Finite size scaling in the two-dimensional *XY* model and generalized universality

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In recent works [S. T. Bramwell, P. C. W. Holdsworth, and J.-F. Pinton, Nature (London) **396**, 552 (1998); S. T. Bramwell *et al.*, Phys. Rev. Lett. **84**, 3744 (2000)], a generalized universality has been proposed, linking phenomena as dissimilar as two-dimensional (2D) magnetism and turbulence. To test these ideas, we performed Monte Carlo simulations of the 2D XY model. We found that the shape of the probability distribution function for the magnetization M is non-Gaussian and independent of the system size—in the range of the lattice sizes studied—below the Kosterlitz-Thoules temperature. However, our results suggest that in the full 2D XY model the shape of these distributions has a slight dependence on temperature—for finite volume—below the lattice-shifted critical temperature $T^*(L)$. This behavior can be explained by using renormalization group arguments and an extended finite-size scaling analysis, and by the existence of bounds for M.

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I. INTRODUCTION

The study of critical phenomena is of great interest not only because it allows the understanding of a large number of very different physical systems, like superfluid helium III, low temperature superconductors, ferromagnetic-paramagnetic systems, turbulent fluids and plasmas, polymers, snowflakes, and earthquakes, but also due to the existence of scale independence of the fluctuations at the critical temperature. In fact, although the underlying intermolecular forces responsible for the existence of phase transitions have a well-defined length scale, the structures they give rise to do not. This leads to the power-law behavior of physical quantities, very close to the critical temperature, which characterizes universality. The main challenge of the theory of critical phenomena is to explain how dissimilar systems exhibit the same critical behavior. Renewed interest in this subject has been raised because in a seminal paper [1] Bramwell, Holdsworth, and Pinton (BHP) argued that turbulence experiments can be explained in terms of a self-similar structure of fluctuations, just as in a finite critical system like the harmonic finite two-dimensional (2D) XY model (2DH XY model). The starting point of this conjecture was the observation that the probability distribution function (PDF) of the injected power fluctuations in a confined shear turbulent flow [2] has the same shape as the PDF of the magnetization in the 2DH XY model. It was also proposed that this analogy should provide an application of finite-size scaling in critical systems with experimental consequences.

In this paper, we report the results of a high precision Monte Carlo study of the full 2D XY model. This computation was carried out over the whole physical range of temperatures. The magnetic susceptibility was computed and the lattice-shifted critical temperature was obtained for different lattice sizes. Scaling laws for the magnetization-temperature ratio were tested. Our results agree with the rigorous findings of Chung [3]. We also found that, below the Berezinskii-Kosterlitz-Thouless temperature T_{BKT}, the shape of the PDF of the magnetization is non-Gaussian and independent of the lattice size, in agreement with previous results [4]. (They also observed corrections to universality for smaller systems containing fewer than 100 spins.) However, we found that the shape of these distributions does depend on the temperature, below $T^*(L)$. In addition, we performed simulations of the 2DH XY model and did not find a temperature dependence in the PDFs.

Recently, a result was reported in Ref. [5], where the full XY model was simulated for systems of up to 64^2 spins. The main result is that, as the system size gets larger, the PDF approaches the universal curve of BHP. We performed a Monte Carlo (MC) simulation with the 2D XY model for lattice sizes $L=10,16,32,64$, and 100 and $T=0.7$ to study this subject. Our preliminary results appear to confirm this claim.

In the preliminary version of this work [6], we reported systematic deviations in the tails of the PDF for finite systems. This fact was acknowledged in [5, p. 9]. These authors argue that "we can only expect agreement between the analytic result and the simulation in the range of temperature sufficiently below T_{BKT} such that vortex pairs do not influence the PDF [4]." However, according to the arguments explained in Refs. [1] and [4], this condition should be satisfied below the lattice-shifted temperature $T^*(L)$, where our simulations were made.

