Evidence for a topological transition in nematic-to-isotropic phase transition in two dimensions

A.I. Fariñas Sanchez\textsuperscript{a,b}, R. Paredes V.\textsuperscript{a} and B. Berche\textsuperscript{b}

\textsuperscript{a} Centro de Física, Instituto Venezolano de Investigaciones Científicas, Apartado 21827, Caracas 1020A, Venezuela

\textsuperscript{b} Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy 1, F-54506 Vandœuvre les Nancy Cedex, France

November 29, 2018

Abstract

The nematic-to-isotropic orientational phase transition, or equivalently the $RP^2$ model, is considered in two dimensions and the question of the nature of the phase transition is addressed. Using powerful conformal techniques adapted to the investigation of critical properties of two-dimensional scale-invariant systems, we report strong evidences for a transition governed by topological defects analogous to the Berezinskii-Kosterlitz-Thouless transition in two-dimensional $XY$ model.

Liquid crystals may be seen as constituted of molecules essentially represented by long rigid rods. From maximization of entropy at high temperatures, all the molecule orientations are equally probable, independently of the neighbouring molecule directions and the system exists in an isotropic phase. At low temperatures a preferential orientation is more favourable in order to minimize interaction terms, and an ordered structure emerges. When order occurs along one space dimension only, the system is said to be nematic. Still at lower temperatures, other ordered phases can appear, e.g. smectic phases.

In a lattice model, each molecule may be represented by a unit vector $\sigma_w$ at site $w$ of a hypercubic lattice $\Lambda$ of linear extent $L$. The $\sigma$’s live in a three-dimensional space attached to each lattice site. In the nematic phase, the preferential direction defines a unit vector, $n$, called the director, and one can measure the deviation of molecule $\sigma_w$ with respect to the director by the scalar product $\sigma_w \cdot n = \cos \theta_w$. Due to the local $Z_2$ symmetry (the rods are not oriented), one cannot distinguish between opposite directions $\theta_w$ and $\theta_w + \pi$, and $\cos \theta_w$ vanishes on average while $\cos^2 \theta_w$ does not. In the disordered phase on the other hand, the angles are measured with respect to any arbitrary direction, and the thermal average of course leads to $\langle \cos \theta_w \rangle = 0$ and $\langle \cos^2 \theta_w \rangle = \frac{1}{3}$, so that $\langle \cos^2 \theta_w \rangle - \frac{1}{3}$ represents a convenient order parameter. In the literature on liquid crystals, one usually defines the local order parameter by the second Legendre polynomial,

$$m(w) = \langle P_2(\sigma_w \cdot n) \rangle = \langle P_2(\cos \theta_w) \rangle. \quad (1)$$

This definition suggests to consider the following Hamiltonian to describe the nematic transition,

$$-\frac{H}{k_B T} = \frac{J}{k_B T} \sum_w \sum_{\mu} P_2(\sigma_w \cdot \sigma_{w+\mu}), \quad (2)$$

where $\mu$ stands for the unit basis vectors of the lattice, $\sigma_w \cdot \sigma_{w+\mu} = \cos(\theta_w - \theta_{w+\mu})$ is the scalar product between neighbouring vectors distant from one lattice spacing, and the interaction term $-JP_2(\sigma_w \cdot \sigma_{w+\mu})$ is reminiscent from a dipole-dipole interaction. This Hamiltonian was introduced by Lebwohl and Lasher [1] as a lattice version of the mean field theory of Maier and Saupe [2], and its success came from its ability to reproduce the weak first order phase transition observed experimentally in the
three dimensional nematic transition \[3\]. In a more abstract context, this Hamiltonian is known as the \(RP^2\) model, since at each lattice site is attached the manifold of directions in 3-dimensional space, also called the real projective space in 3 dimensions \[4\].

