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

Ricardo Paredes V.†, Ana Isabel Fariñas-Sánchez‡ and Robert Botet*

† Instituto Venezolano de Investigaciones Científicas, Centro de Física,
Laboratorio de Física Estadística Apdo. 20632, Caracas 1020A, Venezuela
‡ Universidad Simón Bolívar, Dept Fís, Apdo. 89000, Caracas 1080A, Venezuela
* Laboratoire de Physique des Solides Bât.510, CNRS UMR8502 - Université Paris-Sud, F-91405 Orsay, France

(Dated: August 22, 2008)

PACS numbers: 64.70.M-, 64.60.Bd, 64.70.mf, 05.70.Jk, 05.50.+q

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 \( d \leq 2 \). However, such systems might have another type of transition governed by binding-unbinding topological defects at definite positive temperatures. In this paper, 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 evidences 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.

Systems with global symmetry group \( O(2) \) experience topological transition in the 2-dimensional space. But there is controversy about such a transition for systems with global symmetry group \( O(3) \). In this paper, 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 evidences 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.

On the other hand, Polyakov [5], using renormalization group theory, proved that the 2d Heisenberg model through the hyperscaling law:

\[
\xi \sim \exp(bt^{-1/2}), \quad \xi \sim t^{-\nu},
\]

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 the system susceptibility, \( \chi \), FSS was able to estimate the value of the correlation function exponent \( \eta \) within the temperature range \( T \leq T_{\text{BKT}} \). On a line of critical points, \( \chi \) should scale with the exponent \( \gamma/\nu \), which is related to \( \eta \) through the hyperscaling law:

\[
\gamma/\nu = 2 - \eta. \tag{1}
\]

Using (1), estimation of the values of \( \eta \) was performed [6, 20]. The values appeared to behave similarly to the ones obtained through CT and scaling of the order pa-
rameter, 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 article is to revisit the problem of the possible appearance of BKT-like transition for the 2d LL model. In this model, liquid-crystal molecules are represented by unitary vectors $\vec{\sigma}_i$ situated on the sites, labelled $i$, of a hypercubic lattice $\Lambda$ of length $L$. The Hamiltonian is given by:

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

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 $\mathbf{n}$, called the director, and one can measure the local orientation with respect to the director by: $\hat{\sigma}_i \cdot \mathbf{n} = \cos \theta_i$. 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 $T_{\text{BKT}} = 0.513$, similarly to the transition observed in the 2d XY-model at $T_{\text{BKT}} = 0.893$. 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 \cite{21} in $d = 2$, with periodic boundary conditions at temperatures well below $T_{\text{BKT}}$. A total of $6 \times 10^6$ 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 \cite{20}. Finally, we will analyze the Binder’s cumulant behavior, comparing also with the Heisenberg model.

**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 \cite{22} obtained the value $\beta/\nu = 0.0595$ in excellent agreement with our results. Hyperscaling relation \cite{20} 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 $\chi$ with respective exponents $\beta/\nu = \eta/2 \approx 0.0945$ and $\gamma/\nu \approx 1.868$. But now, the agreement for Eq. \cite{20} 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 \cite{6,20}.

![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 bold circles are the data from \cite{6}. The number of independent realizations used to obtain the bold squares is almost two orders of magnitude larger than in \cite{6}. The hyperscaling relation \cite{20} is not satisfied in the thermodynamic limit by the LL-model at $T = 0.4$.](image)

**First-scaling relation check.** – The first-scaling law \cite{24}:

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

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 \( \Phi_T \) 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 \( T_{\text{BKT}} \) [23]. The definite shape of the scaled distribution is Weibull-like [20] similarly to the \( T_{\text{BKT}} \) case [23].

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.

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 on \( L \) at the critical point [25].

For the XY-model, \( U_4 \) is universal for \( T \leq T_{\text{BKT}} \) [20]. It is checked on the 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 others \( O(2) \) models with \( Z_2 \) symmetry [27, 28].

The behavior of \( U_4 \) is completely different for the LL model. The Binder cumulant decreases with \( L \) in all the domain of temperature explored (\( T > 0.1 \)). No crossing is observed anywhere in Fig. 3 (bottom).
$T = 0.513$. For this reason an apparent QLRO phase may be observed below this temperature.

![Diagram](image_url)

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

**Discussion.** We presented in this paper three strong evidences supporting the idea that the 2d liquid crystals do not have a quasi-long-range order phase, namely:

(a) the hyperscaling [11] 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 can not 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 reference [5] 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 $T_{\text{BKT}}$. However for the LL model the stiffness tends to decrease logarithmically with the system size, similar to the behavior of the fully frustrated anti-ferromagnetic 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 [13], we speculate that the LL model may have a crossover similar to FFAH.

The set of critical-exponents free methods used in this article 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 procedure could be helpful for the Heisenberg model in the $T < 0.1$ domain, to discuss about a possible transition at very low temperature $T < 0.1$.

AIFS and RP like to thank Bertrand Berche for stimulating discussions about the subject of this article.

[1] N.D. Mermin and H. Wagner, Phys. Rev. Lett. 22 1133 (1966).
[2] V.I. Berezinskii, Soviet 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. B 59, 79 (1975).
[6] A.I. Fariñas-Sánchez, PhD Thesis IVIC-UHP (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, Yu Holovatch, J. Phys. A: Math. Theor. 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 [FS12], 514 (1984).
[18] P.A. Lebwohl and G. Lasher, Phys. Rev. A 6, 426 (1973).
[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. (2008).
[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 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, Condensed Matter Theory 8, 723 (2005).
[29] E. Mondal and S. K. Roy, Phys. Lett. A 312, 397 (2003).