Our motivation to study the full 2D XY model was twofold. First of all, as was established by renormalization group studies of José *et al.* [7], the low temperature properties of the full 2D XY model are controlled by the Gaussian fixed point, and therefore it should be expected that the Villain type model studied in Refs. [1] and [4], the 2D XY model, should capture the critical properties of the full model below T_{BKT}. Nevertheless, that result holds only for the infinite volume system. It is therefore not clear *a priori* how important the finite volume corrections are to the renormalization group equations and how slow is the flow toward the fixed point (for instance, there are logarithmic corrections in the lattice size [8]). In this sense, the deviations in the shape of the PDFs between the 2D XY model and the 2DH XY model can be understood as a finite volume effect. Second, the general claim of Ref. [1] is that the universal shape of the PDF for different equilibrium and nonequilibrium systems, such as a coupled planar rotator, Ising and percolation models,

models of forest fires, sand piles, avalanches, and granular media in a self-organized critical state, is a consequence of the properties they share: finite size, strong correlations, and self-similarity. This is the case for the 2D XY model in the low temperature region, which has infinite correlation length in the thermodynamic limit in the whole range below the critical temperature T_{BKT}.

The universality proposed by BHP might go beyond the idea of equivalence classes in Wilson's renormalization group approach [9], by including into a generalized universality class systems sharing the properties of finite size, strong correlations, and self-similarity, even if their dimensions are different.

In [4], the two-dimensional probability distribution for the magnetization is calculated by means of a Monte Carlo simulation in the context of the 2DH XY model. This model is a further simplification of the Villain model [10], where the vortex variable n is not a thermodynamical quantity, but is constrained to the values $n=-1,0,1$. By using diagrammatic techniques, the authors of Ref. [4] showed that this asymmetry in the PDF could be the result of three-spin interactions and higher order corrections.

II. NUMERICAL SIMULATIONS

Here, we consider the 2D XY model, which describes classical planar spins with nearest neighbor interactions, with a Hamiltonian given by

$$H=-J\sum_{\langle i,j\rangle}\cos(\theta_i-\theta_j), \tag{1}$$

where J is the ferromagnetic coupling constant and θ_i is the angle of orientation of the unitary spin vector $\vec{s}_i$. The summation $\langle i,j\rangle$ is over nearest neighbors and the spins are defined on the sites of a square lattice of lattice size L, with periodic boundary conditions. From here on the ratio k_B/J is set equal to unity throughout the paper. This model undergoes a remarkable binding-unbinding topological phase transition, such that the free energy and all its derivatives remain continuous [11], and no long-range order at low temperatures exists, as stated by the Mermin-Wagner theorem [12]. This model has been extensively studied through both numerical and analytical methods [13].

Our simulation was performed on a square lattice of size $L=10$, 12, 16, 22, and 32 respectively. We estimate the MC sweeps needed for thermalization by plotting some observables like magnetization and energy. Typically 10^5 MC sweeps were used to reach thermal equilibrium. For thermal averages we used 5×10^5 spin configurations α_j. Because the 2D XY model has a continuous line of critical points below T_{BKT}, special care was taken to choose statistically independent configurations to evaluate thermal averages of physical observables X. This was achieved by computing its normalized autocorrelation function [14]

$$C(K)=\frac{\langle X_{\alpha_i}X_{\alpha_{i+K}}\rangle-\langle X_{\alpha_i}\rangle\langle X_{\alpha_{i+K}}\rangle}{\langle X^2_{\alpha_i}\rangle-\langle X_{\alpha_i}\rangle^2}, \tag{2}$$

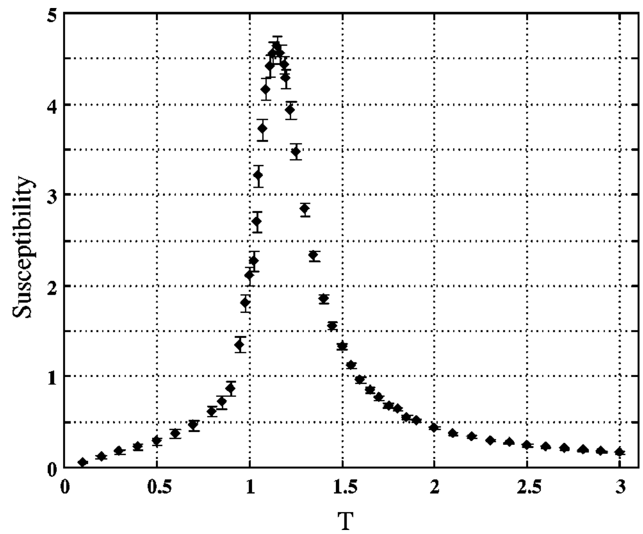

FIG. 1. Susceptibility for $L=16$ in the range $0<T\leqslant 3$. The peak at 1.15 corresponds to the shifted critical temperature. Notice that in all of the figures the axis variables are dimensionless [see text following Eq. (1)].