Like the non linear \(\sigma\)-model, this model possesses generically the symmetry group \(O(n)\) which is non abelian for \(n \geq 3\), and specifically the Lebwohl-Lasher or \(RP^2\) model has a \(O(3)\) symmetry. The question, as it was outstandingly formulated by Kunz and Zumbach \[4\], of the nature of the transition in the \(RP^2\) model in two dimensions is still incompletely solved. The existence of a phase transition (at finite temperature) in two dimensional systems seems connected to the abelian nature of the underlying symmetry group, as both Ising and \(XY\) models are famous examples, unlike the Heisenberg model. On the other hand, according to the Hohenberg-Mermin-Wagner theorem \[5, 6\], models possessing a continuous symmetry group cannot exhibit any finite macroscopic magnetization with no magnetic field applied in dimensions 1 or 2 (we intentionally use the familiar terminology of magnetic systems). The two-dimensional \(XY\) model is the most famous example and it exhibits a non conventional transition \[7, 8, 9\]. In spite of the absence of long-range order (LRO) at low temperatures, the spin-spin correlation function decays algebraically with an exponent which increases monotonically with temperature \[10, 11, 12\] up to a temperature called after Berezinskii, Kosterlitz and Thouless \[13, 14, 15\]. In this critical phase, macroscopic ordering is prevented by collective excitations, namely spin waves which nevertheless do not exclude a coherent orientation of spins at a smaller length scale. Together with the spin waves, localized excitations appear with increasing temperature. These are topological defects associated in pairs, like pairs of opposite charges in the low temperature phase of a two-dimensional Coulomb gas, and they perturb the spin field only locally. This is the usual meaning of the term quasi-long-range order (QLRO). The Berezinskii-Kosterlitz-Thouless transition is governed by unbinding of these defects which completely suppresses any type of long-range order at high temperature, hence the correlation functions decay exponentially like in an ordinary paramagnetic phase. This is the standard scenario of a topological transition. The puzzle becomes confused when one notices that \(XY\) or Heisenberg models in three dimensions display conventional continuous transitions and the \(RP^2\) model exhibits a first order transition while renormalization group treatment of non-linear \(\sigma\) model predicts the absence of any transition at non-zero temperature in \(2d\) (asymptotic freedom in the context of lattice gauge theories \[16\]) and a continuous one in \(3d\) for all the three models. We also have to mention that the \(RP^1\) model (the same as given in equation (2), but with two-component vectors \(\sigma_w\) ) exactly coincides with the \(XY\) model. The question of a possible topological transition in the two-dimensional (non abelian) Lebwohl-Lasher model is thus particularly attracting and was already addressed in previous studies \[17, 18, 19, 20, 4\]. In their remarkable work, Kunz and Zumbach \[4\] concluded in 1992 in favor of such a topological transition scenario, essentially on the basis of qualitative arguments (pairing of topological defects at low temperature where they carry most of the energy in the system, sharp increase of the density of defects and apparent discontinuity of the rotational rigidity modulus at the transition, finite cusp in the specific heat, proliferation of unbinded defects at high temperature). Even though they performed a careful and sizeable study, they were unfortunately not able to decide conclusively between essential singularities or standard power laws - though their preference was for the first case - for the correlation length and the susceptibility when approaching the transition from the high temperature phase. This is essentially due to the limited possibilities of computers ten years ago, since the authors already took care about potential critical slowing down problems as they adapted the Wolff cluster algorithm to the \(RP^{n-1}\) model.

Ten years later, we want to address the same question of the nature of the phase transition of the two-dimensional Lebwohl-Lasher model. Since we believe that the conclusions of Kunz and Zumbach will hardly be improved, even with more powerful facilities, it is necessary to reconsider the problem from a different point of view. We will thus assume the existence of a critical phase at low tempera-
tures and then follow the line of the behaviour of the XY model to predict consequences of the above mentioned assumption, consequences which may be compared easily to numerical results. Of course, the test must discriminate between different scenarios, starting from the confirmation (and thus the characterization) of a topological transition, a conventional continuous transition, a first-order one, or no transition at all. The existence of a scale-invariant low temperature critical phase is characteristic from the first situation. Such a system must thus be conformally invariant at any temperature below the transition $T_{KT}$ (we will abusively keep the terminology adapted to the XY model), so it becomes advantageous to deduce the functional expression of the correlation functions or density profiles in a restricted geometry adapted to numerical simulations from a conformal mapping $w(z)$:

$$\langle \sigma_{w_1} \sigma_{w_2} \rangle = |w'(z_1)|^{-x_\sigma} |w'(z_2)|^{-x_\sigma} \langle \sigma_{z_1} \sigma_{z_2} \rangle. \quad (3)$$

