Two Phase Transitions in the Two-Dimensional Nematic Three-Vector Model with No Quasi-Long-Range Order: Monte Carlo Simulation of the Density of States

B. Kamala Latha[1,*] and V. S. S. Sastry[2]
[1]School of Physics, University of Hyderabad, Hyderabad 500046, India
[2]Centre for Modelling, Simulation and Design, University of Hyderabad, Hyderabad 500046, India

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The presence of stable topological defects in a two-dimensional ($d = 2$) liquid crystal model allowing molecular reorientations in three dimensions ($n = 3$) was largely believed to induce a defect-mediated Berzenskii-Kosterlitz-Thouless-type transition to a low temperature phase with quasi-long-range order. However, earlier Monte Carlo (MC) simulations could not establish certain essential signatures of the transition, suggesting further investigations. We study this model by computing its equilibrium properties through MC simulations, based on the determination of the density of states of the system. Our results show that, on cooling, the high temperature disordered phase deviates from its initial progression towards the topological transition, crossing over to a new fixed point, condensing into a nematic phase with exponential correlations of its director fluctuations. The thermally induced topological kinetic processes continue, however, limited to the length scales set by the nematic director fluctuations, and lead to a second topological transition at a lower temperature. It is argued that in the ($d = 2, n = 3$) system with an attractive biquadratic Hamiltonian, the presence of additional molecular degrees of freedom and local Z_2 symmetry associated with lattice sites together promote the onset of an additional relevant scaling field at matching length scales in the high temperature region, leading to a crossover.

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Two-dimensional ($d = 2$) liquid crystal (LC) models with molecular reorientations in three dimensions ($n = 3$) host stable topological point defects (disclination points) with half integral charge [1] owing to their apolar order parameter (OP) geometry (real two-dimensional projective space RP^2), and are predicted to undergo a topological phase transition [2]. Several Monte Carlo (MC) studies on the Lebwohl-Lasher (LL) model [3] confined to a two-dimensional square lattice were carried out based on the Metropolis algorithm, alluding to a Berenzskii-Kosterlitz-Thouless-type [4–6] topological transition to a low-temperature phase with quasi-long-range order (QLRO) [2,7–11]. This assignment could not be conclusive, however, primarily because of the absence of size-invariant Binder's cumulant [12] at the reported transition temperature [13,14]. Recent comparative analysis of the MC data based on finite size scaling criterion [15] distinguishes the RP^2 systems from other two-dimensional magnetic systems, viz. 2D XY and 2D Heisenberg models, and concludes that the 2D LC systems could only have pseudocritical regions. A plausible conjecture advanced to account for the observed inconsistency has been the presence of an underlying subtle and persistent crossover in the model [11,13,14].

In this context, we examined this model with a different MC sampling procedure: we derived the equilibrium properties of this model by first computing its density of states (DOS) and then constructing equilibrium ensembles. The DOS was obtained with a variant of the MC procedure, entropic sampling technique [16,17], which is geared to access the configuration space uniformly with respect to energy. We used a modified version of the Wang-Landau algorithm [18] augmented with the frontier-sampling [19] technique to enhance its efficacy [20]. We constructed entropic ensembles comprising of microstates distributed uniformly with energy by performing a random walk biased by the DOS of the system. We distinguish the equilibrium ensembles obtained by a reweighting procedure from the entropic ensemble (say, RW ensembles) from those obtained based on Boltzmann sampling (B ensembles) [20], while comparing their equilibrium averages of different physical properties.

We considered a square ($d = 2$) lattice of variable size $L \times L$ ($L = 50, 80, 100, 120, 150$), each lattice site hosting a manifold of directions in three dimensional space ($n = 3$). The interactions are described by the LL Hamiltonian, $H = -\epsilon \sum_{\langle i,j \rangle} P_2(\cos\theta_{ij})$, with the summation covering all the nearest neighbors, and prescribing periodic boundary conditions. P_2 is the second Legendre polynomial and θ_{ij} is the angle between the neighboring molecules. The temperature (T) is reported in reduced units scaled by the coupling strength ϵ. The RW ensembles are constructed from the entropic ensemble [20], in the temperature range of interest

