Logarithmic corrections in the two-dimensional XY model

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Using two sets of high-precision Monte Carlo data for the two-dimensional XY model in the Villain formulation on square $L\times L$ lattices, the scaling behavior of the susceptibility χ and correlation length ξ at the Kosterlitz-Thouless phase transition is analyzed with emphasis on multiplicative logarithmic corrections $(\ln L)^{-2r}$ in the finite-size scaling region and $(\ln\xi)^{-2r}$ in the high-temperature phase near criticality, respectively. By analyzing the susceptibility at criticality on lattices of size up to 512^2 we obtain $r=-0.0270(10)$, in agreement with recent work of Kenna and Irving on the finite-size scaling of Lee-Yang zeros in the cosine formulation of the XY model. By studying susceptibilities and correlation lengths up to $\xi\approx 140$ in the high-temperature phase, however, we arrive at quite a different estimate of $r=0.0560(17)$, which is in good agreement with recent analyses of thermodynamic Monte Carlo data and high-temperature series expansions of the cosine formulation. [S0163-1829(97)00305-6]

I. INTRODUCTION

Ever since the seminal work of Kosterlitz and Thouless (KT) in 1973,[1,2] the two-dimensional (2D) XY model has been the subject of extensive experimental, analytical, and numerical investigations.[3] Physically the interest in this model arises from studies of layers of superconducting materials and films of liquid helium,[4] Josephson-junction arrays,[5] and some magnetic systems.[6] Theoretically the peculiar behavior of the KT phase transition, which is believed to be driven by the unbinding of defect pairs, has attracted much interest. Despite all these efforts, however, the details of the phase transition are not yet fully understood.

In a recent Monte Carlo (MC) simulation study of Lee-Yang partition function zeros, Kenna and Irving[7,8] raised again the question of logarithmic corrections[2,9] to the leading finite-size scaling (FSS) scaling behavior. If the linear lattice size is denoted by L and the multiplicative logarithmic corrections are parametrized as $(\ln L)^{-2r}$, their numerical result is $r=-0.02(1)$, while the standard KT theory would predict quite a different exponent of $r=-1/16=-0.0625$.[2,9] Moreover, by reanalyzing ''thermodynamic'' MC data of Refs. 10 and 11 obtained on lattices with $L>7\xi$, where ξ is the correlation length, Patrascioiu and Seiler[12] obtained an estimate of $r=0.077(46)$, and by analyzing long high-temperature series expansions, Campostrini *et al.*[13] also arrived at positive values in the range $r=0.042(5)$–$0.05(2)$, depending on the quantity considered. While the estimates of the latter two groups are consistent with each other, they are incompatible with the FSS result of Kenna and Irving, which, on the other hand, is somewhat ''closer'' to the theoretical prediction.

All numerical estimates quoted above were obtained in the cosine formulation of the XY model. The purpose of this note is to add further evidence in one or the other direction by analyzing the logarithmic corrections in the Villain formulation[14] of the XY model, which is actually (sometimes implicitly) the starting point of most if not all theoretical investigations.

II. SCALING PREDICTIONS

In the Villain XY model[14] the Boltzmann factor of the cosine formulation, $B_{\cos}=\Pi_{\mathbf{x},i}\exp[\beta_{\cos}\cos(\nabla_i\theta(\mathbf{x}))]$, is replaced by the periodic Gaussian

$$B=\prod_{\mathbf{x},i}\sum_{n=-\infty}^{\infty}\exp\left[-\frac{\beta}{2}(\nabla_i\theta-2\pi n)^2\right], \tag{1}$$

where β is the inverse temperature in natural units, and $\nabla_i\theta=\theta(\mathbf{x}+\mathbf{i})-\theta(\mathbf{x})$ are lattice gradients. A discussion of the relation between the two formulations as well as numerical comparisons can be found in Refs. 14 and 15.

