Monte Carlo investigation of critical properties of the Landau point of a biaxial liquid-crystal system

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Extensive Monte Carlo simulations are performed to investigate the critical properties of a special singular point usually known as the Landau point. The singular behavior is studied in the case when the order parameter is a tensor of rank 2. Such an order parameter is associated with a nematic-liquid-crystal phase. A three-dimensional lattice dispersion model that exhibits a direct biaxial nematic-to-isotropic phase transition at the Landau point is thus chosen for the present study. Finite-size scaling and cumulant methods are used to obtain precise values of the critical exponent $\nu = 0.713(4)$, the ratio $\gamma/\nu = 1.85(1)$, and the fourth-order critical Binder cumulant $U^* = 0.6360(1)$. Estimated values of the exponents are in good agreement with renormalization-group predictions.

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I. INTRODUCTION

According to Landau mean-field theory (MFT) [1], an isolated singular point can exist on any first-order phase-transition line. This point is produced by the vanishing of the coefficient of the cubic term in the expansion of the free energy in powers of the order parameter ϕ, which is

$$f(\phi) = f_0 - h\phi + \tfrac{1}{2}\tau_0\phi^2 + u_3\phi^3 + u_4\phi^4 + u_5\phi^5 + u_6\phi^6 + \cdots . \quad (1)$$

If ϕ is a tensor, the third-order term $u_3\phi^3$ cannot be removed and a first-order transition line is obtained by varying τ_0 and u_3. For the case when $\tau_0 = u_3 = 0$, an isolated singular point arises on the first-order transition line, and at this point the jump in ϕ vanishes. The critical singular point is known as the Landau point.

The presence of the Landau point in the phase diagram of a lattice model for a fluid of biaxial particles was confirmed by Alben [2]. He employed a type of mean-field approximation to obtain the qualitative features of the phase diagram, and he pointed out that mean-field studies are not sufficient to see the special nature of the second-order transition at the Landau point because of strong fluctuations. In his paper, Alben suggested that liquid crystals could be a suitable system to manifest the predicted behavior. A phenomenological description [3–5] of the uniaxial and biaxial nematic phases of liquid crystals can be obtained by a sixth-order Landau–de Gennes free-energy expansion in powers of the symmetric and traceless tensor order parameter $\mathbf{Q}$. The tensor $\mathbf{Q}$ can be written as

$$\mathbf{Q} = \frac{\mathbf{q_0}}{\sqrt{6}}(3\hat{\mathbf{n}} \otimes \hat{\mathbf{n}} - \mathbf{1}) + \frac{\mathbf{q_2}}{\sqrt{2}}(\hat{\mathbf{l}} \otimes \hat{\mathbf{l}} - \hat{\mathbf{m}} \otimes \hat{\mathbf{m}}), \quad (2)$$

where $\{\hat{\mathbf{l}},\hat{\mathbf{m}},\hat{\mathbf{n}}\}$ are the three orthonormal directors that are identified with eigenvectors of $\mathbf{Q}$ corresponding to three real eigenvalues (in the general case of the biaxial phase having $\mathcal{D}_{2h}$ symmetry, the three eigenvalues are different). This simple model predicts a direct $I \leftrightarrow N_B$ second-order transition at the Landau point. In the phase diagram of a liquid-crystal system, the Landau multicritical point exists where biaxial nematic (N_B), uniaxial nematic [$N_{U^\pm}$; for systems of prolate molecules (+) and oblate molecules (−)], and isotropic (I) phases are in equilibrium. At this special critical point, two second-order $N_{U^\pm} \leftrightarrow N_B$ lines meet two first-order $I \leftrightarrow N_{U^\pm}$ lines. In another mean-field type study, Straley [6] generated a topologically identical phase diagram of rectangular hard parallelopipeds. A system of asymmetric ellipsoids interacting with infinite-range forces was studied by Boccara *et al.* [7] to give an identical phase diagram. These studies show that the Landau point, at which a direct $I \leftrightarrow N_B$ second-order transition occurs, corresponds to a given (definite) molecular shape, which can be parametrized by a single molecular biaxiality parameter. At this point, the biaxial molecules are neither very rodlike nor very much disklike (the so called self-dual geometry). Thus in terms of the molecular biaxiality parameters, the location of the Landau point in the phase diagram can be predicted. All the above studies are mean-field type and hence did not take into account fluctuations.

