No quasi-long-range order in a two-dimensional liquid crystal

Ricardo Paredes V.,[1] Ana Isabel Fariñas-Sánchez,[2] and Robert Botet[3]
[1]Centro de Física, Instituto Venezolano de Investigaciones Científicas, Laboratorio de Fisica Estadística Apdo. 20632, Caracas 1020A, Venezuela
[2]Department of Physics, Universidad Simón Bolívar, Apdo. 89000, Caracas 1080A, Venezuela
[3]Laboratoire de Physique des Solides Bât. 510, CNRS UMR8502, Université Paris-Sud, F-91405 Orsay, France

(Received 16 June 2008; published 24 November 2008)

Systems with global symmetry group $O(2)$ experience topological transition in the two-dimensional space. But there is controversy about such a transition for systems with global symmetry group $O(3)$. As an example of the latter case, we study the Lebwohl-Lasher model for the two-dimensional liquid crystal, using three different methods independent of the proper values of possible critical exponents. Namely, we analyze the at-equilibrium order parameter distribution function with (1) the hyperscaling relation; (2) the first-scaling collapse for the probability distribution function; and (3) the Binder's cumulant. We give strong evidence for definite lack of a line of critical points at low temperatures in the Lebwohl-Lasher model, contrary to conclusions of a number of previous numerical studies.

DOI: 10.1103/PhysRevE.78.051706 PACS number(s): 64.70.M−, 05.70.Jk

I. INTRODUCTION

Mermin and Wagner [1] established that no ferromagnetic phase nor any long-range order can appear for systems of continuous symmetry at finite temperature in space dimension $d \leqslant 2$. However, such systems might have another type of transition governed by binding-unbinding topological defects at definite positive temperature T_{BKT} [2–4]. This kind of topological phase transition is called Berezinskii, Kosterlitz, and Thouless (BKT) transition.

The two-dimensional (2D) XY model, with global symmetry group $O(2)$, exhibits such topological transition [4]. Quasi-long-range order (QLRO) appears at low temperatures T, and the order parameter vanishes as a power law at the thermodynamic limit. Due to the QLRO behavior, the system susceptibility χ, that measures the fluctuations of the order parameter, diverges for all temperatures $T \leqslant T_{\text{BKT}}$, and the system is characterized by a line of critical points below the critical temperature T_{BKT}. Close to $T=0$, correlations are dominated by spin-wave solution: In the units system where $k_B=1$ and the coupling factor between magnetic moments is $J=1$, the correlation function exponent, η, depends on the temperature as $\eta = T/2\pi$. Another characteristic behavior of this transition is that at temperatures just above the BKT transition, $t=(T-T_{\text{BKT}})/T_{\text{BKT}} \gtrsim 0$, the correlation length, ξ, diverges as the essential singularity, $\xi \sim \exp(bt^{-1/2})$, that is much stronger than the ordinary second-order transition power law, $\xi \sim t^{-\nu}$.

On the other hand, Polyakov [5], using renormalization group theory, proved that the 2D Heisenberg model, with global symmetry group $O(3)$, does not present any sort of phase transition. An important difference between the two systems above is that the global symmetry group for the XY model is Abelian, while it is not for the Heisenberg model. However, things are not so clear: Numerical evidences were recently given for transition [6–10] in this system, and a possible QLRO phase [6,11] at very low temperatures. In the same spirit, it has also been reported that the 2D fully frustrated antiferromagnetic Heisenberg model presents a cross-over produced by the binding-unbinding of topological defects in a very narrow temperature interval. In this case no QLRO behavior at or below the transition [12,13] has been observed. At present, this controversy on systems with continuous non-Abelian symmetry is not solved.

