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J. Phys. A: Math. Gen. 28 (1995) 3345–3349. Printed in the UK

Critical finite-size scaling of the free energy

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Received 10 March 1995

Abstract. The Privman–Fisher universal amplitude, characterizing the free energy of a finite-sized system at its critical point, is identified as the critical counterpart of the 'number of stable phases' on the coexistence curve. Its value is shown to be determined by the critical-point form of the order parameter distribution, directly accessible to Monte Carlo studies.

Finite-size scaling [1, 2] is an established branch of the theory of phase transitions, of interest in its own right, and essential to the understanding and effective use of Monte Carlo (MC) studies. The literature devoted to this topic is extensive [3]. The specific concern of the present work is the prediction [4] that the (Gibbs) free energy density of a critical system, of volume $V = L^d$, contains a contribution of the form U_0/L^d with U_0 a constant, unique to a universality class, but dependent on sample geometry and boundary conditions. This prediction finds justification in the theory of conformal-invariance [5] which permits the evaluation of the coefficient U_0 in some cases, as do extended scaling arguments [6]. The determination of free energies by MC methods is notoriously awkward, but some MC results for U_0 exist [7]. The results presented here illuminate the physical significance of this quantity, and show that it is available directly to conventional MC sampling studies at criticality. In particular we show that U_0 is a measure of the additional configuration space accessible to a system, at its critical temperature, in the limit of sufficiently small ordering fields; it can be viewed as the critical counterpart of the *number of stable phases* characterizing the associated coexistence curve [8, 9]. The analysis also casts some light on the general structure of the critical probability distribution of the order parameter, which has proved an increasingly useful focus of interest in MC studies of critical behaviour [10–15].

We consider a system in the form of a d-dimensional cube of side L, with periodic boundary conditions. We suppose that the system exhibits a continuous phase transition, associated with a scalar order parameter m, with conjugate field h, such that the phase coexistence boundary lies along the line $h = 0$. We denote by $Z(L, h, t)$ the partition function at reduced temperature $t = (T - T_c)/T_c$. The focus of our interest is an anomalous contribution to the configurational weight, featuring as an *L-independent* multiplicative prefactor in this partition function. More formally, defining a dimensionless free energy by $F \equiv -\ln Z$, the quantity of interest is the free energy anomaly

$$F_a(h, t) \equiv \lim_{L\to\infty} \left\{ F(L, h, t) - L^d \lim_{L\to\infty} \frac{1}{L^d} F(L, h, t) \right\} . \qquad (1)$$

The critical-point value of this anomaly defines the Privman–Fisher coefficient [4] through $U_0 \equiv F_a(h = 0, t = 0)$. Its singular behaviour (for $t = t_- < 0$) at $h = 0$ identifies the line

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of coexistence, with $N_c(h=0,t_-) \equiv \exp\left[-F_a(h=0,t_-)\right]$ giving the number of phases coexisting at $h=0$ [8, 9].

To provide a common framework for understanding and evaluating these quantities we note that the field-dependence of the partition function is expressible in the form

$$Z(L,h,t) = Z(L,0,t)\mathcal{Z}(L,h,t) \tag{2a}$$

with

$$\mathcal{Z}(L,h,t) \equiv \int \mathrm{d}m\ p_{L,t}(m)\mathrm{e}^{hmL^d} \tag{2b}$$

where $p_{L,t}(m)$ is the zero-field probability density (PDF) of the order parameter. It follows that

$$F(L,0,t) = F(L,h,t) + \mathcal{F}(L,h,t) \tag{3a}$$

with

$$\mathcal{F}(L,h,t) \equiv \ln\left[\int \mathrm{d}m\ p_{L,t}(m)\mathrm{e}^{hmL^d}\right] \tag{3b}$$

We analyse these equations on the *assumption* that the Borgs–Kotecky result $F_a(h,t) = 0$ for $h \neq 0$, rigorously established for sufficiently low temperatures, holds for all t. Then, appealing to equations (1) and (3*a*),

$$F_a(h=0,t) = F_a(h_0,t) + \mathcal{F}_a(h_0,t) = \mathcal{F}_a(h_0,t) \tag{4a}$$

with

$$\mathcal{F}_a(h_0,t) = \lim_{L\to\infty}\left\{\mathcal{F}(L,h_0,t) - L^d \lim_{L\to\infty}\frac{1}{L^d}\mathcal{F}(L,h_0,t)\right\} \tag{4b}$$

while h_0 is *any* non-zero field.