where X_{α_i} is the value of X in the configuration α_i at the ith step along the MC path through the configuration space, and the average $\langle\cdots\rangle$ was taken over this particular path of configurations separated by K steps from each other. $C(K)=1$ for $K=0$, but for large enough $K, C(K)$ drops to zero, which means that these configurations become totally uncorrelated. We choose K so that $C(K)$ is less that the recommended value 0.05 [15]. It is well known that, as a critical system approaches the critical temperature, the decorrelation time τ diverges with the power law $\tau\sim\xi^z$, where ξ is the (divergent) correlation length of the system and z is known as the dynamical critical exponent, which is approximately 2 for local-flip algorithms like the Metropolis algorithm. This phenomenon is known as critical slowing down [16]. This means in practice a serious limitation on numerical simulations of critical systems close to a critical point.

III. RESULTS AND DISCUSSION

In Fig. 1 we show MC data for the susceptibility for $L^2=256$ spins, as a function of the temperature. The peak occurs at the value $T_C(16)=1.15$, and corresponds to the temperature at which the correlation length equals L, which is the standard definition of the critical temperature of a finite system. We compute also the errors (standard deviations), which become larger as the critical temperature is approached. Another interesting feature of these errors is that they are larger below T_C. This can probably be explained because of the comparatively larger correlation lengths in this region, which corresponds to a continuous line of critical points with a temperature dependent exponent $\eta(T)$ [17] in the infinite volume limit.

We computed the critical temperature for the lattice sizes $L=10$, 12, 16, 22, 32. For $L=32$ we found an effective transition temperature $T_C=1.08$, in agreement with the value obtained in [18], where the linearized renormalization group

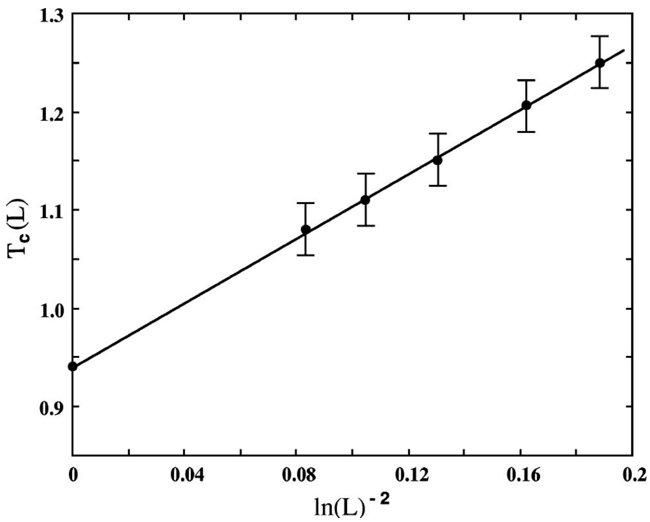

FIG. 2. The shifted critical temperature for different lattice sizes is plotted as a function of the system size.

(RG) equations for the finite size scaling were used. Figure 2 shows $T_C(L)$ as a function of $[\ln(L)]^{-2}$. The values can be described by the finite-size scaling formula [3]

$$T_c(L) \approx T_\infty + \frac{\pi^2}{4c(\ln L)^2}, \tag{3}$$

where T_∞ is the extrapolated value of the critical temperature for infinite volume. Within a few percents, of error, we found that the value of T_∞ agrees with the seemingly exact value 0.892 of the critical temperature T_{BKT} of the Berezinskii-Kosterlitz-Thouless (BKT) phase transition.

The ratio of the mean magnetization to critical temperature is plotted in Fig. 3 as a function of ln(L). These values are compatible with a negative straight line, as suggested in [4] in the context of the harmonic XY model. The values closer to the origin have larger statistical errors, due probably to finite-size effects, which are proportional to ln(L) [3,8].

