# Topological transitions in two-dimensional lattice models of liquid crystals

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The phase diagram of hard-core nematogenic models in three-dimensional space can be studied by means of Onsager's theory, and, on the other hand, the critical properties of continuous interaction potentials can be investigated using the molecular field approach pioneered by Maier and Saupe. Comparison between these treatments shows a certain formal similarity, reflecting their common variational root; on this basis, hard-core potential models can be mapped onto continuous ones, via their excluded volume. Some years ago, this line of reasoning had been applied to hard spherocylinders, hence the continuous potential $G(\tau)=a+b\sqrt{1-\tau^2}$, $b>0$ had been used to define a mesogenic model on a three-dimensional lattice [S. Romano, Int. J. Mod. Phys. B **9**, 85 (1995)]; in the formula, $\tau$ denotes the scalar product between the two unit vectors defining particle orientations. Here we went on by addressing the same interaction potential on a two-dimensional lattice. Our analysis based on extensive Monte Carlo simulations found evidence of a topological transition, and the critical behavior in its vicinity was studied in detail. Results obtained for the present model were compared with those already obtained in the literature for interaction potentials defined by Legendre polynomials of second and fourth orders in the scalar product $\tau$.

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## I. INTRODUCTION AND POTENTIAL MODEL

Several families of classical statistical mechanical spin models, by now extensively studied in the literature, involve $n$-component unit vectors $\mathbf{u}_k$, $n=2,3$, associated with the sites of a two-dimensional lattice, with coordinate vectors $\mathbf{x}_k$; the pair interaction potential is taken to be translationally invariant, restricted to nearest neighbors, and to possess $O(n)$ symmetry at least; in formulas:

$$W = W_{jk} = \epsilon G(\tau), \quad \tau = \tau_{jk} = \mathbf{u}_j \cdot \mathbf{u}_k, \tag{1}$$

where $\epsilon$ denotes a positive quantity, setting temperature and energy scales (i.e., temperature and energy will be expressed in units of $\epsilon$), and $G(\tau)$ is a continuous function of its argument, possessing a minimum when $\tau=1$, so as to produce a fully ordered ground state. By the Mermin-Wagner theorem and its generalizations [1–3], the named models cannot support long-range orientational order at any finite temperature in the thermodynamic limit; on the other hand, in some cases, these studies have shown, and even proven, the existence of a topological phase transition.

The simplest, prototypal case, involves two-component spins (plane rotators, also often called the $XY$ model), parametrized by usual polar angles $\phi_j$, so that $\tau=\cos(\phi_j-\phi_k)$, and coupled by a ferromagnetic (odd) interaction, i.e., $G(\tau)=-\tau$; this model produces the well known and extensively studied Berezinskiĭ-Kosterlitz-Thouless (BKT) transition [4–8], whose existence was proven rigorously by Fröhlich and Spencer [4]: this is a transition to a low-temperature phase possessing slowly decaying (inverse-power-law) correlations, reflected by an infinite susceptibility.

Several other related functional forms of $G(\tau)$, involving two-component spins and sometimes of different parity, have been studied as well (see, e.g., Refs.[9–12]), and often found to produce a similar transition; the even counterparts have been investigated in connection with nematogenic models [11,12]. On the other hand, as discussed in Ref. [8], for a wide class of interaction models involving two-component spins, available mathematical results [4,13–15] entail the existence of a BKT-like transition, as well as a rigorous lower bound on the transition temperature.

Moreover, in some other cases, it was first argued on the basis of simulation results, and later rigorously proven, that the transition to the low-temperature phase may turn first-order [16,17]. Let us also mention that similar rigorous results have been obtained for lattice-gas extensions as well, and even for "liquid" extensions, where particle coordinates $\mathbf{x}_k$ sweep the Euclidean plane $\mathbb{R}^2$ [18,19]; a first-order transition to a BKT phase was studied by simulation in Ref. [20].

Another case studied in the literature involves $n=3$ and ferromagnetic interactions [$G(\tau)=-\tau$, classical Heisenberg model]; does this model support a topological transition as well? No rigorous answer to the question is known to date [21], but various pieces of evidence have been obtained over the years. Various authors (see, e.g., Ref. [22]) have argued that the model does not produce such a transition; the opposite view has been put forward by Patrascioiu and Seiler, in a series of papers starting in the 1990s [23,24]; examples of the resulting debate can be found in or via Refs. [25–28].