The Landau point was investigated by several authors using renormalization-group (RG) methods [8–11]. Vigman *et al.* [8] have shown that the possibility of the existence of the Landau point also remains valid when fluctuations are taken into account. They studied the Landau point by the ϵ expansion method. For their study, they chose a liquid-crystalline system because the order parameter that describes the nematic-isotropic transition in liquid crystals is a symmetric, traceless tensor of rank 2, order 3. In 1978, Vause and Sak [11] extended the theory to order $\epsilon^2, \epsilon = 4 - d$. Apart from the usual critical exponents η (the correlation function exponent) and ν (the correlation length exponent), these authors evaluated a new exponent Δ_3 that determines the shape of the co-existence curve between the isotropic and the uniaxial phases. In their work, they reported that the exponents η and ν are the same as those for the isotropic n-vector model, with $n = 5$ (in three-dimensional space, the nematic order parameter has five independent components). The n-vector model had been studied by Wilson with Feynman-graph

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techniques [12], and the usual critical exponents for the Landau point in liquid crystals with $n = 5$ can be expressed as $\gamma = 1 + \frac{7}{26}\epsilon + \frac{1309}{2197}\epsilon^2 + O(\epsilon^3)$, γ being the susceptibility exponent, and $\eta = \frac{7}{338}\epsilon^2 + O(\epsilon^3)$. The numerical values of these exponents for $\epsilon = 1$ ($d = 3$) are $\gamma = 1.418$ (to order ϵ^2) and $\eta = 0.0207$ (to order ϵ^2). For the correlation-length exponent, the scaling law $\gamma = \nu(2 - \eta)$ is used, and this gives $\nu = 0.716$.

On the experimental front, the realization of the Landau point has long been a challenging task. The recent claims [13,14] of finding the direct $I \leftrightarrow N_B$ transition in thermotropic liquid crystals for bent-core molecules, a new class of liquid crystals, has brought back fresh interest in this field of research. Several theoretical studies and experimental searches for biaxial nematics have been reported, although many open questions still remain to be solved [15]. Computer simulation studies [16,17] have shown that the presence of a strong transverse dipole moment associated with the bent-core molecules splits the Landau point in the phase diagram into a Landau line, and these studies suggest that the formation of a Landau line could help in the detection of biaxial order. The bent-core molecules can be modeled as V-shaped for theoretical studies. Maier-Saupe molecular theory as well as the computer simulation studies predict that the Landau point in the phase diagram for the V-shaped molecules without any permanent dipole moment, and where both mesogenic arms are equivalent, occurs when the interarm angle is at the tetrahedral value [18–20].

Although several computer simulation studies [21,22] close to the Landau point have been reported to find its exact location in the phase diagram and to verify the second-order nature of the $I \leftrightarrow N_B$ phase transition, none of these works investigated the critical properties of the Landau point. To be more specific, to the best of our knowledge there is no such computer simulation study that is involved in extracting the critical exponents for the Landau point.

The purpose of this paper is to estimate the usual critical exponents associated with the Landau multicritical point by Monte Carlo simulation. For this purpose, we have chosen a simple lattice model of symmetric V-shaped biaxial molecules interacting with a second-rank anisotropic pair potential. Monte Carlo (MC) study of such a system has been reported by Bates and Luckhurst [20], and it has been shown that this model contains almost all the features of the biaxial molecule that are essential to its liquid-crystal character. The phase behavior of symmetric V-shaped biaxial molecules is determined by the interarm angle θ. The Landau point in the phase diagram for such a system occurs when $\theta = \theta_C = \cos^{-1}(-1/3)$ [19].