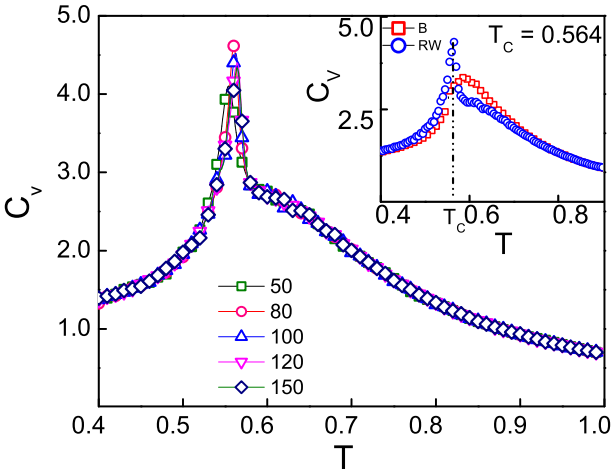

FIG. 1. Temperature variation of specific heat (per site)from RW ensembles at sizes $L = 50$, 80, 100, 120, and 150. Inset shows qualitatively different temperature variations of C_v from RW and B ensembles at $L = 150$.

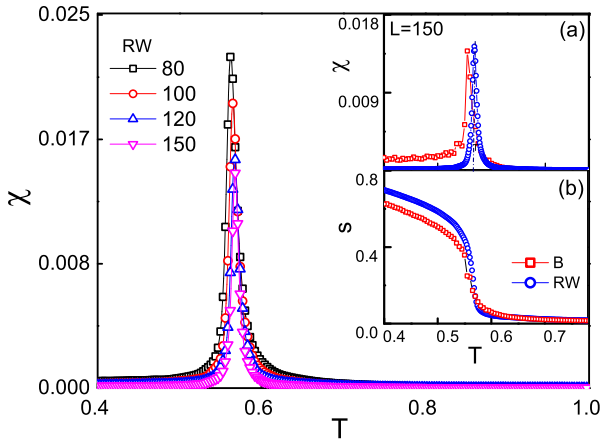

FIG. 2. Temperature variation of nematic susceptibility χ from RW ensembles at sizes $L = 80$, 100, 120, and 150. Insets (a) and (b) depict the comparison of the temperature variations of χ and nematic order S from RW ensembles with B ensembles at $L = 150$.

($T = 0.4$ to 1.0, with a resolution of 0.001). We computed, as a function of T, the averages of energy E, nematic order parameter S, nematic susceptibility χ, as well as Binder's cumulant R_4 associated with S to monitor the transition [20]. In addition, we calculated the topological order parameter μ based on an earlier algorithm [2,10]. Assigning a unit vector at each site $\boldsymbol{x}$ on the square lattice $\boldsymbol{\sigma}(\boldsymbol{x})$ representing the local director orientation in three dimensions ($n = 3$), to each bond $(\boldsymbol{x}, \boldsymbol{y})$ we associate the shortest geodesic connecting the vectors $\boldsymbol{\sigma}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{y})$ on the unit $(n-1)$ sphere, thereby obtaining a map from a closed loop $\mathcal{L}$ on the lattice to a loop on the manifold RP^2. The homotopy class of this map is given by $\mathcal{W}(L) = \prod_{(\boldsymbol{x},\boldsymbol{y})\in\mathcal{L}} \mathrm{sgn}(\boldsymbol{\sigma}(\boldsymbol{x}), \boldsymbol{\sigma}(\boldsymbol{y}))$ the product being sequentially ordered over $\mathcal{L}$. The ensemble average of $\mathcal{W}(L)$ with periodic boundary conditions in place yields μ [2]. Orientational pair correlation function $G(r_{ij}) = \langle P_2(\cos\theta_{ij})\rangle$ was computed (at $L = 150$) at about 40 temperatures covering the temperature range. The averages of E, S, and μ have statistical errors (estimated using the Jack-knife algorithm [21]) typically of the order of 1 in 10^4, while the higher moments (C_v, χ, R_4) are relatively less accurate, estimated to be about 5 in 10^3.

