Pis'ma v ZhETF, vol. 79, iss. 5, pp. 267 – 271

Numerical investigation of logarithmic corrections in two-dimensional spin models

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Submitted 20 January 2004

The analysis of correlation function data obtained by Monte Carlo simulations of the two-dimensional 4-state Potts model, XY model, and self-dual disordered Ising model at criticality are presented. We study the logarithmic corrections to the algebraic decay exhibited in these models. A conformal mapping is used to relate the finite-geometry information to that of the infinite plane. Extraction of the leading singularity is altered by the expected logarithmic corrections, and we show numerically that both leading and correction terms are mutually consistent.

PACS: 05.50.+q, 75.10.–b

A second order phase transition occurs at very special points in the parameter space of a model, i.e. at a fixed point of the renormalization equations. The eigenvalues of the linearized renormalization equations define the scaling dimensions of the corresponding directions related to the scaling fields. Positive eigenvalues are associated to relevant scaling fields while negative ones correspond to irrelevant fields. In some cases, there may exist a line of fixed points along which critical exponents are varying. This occurs when a marginal field (with vanishing scaling dimension) is identified in the model. The scaling dimensions completely characterize the critical properties of the model, e.g. the power laws of the physical quantities. As an example, the correlation functions exhibit an algebraic decay at the fixed point, e.g. for a scaling field density $\phi(\mathbf{r})$,

$$G_\phi(\mathbf{r}_1,\mathbf{r}_2)=\langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle\sim|\mathbf{r}_1-\mathbf{r}_2|^{-\eta_\phi} \quad (1)$$

in two dimensions (η_ϕ should be replaced by $d-2+\eta_\phi$ in arbitrary dimension). In some special cases, this simple behaviour is modified by multiplicative logarithmic terms,

$$G_\phi(\mathbf{r}_1,\mathbf{r}_2)\sim|\mathbf{r}_1-\mathbf{r}_2|^{-\eta_\phi}\times\ln^{\theta_\phi}|\mathbf{r}_1-\mathbf{r}_2|. \quad (2)$$

This situation occurs at the end of a line of fixed points or when the system is perturbed by a marginally irrelevant operator. Examples in two dimensions are given by 4-state Potts model, XY model, or disordered Ising model.

In the case of the q-state Potts model (from now on, we consider the case of the two dimensional problem only), discrete spin variables $\sigma_w=1,2\ldots q$ are located at the sites w of a square lattice (μ specifies the unit lattice vector in the two directions) and interact with nearest neighbours,

$$-\frac{H_q}{k_BT}=K\sum_w\sum_\mu\delta_{\sigma_w,\sigma_{w+\mu}}. \quad (3)$$

The value of the number of states per spin, q, can be seen as a parameter of the model. The special case $q\to 1$ corresponds to the percolation problem and exhibits a second order phase transition. The value $q=2$ corresponds to the Ising model, so when q varies the universality class changes. The transition is of second order as long as $q\le 4$ and the value $q=4$ coincides with the end of the line of fixed points. Along this line, the exponent of the *order parameter correlation function* varies according to [1]

$$\eta_\sigma=\frac{(m+3)(m-1)}{4m(m+1)}, \quad (4)$$

where the value of $m=\pi/\cos^{-1}(\frac{1}{2}\sqrt{q})-1$ parametrizes the number of states. At $q=4$, the correlation function exponent takes the value $\eta_\sigma(q=4)=\frac{1}{4}$. Above $q=4$ the transition becomes of first order. The transition temperature of the $2d$ Potts model is exactly known from duality requirements [2], $K_c=\ln(1+\sqrt{q})$.