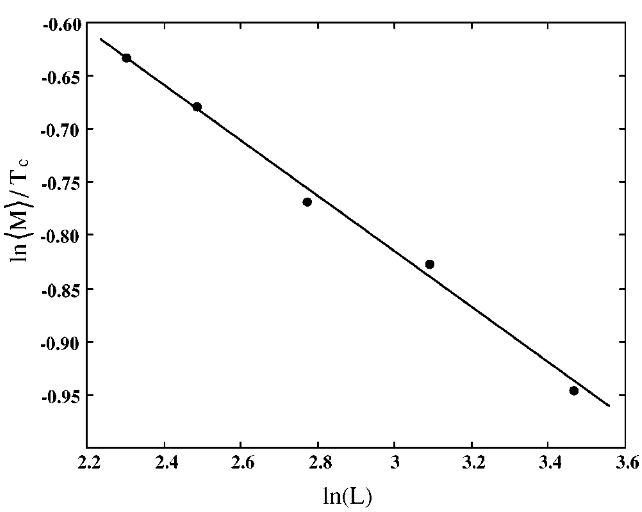

FIG. 3. Scaling relation for the magnetization-temperature ratio as a function of system size.

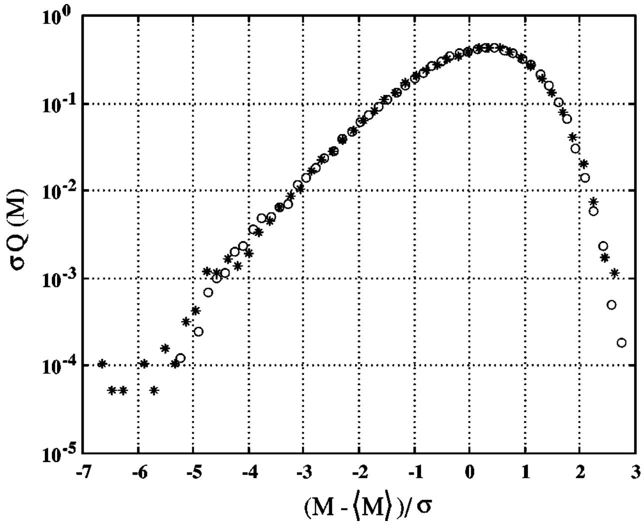

FIG. 4. Plots of $\sigma Q(M)$ vs $(M-\langle M\rangle)/\sigma$ at $T=0.70$ for lattice sizes $L=16$ (○) and $L=32$ (*).

In Refs. [1,4] there are two temperatures that play a central role, $T^*(L)$ and $T_c(L)$, where L is the system size. $T_c(L)$ is the temperature at which the correlation length equals L, and corresponds to the standard definition of the critical temperature for a system. $T^*(L)$ is the shifted T_{BKT} temperature in the sense that at this temperature the vortex distribution renormalizes in a self-similar manner on length scales up to L. This is determined by Monte Carlo simulations as the temperature where the scaling relation for the magnetization $\langle M\rangle \sim L^{-\beta/\nu}$ is satisfied by using the mean-field approximation for $T_{BKT}\sim \pi/2$ (this is the temperature where the renormalized spin-wave stiffness in the infinite system takes the universal value $2/\pi$): $\langle M\rangle = (1/CL^2)^{(1/16)}$, where $C=1.8456$ (see Refs. [3] and [4]). This definition is nevertheless not rigorous because it uses the BKT theory beyond its confirmed validity [3,17]. In fact, according to Cardy [19], the scaling relations of the infinite volume system are valid only in a narrow temperature window $(T-T_{BKT})/T_{BKT}<10^{-2}$.

In Fig. 4 a plot of $\sigma Q(M)$ as a function of $(M-\langle M\rangle)/\sigma$ can be seen, for lattice sizes $L=16$ and $L=32$ at the same temperature $T=0.70$. Here, Q is the PDF of M. These curves have similar shapes to those found in turbulence experiments, but only within a reduced range of temperatures below T_{BKT}. These PDFs can be conveniently compared with the universal form $\Pi(y) = K(e^{b(y-s)-e^{b(y-s)}})^a$ proposed in [1], by plotting the ratio $\sigma Q(M;T)/\Pi(M)$ vs $(M-\langle M\rangle)/\sigma$.