We now present qualitatively differing features of the physical parameters obtained from the two types of sampling procedures, leading to a discussion on the interpretation of our observations. Figure 1 shows an essentially size-independent temperature variation of C_v (per site) as obtained from RW ensembles at different system sizes, indicating an initial development of a broad cusp on cooling, but yielding to an abrupt sharp peak located at $T_c = 0.564$ ($L = 150$). This is to be contrasted with the broad cusp obtained from the B ensemble at the same size (shown in the inset of Fig. 1), which is in accord with the data reported earlier. Figure 2 depicts the temperature dependence of χ from RW ensembles as a function of size. Its temperature variations as obtained from the two ensembles are compared in the inset (a) at $L = 150$. The corresponding order parameters are shown in inset (b). The values of the order parameter S in the low temperature phase were found to decrease with size as computed from the B ensembles (consistent with the QLRO regime), while RW ensembles essentially report its size independence for $L \geq 80$ (not shown here). Low temperature values of the susceptibility also qualitatively differ [inset (a)]: it is nonzero and diverging with size in the B ensembles, while its value quickly tends to zero with the present sampling procedure. Also, the χ peaks in the present study shift slightly towards higher temperature with size, very similar to C_v.

The absence, from the earlier Monte Carlo studies, of a size-invariant Binder's cumulant (R_4) at the predicted transition temperature has been a major obstacle to unambiguously assign the transition as defect mediated, required to explain the observed low temperature QLRO phase [13,14]. From our data based on the DOS, a size-independent cumulant value was obtained at $T = 0.570 \pm 0.001$ (Fig. 3 and inset), providing a confirmatory evidence of a (continuous) transition at this temperature, as also representing the thermodynamic limit of the size-dependent C_v peak position T_c (Fig. 1). We investigate the nature of the low temperature phase by computing the spatial dependences of the orientational correlations of LC molecules at $L = 150$. Variations of $G(r)$ with distance (in lattice units), at different temperatures spanning the window $T = 0.4$ to 0.9, are shown in Fig. 4. Qualitatively differing from the earlier observations of power law variation at low temperatures, $G(r)$ fit very well to exponential decays, leading to the determination of the correlation length $\xi(T)$ (to within

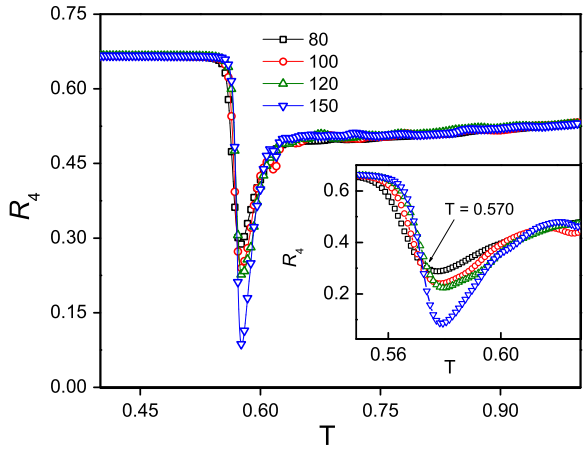

FIG. 3. Temperature variation of Binder's cumulant of the nematic order R_4 from RW ensembles at sizes $L = 80$, 100, 120, and 150. Inset shows the magnified version near the transition.

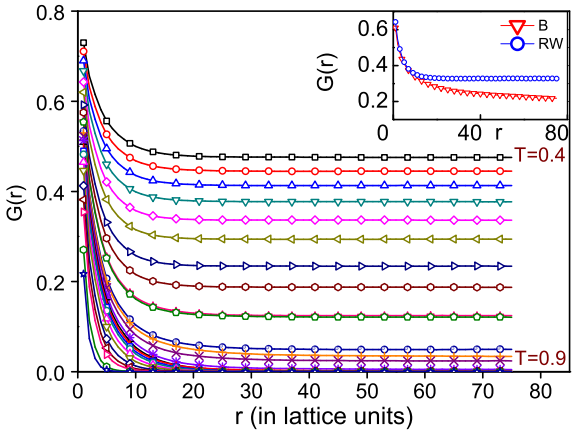

FIG. 4. Variation of the orientational pair correlation function $G(r)$ with lattice distances ($L = 150$) in the temperature range $T = 0.4$ to 0.9. The inset compares the $G(r)$ obtained from B and RW ensembles in the low temperature phase, at $T = 0.5$.