The two-point correlation function $[\vec{s}=(\cos(\theta),\sin(\theta))]$,

$$G(\mathbf{x})\equiv\langle\vec{s}(\mathbf{x})\cdot\vec{s}(\mathbf{0})\rangle=\langle\cos(\theta(\mathbf{x})-\theta(\mathbf{0}))\rangle \tag{2}$$

is predicted to behave at the critical temperature $T_c=1/\beta_c$ as[9]

$$G(\mathbf{x})\propto\frac{(\ln|\mathbf{x}|)^{-2r}}{|\mathbf{x}|^{\eta}}\left[1+\mathcal{O}\left(\frac{\ln(\ln|\mathbf{x}|)}{\ln|\mathbf{x}|}\right)\right], \tag{3}$$

with $r=-1/16$ and $\eta=1/4$. For the power of the logarithmic term we have adopted the notation of Refs. 7 and 8. In the high-temperature phase near criticality, i.e., $0<t\equiv T/T_c-1\ll 1$, this implies for the magnetic susceptibility,

$$\chi=V\left\langle\left(\sum_{\mathbf{x}}\vec{s}(\mathbf{x})/V\right)^2\right\rangle=\sum_{\mathbf{x}}G(\mathbf{x}), \tag{4}$$

a scaling behavior

$$\chi\propto\xi^{2-\eta}(\ln\xi)^{-2r}[1+\mathcal{O}(\ln(\ln\xi)/\ln\xi)], \tag{5}$$

where

$$\xi\propto\exp(bt^{-\nu}) \tag{6}$$

is the correlation length, with $\nu=1/2$ and b being a nonuniversal positive constant. Expressing ξ in terms of t, Eq. (5) can also be written as

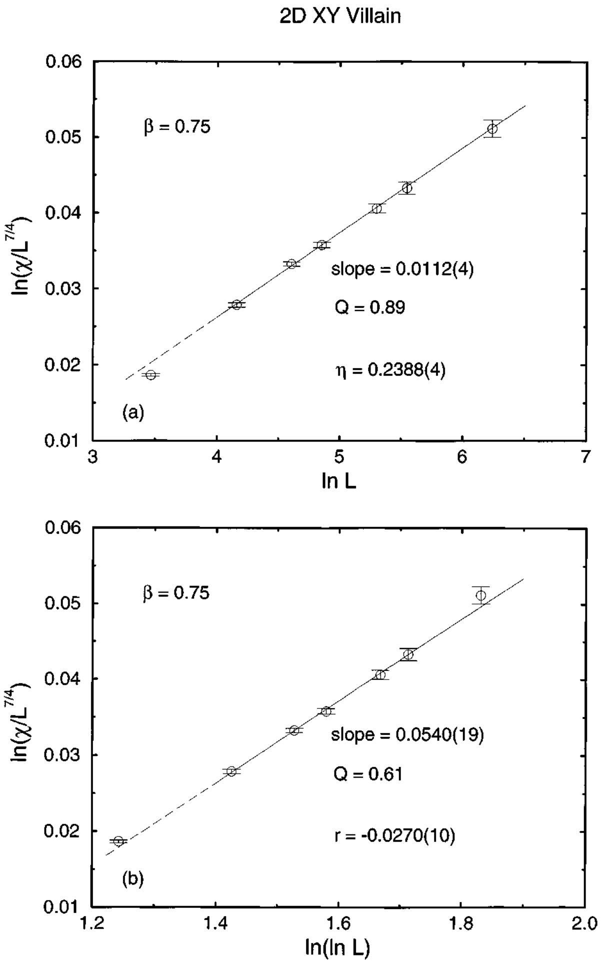

FIG. 1. Finite-size scaling of the susceptibility at criticality. If logarithmic corrections are neglected, the slope in (a) gives $1/4-\eta$. If $\eta=1/4$ is assumed, the slope in (b) yields $-2r$, the exponent of the logarithmic correction.