In contrast to the previous cases, another set of models involves $n=3$ component spins and even interactions; the cases investigated so far are of the form $G(\tau)=-P_M(\tau)$, where $P_M(\cdots)$ denotes Legendre polynomials of even order;

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no rigorous answers are available here either. The case $M=2$ was investigated over the past 25 years [29–41], and various pieces of numerical evidence suggest the existence of such a transition; a recent simulation estimate for the transition temperatures is $\Theta_2=0.548\pm0.002$ [41]; the case $M=4$ was addressed more recently [42,43], and a simulation estimate for the transition temperature is $\Theta_4=0.376\pm0.015$ [42,43]; evidence for a transition of this kind was obtained for some "liquid" counterparts as well [44,45].

Hard-core models of nematogens in three-dimensional Euclidean space are often treated by Onsager theory or extension of it [46–49], based on their excluded volume; in turn, the excluded volume between two hard-core particles is an appropriate continuous function of their mutual orientation; actually, when particles are assumed to possess $D_{\infty h}$ symmetry, the resulting excluded volume is an even function $E(\tau)$ of the scalar product between the two unit vectors defining particle orientations; an explicit expression for this function has been obtained in some cases such as spherocylinders [46,50], cylinders [46,50], and ellipsoids of revolution [50–52]; spherocylinders are the most studied case, with

$$E(\tau) = 8\pi\left(\frac{\lambda D^2}{4} + \frac{D^3}{6}\right) + 2D\lambda^2\sqrt{1-\tau^2}, \tag{2}$$

where $\lambda$ denotes the cylindrical length, and $D$ is the diameter of the cylinder. In turn, in the named (convex) cases, the function $E(\tau)$ possesses its minimum when $\tau=1$, and could be interpreted as pair potential defining a lattice model with nearest-neighbor interactions, or fed into a mean field treatment of the Maier-Saupe (MS-MF) type [53,54]. Upon comparing the equations resulting from the two treatments [54,55], one notices a certain analogy, reflecting their common variational root: it turns out that the reciprocal temperature in a MS-MF approach basically plays the same role as the density in an Onsager treatment. There also exist differences between the two approaches, since the additional constraint of equal pressures and chemical potentials in the two phases must be satisfied for the hard-core case only [46–48]. In other words, a hard-core interaction can be mapped onto a continuous separable potential via its excluded volume, and the latter model is expected to produce a weaker transition than the former. An early example of this idea can be found in Ref. [56], where a continuous pair potential was parametrized so as to fit the excluded volume between two identical hard parallelepipeds for selected reciprocal orientations, i.e., in the six cases where the principal axes of the two inertia tensors were the same, apart from a relabeling. Thus a functional form,

$$G(\tau) = a + b\sqrt{1-\tau^2}, \quad b>0, \tag{3}$$

had been used to define a mesogenic model (the sin model, for short) on a three-dimensional lattice [55]; the square root in Eq. (3) can be expanded in a series of Legendre polynomials of even order, whose expansion coefficients are known in closed form, and their signs are all negative [48,57]; this suggests a possible strengthening of the transition in comparison with the well known Lebwohl-Lasher (LL) model [58,59]. Actually, the numerical values for the coefficients $a$ and $b$ used in Ref. [55] were chosen to be $b=32/(5\pi)$, $a=-8/5$, for ease of comparison, so that, to lowest order in the expansion of Eq. (3), one recovers $-P_2(\tau)$, i.e., the LL model. In the three-dimensional counterpart, the above additional terms were found to make the transition recognizably closer to its MF limit than the LL counterpart [55]. Here we go on to study the same interaction potential on a two-dimensional lattice. Our aim is to gain insights into its critical behavior via extensive Monte Carlo simulations.

The plan of the paper is as follows. In Sec. II we discuss our simulation procedure in detail and define the physical quantities of interest to be computed. Section III presents an analysis of our results and discusses the critical behavior of the model. Comparisons with other models, and especially comments on the transition behavior of the $P_4$ model [42,43], are presented in Sec. IV, also containing a summary and some concluding remarks. Let us finally mention that purely two-dimensional hard-core models, involving uniaxial convex bodies moving in $\mathbb{R}^2$, have been studied as well (see, e.g., Ref. [60] and others quoted therein), and often found to produce evidence of a BKT transition.