We have performed extensive MC simulations in the vicinity of the Landau point for symmetric V-shaped molecules. Throughout our study, θ is set at the tetrahedral value (θ_C). In our model, system molecules are placed at the sites of a simple cubic lattice where they have only orientational degrees of freedom. From the simulated data, relevant thermodynamic quantities have been calculated using the multiple histogram reweighting technique [23]. We then analyzed the reweighted values of thermodynamic quantities for different temperatures by finite-size scaling [24,25] and cumulant methods. The critical temperature has been estimated with high accuracy. The universality of the Landau multicritical point is determined from the values of the critical exponents and by analyzing the value of the fourth-order Binder cumulant at the critical point at the thermodynamic limit.

II. MODEL AND THE OBSERVABLES

We use a lattice model, which is a biaxial generalization of the Lebwohl-Lasher potential [26] as proposed in Ref. [20]. Each arm of the symmetric V-shaped molecules interact with those of the nearest neighbors via a potential that goes like $-P_2(\cos\beta)$, where P_2 is the second Legendre polynomial and β is the angle between the interacting arms. Therefore, the symmetric V-shaped molecules are interacting with six nearest neighbors $\langle ij \rangle$ via the pair potential

$$U_{ij} = -\epsilon \sum_m \sum_n P_2(\cos \beta_{ij}^{mn}), \tag{3}$$

where m,n represent two arms of the ith and jth molecules, respectively, and ϵ is a strength factor that is identical for all interactions between the arms of symmetric V-shaped molecules having the same anisotropy in the interactions. The present lattice model is equivalent [20] to the widely studied dispersion model introduced by Luckhurst *et al.* [27,28]. An extensive Monte Carlo simulation study [29] revealed that the phase diagram for the dispersion model contains the Landau point occurring at $\lambda = 1/\sqrt{6}$, where λ represents the molecular biaxiality parameter. In the present study, the fixed angle θ between two symmetric arms of a V-shaped molecule plays the role of the molecular biaxiality parameter λ, and $\theta = \theta_C$ corresponds to $\lambda = 1/\sqrt{6}$.

To identify nematic phases, second-rank order parameters associated with the long as well as the transverse molecular axes must be defined. Straley [6] introduced four order parameters for the full description of an ordered phase of liquid crystal composed of biaxial particles. Thereafter, several notations [30] have been used to denote the same set of order parameters with different numerical prefactors and symbols. The second-rank orientational order parameters of a rigid biaxial molecule in a biaxial phase expressed in terms of the Saupe ordering matrix [3,20] are directly related with the measurements of the experiments and therefore are widely used. These order parameters are defined by using four independent principal components of the Saupe ordering matrix. Following the prescription of Dunmur and Toriyama [31], order parameters can be expressed in terms of the Saupe ordering matrix as $S = S_{zz}^{ZZ}$, $D = S_{xx}^{ZZ} - S_{yy}^{ZZ}$, $P = S_{zz}^{XX} - S_{zz}^{YY}$, and $\mathcal{C} = (S_{xx}^{XX} - S_{xx}^{YY}) - (S_{yy}^{XX} - S_{yy}^{YY})$, where x,y,z and X,Y,Z denote, respectively, the principal molecular (symmetry) axes and the principal laboratory axes. For a symmetric V-shaped molecule, the z axis is chosen along the vector joining the midpoints of the arms of the molecule, the y axis is chosen along the bisector of the interarm angle, and the x axis is along the perpendicular direction of the plane of the molecule (Fig. 1). The principal axes are labeled so that the biaxiality of the phase is positive, i.e., $S_{zz}^{ZZ} > S_{zz}^{XX} - S_{zz}^{YY} > 0$.

In an isotropic phase, all the order parameters S, D, P, and $\mathcal{C}$ are zero. For a uniaxial phase comprised of uniaxial molecules, only the major order parameter S is nonzero, and the relation $S_{zz}^{XX} = S_{zz}^{YY} = -\frac{1}{2}S_{zz}^{ZZ}$ is maintained. On the other hand, if the molecules are biaxial but the phase is uniaxial, then

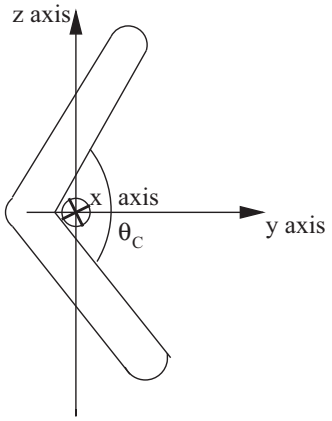

FIG. 1. Schematic diagram of a symmetric V-shaped molecule. The three molecular principal (symmetry) axes are x, y, and z with the x axis normal to the plane of the page.

