Two-scale-factor universality and the ϵ expansion

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A universality hypothesis of Stauffer, Ferer, and Wortis, concerning a relation between the scale factors of the correlation length and of the magnetic field, is proven to order ϵ^2 with $\epsilon=4-d$. Agreement of explicit estimates of the universal quantities with high-T data is discussed.

Many attempts have been made in recent years to confirm the hypothesis of universality for critical phenomena, both by extrapolation of high-temperature-series expansions and by experimental work. Although the universality of the critical exponents is fairly well established, tests of the universality of the scaling functions are still under way, both as regards the scaling function for the equation of state[1–4] and those for the two-point correlation function.[5,6]

These two scaling functions are combined when one studies the two-point correlation function near T_c in a nonzero magnetic field. In Fourier-transformed variables we consider

$$\chi(\vec{q}, t, H) = \langle \sigma^\alpha_{\vec{q}} \sigma^\alpha_{-\vec{q}} \rangle = \sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} \langle S^\alpha_0 S^\alpha_{\vec{R}} \rangle , \qquad (1)$$

where $t=(T-T_c)/T_c$, H is the magnetic field in units of k_BT/m, with m the magnetic moment per spin, while $\sigma^\alpha_{\vec{q}}(\alpha=1,2,\ldots,n)$ is the αth component of the Fourier transform of the "spin" vector $S^\alpha_{\vec{R}}$, namely,

$$\sigma^\alpha_{\vec{q}} = \sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} S^\alpha_{\vec{R}} , \qquad (2)$$

where the summation runs over a d-dimensional cubic lattice with lattice spacing a.

As the critical point is approached $(t\to 0, H\to 0)$, the correlation length ξ_1 (related to the second moment of the correlation function) diverges, and we expect $\chi(\vec{q}, t, H)$ to approach a scaling form.[7] In the critical region, the singular part of the free energy per site may be written in the scaling form

$$F_S \approx C^{-1}(At)^{2-\alpha} f[CH/(At)^\Delta] , \qquad (3)$$

and the resulting equation of state becomes

$$CH/M^\delta \approx h(At/M^{1/\beta}) . \qquad (4)$$

In (3) and (4), M is the magnetization (in units of the saturation magnetization), A and C are scale factors, and α, β, δ, and Δ are the usual critical exponents. The scaling functions $f(y)$ and $h(z)$ are universal, once a proper normalization is adopted. We choose[8]

$$CH/M^\delta = 1 \quad \text{at } t=0 ,$$

$$At/M^{1/\beta} = -1 \quad \text{at } H=0 . \qquad (5)$$

This uniquely defines the scale factors C and A. Similarly, for $H=0$ and $T>T_c$, the correlation length may be written

$$\xi_1(t) \approx f_1 a(At)^{-\nu} , \quad t \ll 1 . \qquad (6)$$

We can now write[9,10]

$$\chi(\vec{q}, t, H) \approx C(At)^{-\gamma} D[\xi_1 q, CH/(At)^\Delta] \qquad (7)$$

for t, aq, $H \ll 1$. The constant f_1 will be determined from the normalization condition

$$D(x,0) = D(0,0)[1-x^2+O(x^4)] , \qquad (8)$$

for small x. With the normalizations (5) and (8), the scaling function $D(x,y)$ is also expected to be universal. Note that our definition of the scale factors is absolute, whereas that of Refs. 9 and 10 is relative to a reference system.[10] With this definition, we are able to calculate the (nonuniversal) coefficients A, C, and f_1, but not the relative factors g, n, and l.

In a recent paper[10] Stauffer, Ferer, and Wortis advanced a hypothesis concerning the universality of the scaling-factor combination

$$X = \rho^s f_1^d / C , \qquad (9)$$

where $\rho^s a^{-d}$ is the particle density per unit volume. They considered the singular part of the free energy for a region of volume ξ_1^d, and postulated that this free energy is universal [see Eqs. (3) and (6)]. Actually, Stauffer *et al.* list values of the combination

$$\overline{X} = t^2 \alpha C_{h=0}\, \xi^d / k_B , \qquad (10)$$

where $C_{H=0}$ is the singular part of the specific heat per unit volume. One easily checks that $\overline{X} = X\alpha A_c C/A^{2-\alpha}$, where $A_c t^{-\alpha}$ is the singular part of the specific heat per site. To obtain X from their values, we note that $A=1/x_0$ and $C=1/h(0)$, where x_0 and $h(0)$ are as defined in Refs. 3 and 4 [they are related to the original function $H/M^\delta = h(t/M^{1/\beta})$]. Extracting values of A and of C from these references, and that of A_c from Ref. 10, we find for $d=3$

$$X(n=1) \simeq 0.48, \quad X(n=3) \simeq 1.25 \quad \text{(series)} \qquad (11)$$

and

$$X(n=1) \simeq 0.35\text{–}1.5, \quad X(n=3) \simeq 0.85\text{–}1.7 \quad \text{(experiment)}. \quad (12)$$