First, we briefly consider this result in the case $t=t_-$ with $t_- < 0$. In this regime, in the limit of large L (specifically, in the limit in which L is large compared with the correlation length ξ), the $h=0$ order parameter distribution is the sum of two Gaussians (see, e.g., [16]):

$$p_{L,t_-}(m) = \frac{1}{2}\frac{1}{\left(2\pi m_\sigma^2\right)^{1/2}}\left[\exp\left(-(m-m_s)^2/2m_\sigma^2\right) + \exp\left(-(m+m_s)^2/2m_\sigma^2\right)\right] \tag{5}$$

where $m_s \equiv \lim_{h\to 0}\lim_{L\to\infty}\langle m\rangle_{L,h,t_-}$ is the equilibrium order parameter and m_σ is defined by $m_\sigma^2 \equiv \langle m^2\rangle_{L,h=0,t} - m_s^2$ and satisfies $m_\sigma^2 = L^{-d}\chi$ with χ the zero-field susceptibility. It then follows from equation (3*b*) that

$$\mathcal{F}(L,h,t_-) = \frac{h^2L^d\chi}{2} + \ln\left\{\frac{\mathrm{e}^{hm_sL^d} + \mathrm{e}^{-hm_sL^d}}{2}\right\} \tag{6}$$

from which (using (4*a*), (4*b*)) one readily finds $F_a(h=0,t_-) = \mathcal{F}_a(h_0,t_-) = -\ln 2$, capturing the result $N_c(h=0,t_-) \equiv \exp\left[-F_a(h=0,t_-)\right] = 2$.

Now consider the case $t=0$ (the critical temperature of the bulk system). It is well established [17, 11, 13] that, for L large compared to microscopic lengths, $p_{L,t=0}(m)\mathrm{d}m \simeq p^\star(x)\mathrm{d}x$ with $x \equiv m/m_\sigma$ and $m_\sigma \equiv \langle m^2\rangle_{L,h=0,t=0}^{1/2} \sim L^{-d/(1+\delta)}$, where δ is the equation of state exponent; the function $p^\star(x)$ is unique to a universality class, and in general non-Gaussian. Appealing to equation (3*b*) we then find

$$\mathcal{F}(L,h,t=0) = \ln\left[\int \mathrm{d}x\ p^\star(x)\mathrm{e}^{yx}\right] = \mathcal{F}^\star(y) \tag{7}$$

with $y = hm_\sigma L^d$. Using equation (4*a*) we may then identify

$$U_0 = F_{\rm a}(h=0, t=0) = \lim_{L\to\infty}\left\{\mathcal{F}^\star(y_0) - L^d \lim_{L\to\infty}\frac{1}{L^d}\mathcal{F}^\star(y_0)\right\} \tag{8}$$

with $y_0 = h_0 m_\sigma L^d$. The limiting behaviour of the function $\mathcal{F}^\star(y)$ is controlled by the large x behaviour of $p^\star(x)$, for which we make the following ansatz:

$$p^\star(x) \simeq p_\infty x^\psi \exp\left(-a_\infty x^{\delta+1}\right) \tag{9a}$$

with

$$\psi = \frac{\delta - 1}{2} \tag{9b}$$

while p_∞ and a_∞ are universal constants (implicit in the form of $p^\star$). The structure of the exponential (equation (9*a*)) is suggested by rigorous results for the 2D Ising model [18] and is consistent with MC studies of the Ising universality class [13]; the value assigned to the exponent of the power law prefactor is proposed here (equation (9*b*)), for reasons to become apparent. We note that a prefactor of this structure features in a recently developed theory [19, 20] which argues that the critical order parameter distribution may be related to the stable distributions of probability theory†.