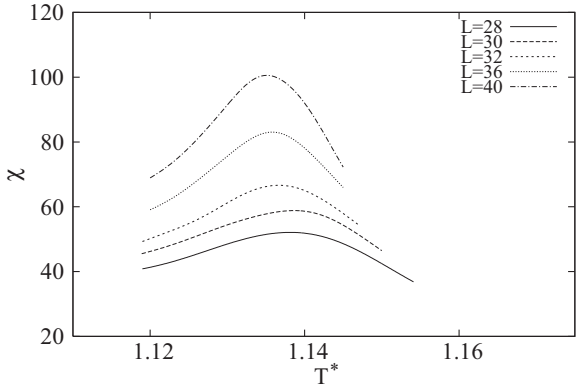

FIG. 2. The susceptibility of biaxial order parameter $\chi(T^*, L)$ generated by multiple histogram reweighting plotted against dimensionless temperature, T^*, for five lattice sizes.

both S and D are nonzero. If the molecules and the phase are both biaxial, then all four order parameters S, D, P, and $\mathcal{C}$ are nonzero. In the limiting case of perfect ordering, $S \to 1$, $D \to 0$, $P \to 0$, and $\mathcal{C} \to 1$. P and $\mathcal{C}$ are the measure of the phase biaxiality of the system. Of these two order parameters, P is independent of molecular biaxiality whereas the other parameter $\mathcal{C}$ depends considerably on it. Considering the extensive simulations involved in extracting critical exponents at the Landau point, we have determined the critical behavior of quantities directly related to $\mathcal{C}$ only.

We point out that the alignment tensor $\mathbf{Q}$ used in the Landau expansion and defined in Eq. (2) is of macroscopic nature. The connection between $\mathbf{Q}$ and the four molecular scalar order parameters S, D, P, and $\mathcal{C}$ for the dispersion model has been described in Refs. [32] and [33].

The observables related to the order parameter, such as the order-parameter susceptibility χ and the reduced fourth-order Binder cumulant U_4, are defined as

$$\chi = \frac{N(\langle \mathcal{C}^2 \rangle - \langle \mathcal{C} \rangle^2)}{T^*} \tag{4}$$

and

$$U_4 = 1 - \frac{\langle \mathcal{C}^4 \rangle}{3\langle \mathcal{C}^2 \rangle^2}, \tag{5}$$

where N is the number of molecules, $T^* = k_B T/\epsilon$ is the dimensionless temperature, and $\langle \cdots \rangle$ denotes the ensemble average.

Another important observable [34] relevant to the present study is the thermodynamic derivative of U_4 with respect to the inverse of temperature, $K = 1/T^*$, and this can be obtained from the relation

$$\frac{dU_4}{dK} = (1 - U_4)\left[\langle E \rangle - 2\frac{\langle \mathcal{C}^2 E \rangle}{\langle \mathcal{C}^2 \rangle} + \frac{\langle \mathcal{C}^4 E \rangle}{\langle \mathcal{C}^4 \rangle}\right]. \tag{6}$$

III. COMPUTATIONAL ASPECTS

We have performed Monte Carlo simulations on simple-cubic lattices consisting of $N = L^3$ particles for five different sizes $L = 28$, 30, 32, 36, and 40 using the conventional METROPOLIS algorithm. Periodic boundary conditions in all directions have been used. In an attempted move, a site is selected randomly at first and then a randomly chosen arm of the V-shaped molecule at that site is rotated following the Barker-Watts method [35] subject to the constraint that the angle between the arms of the molecule is fixed.