The two-dimensional classical XY model is another example of such a scenario, although the transition is in its very nature quite different. The Hamiltonian now describes the interaction of classical two dimensional unit spins, $\boldsymbol{\sigma}_w=(\cos\theta_w,\sin\theta_w)$,

$$-\frac{H_{\rm XY}}{k_BT}=K\sum_w\sum_\mu\boldsymbol{\sigma}_w\cdot\boldsymbol{\sigma}_{w+\mu}. \quad (5)$$

At low temperature, as a consequence of the Mermin-Wagner-Hohenberg theorem [3], there is no finite macroscopic magnetization, but the spin-spin correlation function decays algebraically in the so-called quasi-long-range-ordered phase. The temperature plays the role of a marginal field and the decay exponent η_σ continuously increases up to a limiting value $\eta_\sigma(\mathrm{XY}) = \frac{1}{4}$ at a transition temperature named after Berezinskii-Kosterlitz-Thouless (BKT) [4]. In this low temperature critical phase, ordering is prevented by collective excitations, spin waves, and localized excitations, vortices, which appear in increasing number as the temperature is increased. These latter topological defects are bounded in pairs and the transition to a completly disordered phase with exponential decay of the correlations is reached at the BKT temperature when unbinding of the pairs occurs [5]. The BKT transition thus corresponds to the end of a continuous line of fixed points in the low temperature phase. The transition temperature $K_c \simeq 0.893$, as well as the expression of the temperature dependence of the exponent η_σ are not known exactly. The mechanism of the transition may also be understood from the role of the vortex chemical potential. It is a relevant variable in the low temperature phase, which becomes marginally irrelevant at the BKT transition, thus producing the essential singularities and the logarithmic corrections.

A third example is provided by the random bond Ising model in two dimensions. According to Harris criterion [6], quenched disorder is a relevant variable when the specific heat exponent of the pure system under consideration is positive. In this case, a new fixed point leading to a new universality class is expected. In the case of the $2d$ Ising model, since $\alpha = 0$ in the pure model, randomness is only a marginal variable which could either produce a continuous variation of the exponents with the amplitude of disorder or logarithmic corrections to the unchanged leading critical behaviour if the disorder is eventually marginally irrelevant. After an interesting debate in the eighties [7], the second scenario has been recognized to be correct [8] and the correlation function exponent keeps its value $\eta_\sigma(\mathrm{RBIM}) = \frac{1}{4}$. The Hamiltonian is the one given in Eq.(3), with $q = 2$ and with random nearest neighbour interactions $K_{w,\mu}$ along the bonds between sites w and $w + \mu$. When these couplings are taken from a binary probability distribution with equal probabilities for both strengths, $\mathcal{P}[K_{w,\mu}] = \frac{1}{2}\prod_{w,\mu}[\delta(K_{w,\mu} - K_1) + \delta(K_{w,\mu} - K_2)]$, the critical temperature follows from duality, $(\exp(K_1^c) - 1)(\exp(K_2^c) - 1) = q$ $(= 2$ here).

All these models have the common property that the order parameter correlation function G_σ is expected, from renormalization group arguments, to behave according to Eq.(2) with $\theta_\sigma = \frac{1}{8}$ (XY-model) and $-\frac{1}{8}$ (Potts model and RBIM) [8–10]. One may then define a local effective exponent $\eta_{\mathrm{eff}}(r)$ $(r = |\mathbf{r}_1 - \mathbf{r}_2|)$,

$$\eta_{\mathrm{eff}}(r) = -\frac{d\ln G_\sigma(r)}{d\ln r} = \eta_\sigma - \frac{\theta_\sigma}{\ln r}. \qquad (6)$$