In Fig. 5, seven such curves, successively shifted by factors of 10 to separate them, are displayed for $L=16$ and $T=0.40,0.80,0.90,0.93,0.95,1.00$, and 1.05. Since $T^*(16)=0.94$, the first four values are below T^*. From the lower four curves of this plot it can be seen that when T is increased these ratios change consistently, showing the dependence of $Q(M;T)$ on the temperature. Despite the fact that our results could be affected by statistical effects, the deviations of the PDFs from the BHP distribution display a systematic trend below $T^*(L)$. This is a good reason to believe

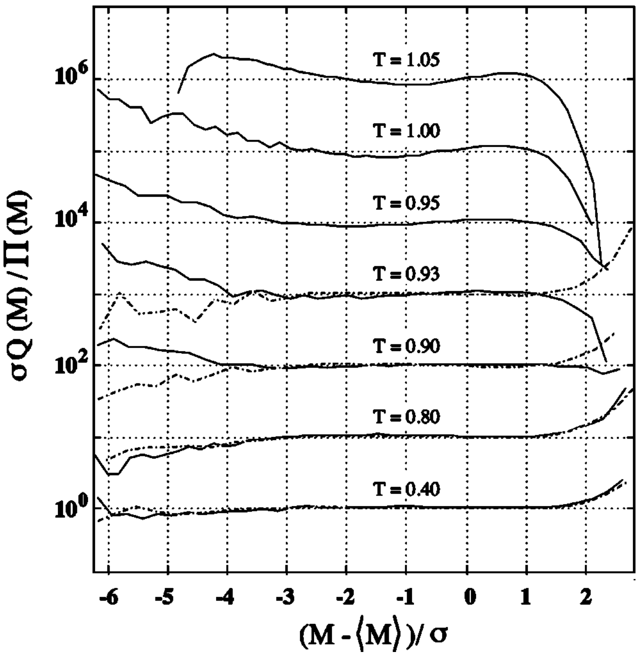

FIG. 5. $\sigma Q(M)/\Pi(M)$ ratios for seven values of temperature. The dashed curves correspond to the 2DH XY model (see text).

that these effects are not artifacts of the simulations. The rightmost part of these curves is raised, probably due in part to the upper bound $M=1$. Note that temperature effects are not observed in our results for the $2DH\ XY$ model, as can be seen in the four dashed curves in Fig. 5, at temperatures below T^*.

Above T^* the departures of the PDF from the universal BHP curve are even more pronounced, but this is not in conflict with the BHP results, because here the population of spin vortex pairs begins to increase. This happens because the system volume occupied by these vortices no longer contributes to the magnetization, which leads to a depleted probability density. This can be appreciated in the central and rightmost parts of the two upper curves.

The peaks are due to the bounds in the magnetization $0<M<1$. At $T=1.05$ this effect is greatly enhanced, and the leftmost part of the curve shows even more clearly the effect of the lower bound $M=0$. Concerning turbulent flows, we do not expect this type of bounding effect in the statistics of injected power. In principle, there are no limits to the fluctuations of such a quantity, and negative values are not excluded, meaning that the flow is delivering power to the driving system. Although this type of event is expected to be very unlikely, they are not forbidden.

We believe that in the full 2D XY model the temperature dependence of the PDF is not really a surprising result. The deviations in the shape of the PDFs between the 2D XY model and the 2DH XY model for finite volume can be understood by using the RG theory as follows. Let us consider the action represented by a point in the infinite dimensional space of couplings corresponding to multispin interactions. Repeated RG transformations move this point in the space of coupling constants, which generates the renormalized trajectory. The partition function is invariant under renormalization group transformations, and hence the physics of the system is the same along the renormalized trajectory.

In the XY model, the renormalization group trajectories flow into the Gaussian line of fixed points, at some particular value of the coupling $K(\infty)$, which is called the stiffness and depends on the temperature [17]. It turns out that the multispin interaction terms appearing in the action are irrelevant at the Gaussian fixed point, and therefore the low temperature properties of the model are controlled by this Gaussian fixed point.