## II. COMPUTATIONAL ASPECTS

Simulations were carried out using periodic boundary conditions in order to neglect possible surface effects; different sample sizes were examined ($N=L^2$, $L=40,60,80,100,120,160$), and calculations were carried out in cascade, in order of increasing temperature; each cycle (or sweep) consisted of $2N$ Monte Carlo (MC) steps, including a sublattice sweep [61,62]. Equilibration runs took between 25 000 and 250 000 cycles, and production runs took between 250 000 and 1 250 000; subaverages for evaluating statistical errors were calculated over macrosteps consisting of 1000 cycles. Different random-number generators were used, as discussed in Ref. [62].

Calculated quantities include mean potential energy $U$ in units $\epsilon$ per particle (and hence, for graphical convenience, its value scaled by the corresponding ground-state quantity $U_0=-16/5$, i.e., $U_N=U/U_0$), as well as configurational heat capacity; long-range order parameters were defined and calculated via the appropriate ordering tensors, as discussed in detail elsewhere [63–66], and are expected to go to zero at all finite temperatures in the thermodynamic limit. Alternatively and equivalently, the second-rank order parameter and the associated susceptibility can be worked out as follows: let

$$F = \sum_{j=1}^{N}\sum_{k=1}^{N} P_2(\mathbf{u}_j\cdot\mathbf{u}_k); \tag{4}$$

then the simulation estimate for the second-rank order parameter is

$$\bar{P}_2 = \frac{1}{N}\langle\sqrt{F}\rangle, \tag{5}$$

and its associated susceptibility reads [30,36] (but see also Sec. IV)

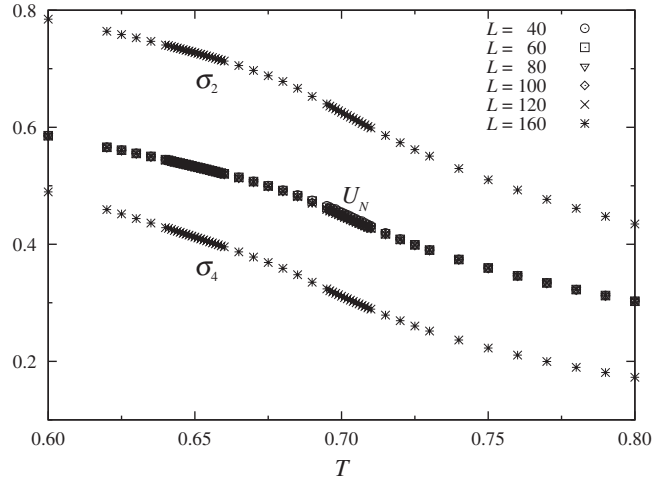


FIG. 1. Simulation results for the scaled potential energy $U_N = U/U_0$, as well as short-range order parameters $\sigma_2$ and $\sigma_4$ obtained with the largest sample size. Unless otherwise stated or shown, here and in the following figures, statistical errors fall within symbol sizes.

$$\chi = \frac{1}{N}\beta\langle F\rangle, \quad \beta = 1/T; \tag{6}$$

notice that, for a finite sample, $\chi \leq \beta N$. By the addition theorem for spherical harmonics, the double sums appearing in Eq. (4) can actually be calculated [67] as linear combinations of the squares of the computationally less demanding quantities

$$\xi_m = \sum_{j=1}^{N} \mathrm{Re}[C_{2,m}(\mathbf{u}_j)], \quad \eta_m = \sum_{j=1}^{N} \mathrm{Im}[C_{2,m}(\mathbf{u}_j)]; \tag{7}$$

here $m=0,1,2$, $C_{2,m}(\cdots)$ are modified spherical harmonics, and Re and Im denote real and imaginary parts, respectively; in turn, each spherical harmonics is a suitable polynomial constructed in terms of Cartesian components of the corresponding unit vector (see, e.g., Ref. [68]). We also evaluated the so-called short-range order parameters [65,69]

$$\sigma_M = \langle P_M(\tau)\rangle, \quad M = 2,4, \tag{8}$$

measuring correlations between nearest-neighboring particles.