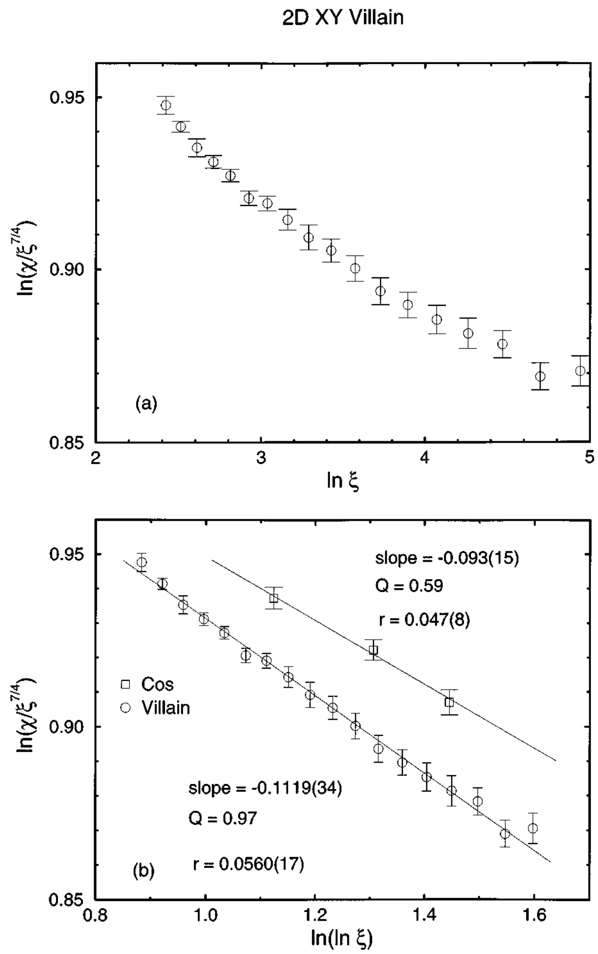

FIG. 2. Test of the scaling relation $\chi\propto\xi^{2-\eta}(\ln\xi)^{-2r}$ in the range $\xi\approx 10\cdots 140$, rewritten as $\ln(\chi/\xi^{7/4})=\text{const}+(1/4-\eta)\ln\xi-2r\ln(\ln\xi)$. The linear behavior in (b) shows that the data are compatible with $\eta=1/4$. As is already obvious from (a), the exponent r must then be positive, in disagreement with the theoretical prediction $r=-1/16$.

$$\chi\propto\xi^{2-\eta}t^{2\nu r}[1+\mathcal{O}(t^{\nu}\ln t)]. \tag{7}$$

Very close to T_c Eq. (5) cannot hold for a finite system with linear size $L\ll\xi$. Here ξ has to be replaced by L, and we expect to observe a FSS behavior

$$\chi\propto L^{2-\eta}(\ln L)^{-2r}[1+\mathcal{O}(\ln(\ln L)/\ln L)]. \tag{8}$$

In numerical simulations it proved to be very difficult to verify the KT scaling laws unambiguously. However, if one rejects a power-law ansatz with unnaturally large exponents and large confluent correction terms, then, among the two alternatives, a pure power-law or the exponential KT divergences, the KT predictions are clearly favored. This is the conclusion of most numerical studies of the cosine formulation[10,11] and, with even stronger evidence, also of the Villain formulation[16] considered here. In this note we shall therefore not study this fundamental question again. We rather assume Eqs. (5)–(8) to be qualitatively valid and try to determine the exponents η, ν, and r. Unfortunately even this goal is far too ambitious, since a precise determination of all three critical exponents together with the (nonuniversal) value of β_c would require much more accurate data than one can hope to generate with present day techniques. We therefore hold the exponents $\nu=1/2$ and $\eta=1/4$ fixed at their theoretically predicted values and ask if any deviation of the data from the leading scaling behavior can be explained by the logarithmic corrections in Eqs. (5) and (8).