For each lattice size, simulations for several values of T^* (at least six temperatures) in the vicinity of the transition region have been carried out for generating a one-dimensional histogram $N(E)$ and three constant energy averages—$\langle \mathcal{C} \rangle(E)$, $\langle \mathcal{C}^2 \rangle(E)$, and $\langle \mathcal{C}^4 \rangle(E)$. From these four one-dimensional arrays, we calculate all thermodynamic quantities of interest.

The maximum autocorrelation time of the system for the largest system size, $L = 40$, is 1500 Monte Carlo steps per site (MCS) corresponding to the energy variable, whereas it is 6970 MCS corresponding to the order-parameter variable. MC runs with, at least, 9×10^6 MCS have been performed for a single temperature for the larger lattices, which took about 90 h of CPU time for $L = 40$, where the simulations were performed on Intel Core i7 processors clocked at 3.2 GHz.

Since the energy in this model is continuous, we need to divide the whole energy range ($E_{\min}/N = -4.0$ and $E_{\max}/N = 0$) into bins of appropriate width. For example, the energy bin-width per particle for $L = 40$ is set to 3.125×10^{-5}. We also checked using ten times finer bins that this binning

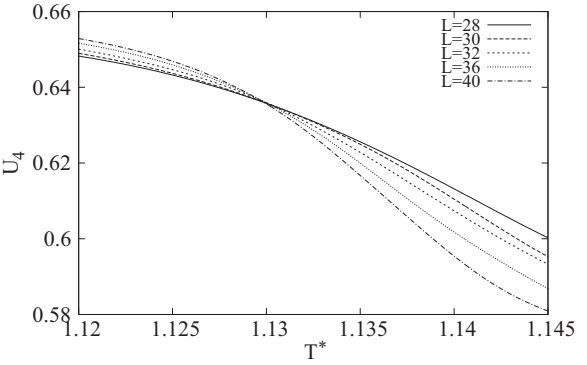

FIG. 3. The Binder cumulant $U_4(T^*, L)$ generated by the multiple histogram reweighting plotted against dimensionless temperature, T^*, for five lattice sizes.

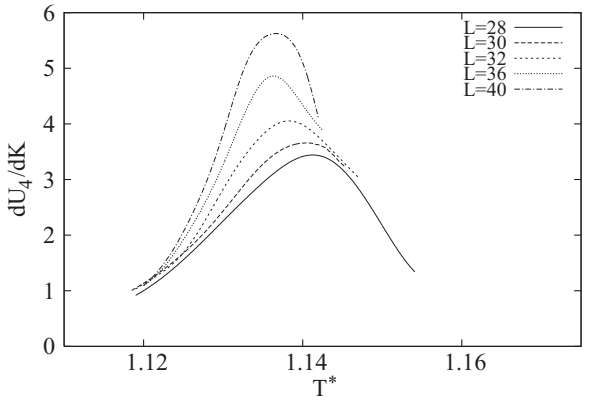

FIG. 4. The derivative of the Binder cumulant dU_4/dK is plotted as a function of the dimensionless temperature, T^*, for five lattice sizes.

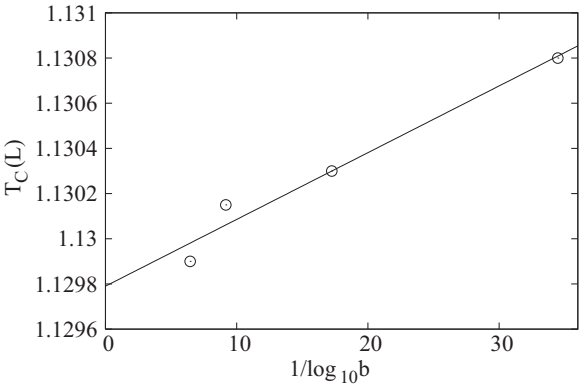

FIG. 6. Extrapolation of the temperature values of the crossings of the $L = 28$ curve of U_4 with all other curves against the inverse logarithm of $b = L'/L$. The critical temperature $T_C = 1.1298 \pm 0.0001$.

is small enough to ensure negligibly small discretization error. Various thermodynamic quantities have been computed using the multiple-histogram reweighting method proposed by Ferrenberg and Swendsen [23].