To make this formula more explicit, let us put some typical numbers. Suppose that we want to produce numerical simulations, in order to check Eq.(2), with let say a relative accuracy of $\Delta\eta/\eta_\sigma = |\theta_\sigma|/\eta_\sigma \ln r = 10^{-2}$. The exponent $|\theta_\sigma|$ might be estimated to be of the order of the value of η_σ, so that one has to reach values of r as large as $r \simeq \exp((\Delta\eta/\eta_\sigma)^{-1}) \simeq 10^{43}$! Even with a value of $|\theta_\sigma| = \frac{1}{8}$, one still needs a sample much larger than $L > 10^{21}$ in order to reach distances between spins which are large enough to become sensitive to the presence of the log in Eq.(2). This is definitely not possible and that might be the reason why it was almost impossible to produce reliable data[1)] to corroborate Eq. (2). The strategy is thus to accept the leading behaviour (the value of η_σ as predicted by RG), and to extract the value of θ_σ. This is also a difficult route, and contradictory results were reported in the literature. In the case of the XY-model for example, fixing $\eta_\sigma = \frac{1}{4}$ and using Monte Carlo simulations (susceptibility and correlation length data), Kenna and Irving [11] reported a value close to $\theta_\sigma \simeq 0.046(20)$, Janke [12] obtained $\theta_\sigma \simeq 0.054(2)$ from data at criticality, or $\theta_\sigma \simeq -0.112(4)$ using high temperature data. Also with high temperature data, Patrascioiu and Seiler [13] obtained $\theta_\sigma \simeq -0.154(92)$ and from strong coupling expansion Campostrini et al. [14] had results depending on the lattice symmetry, $\theta_\sigma \simeq -0.090(6)$ to $-0.084(12)$[2)]. There are even more controversial results reported by Balog et al. [15] who suggest $\theta_\sigma = 0$ plus additive corrections, or Kim [16] who is in favor of ordinary scaling rather than essential singularities. We are not aware of any direct verification of the presence of logarithmic terms directly in the correlation function in the case of 4-state Potts-model or disordered Ising model, but logarithmic terms have been found to be compatible with finite-size scaling data of susceptibility and specific heat [17] in the 4-state Potts-model and in the random bond Ising model [18].

There are conceptual difficulties with the above-mentioned approach applied to numerical simulations. First, the maximum available linear extent of a lattice is of the order of $L = 10^3$, and due to boundary effects, only a fraction (let say 1/4th of the lattice) can be used.

1) Both by simulations and by series expansions.

2) In the literature, θ_σ is often referred to as $-2r$.

As a consequence, the value of η_σ is strongly altered by the log-correction in Eq.(6) [3]. Keeping a fixed $\eta_\sigma = \frac{1}{4}$ means that we attribute all the deviation of numerical data to the existence of θ_σ, but again, this correction is only an effective one, since the log term in the correlation function (2) is only the first of a series and the next term (see e.g. Ref. [10, 17]) will affect in a similar manner the value of θ_σ and make it an effective one [4]. A second objection comes from the appearence of a typical length scale which has strong influence in the correction to scale-invariant behaviour. Usually, one does not have to take care to the unit length, since the physical quantities exhibit scale invariance at criticality. Strictly speaking, this is no longer true when a correction to scaling (e.g. a logarithm) is present, and the above expressions for the correlation functions should be rewritten with respect to some scale factor a. This factor is related to the lattice spacing, but as well to some physics of the problem, like the size of vortex pairs in the XY-model or the typical disorder length in the RBIM, it is thus non universal and depends on the model. The local exponent becomes

$$\eta_{\mathrm{eff}}(r) = \eta_\sigma - \frac{\theta_\sigma}{\ln r/a}. \tag{7}$$

What is important to notice here is the fact that the value of a determines the amplitude of variations of the effective exponent $\eta_{\mathrm{eff}}(r)$. According to these observations, it is probably already a good result to only predict a correct sign for the correction exponent θ_σ, and we have no stronger ambition in this paper.

We propose a different approach which is almost free from boundary effects and enable us to work with the asymptotic expression of the correlation function in the infinite plane. The simulations [5] are performed inside a finite system, but the functional expression of the correlation function inside such a system is predicted by a convenient conformal mapping. This method has been applied with success to magnetization profiles in the case of the pure XY-model [19] and was extensively used in the case of disordered Potts-models [20] in two dimensions where it was shown to provide quite accurate results. More problematic is the fact that we apply a method which is known to be valid at a really scale-invariant fixed point, i.e. in the absence of corrections to scaling which break (at the correction level) dilatation symmetry. In the following, we consider systems of reasonable sizes (L up to 256), the asymptotic regime $r \to \infty$, $G_\sigma(r) \sim r^{-\eta_\sigma}$, is thus far from being reached and the variable $\ln r$ only varies within a narrow range. Accordingly, Eq.(2) might be replaced by an algebraic decay with an effective exponent, $G_\sigma(r) \sim r^{-\eta_{\mathrm{eff}}}$, and displays scale invariance, at least in the range of distances under consideration.