Nevertheless, for finite volume the correspondence between the starting action and the fixed point action is a highly nontrivial problem because it amounts to computing exactly the rather involved renormalized trajectory and the corresponding renormalization constants, which have a cumbersome dependence on the temperature. We believe that the existence of these temperature-dependent renormalization constants is responsible for the deviations in the shape of the PDFs between the 2D XY model and the 2DH XY model at finite volume. With the above arguments in mind we now consider the discussion of the dependence of the PDF on the order parameter close to a single critical point $\xi \sim L$, made by Binder in the context of the Ising model [20]. He argued that the PDF does not depend separately on the three variables ξ, L, M, but only on the two scaled combinations L/ξ and $M\xi^{\beta/\nu}$:

$$\begin{aligned} P_L(M) &= \xi^{\beta/\nu}\tilde{P}(L/\xi, M\xi^{\beta/\nu}) \\ &= L^{\beta/\nu}P(L/\xi, ML^{\beta/\nu}). \end{aligned} \tag{4}$$

This expression, based on phenomenological renormalization, is useful to study finite-size scaling. He also argued that in the critical region $\xi \gg L$ $P_L(M)$ is no longer Gaussian. In the scaling region, it is a good approximation to take $P_L(M)$ equal to the PDF proposed by Bramwell *et al.* [The standard deviation σ plays the role of $L^{-\beta/\nu}$ in the BHP distribution; this can be seen by using the standard definitions of the critical exponents and the relation $\sigma = \sqrt{(T/L^2 \chi}$.] This expresion was already used in the first paper of Ref. [4] to drop the L/ξ dependence in the PDF in the low temperature regime. An important point to notice here is that Binder's expression should be valid only in the neighborhood of a single critical point, as originally proposed by Binder. In spite of this fact, and considering that from the point of view of quantum field theory the PDF corresponds to the exponential of minus the constraint effective potential [21], the temperature dependence of the renormalized coupling constants for finite volume mentioned in the discussion above leads therefore to a T dependence of Binder's expression.

To ensure the validity of our conclusions in the range of temperatures below $T^*(L)$, we repeated our simulations increasing the number of MC configurations from 5×10^5 to 10^7 to obtain thermal averages, and noticed no significant changes in the results. As the sensitivity of PDFs is weak in the region of interest, i.e., their wings, we have chosen to plot the skewness and kurtosis versus the temperature of these distributions, as suggested by Chapman *et al.* [22], in

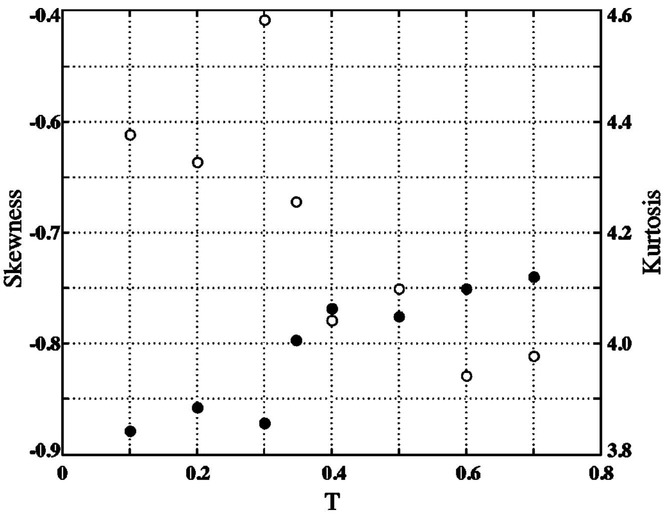

FIG. 6. Skewness (●) and kurtosis (○) of $Q(M)$ as a function of temperature for $0.1 \leqslant T \leqslant 0.7$.

the range $0.1 \leqslant T \leqslant 0.7$. As can be seen in Fig. 6, these plots display a clear trend, which confirms our previous statement regarding the PDF's temperature dependence. The slopes for skewness and kurtosis are 0.26 and -0.88, respectively. The determination of the precise effect of the temperature on these distributions is the object of ongoing analytic and numerical work.

IV. CONCLUSIONS

In conclusion, we found that the probability distribution function of the magnetization in the 2D XY model is independent of the system size—in the range of the lattice sizes studied—but its shape displays a slight but systematic temperature dependence below $T^*(L)$. This temperature dependence can be explained by using RG arguments for finite-volume systems [see discussion above Eq. (4)]. Additionally, there is a contribution coming from the constrained character of the magnetization.

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