Here, $w$ labels the lattice sites in the transformed geometry (the one where the computations are really performed), $z$ are the corresponding points in the original one (usually the infinite plane where $\langle \sigma_{z_1} \sigma_{z_2} \rangle \sim |z_1 - z_2|^{-\eta_\sigma}$ takes the standard power-law expression), and $x_\sigma = \frac{1}{2} \eta_\sigma$ is the scaling dimension associated to the scaling field $\sigma$. The interest of such an approach lies in the full inclusion in the functional expression of the changes due to shape effects. The most famous example is the exponential decay of the correlation functions at criticality along a strip of finite width, unlike the algebraic decay in the infinite plane. For simplicity reasons, it is even more convenient to work with density profiles in a finite system with symmetry breaking fields along some surfaces in order to induce a non vanishing local order parameter in the bulk. In the case of a square lattice $\Lambda$ of size $L \times L$, with fixed boundary conditions along the four edges $\partial \Lambda$, one expects $[21, 22, 23]$

$$m_{FBC}(w) = \langle P_2(\sigma_w \cdot h_{\partial \Lambda(w)}) \rangle_{FBC} \sim |\kappa(w)|^{-\frac{1}{2}} \quad (4)$$

$$\kappa(w) = \text{Im} \left[ \frac{2Kw}{L} \right] \times \left( 1 - \text{sn}^2 \frac{2Kw}{L} \right) \left( 1 - k^2 \text{sn}^2 \frac{2Kw}{L} \right)^{-\frac{1}{2}} \quad (5)$$

where $FBC$ specifies that the boundary conditions are fixed. This expression easily follows from the expression of the order parameter profile decaying in the upper half-plane from a distant surface of spins constantly fixed in a given direction, $m(z) = \langle P_2(\sigma_z \cdot h_{\partial \Lambda(z)}) \rangle_{UHP} \sim y^{-x_\sigma}$, and from the conformal transformation of the upper half-plane (UHP) $z = x + iy$ ($0 \leq y < \infty$) inside a square $w = u + iv$ of size $L \times L$ ($-L/2 \leq u \leq L/2$, $0 \leq v \leq L$) with open boundary conditions along the four edges, realized by a Schwarz-Christoffel transformation $[24]$.

$$w(z) = \frac{L}{2K} F(z, k), \quad z = \text{sn} \left( \frac{2Kw}{L} \right). \quad (6)$$

Here, $F(z, k)$ is the elliptic integral of the first kind, $\text{sn} (2Kw/L)$ the Jacobian elliptic sine, $K = K(k) = F(1, k)$ the complete elliptic integral of the first kind, and the modulus $k$ depends on the aspect ratio of $\Lambda$.

Our strategy is now to fit numerical data of the order parameter profile against expression (4). Like in the previous study of Kunz and Zambuck $[4, 20]$ the resort to a cluster update algorithm is necessary in order to prevent the critical slowing down, all the spins of clusters (build through intermediate bond variables) being updated simultaneously. The algorithm becomes particularly efficient if the percolation threshold of the bond process occurs at the transition temperature of the spin model, which ensures the updating of clusters of all sizes in a single MC sweep. For $O(n)$ models, Ising variables are defined in the Wolff algorithm by the sign of the projection of the spin variables along some random direction. The bonds are then introduced through the Kasteleyn-Fortuin random graph representation $[25]$. When one uses fixed boundary conditions, a difficulty occurs and the Wolff algorithm should become less efficient, since close to criticality the unique cluster will often reach the boundary and no update is made in this case. This is circumvented by the following trick: even when the cluster reaches the fixed boundaries, it is updated - and so are the boundary spins - and the order parameter profile is then measured with respect to the new direction of the boundary spins, $m_{FBC}(w) = \langle P_2(\sigma_w \cdot h_{\partial \Lambda}) \rangle_{FBC}$. Using this procedure, we studied systems of size $48 \times 48$ up to $200 \times 200$. For the measurement of
the order parameter profile, we discarded $10^6$ Wolff sweeps for thermalization, and the measurements were performed on $10^6$ production sweeps. For reasons which are made obvious below, the energy density required a better statistics and the measurements were obtained over $16.10^6$ sweeps.