Kunz and Zumbach (KZ) [14] performed an intensive Monte Carlo study of the 2D RP^2 model, which has the global symmetry group $O(3)$ and the local symmetry group Z_2. The model describes the isotropic-nematic transition of a liquid crystal. KZ concluded with BKT-like transition from analysis of energy, specific heat and topological quantities. But the correlation length behavior for $t \gtrsim 0$ was not proven to be either of the power-law or of the essential singularity type. Ten years later, the problem of phase transitions for liquid crystals in $d=2$ was complemented [6,15,16] using the powerful techniques of conformal transformations (CT) [17] and finite size scaling (FSS) [6,16]. The Lebwohl-Lasher (LL) [18] was preferred to the RP^2 model though sharing the same symmetries. These studies concluded with a BKT-like transition and a QLRO phase below the BKT temperature estimated by KZ [14] to be $T_{\text{BKT}}=0.513$. At low temperatures, a spin-wave dependence $\eta \propto T$ was obtained. To support this conclusion Dutta and Roy [19] showed that the transition is driven by topological stable points defects known as $\frac{1}{2}$-disclination points.

Using FSS for the system susceptibility, χ, it is possible to estimate the value of the correlation function exponent η within the temperature range $T \leqslant T_{\text{BKT}}$. On a line of critical points, χ should scale with the exponent γ/ν, which is related to η through the hyperscaling law

$$\gamma/\nu = 2 - \eta. \quad (1)$$

Using (1), estimation of the values of η was performed [6,20]. The values appeared to behave similarly to the ones obtained through CT and scaling of the order parameter, but there is a discrepancy of about 5% between both results. The origin of such difference was tentatively explained arguing that the system sizes were far from the thermodynamic limit and the number of independent realizations were too small to reach good statistics.

The purpose of this paper is to revisit the problem of the possible appearance of quasi-long-range order for the 2D LL model. In the LL model, liquid-crystal molecules are represented by unitary three-dimensional (3D) vectors $\vec{\sigma}_i$ situated on the sites, labeled i, of a hypercubic lattice Λ of length L. The Hamiltonian is given by

$$-\beta H = \sum_i \sum_\delta P_2(\vec{\sigma}_i \cdot \vec{\sigma}_{i+\delta}), \qquad (2)$$

where $\beta = 1/T$, P_2 is the second Legendre polynomial and the interaction is between nearest neighbors. The appearance of the P_2 function in (2) comes from the Z_2 local symmetry. In the nematic phase, the preferential direction is characterized by the unit vector **n**, called the director, and one can measure the local orientation with respect to the director by $\vec{\sigma}_i \cdot \mathbf{n} = \cos\theta_i$. Then, the local order parameter is defined by $m(i) = \langle P_2(\cos\theta_i)\rangle$. Whenever the system is completely ordered, $m(i) = 1$.

Therefore, we start from the hypothesis that the 2D LL model experiments BKT transition at $T_{\mathrm{BKT}} = 0.513$, similar to the transition observed in the 2D XY model at $T_{\mathrm{BKT}} = 0.893$. Below such critical temperature a line of critical points should be observed in both models. To validate this point, we performed Monte Carlo simulations using the Wolff algorithm [21] in $d = 2$, with periodic boundary conditions at temperatures well below T_{BKT}. A total of 6×10^6 independent realizations were performed for each system size and each temperature for both models. Then we found estimates of the order parameter probability distribution function (PDF), and estimation of the validity for the hyperscaling relation (1). Finally we will analyze the Binder's cumulant behavior, comparing also with the Heisenberg model.

II. HYPERSCALING RELATION CHECK

For the XY model at $T = 0.6$, we observe that both the order parameter and the susceptibility have power-law behavior, $\langle m\rangle \sim L^{-\beta/\nu}$ and $\chi \sim L^{\gamma/\nu}$, respectively. For the XY system the exponents obtained were $\beta/\nu = \eta/2 \approx 0.058$ and $\gamma/\nu \approx 1.877$. With use of the CT method, Berche *et al.* [22] obtained the value $\beta/\nu = 0.0595$ in excellent agreement with our results. Hyperscaling relation (1) is satisfied with error smaller than 0.4%.