– The upper complex plane $\Im\mathrm{m}\,\zeta \geq 0$ is mapped inside a square $-L/2 \leq \Re\mathrm{e}\, w \leq L$, $0 \leq \Im\mathrm{m}\, w \leq L$ through the Schwarz-Christoffel conformal mapping $\zeta = \mathrm{sn}(2\mathrm{K}w/L)$.

– In order to relate this finite geometry to an original infinite plane (with complex variable z), one may use the Schwarz transformation $\zeta = z^{1/2}$ which has the effect of a folding of opposite edges of the square two by two [21] as shown in Fig.1.

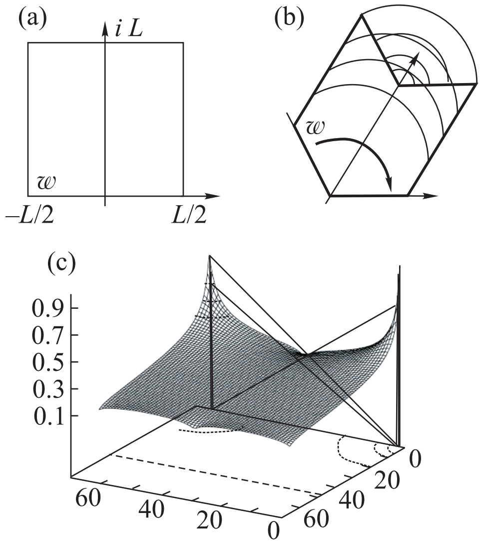

Fig.1. (a) Conformal mapping of the infinite complex plane inside a square w. (b) Sketch which shows how the boundary conditions (BC) follow from the folding ("pillow" geometry). c) Example of the profile of the correlation function between the upper right corner and other points in the square with these particular BC

There, the effect of the conformal mapping,

$$G_\sigma(w_1, w_2) \sim |w'(z_1)|^{-\frac{1}{2}\eta_\sigma} |w'(z_2)|^{-\frac{1}{2}\eta_\sigma} G_\sigma(z_1, z_2), \tag{8}$$

is just to define a rescaled distance variable, called $\kappa(w_1, w_2)$, in terms of which one recovers inside the square with these special boundary conditions, a simple power law for the correlation function:

[3] With $\theta_\sigma = \pm\frac{1}{8}$ and simulations available up to relative distances as large as $r = 500$, one can at most reach values of η_σ in the range $0.23 - 0.27$.

[4] Using the expression $G(r) \times r^{1/4} \sim \ln^{1/8} r \times (1 + \frac{1}{16}\frac{\ln\ln r}{\ln r})$ given in Ref. [10] for the BKT transition and again with $r \simeq 500$, we get $\theta_\sigma(r) = \theta_\sigma + \frac{1}{16}\frac{1-\ln\ln r}{\ln r + (\ln\ln r)/16} \simeq 0.117$.

[5] Standard Wolff cluster algorithms.

$$G_\sigma(w_1, w_2) \sim [\kappa(w_1, w_2)]^{-\eta_{\rm eff}}, \qquad (9)$$

$$\kappa(w_1, w_2) = |w'(z_1)|^{\frac{1}{2}} |w'(z_2)|^{\frac{1}{2}} |z_1 - z_2|, \qquad (10)$$

where

$$|w'(z)| = \frac{L}{4{\rm K}} \left| {\rm cn}(2{\rm K}w/L){\rm dn}(2{\rm K}w/L){\rm sn}(2{\rm K}w/L) \right|^{-1}$$

and $G_\sigma(z_1, z_2)$ is the correlation function in the plane (with $z = {\rm sn}^2(2{\rm K}w/L)$). Here, ${\rm cn}x$, ${\rm dn}x$ and ${\rm sn}x$ are the Jacobi elliptic functions, L the linear size of the lattice, and ${\rm K} \simeq 1.58255$ is a constant related to the aspect ratio of the system.

