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Effect of an external magnetic field on the nematic-isotropic phase transition in mesogenic systems of uniaxial and biaxial molecules: A Monte Carlo study

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We determine the nematic-isotropic coexistence curve terminating at the critical point in a temperature-external field phase diagram for nematic liquid crystals with positive diamagnetic anisotropy, where the molecules are either perfectly uniaxial or biaxial using computer simulation of a lattice model. The coexistence curve is much steeper than that predicted by the standard Landau–de Gennes and Maier-Saupe mean-field theories. For the uniaxial system the critical magnetic field is estimated to be one order of magnitude lower than the mean-field estimate but of the same order of magnitude as the experimental measurement. Our study shows that molecular biaxiality could reduce the critical field strength significantly.

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I. INTRODUCTION

The effect of an external field on the nematic-isotropic (N-I) phase transition has long been an active area of research because of its fundamental importance [1–11]. An external field makes the normally weak first-order N-I transition even weaker, shifts the transition temperature T_{NI} to a higher value, and induces a weak orientational order in the isotropic phase resulting in an anisotropic phase known as the paranematic (pN) phase. With an increase in the field strength, the difference between the N and I (or pN) phases decreases and finally vanishes at a critical point, above which the N and I (or pN) phases are indistinguishable. This critical end point is analogous to the critical points observed in liquid-vapor and ferromagnetic systems [12].

Four decades ago Wojtowicz and Sheng [3] extended the Maier-Saupe (MS) mean-field theory (MFT) to investigate the effect of an external magnetic field on the N-I transition. These authors considered nematic liquid crystals composed of uniaxial molecules with positive diamagnetic anisotropy and obtained the temperature–magnetic-field phase diagram, which shows the existence of a critical end point. Similar investigations have also been carried out within the framework of Landau–de Gennes (LdG) phenomenological mean-field theory [13] and these too predict a quadratic variation of T_{NI} with the external field B. The mean-field estimate of the critical magnetic field is ~1000 T [3,4], which is outside the range attainable in a laboratory.

In similar mean-field calculations using an external electric field the predicted critical field is $\sim 10^8$ V/m [3,4] which is experimentally attainable. The first such determination of the critical point in a calamitic nematic (4-pentyl-4′-cyanobiphenyl) was done by Lelidis and Durand [10], who observed the critical electric field to be 1.41×10^7 V/m (the equivalent magnetic-field strength is ~140 T) and the shift in T_{NI} in similar studies [8,10,14] was a measurable quantity. Few such observations have been reported where magnetic-field-induced effects have been studied. Rosenblatt [11] was the first to observe a shift in T_{NI} in octylcyanobiphenyl (8CB), albeit by a few millikelvin, using a magnetic-field of strength 14.8 T. One reason behind such a small change in the transition temperature is the relatively low value of the diamagnetic anisotropy of the traditional calamitic mesogenic molecules.

The above features of the N-I transition in the presence of a magnetic field have also been confirmed by early Monte Carlo (MC) studies. A series of such important work was done three decades ago by Luckhurst *et al.* [15] using a Lebwohl-Lasher (LL) [16] lattice MC simulation. More recently, Warsono *et al.* [17] reported lattice simulation using a Zwanzing model of discrete orientations [18] and this simple model also has shown the existence of a magnetic-field-induced N-pN transition and a critical field.

A recent experimental observation of a magnetic-field-induced first-order I-N transition by Ostapenko *et al.* [19] in a different class of liquid crystals has created fresh excitement in this area of research. These investigators observed a shift in T_{NI} as high as ~0.8 K at $B = 23$ T, but could not detect the existence of a critical end point, although a magnetic field up to 31 T was used. The bent-core compounds exhibit a number of fascinating phenomena in liquid-crystal science, for example, the formation of the long-sought biaxial nematic phase in thermotropic liquid crystals [20,21]. For the purpose of this paper it is sufficient to note that the bent-core molecules are highly biaxial. It has also been observed that the N-I transition in a system composed of such molecules is more weakly first order than that observed in systems made up of calamitic molecules [22].

The first theoretical study of the effect of molecular biaxiality on the N-I transition in the presence of a magnetic field was reported by Remler and Haymet [7], who also used a MFT. It is evident from this work that as the degree of molecular biaxiality is increased the critical field strength drops rapidly and for a given field strength the shift in T_{NI} is higher in uniaxial nematics composed of biaxial molecules.

In a recent study Trojanowski *et al.* [23] extended an earlier work by Gramsbergen *et al.* [6] to investigate the effect of an external field on uniaxial N-I (pN) as well as biaxial N–uniaxial N phase transitions. These authors have used the phenomenological LdG theory and also a MS-type MFT using

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the so-called dispersion model [24] of interaction between biaxial molecules. A limited amount of MC simulation using the dispersion model was also performed to check the consistency of the results. The part of the findings relevant to the present paper is that in an uniaxial nematic composed of biaxial molecules having a fixed value of the biaxiality parameter $\lambda = 0.3$ (to be elaborated later) both MFT and MC simulation predict a N-pN coexistence curve that is linear in the T-B^2 plane and ends at a critical point. The MC study is only qualitative in predicting the critical point since an estimate of a rather broad range of the critical magnetic field (for a given value of the anisotropic molecular susceptibility) is given.