For the LL model at $T = 0.4$, we obtained again excellent power laws for $\langle m\rangle$ and χ with respective exponents $\beta/\nu = \eta/2 \approx 0.0945$ and $\gamma/\nu \approx 1.868$. But now, the agreement for Eq. (1) is poor and about 3% (one order of magnitude larger than for the XY case). The actual increase of the number of independent realizations does not really improve the results obtained previously [6,20].

We shall use now an alternative method to check the hyperscaling relation. Let us introduce σ as the standard deviation of the order parameter. One has $\sigma^2 \propto \chi/L^d$, then σ scales with the system size as $\sigma \sim L^{\gamma/2\nu - 1}$ for the 2D systems. Therefore, the ratio $\langle m\rangle/\sigma$ should be a constant whenever the hyperscaling relation (1) is satisfied. The great advantage for using this ratio is that previous estimation of the exponents is not necessary to check (1). In Fig. 1, $\langle m\rangle/\sigma$ is plotted versus L^{-1} for the XY (above) and the LL (below) models in the low-temperature domain.

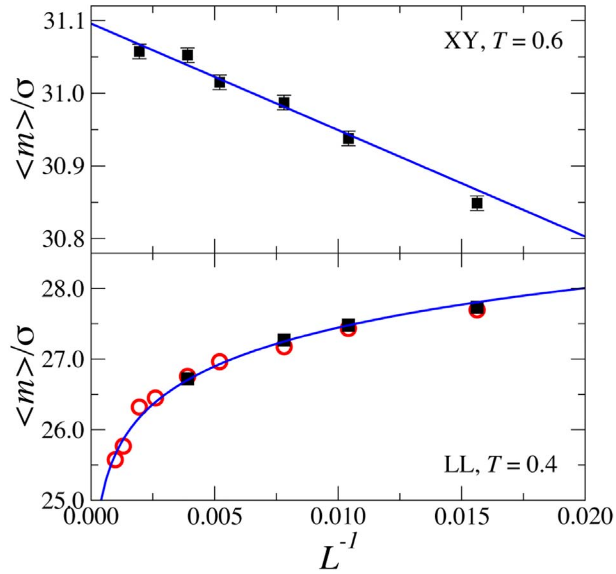

FIG. 1. (Color online) $\langle m\rangle/\sigma$ is plotted vs L^{-1} for the XY model at $T = 0.6$ (top) and for the LL model at $T = 0.4$ (bottom). A linear fit is obtained for the XY model ($\langle m\rangle/\sigma = 31.1 - 16.4/L$). A power-law fit shows that no saturation is observed for the LL model. Both fits are shown as bold lines. The circles are the data from [6]. The number of independent realizations used to obtain the bold squares is almost two orders of magnitude larger than in [6]. The hyperscaling relation (1) is not satisfied in the thermodynamic limit by the LL model at $T = 0.4$.

For the XY model, the ratio is seen to saturate at the thermodynamic limit to a value $\langle m\rangle/\sigma \simeq 31.1$.

For the LL model, power law is the best fit consistent with our data for $\langle m\rangle/\sigma$ versus L. The ratio does not saturate to a finite value and we conclude that the hyperscaling relation (1) does not hold in this case.

Similar behavior was observed for the XY model at $T_{\mathrm{BKT}} = 0.893$ [23] and for the LL model at $T_{\mathrm{BKT}} = 0.513$ [20].

III. FIRST-SCALING RELATION CHECK

The first-scaling law [24]:

$$\langle m\rangle P(m) = \Phi_T(z_1) \quad \text{with } z_1 \equiv \frac{m}{\langle m\rangle}, \qquad (3)$$

should be satisfied anywhere on the line of critical points below the BKT transition. In (3), $P(m)$ denotes the order parameter PDF. The scaling function Φ_T depends only on the actual temperature. Here too, one great advantage of the first-scaling law is that Eq. (3) does not require knowledge of any critical exponent. In Fig. 2 the order parameter PDF is plotted in the first-scaling form for both models.