The integral of interest in equation (7) may be written in the form $\mathcal{F}^\star(y) = \ln\left[\int \mathrm{d}x\, \mathrm{e}^{g_y(x)}\right]$ with $g_y(x) = \ln p^\star(x) + yx$. For sufficiently large y it is dominated by a maximum of $g_y(x)$, at $x = x_{\rm s}$ say. Then

$$\mathcal{F}^\star(y) = g_y(x_{\rm s}) + \ln\sqrt{\frac{2\pi}{|\, g_y''(x_{\rm s})\,|}} + \mathrm{O}(y^{-(1+1/\delta)})\,. \tag{10}$$

Solving $g_y'(x_{\rm s}) = 0$ for $x_{\rm s}$, and substituting yields

$$\mathcal{F}^\star(y) \simeq b_\infty y^{1+1/\delta} + \tfrac{1}{2}\ln\left[\frac{2\pi p_\infty^2}{a_\infty\delta(\delta+1)}\right] + \left[\psi - \frac{\delta-1}{2}\right]\ln x_{\rm s} \tag{11}$$

where b_∞ is a constant. The proposed value for ψ (equation (9*b*)) ensures that the coefficients of the two $\ln x_{\rm s}$ terms cancel, removing a logarithmic dependence on system size that would otherwise result (since $x_{\rm s} \sim y^{1/\delta}$). Recognizing that $y_0^{1+1/\delta} = (h_0 m_\sigma L^d)^{1+1/\delta} \sim L^d$ and appealing to equations (8) and (11) we find

$$U_0 = \tfrac{1}{2}\ln\left[\frac{2\pi p_\infty^2}{a_\infty\delta(\delta+1)}\right]\,. \tag{12}$$

Although this result is illuminating in that it exposes, analytically, the factors controlling U_0, the value of this amplitude is more reliably determined by direct calculation of the function $\mathcal{F}^\star(y)$ through numerical integration of equation (7), using MC results for $p^\star(x)$. Figure 1 shows results for the 2D Ising universality class obtained using the form of $p^\star(x)$ established in studies of both lattice-based spin models [13] and 2D fluids [14]. The inset shows the function $\mathcal{F}^\star(y)$ plotted against $y^{1+1/\delta}$, with the assignment $\delta = 15$ [21]. The convergence to the large-y form indicated by equation (11) is apparent, occurring within the interval in which $hL^{d\delta/(1+\delta)} \lesssim 1$; the value of U_0 is given by extrapolating the limiting linear form back to $y = 0$. The result of this extrapolation depends upon the interval in which the 'limiting' linear behaviour is deemed to hold. The main figure shows the result (for

† However, this theory also suggests the existence of further non-universal contributions to the order parameter distribution, falling off as a *power* at large x and thus asymptotically dominant. Further MC studies of the large-x regime are clearly called for.