## III. RESULTS

Simulation estimates for the potential energy were found to evolve with temperature in a gradual and continuous way, and to be independent of sample size; results for the short-range quantities $\sigma_M$ followed the same pattern (Fig. 1), showing the expected decrease of nearest-neighbor correlations with increasing temperature. The three named quantities showed a change of the slope of their curves at about $T=0.7$. This change of the slope for the energy is investigated further through the behavior of the specific heat, whose results showed a peak at about $T \approx 0.7$ and a slightly more pronounced sample-size dependency around the same temperature (Fig. 2). Notice that the specific heat did not develop a divergence at the indicated temperature. Simulation results for $\bar{P}_2$ and $\bar{P}_4$ were found to decrease with temperature, and, at each temperature, with increasing sample size, (Figs. 3 and 4, respectively); moreover, they showed a recognizable amount of finite-size order setting in at $T \lesssim 0.66$.

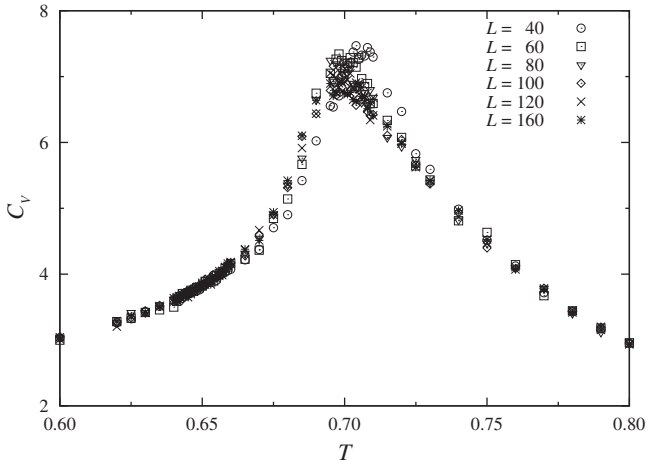


FIG. 2. Simulation results for the configurational specific heat, obtained with different sample sizes. The statistical errors, not shown here, range between 1 and 5 %.

At all investigated temperatures simulation results for the order parameters $\bar{P}_M$, $(M=2,4)$ exhibited a power-law decay with increasing sample size. They were well fitted by the respective relations

$$\ln \bar{P}_M = -b_{M1} \ln L + b_{M0}, \quad b_{M1} > 0 \tag{9}$$

for a given temperature. Furthermore, the coefficients $b_{M1}(T)$ were found to increase with $T$ for higher temperatures and proportional to $T$ to within statistical errors in the low-temperature region. The results obtained from Eq. (9) show that both order parameters vanish at the thermodynamic limit, i.e., $L \to \infty$ in conformity with the Mermin-Wagner theorem. Such a behavior is in agreement with the spin wave theory developed for the magnetization in the case of the

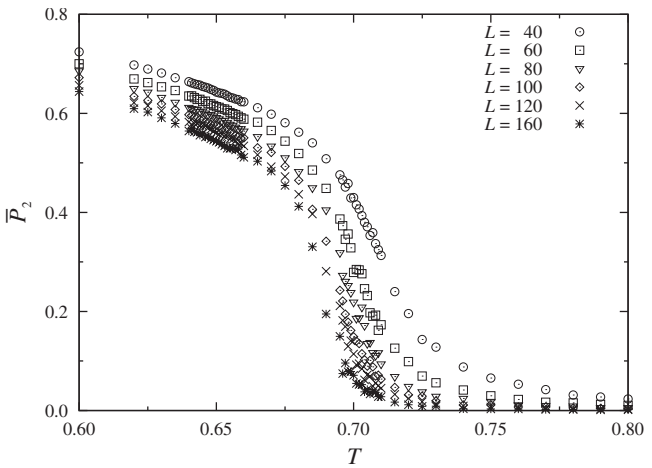


FIG. 3. Simulation results for the second-rank order parameter $\bar{P}_2$ obtained with different sample sizes.