For the XY model, the three curves exhibit almost perfect collapse. Relation (3) is clearly satisfied at $T = 0.6$. Similar behavior was observed previously for the XY model at T_{BKT} [23]. The definite shape of the scaled distribution is Weibull-like [20] similar to the T_{BKT} case [23].

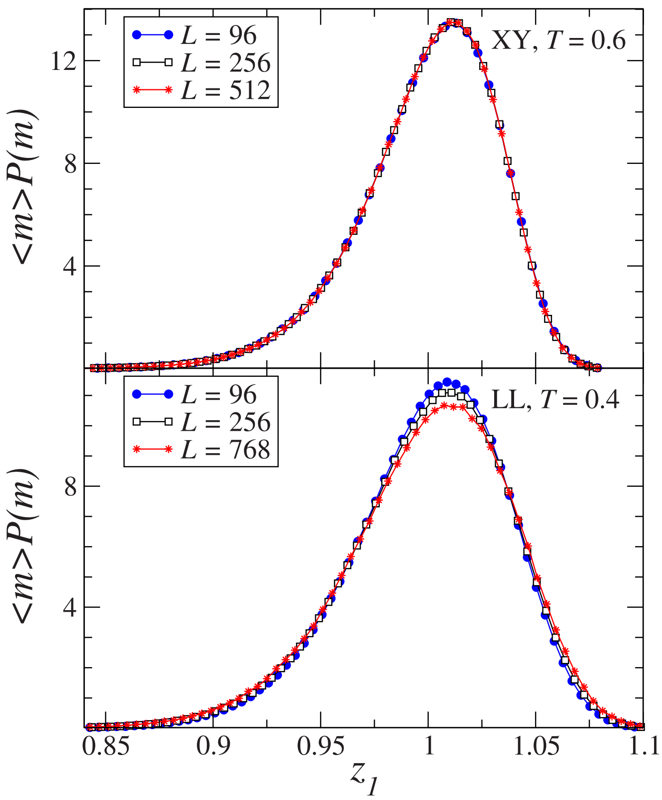

FIG. 2. (Color online) Order parameter PDF for the *XY* model at $T=0.6$ (top) and the LL model at $T=0.4$ (bottom) in the first-scaling form. A perfect collapse is observed for the *XY* model. This is not the case for the LL model. The $L=768$ data are from [6], with 9×10^4 independent realizations. It is clear from this figure that the number of independent realizations used in [6] was large enough to realize the first-scaling law. No self-similarity is observed for the LL model at $T=0.4$.

For the LL model, collapse is not realized in Fig. 2. As the system size is increased, the scaled distributions tend to separate for $T=0.4$. This is evidence that the LL model is not at a critical point for this temperature.

IV. BINDER'S CUMULANT CHECK

For a continuous phase transition the Binder's cumulant,

$$U_4 = 1 - \frac{\langle m^4\rangle}{3\langle m^2\rangle}, \tag{4}$$

is known to be a universal quantity independent of L at the critical point [25].

For the *XY* model, U_4 is universal for $T\leq T_{\mathrm{BKT}}$ [26]. It is checked in Fig. 3 where U_4 is plotted for this model (above). For the *XY* model a crossing point is observed near the reported BKT temperature. For temperatures below the crossing point, the U_4 grows with the system size. All the curves are expected to collapse in this interval when $L\to\infty$. It is faster when the temperature is small [20]. On the other hand, the U_4 above the crossing point, decreases with increasing L. This type of behavior is observed in other $O(2)$ models with Z_2 symmetry [27,28].