IV. RESULTS AND DISCUSSION

We first present some raw simulation data displaying how the various observables of interest depend on temperature and system size. In Fig. 2 , the susceptibility χ corresponding to the biaxial order parameter $\mathcal{C}$ is plotted versus T^* for various system sizes. We observe that χ shows a maximum, which becomes more pronounced as L increases. Also the peak position shifts toward the lower values of T^* as L increases.

The fourth-order Binder cumulant U_4 is plotted in Fig. 3 for various system sizes. We observe that the curves for the cumulant approximately cross each other at a single point. This exhibits the typical behavior of the cumulants near a continuous phase transition. The thermodynamic derivative dU_4/dK is determined using Eq. (6), and we plot it in Fig. 4 as a function of T^* with increasing system size L. The derivative shows a maximum at the transition.

In the vicinity of the critical point, the reduced fourth-order cumulants U_4 show a strong dependence of the system sizes (see Fig. 3). However, at the critical point the cumulants adopt a nontrivial value U^*, known as the critical Binder cumulant, which does not depend on system sizes in the scaling limit. From the value of U^*, we can identify the universality class of the continuous transition. The crossings of the $U_4(L,T^*)$ curves (see Fig. 3) give a first estimate of U^* and the critical temperature T_C, which are 0.63 and 1.13, respectively. To get more precise values of these quantities from our simulation data, we have used an extrapolation procedure, which is necessary due to the presence of finite-size corrections to scaling.

Four data points are obtained from the crossings of the $L = 28$ curve with the others (see Fig. 5) having a higher L value (L'), and these are used for two straight-line fits (Figs. 6 and 7). The first extrapolation leads to an estimate of the critical temperature $T_C = 1.1298 \pm 0.0001$ at the thermodynamic limit. A similar analysis of the variation of cumulant crossings gives an accurate estimate of the critical Binder cumulant $U^* = 0.6360 \pm 0.0001$. As far as we know, there are no

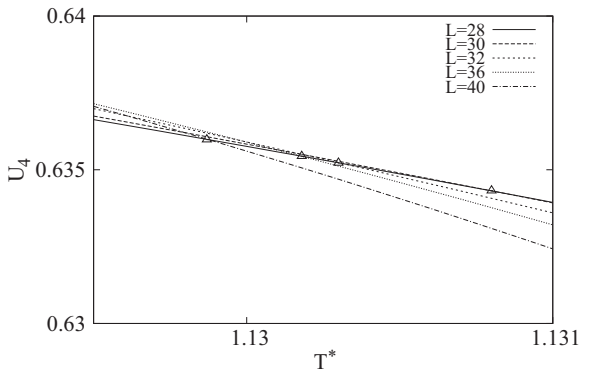

FIG. 5. Plot of $U_4(T^*,L)$ vs T^* for several lattice sizes. For increasing lattice size, a shift of the intersection toward higher values of U_4 becomes visible as a larger scale is chosen. The intersections with the cumulant for $L = 28$ are shown by triangles.

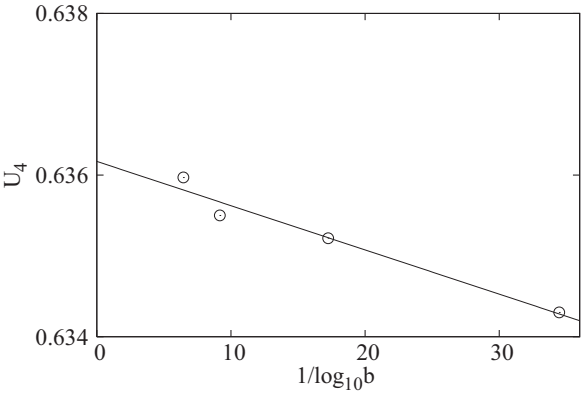

FIG. 7. Extrapolation of the fourth-order Binder cumulant values of the crossings of the $L = 28$ curve of U_4 with all other curves against the inverse logarithm of $b = L'/L$. The critical Binder cumulant $U^* = 0.6360 \pm 0.0001$.