about 1% error). The inset compares $G(r)$ obtained from RW and B ensembles at $T = 0.5$ (low-temperature phase), at $L = 150$. The B-ensemble data require a power law for a satisfactory fit, as concluded by the earlier studies. The presence of a single length scale in the system at any temperature is the major indicator signaling a qualitative departure from the current interpretation of the low temperature phase in terms of QLRO.

We show the temperature variation of $\xi(T)$ in Fig. 5. Starting from the high temperature side, $\xi(T)$ initially tends to diverge, but deviates away near $T \approx 0.6$ to form a cusp at 0.564. We analyze the high temperature data [$\xi(T)$ vs T in Fig. 5] assigning its divergence as due to the temperature dependent kinetics of the unbound defects, given by $\xi(T) \sim \exp[A/(T - T_{U_\xi})^{1/2}]$ in the mean-field limit [4–6]. Here, T_{U_ξ} is the limiting temperature, determined from the high temperature $\xi(T)$ divergence, for the unbound defects to exist and A is a constant. The present data fit to this expression very satisfactorily until about $T \simeq 0.6$ (Fig. 5), yielding an estimate of the unbinding transition temperature $T_{U_\xi} = 0.471 \pm 0.005$. This implies that, but for the interruption by the transition at T_c, the system would have proceeded to a direct topological transition with the broad C_v cusp terminating its critical contribution in the neighborhood of T_{U_ξ} as a weak essential singularity. The departure of the observed ξ from its expected divergence (shown as dotted line in Fig. 5), forming a cusp at $T_c = 0.564$, as well as concomitant development of a sharp C_v peak at the same temperature show a crossover of the system towards a new fixed point from its initial progression towards a topological transition. The inset of this figure shows the differences in the energies (per site) as computed by the two MC procedures in the crossover region. The Metropolis algorithm accesses lower energy microstates in locating the regions of equilibrium ensembles, while ensembles based on the density of states computation sample relatively higher energy microstates, both being guided, however, by the same requirement of free energy minimization.

Figure 6 depicts the temperature variation of a related topological parameter δ [$=(1-\mu)/2$] and C_v at $L = 150$. $\delta \to 1/2$ at high temperatures above the topological transition, decreasing steadily on decreasing the temperature with a nonzero value at the topological transition. The inflexion point of this parameter seems to indicate the topological transition temperature [2]. We determined this temperature to be at $T_{U_\delta} = 0.483$ (± 0.002) at $L = 150$, by locating the peak of the temperature derivative of δ with a local Gaussian fit (Fig. 6). In Fig. 7 we show the temperature variation of δ at different sizes and plot the derived transition temperatures T_{U_δ} as a function of L^{-2} in the inset.

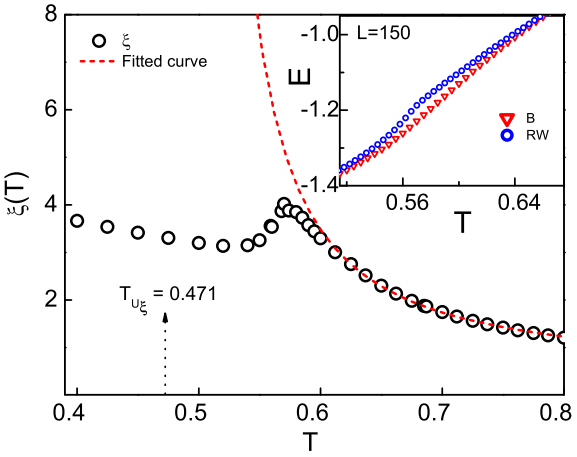

FIG. 5. Variation of correlation length ξ as a function of temperature. The dotted line represents the extrapolated divergence of ξ based on high temperature data (see text). Inset shows the variation of energy with temperature near the peak position from both the ensembles.