The introduction of the ϵ-expansion technique[11,12] has improved our understanding of critical phenomena and led to explicit expressions, to orders ϵ^3 and ϵ^2 ($\epsilon = 4 - d$), for the critical exponents and for the scaling function $h(x)$.[8,12] In recent work[13] the scaling function of the correlation function in zero magnetic field, $D(x, 0)$, has also been calculated to order ϵ^2. In the present paper we combine these two studies with an additional calculation, to order ϵ^2, of the four-spin correlation function, in order to derive an ϵ expansion for X. To order ϵ^2, the result is found to be cutoff independent, and therefore universal. However, it is not clear if this will remain true in order ϵ^3.

Explicitly we find

$$\frac{1}{X(n)} = \frac{C}{\rho^s f_1^d} = \frac{\epsilon d}{K_d(n+8)}\left[1 + \epsilon\left(\frac{9n+42}{(n+8)^2} + \frac{3\ln(16/27)}{2(n+8)}\right)\right] + O(\epsilon^3) , \quad (13)$$

where

$$K_d^{-1} = 2^{d-1}\pi^{d/2}\Gamma(\tfrac{1}{2}d) = 8\pi^2[1 - \tfrac{1}{2}\epsilon(\ln 4\pi + 1 - C_E)] + O(\epsilon^2) , \quad (14)$$

while C_E is Euler's constant. Substituting the ϵ expansion of K_d^{-1} from (14) into (13) and putting $\epsilon = 1$ yields

$$X(n=1) \simeq 0.58, \quad X(n=3) \simeq 1.73. \quad (1$$

The final values are somewhat different if one uses K_3 in (13). One must also note that the convergence of ϵ expansions is still generally questionable. Thus the values (15) may be taken as rough estimates. As such, their agreement with the values from series (11) and from experiments (12) is quite satisfactory. Moreover, it is also possible that the ϵ^3 terms in (13) will be nonuniversal, leading to a nonuniversality of X.[14] Until these questions are settled, more precise experiments [the large spread of values in (12) is a result of the spread of values for different materials, plus the experimental errors[10]] and series (the scatter of values of $\alpha C_{H=0}$ for $n = 3$ is quite large) may be quite helpful.

To derive the result (13) we first note that the constant C is directly related to the four-spin correlation function,

$$\langle\sigma_0\sigma_0\sigma_0\sigma_0\rangle_c = \frac{\partial^2\chi}{\partial H^2}\bigg|_{H=0,\,q=0} = C^3(At)^{-\gamma-2\Delta}\frac{\partial^2}{\partial y^2}D(0,y)\bigg|_{y=0}, \quad (16)$$

where the subscript c means "connected."

The small-y behavior of $D(0, y)$ follows from the large-z behavior of $h(z)$,[3,4,8] namely,

$$h(z) \approx z^\gamma(h_1 + h_2 z^{-2\beta} + \ldots) \text{ as } z \to \infty , \quad (17)$$

which leads to

$$D(0,0) = \frac{1}{h_1} \quad (18)$$

and

$$\frac{\partial^2}{\partial y^2}D(0,y)\bigg|_{y=0} = \frac{-6h_2}{h_1^4} . \quad (19)$$

Defining r as the inverse susceptibility at $H = 0$, that is,

$$r = \frac{1}{\chi(0,t,0)} \approx C^{-1}h_1(At)^\gamma , \quad (20)$$

(16) now becomes

$$\langle\sigma_0\sigma_0\sigma_0\sigma_0\rangle_c \approx -6h_2h_1^{-4}C^3(Cr/h_1)^{-1-2\Delta/\gamma} = -6h_2h_1^{(\epsilon/2)-\eta}C^{(\epsilon/2)-1-\eta}r^{(\epsilon/2)-4-\eta} + O(\epsilon^3), \quad (21)$$

where the known ϵ expansions for the exponents[8,11,12] have been used.