The main advantage of this technique is that one lattice size L is in principle sufficient (provided it is large enough), since the shape effects are included in the conformal mapping and the method is not much sensitive to finite-size effects. The effect of discretization of the lattice is only appearent at the scale of a few lattice spacings. One more advantage is the fact that all the information encoded in the correlation function is used, since *all* the points w inside the square enter the fit (see Fig.2). Now, as we noticed above, it is necessary to

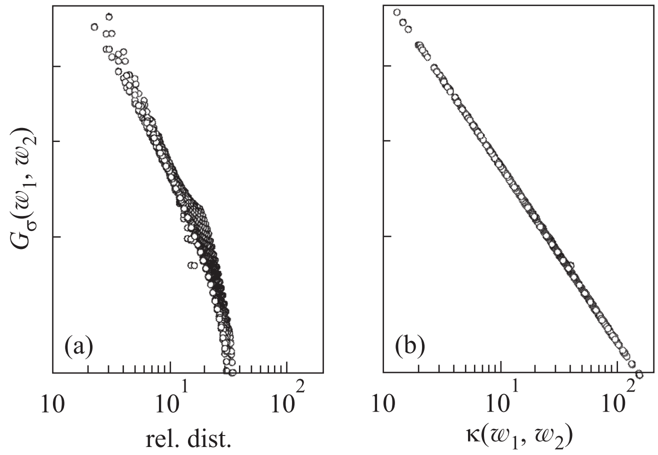

Fig.2. (a) Log-log plot of the correlation function $G_\sigma(w_1, w_2)$ of the XY-model *vs* the relative distance in the original square geometry for a system of size 32^2. (b) Same data plotted now *vs* the rescaled relative distance $\kappa(w_1, w_2)$.

take into account the existence of the logarithmic term if we want to understand the leading singularity. In order to emphasize this comment, let us discuss briefly the results presented in Fig.3 for $L = 32$ to 256 in the case of XY, 4-state Potts and random-bond Ising models. We show the log-log plot of $G_\sigma(w_1, w_2)$ with respect to the rescaled distance $\kappa(w_1, w_2)$ for the three models under consideration. One observes the remarkable linear regime (on this log-log scale) over the whole range of variables, and in particular no boundary effects, as these

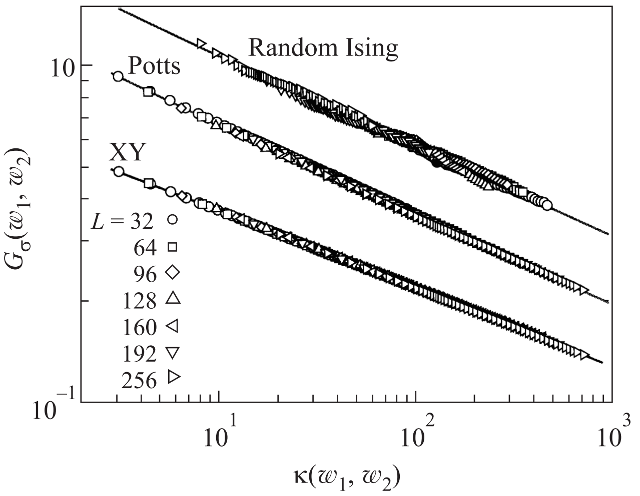

Fig.3. Log-log plot of the correlation function inside the square, $G_\sigma(w_1, w_2)$ as a function of the convenient rescaled variable $\kappa(w_1, w_2)$ (for sizes from $L = 32$ to $L = 256$ for the three models under consideration)

were included in the conformal mapping. Nevertheless, while the expected slopes should all be equal to the same $\eta_\sigma = \frac{1}{4}$, a deviation from this value is suspected. Then, a power law fit leads to leading singularities with exponents[6] $\eta_{\rm eff}({\rm XY}) \simeq 0.233(3)$, $\eta_{\rm eff}({\rm PM}) \simeq 0.264(6)$ and $\eta_{\rm eff}({\rm RBIM}) \simeq 0.265(14)$ (there is a slight variation, depending on the size). All these results are in poor agreement with the exact result $\frac{1}{4}$. This is a clear evidence that the logarithmic correction has to be taken into account.