In order to underscore the existence of a line of marginal fixed points in the low temperature phase, we first check qualitatively the expression of the energy-energy correlations from the behaviour of the energy density profile. The energy density at site $w$ is for example defined as the average value of the energies of the four links reaching $w$:

$$
\varepsilon_w = \frac{1}{2d} \sum_{\mu} [P_2(\sigma_{w-\mu} \cdot \sigma_w) + P_2(\sigma_w \cdot \sigma_{w+\mu})].
$$ (7)

The existence of a regular contribution in the energy density makes the calculation a bit more subtle than what presented in equation (4). This regular contribution $\langle \varepsilon_0(T) \rangle$ which depends on $T$ cancels after a suitable difference between profiles obtained with different conditions at the boundaries (free (fbc) and fixed (Fbc) boundary conditions). Although it makes the numerical computation longer in order to reach some satisfactory accuracy, this makes possible to extract the singularity associated to the energy density:

$$
\langle \varepsilon_{z_1} \varepsilon_{z_2} \rangle_{Fbc} = \langle \varepsilon_0(T) \rangle + B_{Fbc}(T)y^{-\eta_c(T)/2}; \quad \langle \varepsilon_{z_1} \varepsilon_{z_2} \rangle_{Fbc} = \langle \varepsilon_0(T) \rangle + B_{Fbc}(T)y^{-\eta_c(T)/2}.
$$ (8)

This is clearly illustrated in figure 1 where convergence towards the same temperature-dependent constant $\langle \varepsilon_0(T) \rangle$ is shown, with amplitudes of the singular terms having opposite signs, therefore a simple difference of the quantities measured in the square geometry,

$$
\Delta \varepsilon(w) = \langle \varepsilon_w \rangle_{Fbc} - \langle \varepsilon_w \rangle_{fbc} \sim \Delta B \times [\kappa(w)]^{-\frac{1}{2}y (T)}
$$ (10)

leads to the value of the thermal scaling dimension $\eta_c(T)$. The right part in figure 1 presents a log-log plot of the difference $\Delta \varepsilon(w)$ vs $\kappa(w)$ at two temperatures below $T_{KT}$ and one above which shows that the functional expression used is no longer valid, as expected, in the paramagnetic phase. Due to the strong fluctuations, in the QLRO phase the data scatter around straight lines which represent the slopes $[\kappa(w)]^{-2}$. This figure, though not definitely conclusive, confirms that the exponent of the decay of energy-energy correlations keeps a constant value $\eta_c(T) = 4$ in the low-temperature phase of the $RP^2$ model, confirming that like in the case of the $XY$ model, the temperature is a marginal field, responsible for the existence of a critical line in the whole low-temperature phase. It thus implies a thermal scaling exponent $x_\varepsilon = d - y_t = 2$ which ensures a vanishing RG eigenvalue $y_t = 0$ (up to $T_{KT}$ where it is consistent with an essential singularity of $\xi$ above the KT point, as suspected by Kunz and Zumbach [4]).

The energy-energy correlation function in the plane should thus decay algebraically as

$$
\langle \varepsilon_{z_1} \varepsilon_{z_2} \rangle \sim |z_1 - z_2|^{-\eta_c},
$$ (11)

with $\eta_c(T) = 2x_\varepsilon = 4 \forall T < T_{KT}$.

---

**Fig. 1:** MC simulations of the 2d $RP^2$ model inside a square of $100 \times 100$ spins ($16.10^6$ MC sweeps after cancellation of $10^6$ for thermalization). Several temperatures below the transition temperature are shown, and one above ($T = 0.6$). Left: local energy density vs the rescaled variable $\kappa(w)$. Right: log-log plot of the difference $\Delta \varepsilon(w)$.

From the existence of a marginal line, one may suspect that the other scaling dimensions should continuously vary with the marginal field. The order parameter profile thus has to obey equation (4) in the whole low temperature phase, but with an exponent $\eta_c(T)$ which depends on $T$. Equivalently,
a log-log plot of \( m_{Bsc}(w) \) vs \( \kappa(w) \) must display straight lines with different slopes below \( T_{KT} \). This is exactly what is observed in figure 2. Again, the curves start to deviate from the straight line when the system enters the high temperature phase.

The slopes measured in figure 2 are reported as a function of the temperature in figure 3.

Another signature of this mechanism is the behaviour of the rotational rigidity modulus. This latter quantity generalizes the helicity modulus \( \Upsilon \) in the \( XY \) model, which measures the quadratic response in the free energy of the system to a twist across the sample. This is generalized to the \( RP^2 \) model by measuring the change in free energy when a rotation of angle \( \phi \) around some axis in spin space is applied to the system:

\[
F(\phi) - F(0) = \Sigma \phi^2 + O(\phi^4).
\]

This expression defines the rotational rigidity modulus \( \Sigma \). In the \( XY \) model, there exists a universal relation between the helicity modulus and the correlation function exponent, \( \eta_{\sigma} = k_B T / 2\pi J \Upsilon \) [26], which appears as a consequence of the Kosterlitz recursion relations. In the Lebwohl-Lasher model, the same type of behaviour is checked in figure 4 where one observes a linear dependence (the larger the system size, the better the linear behaviour) of \( \eta_{\sigma} \) with \( T/\Sigma \), correctly fitted at low temperatures by \( \eta_{\sigma} = 0.117 k_B T / J \Sigma \).

