute for Theoretical Physics, University of California, Santa Barbara. He gratefully acknowledges the hospitality and support of I.T.P.

8. APPENDIX

Some technical details are presented in this Appendix.

The renormalized $\Gamma_{R,1}(t(\rho), m(\rho), u(\rho), \kappa\rho, L)$ is given in $d=4$ by

$$
\begin{aligned}
[\Gamma_{R,1}]_{d=4} = {} & \frac{S_d}{8} T^2 \left[\frac{1}{2} - \ln\frac{T}{(\kappa^2\rho^2)}\right] - \frac{S_d}{4}\rho^4 t^2(\rho) \\
& + \frac{S_d}{8} T^2 E_1(\omega) - \frac{1}{2L^4}[E_1(\omega) + \ln\omega + \gamma] - \frac{1}{4L^4}(1 - e^{-\omega}) \\
& - \frac{\omega}{4L^4} e^{-\omega} + \frac{1}{2L^4}\int_1^\infty \frac{dx}{x}(1 - e^{-\omega x})[X^4(\pi x) - 1] \\
& + \frac{1}{2L^4}\int_1^\infty dx\; x(1 - e^{-\omega/x})[X^4(\pi x) - 1]
\end{aligned}
\tag{A1}
$$

where

$$
T \to T(\rho) \equiv \rho^2 t(\rho) + \frac{1}{2} u(\rho)\, m^2(\rho)
$$

$$
\omega \equiv L^2 T(\rho)/4\pi
$$

and where $X(x)$ has been defined in (3.6), $E_1(z)$ has been given in (3.10) and γ is Euler's constant. Derivatives

$$
a_1 = \frac{\partial \Gamma_{R,1}}{\partial m^2(\rho)} \qquad \text{and} \qquad a_2 = \frac{\partial^2 \Gamma_{R,1}}{\partial [m^2(\rho)]^2}
$$

evaluated at $m^2(\rho^*) = \langle m^2(\rho^*)\rangle$ are required for the specific heat; the choice of ρ^* has been discussed in Section 4. These derivatives are easily converted to derivatives with respect to $T(\rho)$. Then the singular part of the specific heat, which is evaluated numerically in Section 5, has the form

$$\frac{C}{L^4}=\frac{1}{4}\left[\frac{u(\rho^*)}{u}\right]^{2/3} L^4[\langle m^4(\rho^*)\rangle-\langle m^2(\rho^*)\rangle^2]$$
$$+\frac{1}{u}\left[\left(1-\frac{3}{2}S_d u\ln\rho^*\right)^{1/3}\right]-\left[\frac{u(\rho^*)}{u}\right]^{2/3}\left[\frac{\partial^2\tilde{\Gamma}_{R,1}}{\partial T(\rho)^2}\bigg|_*\right]$$
$$-\frac{S_d}{2}\left[\frac{u(\rho)}{u}\right]^{2/3}+\frac{1}{16}u^2(\rho^*)\left[\frac{u(\rho^*)}{u}\right]^{2/3}$$
$$\times\left\{\frac{1}{2}\left[L^2\frac{\partial\tilde{\Gamma}_{R,1}}{\partial T(\rho)}\right]^2-\frac{\partial^2\tilde{\Gamma}_{R,1}}{\partial T(\rho)^2}\right\}_* L^8\langle[m^2(\rho^*)]^4\rangle_c \tag{A2}$$

where $\tilde{\Gamma}_{R,1}$ is $\Gamma_{R,1}$ without the term $S_d\rho^4t^2/4$. In the final expression derivatives, as indicated by $|_*$, are evaluated at

$$T(\rho^*)=\rho^{*2}t(\rho^*)+\tfrac{1}{2}u(\rho^*)\langle m^2(\rho^*)\rangle$$

and $\langle\ \rangle_c$ means cumulant average. The terms without $\tilde{\Gamma}_{R,1}$ belong to the renormalized mean field theory. Finally it should be recalled that

$$\langle m^{2j}(\rho^*)\rangle=[u(\rho^*)L^4]^{-j/2}D_j\left[\frac{\rho^{*2}t(\rho^*)L^2}{u(\rho^*)^{1/2}}\right] \tag{A3}$$

as is (2.7).

