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Logarithmic Corrections to Scaling in the XY_2 -Model

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We study the distribution of partition function zeroes for the XY -model in two dimensions. In particular we find the scaling behaviour of the end of the distribution of zeroes in the complex external magnetic field plane in the thermodynamic limit (the Yang-Lee edge) and the form for the density of these zeroes. Assuming that finite-size scaling holds, we show that there have to exist logarithmic corrections to the leading scaling behaviour of thermodynamic quantities in this model. These logarithmic corrections are also manifest in the finite-size scaling formulae and we identify them numerically. The method presented here can be used to check the compatibility of scaling behaviour of odd and even thermodynamic functions in other models too.

1. KOSTERLITZ-THOULESS SCALING

The partition function for the d -dimensional $O(n)$ non-linear σ -model is

$$Z_L(\beta, h) = \int_{S_{n-1}} \prod_{i \in \Lambda} d\sigma_i e^{\beta \sum_{\langle i, j \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i}, \quad (1)$$

where L denotes the linear extent of the lattice Λ , β is the Boltzmann factor and h is the reduced external field. The n -component spin σ_i has unit modulus. In the case of $d = n = 2$ this is the plane rotator or XY -model and has a phase transition at $(\beta, h) = (\beta_c, 0)$ which is caused by the binding and unbinding of vortices.

An approximate renormalization group approach indicates unusual scaling behaviour of the thermodynamic functions as criticality is approached from the disordered phase [1]. In terms of the reduced temperature $t = 1 - \beta/\beta_c$, the scaling behaviour of the correlation length, susceptibility and the specific heat is given in [1] as

$$\xi_\infty(t) \sim e^{at^{-\nu}}, \quad (2)$$

$$\chi_\infty(t) \sim \xi_\infty^{2-\eta_c}, \quad (3)$$

$$C_\infty(t) \sim \xi_\infty^{\tilde{\alpha}} + \text{constant}, \quad (4)$$

where for $t > 0$, $\nu = 1/2$, $\eta_c = 1/4$ and $\tilde{\alpha} = -d = -2$. The aim of this work is to argue that the latter two scaling formulae are incompatible as they stand. To this end, a method is presented

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by which odd and even thermodynamic functions (like (3) and (4)) can be related and expressed in terms of partition function zeroes. Using certain reasonable assumptions regarding finite-size scaling, it is shown that there have to exist multiplicative logarithmic corrections to (3) and (4). This method can be applied to any model.

2. LEE-YANG ZEROES

For the XY_2 -model the zeroes in the complex external field strength plane are on the imaginary axis [2,3]. Expressing the partition function in terms of its Lee-Yang zeroes (denoted $z_j(\beta)$),

$$Z_L(\beta, h) = \rho_L(\beta, h) \prod_j (h - iz_j(\beta)), \quad (5)$$

where ρ_L is a non-vanishing function of h related to the spectral density and contributes only to the regular part of the free energy. The singular part of the free energy corresponds to

$$f_L(\beta, h) = L^{-d} \sum_j \ln(h - iz_j(\beta)). \quad (6)$$

This can be written as

$$f_L(\beta, h) = \int_{z=-R}^R \ln(h - iz) g_L(\beta, z) dz, \quad (7)$$

in which R is an appropriate cutoff and the density of zeroes, $g_L(\beta, z)$ is given by

$$g_L(\beta, z) = L^{-d} \sum_j \delta(z - z_j(\beta)) = \frac{\partial G_L(\beta, z)}{\partial z}. \quad (8)$$

Here G_L is the cumulative density of zeroes. The distribution of zeroes is symmetric in the real h -axis and the (cumulative) density of zeroes is zero up to the Yang–Lee edge. This allows one to write the singular part of the free energy in the thermodynamic limit as [4–6]

$$f_\infty(\beta, h) = -2 \int_{z_1(\beta)}^R \frac{z}{h^2 + z^2} G_\infty(\beta, z) dz \quad , \quad (9)$$

where $z_1(\beta)$ is the position of the Yang–Lee edge.

This leads to an expression for χ_∞ in terms of the cumulative density of zeroes and the edge. Following [4,5] this gives (independent of the model under consideration provided it obeys the Lee–Yang theorem)

$$G_\infty(\beta, z) = \chi_\infty(\beta, z) z_1^2(\beta) \Phi\left(\frac{z}{z_1(\beta)}\right) \quad , \quad (10)$$

where Φ is unknown. The specific heat can also be written in terms of z_1 and G_∞ [4–6];

$$C_\infty(\beta) = -2 \int_{z_1(\beta)}^R z^{-1} \frac{\partial^2 G_\infty}{\partial \beta^2} dz \quad . \quad (11)$$

3. SCALING AND CORRECTIONS

Assume the following modified Kosterlitz–Thouless (KT) scaling behaviour for the singular parts of the thermodynamic functions:

$$\chi_\infty(t) \sim \xi_\infty^{2-\eta_c} t^r \quad , \quad (12)$$

$$C_\infty(t) \sim \xi_\infty^{\tilde{\alpha}} t^q \quad . \quad (13)$$

Assume, furthermore, the edge scales as

$$z_1(t) \sim \xi_\infty^\lambda t^p \quad . \quad (14)$$

Putting these in (10) and (11) gives [6]

$$\lambda = \frac{1}{2}(\tilde{\alpha} - 2 + \eta_c), \quad p = \frac{1}{2}(q - r) + 1 + \nu, \quad (15)$$

Thus the scaling behaviour of the Yang–Lee edge has multiplicative logarithmic corrections even if χ_∞ and C_∞ have not.