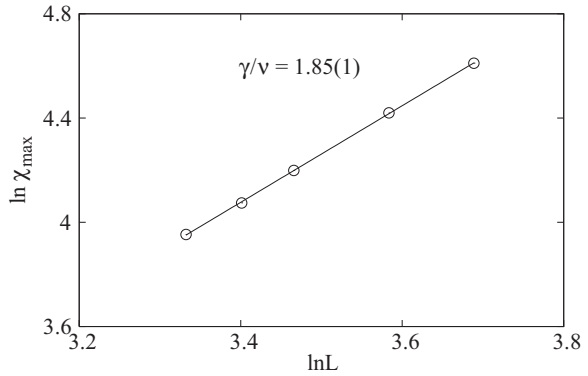

FIG. 8. Variation of $\ln \chi_{\max}$ with $\ln L$ (slope, $\gamma/\nu = 1.85 \pm 0.01$).

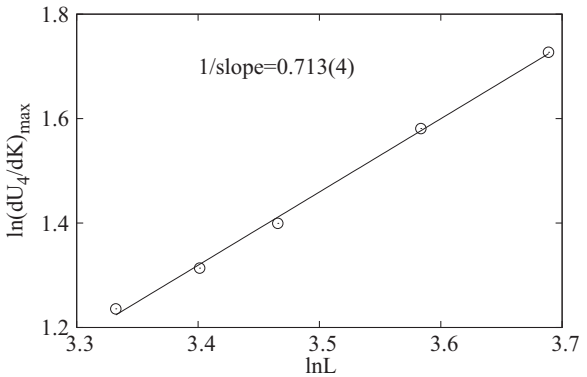

FIG. 9. $\ln(dU_4/dK)_{\max}$ vs $\ln(L)$. The exponent $\nu = 0.713 \pm 0.004$.

previous results for U^* at the Landau point with which we can compare our estimate. We only mention that this is a little higher than the universal value of U^* for the conventional Heisenberg-like transition ($U^* \approx 0.62$), which corresponds to $n = 3$. Also, for the Ising-like transition, $U^* \approx 0.46$ in three dimensions ($n = 1, d = 3$) [34].

The finite-size scaling analysis of various thermodynamic quantities has been performed by the standard method [24] to estimate the critical exponents.

The susceptibility peak $\chi_{\max}$ scales as

$$\chi_{\max} \propto L^{\gamma/\nu}. \tag{7}$$

The slope of the straight line in the log-log plot of $\chi_{\max}(L)$ (Fig. 8) gives the value of the ratio $\gamma/\nu = 1.85 \pm 0.01$.

Determination of the correlation-length exponent from the usual MC simulation data is quite a difficult task. Use of the derivative of the Binder cumulant improves the situation. The maximum value of dU_4/dK has a nice scaling property, that it scales as $L^{1/\nu}$. In Fig. 9 we plot $(dU_4/dK)_{\max}$ as a function of system size on a log-log scale. The linear fit of the logarithm of the derivatives as a function $\ln L$ yields $\nu = 0.713 \pm 0.004$. This is remarkably close to the ϵ-expansion prediction (to order ϵ^2) $\nu = 0.716$ [12]. Taking the product of the MC estimates of γ/ν and ν, we obtain $\gamma = 1.319$, which is a little lower than the ϵ-expansion prediction (to order ϵ^2) $\gamma = 1.418$.

V. CONCLUSION

We have shown that the multiple-histogram reweighting technique and finite-size scaling analysis allow us a precise determination of the critical exponents $\nu = 0.713(4)$, $\gamma = 1.319$, and the fourth-order critical Binder cumulant $U^* = 0.6360(1)$ at the Landau point. Our simulation results confirm that the $I \leftrightarrow N_B$ transition predicted by the dispersion model belongs to the 3D-isotropic Heisenberg universality class with order-parameter dimensionality $n = 5$ as predicted earlier by renormalization-group methods [9,12].