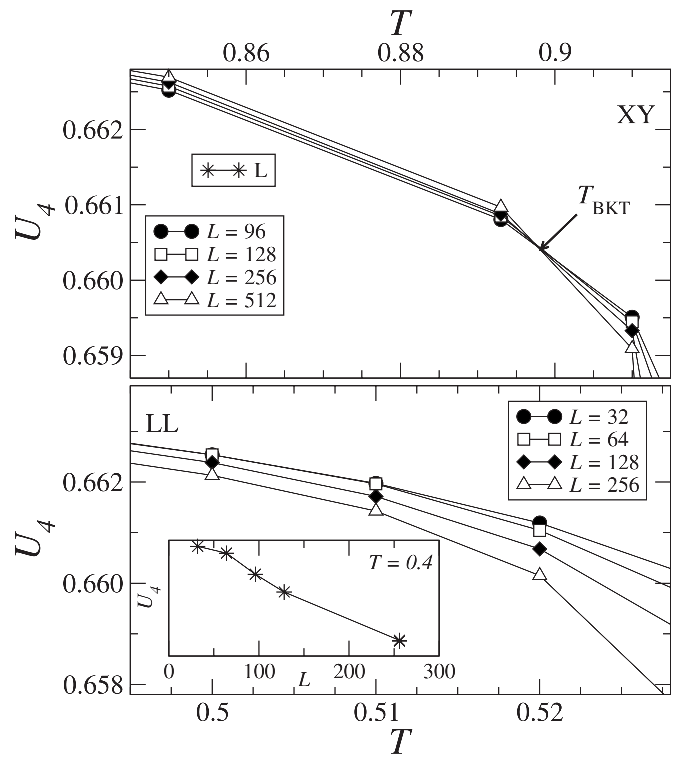

FIG. 3. The Binder cumulant vs the temperature for the *XY* model $T=0.6$ (top) and the LL model (bottom). The number of independent realizations is 10^5 for each T and L. No crossing is observed for the LL model. Therefore, no evidence of any phase transition is observed for the LL model. Values of the Binder cumulant for $T=0.4$ are shown in the inset as a function of the system size. We used 6×10^6 independent realizations to obtain each point, so that the error bars are much smaller than the symbol size.

The behavior of U_4 is completely different for the LL model. The Binder cumulant decreases with L in all of the domains of temperature explored ($T>0.1$). No crossing is observed anywhere in Fig. 3 (bottom).

To complement the discussion, we study the Binder cumulant behavior for the Heisenberg model at $T>0.1$. It is seen to behave very similarly to the 2D LL model, as no crossing is observed (see Fig. 4). Then we can conclude that in the low-temperature range, the LL model must have very large (but not infinite) correlation length, that suddenly begin

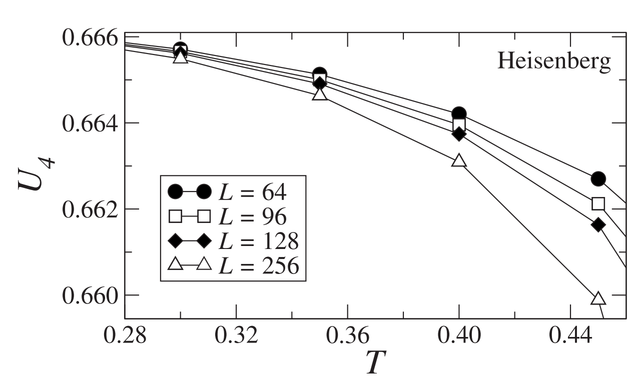

FIG. 4. The 2D Binder cumulant for the Heisenberg model exhibits the same type of behavior as for the LL model (see Fig. 3).

to decrease in the neighborhood of $T=0.513$. For this reason an apparent QLRO phase may be observed below this temperature.

V. DISCUSSION

We presented in this paper three strong evidences supporting the idea that the Lebwohl-Lasher liquid crystal in 2D does not have a quasi-long-range order phase, namely,

(a) the hyperscaling (1) is not satisfied;

(b) the first-scaling collapse (3) does not hold;

(c) the Binder cumulant (4) does not exhibit any crossing point.

Then this system cannot experience a transition of the BKT type.