4. FINITE-SIZE SCALING

Finite-size scaling (FSS) [7] allows one to find the volume dependency of thermodynamic quan-

ties at β_c from their thermodynamic limit scaling behaviour. Its general form (valid in all dimensions including the upper critical one) is [8]

$$\frac{P_L(0)}{P_\infty(t)} = F_P\left(\frac{\xi_L(0)}{\xi_\infty(t)}\right) \quad , \quad (16)$$

where $P_L(t)$ is some thermodynamic function at reduced temperature t for a system of extent L and F_P is unknown. For the XY_2 -model $\xi_L(0) \propto L$ [9]. Applying (16) to (12) and (14) gives

$$\chi_L(0) \sim L^{2-\eta_c} (\ln L)^{-\frac{r}{\nu}} \quad , \quad (17)$$

$$z_1(L) \sim L^{\frac{1}{2}(\tilde{\alpha}-2+\eta_c)} (\ln L)^{-\frac{1}{\nu}(\frac{q-r}{2}+1+\nu)} \quad . \quad (18)$$

The finite-volume counterpart of (10), relating the susceptibility and the zeroes, is (from (6))

$$\chi_L(0) = L^{-d} \sum_j z_j(L)^{-2} \approx L^{-d} z_1(L)^{-2} \quad , \quad (19)$$

where it has been assumed that the lowest lying zero has the dominant effect. This gives

$$\tilde{\alpha} = -d = -2, \quad q = -2(1 + \nu) = -3. \quad (20)$$

Thus the scaling behaviour of the singular part of the specific heat indeed exhibits multiplicative logarithmic corrections.

5. NUMERICAL RESULTS

The above arguments have yielded no information on the odd correction exponent r . Careful renormalization group (RG) considerations give $r = -1/16$ [10]. Our task now is to identify r numerically. To this end we use the FSS of the Lee–Yang zeroes. Accepting the KT predictions for ν , η_c and $\tilde{\alpha}$ for $t > 0$, (18) gives

$$z_1(L) \sim L^{-\frac{15}{8}} (\ln L)^r \quad . \quad (21)$$

A Wolff algorithm [11] was used to simulate the XY -model on square lattices of sizes $L = 32, 64, 128$ and 256 . The critical β -value was found to be 1.11(1) from phenomenological RG methods [12]. The results for the lowest lying zeroes at $\beta = 1.11$ are $z_1(L) = 0.0023348(7)$, $0.0006350(2)$, $0.00017279(5)$ and $0.000047062(13)$ for $L = 32, 64, 128$ and 256 . Details on the numerics and the determination of β_c and the zeroes

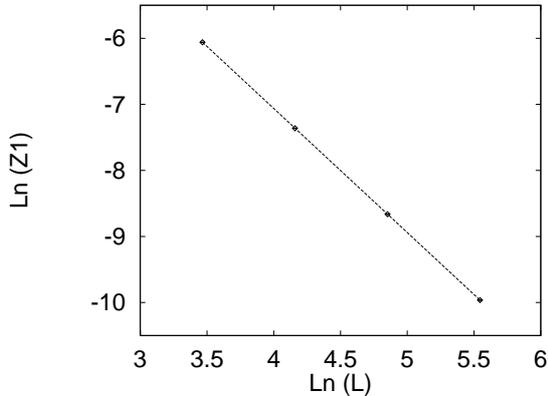


Figure 1. Leading FSS of Lee–Yang Zeroes.

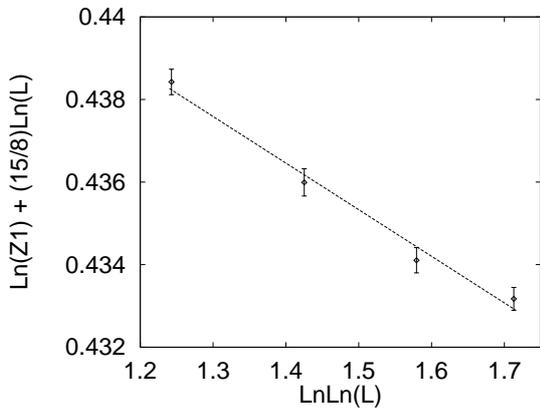


Figure 2. Corrections to FSS of Lee–Yang Zeroes.

will be given in a forthcoming publication [6]. In the absence of any corrections, the slope of Figure 1 should give the leading power-law FSS exponent. In fact the slope is $-1.8777(4)$, the deviation from the KT value of $-15/8 = -1.875$ being due to the presence of logarithmic corrections. To identify these, and the correction exponent r in (21), $\ln(z_1 L^{15/8})$ is plotted against $\ln \ln L$ in Figure 2. A straight line is identified. Its slope is $-0.012(1)$. Thus we have strong evidence for a non-zero value of r , albeit not in agreement with the RG predictions of $-1/16 = -0.0625$ from [10].

6. CONCLUSIONS

Theoretical arguments checking the consistency of the scaling behaviour of odd and even thermodynamic functions at a KT phase transition have been presented. The generally used scaling formulae have to be modified by multiplicative corrections. These are identified analytically for the specific heat and numerically for the susceptibility. This numerical identification comes via an analysis of Lee–Yang zeroes, the FSS of which is linked to that of the susceptibility.

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