III. RESULTS

In Ref. 16 we have reported high-precision MC simulations of the Villain model (1), using the single-cluster update algorithm and improved estimators for the two-point correlation function. This enabled us to obtain on a 1200^2 square lattice data for the correlation length up to $\xi\approx 140$. Since $L>8\xi$ this value should be a very good approximation of the thermodynamic limit. By performing fits of ξ to the KT prediction (6) and of χ to Eq. (5) (without the logarithmic term) with four free parameters (the prefactor, b, ν, and β_c) we obtained $\beta_c=0.752(5)$ and $\nu=0.48(10)$. The estimate of β_c is in very good agreement with the more precise value of $\beta_c=0.7524(7)$ obtained in Ref. 17 from a study of the dual discrete Gaussian model (see also Ref. 18). Using the ansatz (7), i.e., including the theoretically predicted correction $t^{-1/16}$ did not improve the quality of the fits.

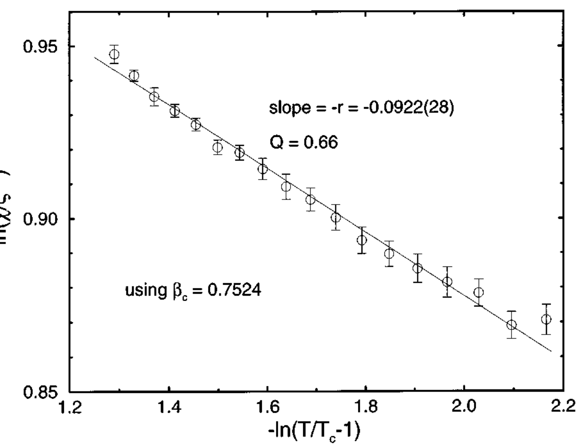

FIG. 3. Test of scaling similar to Fig. 2, but with $\ln\xi$ replaced by $t=T/T_c-1$ [cf. Eq. (6)].

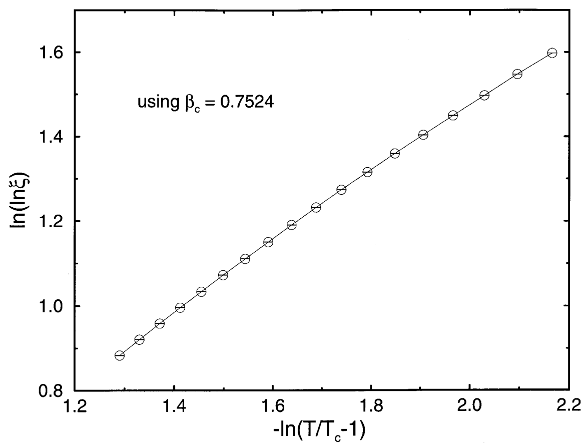

FIG. 4. Correlation length vs reduced temperature. In the range $\xi\approx 10\cdots 140$ the slope is effectively about 0.8, while asymptotically it should approach $\nu=0.5$ according to Eq. (6).

Further data of the susceptibility at criticality on lattices with up to 512^2 sites showed a clear scaling behavior for $L\geqslant 100$, $\chi\propto L^{2-\eta}$, with $\eta=0.2495\approx 1/4$ at $\beta=0.74$, and $\eta=0.2389(6)\neq 1/4$ at $\beta=0.75$. This is obviously not consistent with the prediction that $\eta=1/4$ *at* β_c. Since the estimate of β_c from two completely independent simulations agreed so well we concluded in Ref. 16 that $\eta(\beta_c)\neq 1/4$, in disagreement with the KT prediction. To reconcile simulations and theory we speculated that the scaling curve for χ might still change for much larger system sizes, but this is of course not very convincing. Mainly based on our negative experience with the $t^{-1/16}$ correction in the $\chi(T)$ fits, we did not try, however, to attribute the observed discrepancy to logarithmic corrections.

The data at $\beta=0.75$ and a fit in the range $L\geqslant 64$ according to $\ln(\chi/L^{7/4})=\text{const}+(1/4-\eta)\ln L$ is reproduced in Fig. 1(a). In Fig. 1(b) we show the same data, but now fix $\eta=1/4$ at the theoretical value and assume that Eq. (8) *with* the logarithmic correction is valid. Since then $\ln(\chi/L^{7/4})=\text{const}-2r\ln(\ln L)$, we expect a straight line when $\ln(\chi/L^{7/4})$ is plotted against $\ln(\ln L)$. As is demonstrated in Fig. 1(b) this is clearly the case. Also shown is a linear fit which is of high statistical quality (goodness-of-fit parameter $Q=0.61$) and yields a slope of 0.0540(19), or