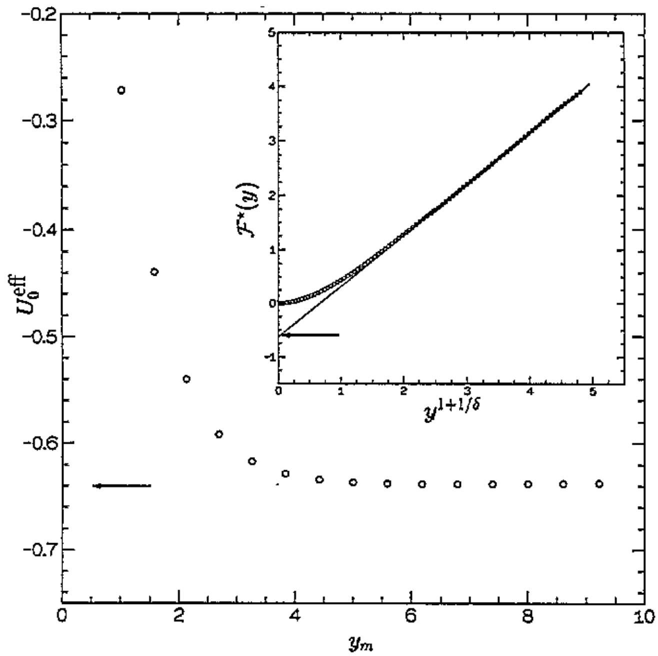

Figure 1. Inset: The field-dependent contribution to the free energy, $\mathcal{F}^*(y)$, at criticality, for the 2D Ising universality class, evaluated from the order parameter PDF [13] using equation (7). Main: The value of the vertical-axis intercept of the linear fit to the data, as function of the y-value that locates the centre of the window of y-values used in the fit. The arrows mark the exact value of the amplitude U_0 for the 2D Ising model [22].

the intercept, and thus the 'effective' U_0) obtained by a fitting procedure using data lying within a window of y-values, as a function of the central y-value in that window. There is excellent agreement with the value $U_0 = -\ln 2 - \ln[(2^{1/4} + 2^{-1/2})/2] = -0.639\,912$ obtained from exact evaluation of the zero-field partition function of the finite-sized 2D Ising model [22]. Figure 2 shows similar results for the 3D Ising universality class, with the presumption $\delta = 4.8$ [23], using the form of $p^*(x)$ established in an independent MC study [15, 19], employing 5×10^7 MC sweeps of a lattice of size 32^3 at the critical coupling $K_c = 0.221\,6595$ [23]. The limiting behaviour suggested by the inset is to be compared with the MC estimates in the range –0.64 to –0.66 obtained in studies of systems up to 24^3 [7]. As regards other dimensionalities, one might note that the double-delta function form of $p^*(x)$ in $d = 1$ [12] implies $U_0 = -\ln 2 = -0.693\ldots$; a droplet-model valid in $d = 1 + \epsilon$ [24] may be analysed to show that $U_0 = -\ln 2\left[1 + O(1/\delta)\right]$. It is then evident that the general closeness of U_0 to $-\ln N_c(0, t_-)$ reflects the significant vestiges of phase coexistence that persist through to the critical point; the amplitude itself measures the additional configurational space which becomes available to the system when the ordering field is reduced below of order $L^{-d\delta/(1+\delta)}$, as the order parameter distribution broadens from a Gaussian centred on $m = m_\sigma x_s$ to the symmetric non-Gaussian form described by $p^*(x)$.

Acknowledgments

I am grateful to Graham Smith for prompting me to think about this problem; and to Nigel Wilding for making available his 3D-Ising PDF data.

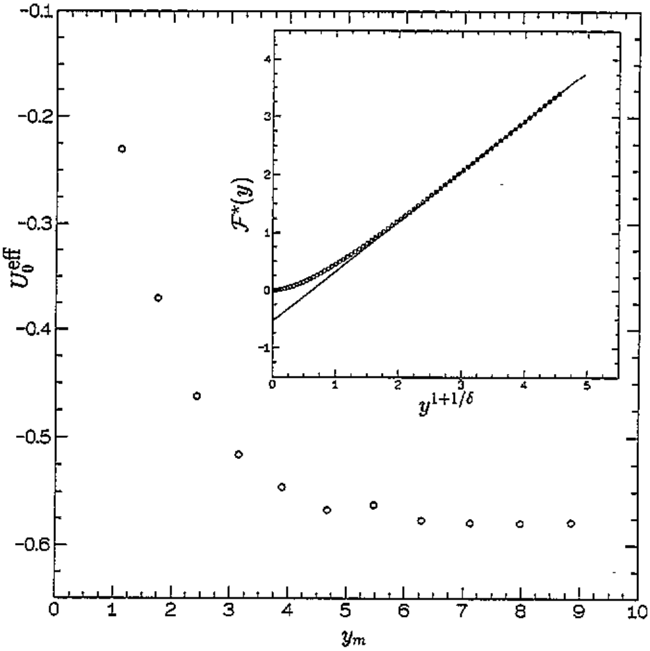

Figure 2. As figure 1, but in the case of the 3D Ising universality class using PDF data from [15, 19].

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