An alternative derivation of (21) follows Wilson's calculation[12] of the "renormalized coupling constant" u_R. We start with the reduced Hamiltonian

$$\overline{\mathcal{H}} = -\int_{\vec q}[r_0 + q^2]\vec\sigma_{\vec q}\cdot\vec\sigma_{-\vec q} - u_0\int_{\vec q}\int_{\vec q'}\int_{\vec q''}(\vec\sigma_{\vec q}\cdot\vec\sigma_{\vec q'})(\vec\sigma_{\vec q''}\cdot\vec\sigma_{-\vec q-\vec q'-\vec q''}) , \quad (22)$$

where $\sigma_{\vec q}$ is a new spin variable, rescaled by a factor $(2dk_BT\rho^s/cJ)^{1/2} \simeq (d\rho^s)^{1/2}$ (J is the nearest-neighbor exchange, c the coordination number), and where $\int_{\vec q}$ means $(2\pi)^{-d}\int d^dq$ with a sharp cutoff at $|\vec q| = \Lambda = \pi$ (we set the lattice constant a equal to unity). This cutoff may also be replaced by other forms (e.g., the one used by Wilson in Ref. 12), and the final results remain unchanged. The parameter r_0 is linear in the temperature T. Using a perturbation expansion in u_0 and in $(r_0 - r)$ one finds

$$\langle\sigma_0\sigma_0\sigma_0\sigma_0\rangle_c = u_R r^{-4} = -24u_0r^{-4}\{1 + 2(n+8)K_du_0 \times [\ln(r/\Lambda^2) + 1] + O(u_0^2)\} . \quad (23)$$

A careful comparison of the exponents of r in (23) and in (21), including the leading-order ϵ^2 terms in both cases, gives[8]

$$K_du_0 = \frac{\epsilon}{4(n+8)}\left[1 + \epsilon\left(\ln\Lambda + \frac{9n+42}{(n+8)^2}\right)\right] + O(\epsilon^3) . \quad (24)$$

Comparison of the coefficients then yields

$$C^{\epsilon/2-1} = h_1^{\epsilon/2}h_2^{-1}\frac{\epsilon}{K_d(n+8)}\left[1 + \epsilon\left(\frac{9n+42}{(n+8)^2} + \frac{1}{2}\right)\right] + O(\epsilon^3) . \quad (25)$$

To this order we thus find that the amplitude C is cutoff independent [note that h_1 and h_2 are universal; see (29)]. Moreover, the result (25) is also independent of the form of the cutoff used.

To calculate X we now need ξ_1. From (20), (22), and (24) one easily finds[13]

$$\chi(\vec{q}, t, 0) = \langle\sigma_{\vec{q}}^{\alpha}\ \sigma_{-\vec{q}}^{\alpha}\rangle \approx \frac{1}{r+q^2} + O(\epsilon^2) \tag{26}$$

(the order-ϵ terms cancel through the definition of r; see Refs. 12 and 13) and hence, using (8),

$$\xi_1 \approx a r^{-1/2} + O(\epsilon^2) = a h_1^{-1/2} C^{1/2} (At)^{-\gamma/2} + O(\epsilon^2)\ , \tag{27}$$

which, together with (6), yields

$$f_1 = h_1^{-1/2} C^{1/2} + O(\epsilon^2)\ . \tag{28}$$

Again, f_1 is cutoff independent to this order! However, to order ϵ^2 f_1 does depend on the cutoff.

The constants h_1 and h_2 are derived from Ref. 8, which gives

$$h_1 = 1 + \frac{3\epsilon}{2(n+8)} \ln\left(\frac{4}{27}\right) + O(\epsilon^2)\ ,$$
$$h_2 = 1 + \frac{\epsilon}{2}\left(1 - \frac{9\ \ln 3}{n+8}\right) + O(\epsilon^2)\ . \tag{29}$$

A combination of (25), (28), (29) and the spin rescaling factor finally leads to the result (13).

The origin of the universality of X to order ϵ^2 thus lies in the cutoff independence of both C and f_1 to orders ϵ^2 and ϵ. To the next orders in ϵ both scale factors have cutoff-dependent contributions. Although the order-ϵ^2 terms in the combination $f_1 C^{-1/(2-\eta)}$ have been explicitly calculated in Ref. 13, an order-ϵ^3 calculation of the coefficient in (21) is not available for the sharp cutoff. [This involves a knowledge of u_0 to order ϵ^3 and a knowledge of the coefficient of $r^{(\epsilon/2)-4-\eta}$ in (21) to order ϵ^2.] Thus one cannot yet reach a definite conclusion regarding the universality of X to order ϵ^3. Even if universality turns out to be broken, one might expect that the deviations from (15) will not be too large.

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