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LETTER TO THE EDITOR

Systems with logarithmic specific heat: finite-size scaling

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Abstract. A detailed study is presented of the finite-size scaling in systems with vanishing critical exponent α, which usually have logarithmic specific heat singularity. The appropriate form of the finite-size hyperuniversality is established. Recent results on complex temperature plane zeros of the partition function are extended to the $\alpha = 0$ case.

We develop a systematic formulation of the finite-size scaling theory for systems with vanishing specific heat exponent α. The two-dimensional Ising model is the most notable example of the logarithmic specific heat divergence as $T \to T_c$. Based on Onsager's (1944) solution, explicit calculations of the specific heat finite-size scaling behaviour have been reported by Ferdinand and Fisher (1969) and by Kleban and Akinci (1983). However, a more general scaling formulation is called for, following several recent developments. Firstly, it is interesting to explore how the hyperuniversality notions (Privman and Fisher 1984) in the finite-size scaling, fit with the emergence of logarithms as $\alpha \to 0$. Indeed, a property of conformal invariance which is even stronger than hyperuniversality hyperscaling, holds for the two-dimensional Ising model (see a review by Cardy (1986) for details). Our analysis will actually apply to any dimension below the upper marginal for finite systems of fixed shape (while the volume, V, may vary) and with *periodic* boundary conditions. Blöte and Nightingale (1982) discussed emergence of logarithms in finite systems, within the real space RG derivation of the finite-size scaling of the free energy. Fisher (1971) formulated a phenomenological finite-size scaling ansatz for the 'logarithmic' case.

Recent results by Glasser *et al* (1986) for the partition function zeros in the complex temperature plane are the second motivation for our study. Their explicit formulae contain combinations of bulk amplitudes (and α) which require delicate limiting procedures as $\alpha \to 0$, and detailed understanding of the finite-size scaling in this limit. We extend the Glasser *et al* formalism to the logarithmic case. Previous studies of the complex temperature zeros for $\alpha = 0$ systems concentrated on their locus and density in the $d = 2$ Ising model (Fisher 1965, Brascamp and Kunz 1974, Abe and Katsura 1970). However, Abe (1967) considered a more general asymmetric-background logarithmic case.

It is convenient to formulate our discussion in terms of the limit $\alpha \to 0$. The finite-size scaling relation for the free energy *density*, measured in units of kT, takes the form

$$f(t, V) \approx b_0 + b_1 t + b_2 t^2 + V^{-1} Y(t(AV)^{1/d\nu}; \ldots) \qquad (1)$$

where $t \equiv (T - T_c)/T_c$. In the scaling term, A is the only non-universal parameter (Privman and Fisher 1984). The undisplayed arguments are system shape ratios. The

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power series in t includes the first few of the *bulk* analytic background contributions; this last identification has been established only for systems with *periodic* boundary conditions (Brézin 1982). The scaling function $Y(\tau)$, with

$$\tau \equiv t(AV)^{1/d\nu} \tag{2}$$

can be expanded in powers of τ for small $|\tau|$. For $\tau \to \pm\infty$ however, we have

$$Y \approx (A_\pm/A)|\tau|^{d\nu}. \tag{3}$$

This limit reproduces the bulk behaviour

$$f_\pm(t, \infty) \approx b_0 + b_1 t + b_2 t^2 + A_\pm |t|^{d\nu} \tag{4}$$

where $\pm$ denotes the free energy density for $t \gtrless 0$, respectively. (Note that $d\nu = 2 - \alpha$ here.) Finally, a convenient normalisation in (1) is provided by the choice (Glasser *et al* 1986)

$$A = [A_+^2 + A_-^2 - 2A_+A_- \cos(\pi\alpha)]^{1/2}. \tag{5}$$

The limit $\alpha \to 0$ in the *bulk* system, and the emergence of the $t^2 \ln(t^{-2})$ contribution to the free energy, are well understood both in the field theoretical (Wegner 1972) and real space (Nightingale and t'Hooft (1974) and references therein) RG formalisms. A recent general scaling discussion is due to Chase and Kaufman (1986). In the limit, the amplitudes $A_\pm$ and b_2 have poles