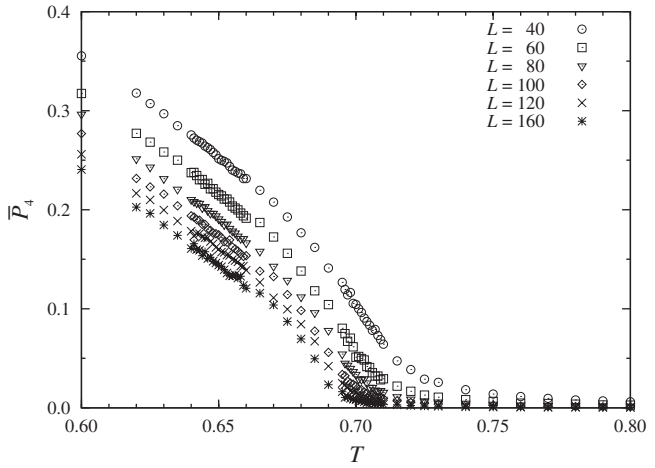


FIG. 4. Simulation results for the fourth-rank order parameter $\bar{P}_4$ obtained with different sample sizes

two-dimensional planar rotator (see Refs. [70,71] and those quoted therein).

Results for ln $\chi$ vs temperature Fig. 5 were found to be independent of sample size when $T \gtrsim 0.71$, and showed a recognizable increase with it (a power-law dependence of $\chi$ on $L$) when $T \lesssim 0.68$. The behaviors of specific heat, order parameters, and nematic susceptibility suggest that the present model undergoes a BKT-like phase transition. According to the BKT theory, in the thermodynamic limit, the susceptibility $\chi$ diverges exponentially while approaching the transition temperature $\Theta$ in the high-temperature region [7], i.e.,

$$\chi \sim a_\chi \exp[b_\chi (T-\Theta)^{-1/2}]; \quad T \to \Theta^+ \tag{10}$$

and remains infinite in the low-temperature region $T<\Theta$. For a finite sample consisting of $N=L^2$ sites, the situation is different, since the susceptibility obeys the constraint $\chi \leq \beta N$; thus $\chi$ is always finite, and its exponential divergence

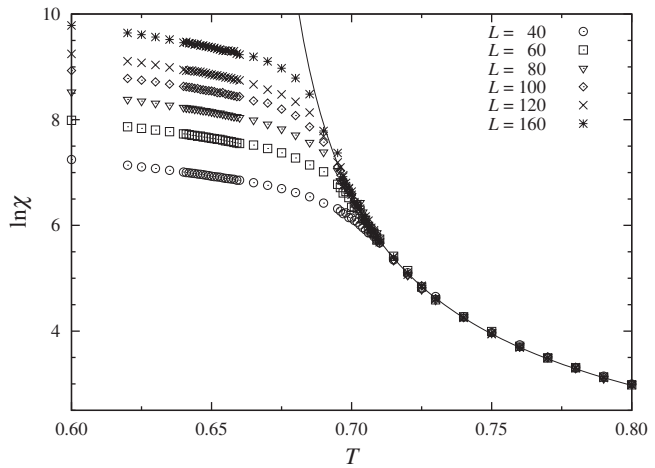


FIG. 5. Simulation results for the logarithm of the nematic susceptibility $\chi$, obtained with different sample sizes; the statistical errors on $\chi$, not shown, range up to 3%. The solid curve is obtained by fitting to Eq. (10) with data corresponding to $L=160$.

TABLE I. Results obtained from the linear fit of the simulation data of the susceptibility, for some selected temperatures, using the expression $\chi(T)=c_\eta L^{2-\eta}$ following Eq. (11).

| $T$ | $\eta$ | ln $c_\eta$ |
|---|---|---|
| 0.648 | $0.243 \pm 0.005$ | $0.47 \pm 0.02$ |
| 0.649 | $0.244 \pm 0.005$ | $0.46 \pm 0.02$ |
| 0.650 | $0.246 \pm 0.005$ | $0.46 \pm 0.02$ |
| 0.651 | $0.247 \pm 0.007$ | $0.46 \pm 0.03$ |
| 0.652 | $0.249 \pm 0.005$ | $0.45 \pm 0.02$ |
| 0.653 | $0.263 \pm 0.003$ | $0.51 \pm 0.02$ |
| 0.654 | $0.270 \pm 0.009$ | $0.53 \pm 0.04$ |

in the transition region is rounded, because of the important finite-size effects.