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[1] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, 2nd ed. (Pergamon, Oxford, 1969).
[2] R. Alben, Phys. Rev. Lett. **30**, 778 (1973).
[3] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals*, 2nd ed. (Clarendon, Oxford, 1993).
[4] E. F. Gramsbergen, L. Longa, and W. H. de Jeu, Phys. Rep. **135**, 195 (1986).
[5] D. Allender and L. Longa, Phys. Rev. E **78**, 011704 (2008).
[6] J. P. Straley, Phys. Rev. A **10**, 1881 (1974).
[7] N. Boccara, R. Mejdani, and L. de Seze, J. Phys. **38**, 149 (1977).
[8] P. B. Vigman, A. I. Larkin, and V. M. Filev, Sov. Phys. JETP **41**, 944 (1975).
[9] R. G. Priest and T. C. Lubensky, Phys. Rev. B **13**, 4159 (1976).
[10] C. Vause and J. Sak, Phys. Lett. A **65**, 183 (1978).
[11] C. Vause and J. Sak, Phys. Rev. B **18**, 1455 (1978); **18**, 4842 (1978).
[12] K. G. Wilson, Phys. Rev. Lett. **28**, 548 (1972).
[13] B. R. Acharya, A. Primak, and S. Kumar, Phys. Rev. Lett. **92**, 145506 (2004).
[14] L. A. Madsen, T. J. Dingemans, M. Nakata, and E. T. Samulski, Phys. Rev. Lett. **92**, 145505 (2004).
[15] *Biaxial Nematic Liquid Crystals*, edited by G. R. Luckhurst and T. J. Sluckin (Wiley, Oxford, 2015).
[16] M. A. Bates, Chem. Phys. Lett. **437**, 189 (2007).
[17] N. Ghoshal, K. Mukhopadhyay, and S. K. Roy, Liq. Cryst. **39**, 1381 (2012).
[18] P. I. C. Teixeira, A. J. Masters, and B. Muldar, Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A **323**, 167 (1998).
[19] G. R. Luckhurst, Thin Solid Films **393**, 40 (2001).

[20] M. A. Bates and G. R. Luckhurst, Phys. Rev. E **72**, 051702 (2005).
[21] M. P. Allen, Liq. Cryst. **8**, 499 (1990); P. J. Camp and M. P. Allen, J. Chem. Phys. **106**, 6681 (1997).
[22] C. Chiccoli, P. Pasini, F. Semeria, and C. Zannoni, Int. J. Mod. Phys. C **10**, 469 (1999).
[23] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988); **63**, 1195 (1989).
[24] D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge University Press, Cambridge, 2000), Chap. 4.
[25] *Monte Carlo Methods in Statistical Physics*, edited by M. E. J. Newman and G. T. Barkema (Clarendon, Oxford, 1999), Chap. 8.
[26] P. A. Lebwohl and G. Lasher, Phys. Rev. A **6**, 426 (1972).
[27] G. R. Luckhurst, C. Zannoni, P. L. Nordio, and U. Segre, Mol. Phys. **30**, 1345 (1975).
[28] G. R. Luckhurst and S. Romano, Mol. Phys. **40**, 129 (1980).
[29] F. Biscarini, C. Chiccoli, P. Pasini, F. Semeria, and C. Zannoni, Phys. Rev. Lett. **75**, 1803 (1995).
[30] R. Rosso, Liq. Cryst. **34**, 737 (2007).
[31] D. Dunmur and K. Toriyama, in *Physical Properties of Liquid Crystals*, edited by D. Demus, J. Goodby, G. W. Gray, H.-W. Spiess, and V. Vill (Wiley-VCH, Weinheim, 1999), Chap. IV.
[32] L. Longa and G. Pajak, Liq. Cryst. **32**, 1409 (2005).
[33] K. Trojanowski, D. W. Allender, L. Longa, and L. Kusmierz, Mol. Cryst. Liq. Cryst. **540**, 59 (2011).
[34] C. Holm and W. Janke, Phys. Rev. B **48**, 936 (1993).
[35] J. A. Barker and R. O. Watts, Chem. Phys. Lett. **3**, 144 (1969).