In Section 6 the modifications for dealing with $d=4-\varepsilon$ were described. A general formulation is possible (as noted) which goes over to the $d=4$ results. For simplicity, as long as one does not intend to study the limiting behavior as $\varepsilon\to 0$, one may set $u=u^*$, the fixed-point value. Then in place of (A2) one finds the dimensionless quantity

$$\frac{\kappa^\varepsilon C}{L^d}=(\rho^*\kappa L)^\varepsilon(\rho^*)^{-\alpha/\nu}\left\{\frac{1}{4}[\langle x^4\rangle-\langle x^2\rangle^2]-L^{d-4}\frac{\partial^2\Gamma_{R,1}}{\partial T(\rho)^2}\bigg|_*\right.$$
$$\left.+\frac{u^{*2}}{16}\left\{\frac{1}{2}\left[L^{d-2}\frac{\partial^2\Gamma_{R,1}}{\partial T(\rho)}\right]^2-L^{d-4}\frac{\partial^2\Gamma_{R,1}}{\partial T(\rho)^2}\right\}_*\cdot\langle(x^2)^4\rangle_c\cdot(\rho^*\kappa L)^{2\varepsilon}\right\}$$
$$+\frac{S_d}{4\alpha}\left(1+\frac{\varepsilon}{3}\right)(\rho^*)^{-\alpha/\nu} \tag{A4}$$

Once again the symbol * implies derivatives are evaluated at

$$T(\rho^*)=\rho^{*2}t(\rho^*)+\tfrac{1}{2}u^*(\kappa\rho^*)^\varepsilon\langle m^2(\rho^*)\rangle$$

It is straightforward to verify

$$\left[L^{d-2}\frac{\partial\Gamma_{R,1}}{\partial T(\rho)}\right]\quad\text{and}\quad\left[L^{d-4}\frac{\partial^2\Gamma_{R,1}}{\partial T(\rho)^2}\right] \tag{A5}$$

became functions of $L^2\rho^{*2}t(\rho^*)$ alone. Explicitly the averages $\langle x^n \rangle$ are computed according to the probability distribution

$$\exp\left\{-\frac{1}{2}L^2\rho^{*2}t(\rho^*)x^2 - \frac{1}{4!}u^*(\rho^*\kappa L)^{\varepsilon}x^4\right\} \tag{A6}$$

so that the cumulants also depend only on that combination. Substitution of $\rho^* = (\kappa L)^{-1}$ yields the scaling form given in Eq. (6.5). The explicit form of the scaling function is found numerically using, as in (4.11),

$$\rho^{*2}t(\rho^*)L^2 + \frac{u^*}{2}(\rho^*\kappa L)^{\varepsilon}\langle x^2 \rangle + 1 = (\rho^*\kappa L)^2 \tag{A7}$$

which implies

$$\rho^* = (\kappa L)^{-1}\ R(tL^{1/\nu})$$

The "universal" scaling function $X(y)$ for the specific heat has been plotted in Fig. 4. See the text for further discussion.

REFERENCES

1. M. E. Fisher and M. N. Barber, *Phys. Rev. Lett.* **28**:1516 (1972).
2. K. Binder, ed., *Monte Carlo Methods in Statistical Physics* (Springer, New York, 1979), and references therein.
3. K. K. Mon and D. Jasnow, *Phys. Rev. A* **30**:670 (1984).
4. E. Brézin, *J. Phys. (Paris)* **43**:15 (1982).
5. M. N. Barber and M. E. Fisher, *Ann. Phys.* **77**:1 (1973).
6. S. Singh and R. K. Pathria, *Phys. Rev. B* **31**:4483 (1985).
7. J. Rudnick, unpublished.
8. L. Schwartz, *Mathematics for the Physical Sciences* (Addison-Wesley, Reading, Massachusetts, 1966), Chap. 5.
9. Milton Abramowitz and Irene A. Stegun, eds. *Handbook of Mathematical Functions with Formulae, Graphs, and Mathematical Tables* (Dover, New York, 1972).
10. E. Brézin, J. C. LeGuillou, and J. Zinn-Justin, in *Phase Transitions and Critical Phenomena*, Vol. 6, C. Domb and M. S. Green, eds. (Academic, New York, 1976); D. J. Amit *Field Theory*, the *Renormalization Group* and *Critical Phenomena* (McGraw-Hill, New York, 1978).
11. J. Rudnick and D. Nelson, *Phys. Rev. B* **13**:2208 (1976).
12. E. Brézin and J. Zinn-Justin, preprint.