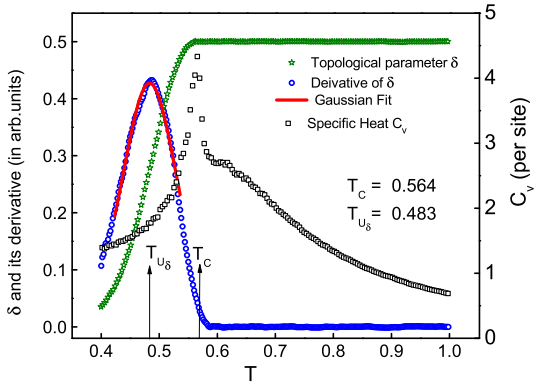

FIG. 6. Temperature variation of topological parameter δ (stars) and of its derivative (circles) superposed on the specific heat C_v profile (squares). Solid line indicates a local Gaussian fit to the cusp of the derivative.

The data seem to conform to finite size scaling reasonably well, yielding $T_{U_\delta} = 0.475$ (± 0.002) in the thermodynamic limit. This temperature was estimated earlier from the divergence data of $\xi(T)$ in the high temperature region, to be $T_{U_\xi} = 0.471$ (± 0.005).

The present LC system ($d = 2$ and $n = 3$ model, with apolar site directors coupled through LL interaction) differs qualitatively from two related models. The ($d = 2$ and $n = 2$) LC system is formally equivalent to the 2D XY model with known critical behavior [8]. The 2D Heisenberg model with polar site variables does not host stable topological defects since $n = 3$ facilitates escape to the third dimension (owing to the integer charge of defects), negating any transition at finite temperatures [22]. The present LC system on the other hand hosts topological defects, which are stable against such an escape even with $n = 3$ due to their half-integral charge [1]: any attempt to escape leads to a more singular line defect extending from the defect core. Further, the LL

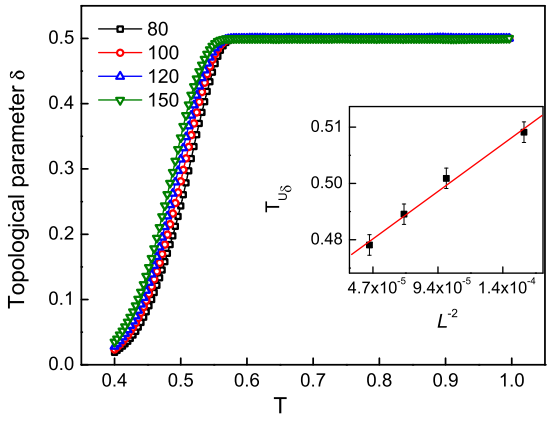

FIG. 7. Temperature variation of topological parameter δ from RW ensembles for sizes $L = 80$, 100, 120, and 150. The inset shows the finite size scaling of T_{U_δ}.

interaction implies isotropy with respect to the splay, twist, and bend distortions, ruling out the existence of higher order fundamental topological groups, negating other interesting defect structures within this system. More complex LC models are required to manifest higher order topological defects, like in cholesteric and biaxial nematics under specific anchoring conditions [23], and LC media with colloidal inclusions [24–26].

In the current LC system the local directors (with Z_2 symmetry) are coupled by the attractive biquadratic LL interaction with a potential to promote orientational order, its cooperative manifestation, however, being hindered by the very short correlation lengths at higher temperatures. But as the correlation length set by the defects diverges on cooling, it matches typical nearest neighbor distances of the site directors (in lattice units), and the LL interaction with the circumstance $n = 3$, seems to promote critical fluctuations of the nematic order resulting in a qualitative deviation of $\xi(T)$ from its divergent path (Fig. 5). This is in sharp contrast to the $n = 2$ LC model in two dimensions exhibiting the classical Berzenskii-Kosterlitz-Thouless pretransitional behavior. The length scales at lower temperatures are now set by the director fluctuations facilitated by extending the dimension of n to three (and not by the defect mediated mechanism), introducing a new relevant scaling field. We interpret the simultaneous occurrence of a sharp C_v peak and size-invariant R_4 value as manifestations of a crossover culminating in a transition at T_c (=0.570 in the thermodynamic limit) to a curious nematic phase. The nematic clusters in this medium, with their coherence length being set by the underlying order director fluctuations, however, are different in that they still host topological defects with their associated dynamics. The unbounded defects within the clusters continue to exist until the second topological transition takes place at T_{U_δ} (= 0.475). The present study thus points to two distinct fixed points in this system, alluding to a new universality class of this model.