$$b_2 \approx -(2a/\alpha) + B_2 \tag{6}$$

$$A_\pm \approx (2a/\alpha) + B_\pm \qquad a \geqslant 0 \tag{7}$$

but

$$b_0 \approx B_0 \qquad \text{and} \qquad b_1 \approx B_1 \tag{8}$$

with corrections (in (6)-(8)) of $O(\alpha)$. Small-α expansion of (4) leads to the limiting form

$$f_\pm(t, \infty) \approx B_0 + B_1 t + (B_2 + B_\pm)t^2 + at^2 \ln(t^{-2}). \tag{9}$$

In the finite system case, we can formally separate the bulk singularity by defining

$$X_\pm(\tau) = Y(\tau) - (A_\pm/A)|\tau|^{d\nu} \tag{10}$$

(compare (3)). Then

$$f(t, V) \approx b_0 + b_1 t + b_2 t^2 + A_\pm |t|^{d\nu} + V^{-1} X_\pm(t(AV)^{1/d\nu}) \tag{11}$$

but the new scaling functions $X_\pm(\tau)$ are no longer regular for small $|\tau|$ which is the regime of strong finite-size effects. It is plausible to conjecture that the finite-size term in (11) has a smooth limit as $\alpha \to 0$. Indeed, according to Brézin (1982), restricting system size (which can be viewed as discretising momentum variables in the field theoretical RG formalism and thus effectively introducing an infrared cutoff) 'commutes' with the finite lattice spacing (ultraviolet cutoff) related regularisations. This feature is explicit in the real space RG (Blöte and Nightingale 1982) and was also checked in the low-order $\sqrt{\varepsilon}$-expansion calculations by Brézin and Zinn-Justin (1985) and by Rudnick *et al* (1985). Now according to relations (5) and (7) we have, in the $\alpha \to 0$ limit,

$$A \equiv [(B_+ - B_-)^2 + (2\pi a)^2]^{1/2} \tag{12}$$

which is finite. In summary, we propose the following scaling for the $\alpha \equiv 0$ case:

$$f(t, V) \approx B_0 + B_1 t + (B_2 + B_\pm)t^2 + at^2 \ln(t^{-2}) + V^{-1} X_\pm(t(AV)^{1/2}) \qquad (13)$$

with A given by (12).

To proceed, let us define a universal parameter p via

$$p \equiv (1 - A_+/A_-)/\alpha. \qquad (14)$$

This quantity has been used in fitting experimental data in $d = 3$: see Chase and Kaufman (1986) for further discussion and literature. Indeed, $p(\alpha)$ has a smooth limit

$$P \equiv p(\alpha = 0) \qquad (15)$$

which is the linear coefficient in the expansion

$$A_+/A_- = 1 - P\alpha + O(\alpha^2). \qquad (16)$$

By (7), we have

$$P \equiv (B_- - B_+)/(2a) \qquad (17)$$

and so

$$A/a = 2(P^2 + \pi^2)^{1/2}. \qquad (18)$$

The ratio a/A is then universal. By inspection of the defining relations (5) and (7), one concludes that $B_\pm/A$ (and $A_\pm/A$) are also universal. In terms of $\tau \equiv t(AV)^{1/2}$, we now represent the logarithmic term in (13) as

$$at^2 \ln(t^{-2}) = at^2 \ln(AV) + V^{-1}(a/A)\tau^2 \ln(\tau^{-2}). \qquad (19)$$

The $B_\pm t^2$ term in (13) can also be represented in terms of τ as $V^{-1}(B_\pm/A)\tau^2$. We can absorb the terms with the universal coefficients a/A and $B_\pm/A$ in the definition of the finite-size scaling function. Relation (13) is replaced by

$$f(t, V) \approx B_0 + B_1 t + [a \ln(AV) + B_2]t^2 + V^{-1} W(t(AV)^{1/2}). \qquad (20)$$