To conclude, we mention that the most remarkable feature is a complete analogy with the two-dimensional \( XY \) model [22] where the transition is mediated by the defects. The exponent \( \eta_{\varepsilon} \) keeps a
constant value while $\eta$, associated to the order parameter, starts from zero at $T = 0$ and increases linearly with $T$ at low temperatures where a spin wave approximation should capture the essentials of the behaviour of the system. The influence of pairs of topological defects, which would appear in increasing number when the temperature increases, is probably responsible for the deviation from the spin wave approximation and of the sharper increase of $\eta$, and the transition is presumably completely governed by unbinding of these defects, like in the Kosterlitz-Thouless scenario. The order parameter exponent at the transition $k_B T_{KT}/J \simeq 0.52$ takes a value $\eta(T) \simeq 0.40(2)$. The relation between rotational rigidity modulus and the exponent $\eta(T)$ also seems completely coherent with what happens in the XY model, giving one more evidence of the topological nature of the transition.

Acknowledgement: This work is supported by the french-venezuelian PCP program ‘Fluides pétroliers’. Support from the CINES under project e20020622309 is also gratefully acknowledged.

References

[1] P.A. Lebwohl and G. Lasher, Phys. Rev. A 6 (1973) 426.
[2] W. Maier and A. Saupe, Z. Naturforsch. 14A (1959) 882.
[3] Z. Zhang, O.G. Mouritsen and M. Zuckermann, Phys. Rev. Lett. 69 (1992) 2803.
[4] H. Kunz and G. Zumbach, Phys. Rev. B 46 (1992) 662.
[5] N.D. Mermin and H. Wagner, Phys. Rev. Lett. 22 (1966) 1133.
[6] P.C. Hohenberg, Phys. Rev. 158 (1967) 383.
[7] J.M. Kosterlitz and D.J. Thouless, Prog. Low Temp. Phys 78 (1978) 371.
[8] D.R. Nelson, in Phase Transitions and Critical Phenomena, ed. by C. Domb and J.L. Lebowitz, Academic Press, London 1983, p. 1.
[9] C. Itzykson and J.M. Drouffe, Statistical field theory, Cambridge University Press, Cambridge 1989, vol. 1.
[10] T.M. Rice, Phys. Rev. 140 (1965) A 1889.
[11] F. Wegner, Z. Phys. 206 (1967) 465.
[12] G. Sarma, Solid State Comm. 10 (1972) 1049.
[13] V.L. Berezinskii, Sov. Phys. JETP 32 (1971) 493.
[14] J.M. Kosterlitz and D.J. Thouless, J. Phys. C 6 (1973) 1181.
[15] J.M. Kosterlitz, J. Phys. C 7 (1974) 1046.
[16] J.B. Kogut, Rev. Mod. Phys. 51 (1979) 659.
[17] S. Duane and M.B. Green, Phys. Lett. B 103 (1981) 359.
[18] S. Solomon, Y. Stavans and E. Domany, Phys. Lett. B 112 (1982) 373.
[19] C. Chiccoli, P. Pasini and C. Zannoni, Physica A 148 (1988) 298.
[20] H. Kunz and G. Zumbach, Phys. Lett. B 257 (1991) 299.
[21] T.W. Burkhardt and T. Xue, Nucl. Phys. B354 (1991) 653.
[22] B. Berche, A.I. Fariñas Sanchez and R. Paredes V., Europhys. Lett. 60 (2002) 539.
[23] B. Berche, J Phys. A 36 (2003) 585.
[24] M. Lavrentiev and B. Chabat, Méthodes de la théorie des fonctions d’une variable complexe, Mir, Moscou 1972, Chap. VII.
[25] C.M. Fortuin and P.W. Kasteleyn, Physica 57 (1972) 536.
[26] D.R. Nelson and J.M. Kosterlitz, Phys. Rev. Lett. 39 (1977) 1201.