Fig.4 shows a semi-log plot of the *rescaled* correlation function $f(|z_{12}|) = G_\sigma(w_1, w_2) \times [\kappa(w_1, w_2)]^{\eta_\sigma}$ against the relative distance $|z_2 - z_1|$ in the infinite plane geometry. One observes empirically that the expected behaviour $f(|z_{12}|) \sim A(\ln(|z_{12}|/a))^{\theta_\sigma}$ according to Eq.(2) is in fact linear in this scale, that is

$$f(|z_{12}|) \sim B_0 + B_1 \ln |z_{12}|. \qquad (11)$$

This is coherent with the logarithmic correction provided that the dimensionless inverse typical length scale a^{-1} is larger than any of the accesible relative dimensionless distances at the sizes available, $a^{-1} \gg \max |z_{12}|$. Under these conditions, the logarithmic correction yields

$$f(|z_{12}|) \sim A(\ln(a^{-1}))^{\theta_\sigma} \left(1 + \frac{\theta_\sigma}{\ln(a^{-1})} \ln |z_{12}| \right), \quad (12)$$

i.e. θ_σ appears in the ratio $B_1/B_0 = \theta_\sigma / \ln(a^{-1})$. The slope B_1 in Eq. (11) is positive if $\theta_\sigma > 0$ and negative otherwise.

[6] Statistics over the 7 values of size L for each model.

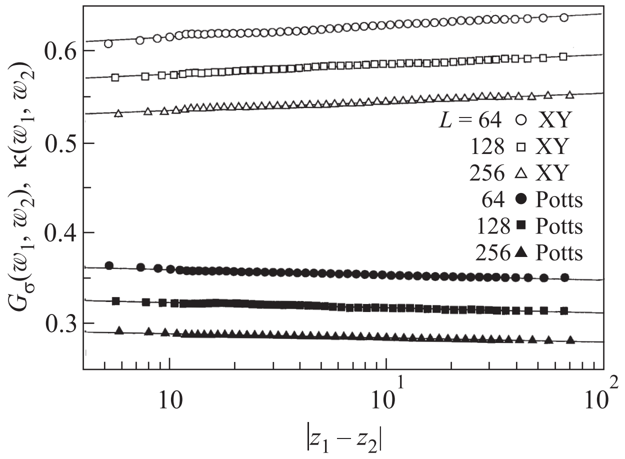

Fig.4. Semi-log plot of the rescaled correlation function for XY- and Potts-models *vs* relative distance in the plane geometry ($L = 256$). The slope B_1 is positive for XY-model and negative in the 4-state Potts-model

As we have mentioned previously, the accessible lattice sizes are too small, so that we do not expect any precise determination of the correction exponent θ_σ. More dramatic is the fact that the θ_σ exponent appears in our expressions mixed with the non universal length scale a from which a reliable value would hardly be extracted. Nevertheless, what is shown in Fig.4 is that a logarithmic correction is consistent with the data for both XY- and 4-state Potts-models, that the signs of the exponents of the log terms are opposite for both models and that their absolute values are quite close to each other (see table). In the case of the disordered Ising model, a quantitative analysis is made difficult due to the fluctuations introduced by the disorder average, but the leading exponent $\eta_{\rm eff}$ was compatible with a negative correction exponent θ_σ, as expected.

Values of the effective exponents deduced from fits of the curves shown in Figs.3 and 4. In the case of RBIM, the value of B_1/B_0 is roughly 3 times larger than for Potts (same sign), but strongly fluctuating

	$\eta_{\rm eff}$			$\theta_\sigma/\ln(a^{-1})$	
L	XY	Potts	RBIM	XY	Potts
64	0.231	0.268	0.259	0.0087	−0.0075
128	0.233	0.266	0.287	0.0077	−0.0081
256	0.234	0.260	0.255	0.0072	−0.0074

We gratefully acknowledge Ralph Kenna for stimulating discussions. We thank the Twinning program between the CNRS and the Landau Institute which made possible this pleasant cooperation. Partial support from RFBR is acknowledged.

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