From FSS analysis, Mondal and Roy [29] concluded that the LL model should present a continuous transition at $T=0.548$. The lack of crossing event for the Binder cumulant behavior (as observed in Fig. 3) definitely suggests that this is not the case. In Refs. [6,20] the stiffness and the susceptibility are studied as functions of temperature T and system size L for the LL and the XY models. For the XY model the stiffness saturates to finite value below T_{BKT}. However, for the LL model the stiffness tends to decrease logarithmically with the system size, similar to the behavior of the fully frustrated antiferromagnetic Heisenberg model (FFAH) [13]. On the other hand, the susceptibility for the LL model changes its functional form in a small region of temperature around $T=0.513$. This is also observed in the FFAH [13]. Then for this reason, and knowing the fact that topological defects are stable [19], we speculate that the LL model may have a crossover similar to FFAH.

The set of critical-exponents free methods used in this paper can be used to explore any thermodynamic systems and to identify possible critical points. The hyperscaling relation and the first-scaling law are of great utility to identify whether a system is or is not at a critical point. In particular, such a procedure could be helpful for the Heisenberg model in the $T<0.1$ domain, to discuss a possible transition at very low temperature [6–10].

ACKNOWLEDGMENT

A.I.F-S. and R.P. thank Bertrand Berche for stimulating discussions about the subject of this paper.

[1] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[2] V. I. Berezinskii, Sov. Phys. JETP **34**, 610 (1971).

[3] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

[4] J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).

[5] A. M. Polyakov, Phys. Lett. **59B**, 79 (1975).

[6] A. I. Fariñas-Sánchez, Ph.D. thesis, Instituto Venezolano de Investigaciones Científicas, Caracas, Venezuela, 2004; Ph.D. thesis, Université Henri Poincaré–Nancy 1, France, 2004.

[7] F. Niedermayer, M. Niedermaier, and P. Weisz, Phys. Rev. D **56**, 2555 (1997).

[8] A. Patrascioiu and E. Seiler, Phys. Rev. Lett. **74**, 1920 (1995); J. Stat. Phys. **106**, 811 (2002); Phys. Rev. B **54**, 7177 (1996); Phys. Rev. D **57**, 1394 (1998).

[9] A. Patrascioiu, Europhys. Lett. **54**, 709 (2001).

[10] M. Aguado and E. Seiler, Phys. Rev. D **70**, 107706 (2004).

[11] O. Kapikranian, B. Berche, and Yu Holovatch, J. Phys. A **40**, 3741 (2007).

[12] H. Kawamura and M. Kikuchi, Phys. Rev. B **47**, 1134 (1993).

[13] M. Wintel, H. U. Everts, and W. Apel, Phys. Rev. B **52**, 13480 (1995).

[14] H. Kunz and G. Zumbach, Phys. Lett. B **257**, 299 (1991); , Phys. Rev. B **46**, 662 (1992).

[15] A. I. Fariñas Sánchez, R. Paredes, and B. Berche, Phys. Lett. A **308**, 461 (2003).

[16] R. Paredes, A. I. Fariñas-Sánchez, and B. Berche, Rev. Mex. Fis. **52**, 181 (2006).

[17] J. L. Cardy, Nucl. Phys. B **240**, 514 (1984).

[18] P. A. Lebwohl and G. Lasher, Phys. Rev. A **6**, 426 (1972).

[19] S. Dutta and S. K. Roy, Phys. Rev. E **70**, 066125 (2004).

[20] A. I. Fariñas-Sánchez, R. Paredes V., and R. Botet (unpublished).

[21] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).

[22] B. Berche, A. I. Fariñas-Sánchez, and R. Paredes, Europhys. Lett. **60**, 539 (2002).

[23] R. Paredes V. and R. Botet, Phys. Rev. E **74**, 060102(R) (2006).

[24] R. Botet, M. Płoszajczak, and V. Latora, Phys. Rev. Lett. **78**, 4593 (1997).

[25] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).

[26] D. Loison, J. Phys.: Condens. Matter **11**, L401 (1999).

[27] A. I. Fariñas-Sánchez, R. Paredes, and B. Berche, Phys. Rev. E **72**, 031711 (2005).

[28] B. Berche and R. Paredes, Condens. Matter Theor. **8**, 723 (2005).

[29] E. Mondal and S. K. Roy, Phys. Lett. A **312**, 397 (2003).