We are benefited by insights from the earlier studies on magnetic systems with similar topology: two-dimensional fully frustrated antiferromagnetic Heisenberg system on a triangular lattice (HAFT model) [27]: the phenomenon of director fluctuations in the present $n = 3$ system in limiting the high temperature divergence of the correlation length is strikingly similar to the role of spin-wave fluctuations in condensing this magnetic system to a low temperature spin gel phase. Accordingly we refer to the low temperature ordered LC phase hosting topological defects as the nematic gel phase.

The failure of the earlier MC studies to associate a size-invariant Binder's cumulant at the proposed transition temperature seems to be justifiably conjectured as due to an underlying crossover, but the Boltzmann sampling method could not access the higher energy microstates apparently needed in this temperature region (inset of Fig. 5)

to locate the true minimum free energy configurations, thus missing to detect the crossover phenomenon.

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*Corresponding author.
kklata@gmail.com

[1] N. D. Mermin, Rev. Mod. Phys. **51**, 591 (1979).
[2] H. Kunz and G. Zumbach, Phys. Rev. B **46**, 662 (1992).
[3] P. A. Lebwohl and G. Lasher, Phys. Rev. A **6**, 426 (1972).
[4] V. L. Berezenskii, Sov. Phys. JETP **32**, 493 (1971).
[5] V. L. Berezenskii, Sov. Phys. JETP **34**, 610 (1972).
[6] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[7] C. Chiccoli, P. Pasini, and C. Zannoni, Physica (Amsterdam) **148A**, 298 (1988).
[8] B. Berche and R. Paredes, Condens. Matter Phys. **8**, 723 (2005).
[9] E. Mondal and S. K. Roy, Phys. Lett. A **312**, 397 (2003).
[10] S. Dutta and S. K. Roy, Phys. Rev. E **70**, 066125 (2004).
[11] S. Shabnam, S. D. Gupta, and S. K. Roy, Phys. Lett. A **380**, 667 (2016).
[12] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[13] V. R. Paredes, A. I. Farinas-Sanchez, and R. Botet, Phys. Rev. E **78**, 051706 (2008).
[14] A. I. Farinas-Sanchez, R. Botet, B. Berche, and R. Parades, Condens. Matter Phys. **13**, 13601 (2010).
[15] Y. Tomita, Phys. Rev. E **90**, 032109 (2014).
[16] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
[17] F. Wang and D. P. Landau, Phys. Rev. E **64**, 056101 (2001).
[18] D. Jayasri, V. S. S. Sastry, and K. P. N. Murthy, Phys. Rev. E **72**, 036702 (2005).
[19] C. Zhou, T. C. Schulthess, S. Torbrugge, and D. P. Landau, Phys. Rev. Lett. **96**, 120201 (2006).
[20] B. K. Latha, R. Jose, K. P. N. Murthy, and V. S. S. Sastry, Phys. Rev. E **92**, 012505 (2015).
[21] B. K. Latha, G. Sai Preeti, K. P. N. Murthy, and V. S. S. Sastry, Comput. Mater. Sci. **118**, 224 (2016).
[22] A. Pelissetto and E. Vicari, Phys. Rep. **368**, 549 (2002).
[23] P. J. Ackerman and I. I. Smalyukh, Phys. Rev. X **7**, 011006 (2017).
[24] D. Seč, S. Čopar, and S. Žumer, Nat. Commun. **5**, 3057 (2014).
[25] F. Serra, Liq. Cryst. **43**, 1920 (2016).
[26] A. Humpert, S. F. Brown, and M. P. Allen, Liq. Cryst. **45**, 59 (2018).
[27] H. Kawamura, A. Yamamoto, and T. Okubo, J. Phys. Soc. Jpn. **79**, 023701 (2010).