$$r=-0.0270\pm 0.0010, \tag{9}$$

in good agreement with the estimate of $r=-0.02(1)$ from the FSS of Lee-Yang zeros in Refs. 7 and 8. To summarize this subsection, by allowing for logarithmic corrections we can reconcile the numerical estimate of $\beta_c\approx 0.752$ with the KT prediction $\eta(\beta_c)=1/4$. The value of the exponent r, however, is clearly *not* in agreement with the theoretical prediction $r=-1/16=-0.0625$.

Let us next consider the scaling behavior of the thermodynamic data near criticality in the high-temperature phase. In Ref. 16 we neglected logarithmic corrections in Eq. (5) and tested the relation $\ln\chi/\xi^{7/4}=\text{const}+(1/4-\eta)\ln\xi$ graphically. This plot is reproduced in Fig. 2(a). We see that the curve has a negative slope, corresponding to $\eta>1/4$. We also observe, however, that the data are curved and that for large ξ the slope decreases. By defining η^{eff} from the local slopes, we obtained at the scale of $\xi\approx 110\ldots 140$ an estimate of $\eta^{\text{eff}}\approx 0.267$. Notice that this effective η is *above* 1/4, while from FSS without logarithmic corrections we would have extracted an effective η that is *smaller* than 1/4. In Fig. 2(b) we show the same data, but similar to Fig. 1 we now again fix $\eta=1/4$ at the theoretical value and assume that Eq. (5) *with* the logarithmic correction is valid. Since then $\ln(\chi/\xi^{7/4})=\text{const}-2r\ln(\ln\xi)$, we expect a straight line when $\ln(\chi/\xi^{7/4})$ is plotted against $\ln(\ln\xi)$. This is indeed the case, and from the fit over all available data points (with $Q=0.97$) we obtain

$$r=0.0560\pm 0.0017, \tag{10}$$

in qualitative agreement with the results in Refs. 12 and 13, which are also derived from the approach to criticality in the high-temperature phase. The value (10) is clearly different from Eq. (9), and is very far from the theoretical estimate $r=-1/16=-0.0625$. In retrospective this ''explains'' why we did not observe any improvement when trying fits of $\chi(T)$ *with* the t^r correction fixed to the theoretical prediction $t^{-1/16}$.

We repeated the analysis leading to the Villain model estimate (10) also with the three data points for the cosine model in Ref. 16 (with $\xi\approx 21$, 40, and 70) and obtained a compatible value of $r=0.047(8)$. Furthermore, using the more extensive data sets of Refs. 10 and 11 we find consistent values of $r=0.050(10)$ and $r=0.049(10)$, respectively.

We also tried to use the scaling form (7) which requires as input information the value of β_c. Using the most accurate estimate of $\beta_c=0.7524$ we find the result shown in Fig. 3. Again the linear scaling looks almost perfect, but from the slope we now read off an even larger value of $r=0.0922(28)$. Qualitatively this can be understood as follows. Going from Eq. (5) to Eq. (7) we replace $\ln\xi$ by $t^{-\nu}=t^{-1/2}$. Asymptotically this follows from the scaling behavior of ξ in Eq. (6). This implicitly assumes, however, that the constant in the proper relation, $\ln\xi=\text{const}+bt^{-\nu}$, can be neglected. If t is not really asymptotically small, this is not justified. In fact, the plot of $\ln(\ln\xi)$ vs $-\ln t$ in Fig. 4 does show effectively an almost linear behavior, but with a slope completely different from the asymptotic value $\nu=1/2$.