In the critical region, i.e., in the vicinity of the BKT temperature, the correlation length becomes comparable in magnitude with the linear size $L$ of the system. In this case, the exponential divergence of the susceptibility is rounded in the critical region, but the divergence persists in the behavior of $\chi$ at higher temperatures, where the correlation length is smaller than the linear system size and finite-size effects can be neglected. We first fitted our MC results obtained for the largest sample size and for temperatures in the range $0.698 \lesssim T \lesssim 0.760$ to Eq. (10), and obtained evidence of the exponential divergence of the susceptibility (see Fig. 5), and an estimated transition temperature $\Theta=0.66 \pm 0.01$, with $a_\chi = 0.46 \pm 0.11$ and $b_\chi = 1.38 \pm 0.08$.

Our results were checked by using data on a wider range of temperatures extending up to $T=0.80$. This yielded a consistent result. In the following we refine our results using a more elaborate method, i.e., finite-size scaling theory, and apply it in the temperature region where the singularity of $\chi$ is rounded. Then, the correlation length $\xi$ is proportional to the size of the sample, $\xi \sim L$. From the behavior of the susceptibility $\chi \sim \xi^{2-\eta}$, with $\eta = 1/4$ [7], we have

$$\chi(\Theta) \sim L^{2-\eta}. \tag{11}$$

In this expression we have ignored the "analytic" corrections emanating from the background, expected to contribute with small corrections to the finite-size scaling expressions.

The temperature region $0.65 \lesssim T \lesssim 0.67$, was explored in greater detail, first by carrying out a linear fit of ln $\chi$ vs ln $L$ and extracting $\eta$ from the slope. Our estimations for some temperatures are presented in Table I along with the associated coefficient $c_\eta$ according to $\chi(T)=c_\eta L^{2-\eta}$. A nonlinear square fit was attempted as well, and yielded results consistent with these ones. Thus the transition temperature is estimated to be $\Theta=0.650 \pm 0.002$, in agreement with the above mentioned result obtained by fitting the data of the susceptibility, corresponding to the largest sample size, in the high-temperature region; at this temperature the value of $\eta$ is expected to be $\frac{1}{4}$ to within statistical errors. Thus the present model exhibits a BKT-like phase transition. Notice that for this model the maximum of the specific heat occurs at a temperature about 7% higher than the critical point.

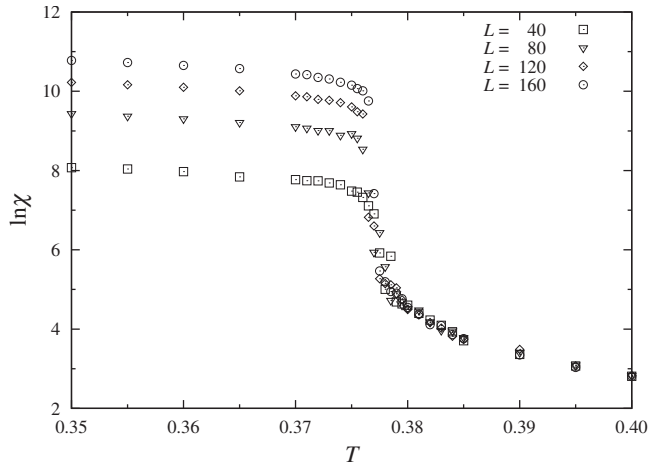


FIG. 6. Simulation results for the logarithm of the nematic susceptibility $\chi$ for the $-P_4$ model; the statistical errors on $\chi$, not shown, range up to 3%.

## IV. COMPARISON WITH OTHER MODELS AND CONCLUSIONS

In this section we compare results for the transitional behavior resulting from the present interaction model with those obtained for the above mentioned pair potentials. i.e., of the form $-P_M(\tau)$, with $M=2,4$. Both a *BKT* (see, e.g., Ref. [36]) a second-order scenario [41] have been proposed in the literature for the $-P_2(\tau)$ model; furthermore, some remarks are appropriate about the transitional behavior of the $-P_4$ model as well, for which evidence of a first-order transition has been produced [42,43].