The combined scaling function $W(\tau)$ must be *regular at the origin* similar to $Y(\tau)$ in (1), since the other leading terms in (20) have no explicit singularities at $t = 0$. The scaling term in (20) is *shape dependent*; it has a hyperuniversal form (Privman and Fisher 1984) with a single non-universal amplitude. Specifically, the $W(0)V^{-1}$ term in the free energy *at* T_c has a universal (shape-dependent) amplitude $W(0)$. The large-τ behaviour of $W(\tau)$ is given by

$$W(\tau) = (a/A)\tau^2 \ln(\tau^{-2}) + (B_\pm/A)\tau^2 + o(\tau^2) \qquad (21)$$

for $\tau \to \pm\infty$, respectively. Finally, note that we did not consider corrections to the leading scaling-plus-background terms in relation (20): see Ferdinand and Fisher (1969) and Kleban and Akinci (1983) for explicit results for the $d = 2$ Ising model. These authors studied specific heat which is given essentially by the second-T derivative of (20). Some further results on corrections were obtained by Barber (1983).

The finite-size relation (20) involves the non-universal amplitudes B_0, B_1, B_2 and a and the universal scaling function $W(\tau)$. Three other amplitudes entering in (20) and (21) are $B_\pm$ and A which are related universally to a. The form (20) is applicable in the case of $a = 0$ (no logarithmic divergence) since the metric factor A is well defined (see (12)). It is, however, obvious that one can redefine the scaling function W to have a as a metric factor (provided $a \neq 0$), which means having *both* (AV) dependences in (20) replaced by (aV) dependences. Our formulation can also be extended to higher-order logarithmic anomalies appearing at $\alpha = -1, -2, \ldots$ (see Chase and Kaufman (1986) and references therein).

Turning to the complex temperature zeros of the partition function, let n label the $\mathrm{Re}(t) > 0$ zeros: $n = 1, 2, 3, \ldots, \mathrm{O}(AV)$. Note that the dimensionless product AV is of the order of number of particles in a system. For $1 \ll n \ll AV$ an explicit asymptotic expression for the nth zero, t_n, can be derived from finite-size scaling relations (see Glasser *et al* 1986). Their analysis can be extended to the logarithmic case by using relations (20), (21), etc. We will not report the details but list central results, since they all can be obtained by the $\alpha \to 0$ limit of the $\alpha \neq 0$ relations. Firstly, *all* the $n \ll AV$ zeros *scale* according to

$$t_n \approx \tau_n (AV)^{-1/2} \tag{22}$$

where A is given by (18), while τ_n are the roots of

$$\exp[-W(\tau)] = 0. \tag{23}$$

For $n \gg 1$, we have the asymptotic relation

$$\tau_n \approx \sqrt{2\pi n}\, \exp[\mathrm{i}(\pi - \phi)]. \tag{24}$$

The angle ϕ defines the slope of the asymptotic accumulation line of zeros, with respect to the negative-t axis. For general α, it is given by

$$\tan[(2-\alpha)\phi] = [\cos(\pi\alpha) - A_-/A_+]/\sin(\pi\alpha) \tag{25}$$

(see Itzykson *et al* 1983). The $\alpha \to 0$ limit of (25) is straightforward (as opposed to that for the amplitude A):

$$\tan(2\phi) = -P/\pi. \tag{26}$$

An equivalent equation was derived by Abe (1967); note, however, that his range of angle values (his equation (3.8)) is incorrect. Typically, $\frac{1}{4}\pi \leq \phi \leq \frac{1}{2}\pi$. For the symmetric-background logarithmic singularity, $B_+ = B_-$, as in the $d = 2$ Ising model, the scaling predictions (22), (24)-(26) and (12) can be summarised in the simple expression

$$t_n \approx \mathrm{i}(n/(aV))^{1/2} \qquad \text{for } B_+ = B_-. \tag{27}$$

In summary, we have presented a systematic formulation of the finite-size scaling behaviour for systems with logarithmic specific heat ($\alpha = 0$), with restriction to periodic boundary conditions. Our results include identification of the hyperuniversal scaling properties for this case, and study of the complex temperature zeros.

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