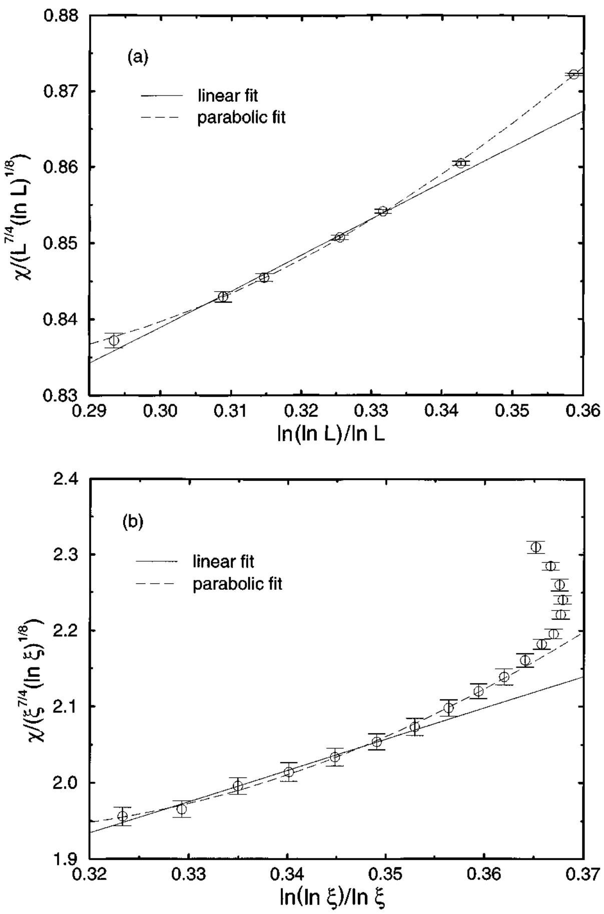

FIG. 5. Test for additive logarithmic corrections in (a) the data at criticality and (b) the thermodynamic data. Here the exponents η and r are assumed to take the theoretically predicted values $\eta=1/4$ and $r=-1/16$.

Finally it was of course tempting to enquire if the observed discrepancies between the numerical data and the theoretical expectations can be blamed on the additive logarithmic corrections in Eqs. (5) and (8). To test this possibility we have replotted in Fig. 5 the data at criticality in the form $\chi/L^{2-\eta}(\ln L)^{-2r}$ vs $\ln(\ln L)/\ln L$ and the thermodynamic data in the form $\chi/\xi^{2-\eta}(\ln\xi)^{-2r}$ vs $\ln(\ln\xi)/\ln\xi$, assuming the theoretically predicted values of η and r. The double valuedness in Fig. 5(b) is caused by the fact that $f(\xi)=\ln(\ln\xi)/\ln(\xi)$ assumes a maximum $f_{\max}=1/e\approx 0.3679$ at $\xi_{\max}=e^e\approx 15.15$. We see that both the data for $L>64$ or $\xi>40$ can be well fitted with a simple linear function. With a parabolic ansatz the acceptable fit range can even be extended to smaller values of L or ξ. From Fig. 5 it is obvious, however, that we are still too far away from the truly asymptotic region $x\rightarrow 0$ to take this as a convincing evidence that additive logarithmic corrections can reconcile simulations and theory.

IV. DISCUSSION

In summary we have shown that, when multiplicative logarithmic corrections are taken into account, numerical simulation data of the 2D XY Villain model are quite consistent with the leading KT predictions even at a quantitative level with critical exponents fixed to the theoretical values of $\nu=1/2$ and $\eta=1/4$. Estimates of the logarithmic correction exponent r, however, turn out to be quite inconsistent. Scaling analyses in the FSS region yield a negative ($r\approx-0.03\cdots-0.02$) and analyses in the high-temparature phase a positive ($r\approx 0.04\cdots 0.08$) value, both being quite different from the theoretical prediction of $r=-1/16=-0.0625$. This is obviously related to the fact that analyses neglecting logarithmic corrections tended to estimate $\eta>1/4$ using thermodynamic data and $\eta<1/4$ in the FSS region. We have no good explanation for this observation other than the common, but unfortunately probably correct statement[19,20] that the studied system sizes are still much too small to resolve these discrepancies.

Note added in proof. Similar observations have recently been reported by J. Salas and A. D. Sokal (unpublished) for the logarithmic corrections at the phase transition of the two-dimensional four-state Potts model.

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