Notice that the authors of Refs. [41–43] had used a different definition of susceptibility, which appears to correspond to

$$\chi' = \frac{1}{N}\beta(\langle F\rangle - \langle\sqrt{F}\rangle^2) \tag{12}$$

in our symbols [see also Eq. (6)]; this definition seems to be appropriate for an ordered phase, where $\bar{P}_2>0$ (see the discussion for the magnetic case in Refs. [72,73]), and did not produce results diverging with sample size *below* the transition temperature. This difference is likely to explain, at least partly, the difference in transition character which the authors of Ref. [41] point out. [As a minor point, notice also that, since $|P_m(t)|\leq 1, m\in\mathbb{N}$, $-1\leq t\leq +1$ [74], Eq. (6) and Fig. 7 in Ref. [41] disagree by orders of magnitude, i.e., a factor $N$ seems to be missing in Eq. (6); the same remarks appear to apply to Eqs. (6)–(8) and Fig. 14 in Ref. [43].]

We ran additional simulations for the $-P_4$ model (using $L=40,80,120,160$) and found results suggesting a slowly developing discontinuity of potential energy, as well as of long- and short-range order parameters, around the estimated transition temperature proposed in Refs. [42,43]; moreover, our results for $\chi$ (Fig. 6) were found to be independent of sample size above this temperature, and to exhibit a recognizable power-law increase with $L$ below it. Thus it seems likely that the two-dimensional $-P_4$ model actually supports a *first-order transition* [42,43] *to a low-temperature BKT phase*; examples of this type of transition are also known for magnetic models of the saturated-lattice type, as well as for some lattice-gas counterparts of them, as mentioned in the Introduction.

Now we turn to quantitative comparison between the three models; this can be realized by considering the ratios between transition temperatures and ground-state energies: the values are $0.279\pm0.001$ for the $-P_2$ model [41], $0.188\pm0.008$ for the $-P_4$ model [42,43], and $\approx 0.2$ in the present case. As for the counterparts associated with a three-dimensional lattice, where a discontinuous ordering transition takes place, the corresponding ratios are 0.3744 for the $-P_2$ model [75–79], $0.2178\pm0.0002$ for the $-P_4$ model [66,80], $0.257\pm0.001$ for the sin model [55]. In both cases the ratio recognizably decreases upon going from the second-rank model to the fourth-rank one, and, to a lesser extent, upon going from the $P_2$ to the sin model.

This trend can be correlated with known aspects of the interaction models. On the one hand, in comparison with $-P_2$, the sin model produces a greater separation between maximum and minimum [$(32/5\pi)$ vs $(3/2)$], but also a broader minimum; on the other hand, the separation between maximum and minimum for $-P_4$ is (10/7) vs (3/2) for $P_2$ and, moreover, the $P_4$ model possesses a secondary minimum at $\tau=0$, where $P_4(0)=(3/8)$ [66,80], mildly disfavoring the mutual parallel orientation of the interacting pair at finite temperature.

To summarize, we have studied via extensive Monte Carlo simulation the critical properties of a two-dimensional lattice spin model, involving three-component unit vectors, and whose interaction potential is restricted to nearest neighbors and defined by the above Eq. (3); as discussed in Sec. I, its counterpart associated with a three-dimensional lattice can be obtained via the mutual excluded volume between two hard spherocylinders, thus defining a mapping and, so to speak, a bridge, between the Onsager and the MS-MF treatments.

We have computed a number of thermodynamic quantities in order to characterize the critical behavior of the present model. Both potential energy and short-range order parameters were found to be independent of sample size and showed a smooth and gradual decrease with the temperature. The behaviors of specific heat, of order parameters $\bar{P}_2$ and $\bar{P}_4$, and especially of the susceptibility $\chi$, suggested a BKT-like phase transition. The transition temperature was determined by analyzing the data obtained for the susceptibility. This is $\Theta=0.650\pm0.002$. The maximum of the specific heat was found to be at a temperature higher than $\Theta$, as is the case for systems exhibiting a BKT-like transition. Note that the two-dimensional $-P_2$ model may exhibit a second-order phase transition, while its $-P_4$ counterpart appears to support a first-order phase transition to a low-temperature BKT phase. Quantitative comparisons between the three pair interaction potentials have been carried out, and correlations with known aspects of the models have been found.

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