Very recently To *et al.* [25] performed an elaborate study of the effect of variation of the molecular biaxiality parameter λ on the N-pN transition. Although these authors have used the same dispersion potential as that used in Ref. [23], their mean-field approach is significantly different. An important finding in this work is that the difference between T_{NI} and T_{-} (the supercooling limit of the isotropic phase) depends on λ and that from a knowledge of the difference between these temperatures one can estimate the angle between the arms of a bent-core molecule (and vice versa). They are also of the opinion that Ostapenko *et al.* [19] have been rather unlucky in not observing the critical point in the particular system they studied with the magnetic field going up to 31 T.

In the present paper we report an extensive Lebwohl-Lasher-like MC study of the effect of an external magnetic field on the uniaxial nematic–paranematic transition for systems composed of both uniaxial ($\lambda = 0$) and biaxial ($\lambda = 0.2$) molecules having positive diamagnetic anisotropy. We have used a lattice model with the same dispersion potential as in Refs. [24,26] and have used different system sizes to perform finite-size-scaling analysis [27,28] in order that observables can be determined in the thermodynamic limit. This approach also enables us to minimize the errors characteristic in mean-field predictions resulting from the neglect of fluctuations. Also, to improve the reliability of our results we have performed multiple histogram reweighting (MHR) [29] of our data. Our predictions are the same as those in the MFT results discussed above with perhaps a little more realistic estimate of the critical field for the molecular biaxiality we have used. One of our important observations is that the coexistence curve (N-pN) in the T-B^2 plane is quadratic for both $\lambda = 0$ and 0.2 instead of being linear as predicted by all forms of MFT.

II. MODEL

We consider a system of biaxial prolate molecules possessing D_{2h} symmetry (boardlike), whose centers of mass are associated with a simple-cubic lattice and subjected to an external magnetic field. The total energy of the system is the sum of two terms: (i) a dispersion potential term that takes into account the interaction between all nearest-neighbor pairs of molecules and (ii) a field term that represents the interaction of each molecule with the external field. We use the dispersion potential [24,26] between two identical neighboring molecules (say ith and jth molecules)

$$U_{ij}^{\text{disp}} = -\epsilon_{ij}\big\{R_{00}^{2}(\Omega_{ij}) + 2\lambda\big[R_{02}^{2}(\Omega_{ij}) + R_{20}^{2}(\Omega_{ij})\big] + 4\lambda^{2}R_{22}^{2}(\Omega_{ij})\big\}. \tag{1}$$

Here $\Omega_{ij} = \{\phi_{ij},\theta_{ij},\psi_{ij}\}$ denotes the triplet of Euler angles defining the relative orientation of the two molecules; we have used the convention used by Rose [30] in defining the Euler angles. In addition, ϵ_{ij} is the strength parameter, which is assumed to be a positive constant ϵ when the particles i and j are nearest neighbors and zero otherwise, and R_{mn}^{L} are combinations of symmetry-adapted (D_{2h}) Wigner functions

$$R_{00}^{2} = \frac{3}{2}\cos^{2}\theta - \frac{1}{2}, \tag{2}$$

$$R_{02}^{2} = \frac{\sqrt{6}}{4}\sin^{2}\theta\cos 2\psi, \tag{3}$$

$$R_{20}^{2} = \frac{\sqrt{6}}{4}\sin^{2}\theta\cos 2\phi, \tag{4}$$

$$R_{22}^{2} = \frac{1}{4}(1+\cos^{2}\theta)\cos 2\phi\cos 2\psi - \frac{1}{2}\cos\theta\sin 2\phi\sin 2\psi. \tag{5}$$

The parameter λ is a measure of the molecular biaxiality and for the dispersion interactions it can be expressed in terms of the eigenvalues (ρ_1,ρ_2,ρ_3) of the polarizability tensor $\boldsymbol{\rho}$ of the biaxial molecule $\lambda = \sqrt{3/2}(\rho_2 - \rho_1)/(2\rho_3 - \rho_2 - \rho_1)$. The condition for the maximum biaxiality (also known as the self-dual geometry) is $\lambda = \lambda_C = 1/\sqrt{6}$. Here $\lambda < \lambda_C$ corresponds to the case of prolate molecules, whereas $\lambda > \lambda_C$ corresponds to oblate molecules. This dispersion model can successfully reproduce both the uniaxial and the biaxial orientational orders and various order-disorder transitions as a function of temperature and molecular biaxiality [26].

In our simulations we consider two cases: In one case $\lambda = 0$ and the pair potential takes the usual LL form [16] for nematic liquid crystals of perfectly uniaxial molecules, which has been extensively studied by Zhang *et al.* [31]; in the other case we choose $\lambda = 0.2$, which represents a biaxial system composed of prolate biaxial molecules. For the LL model there is a single weak first-order N-I transition at a dimensionless temperature ($T = kT_K/\epsilon$, T_K being the temperature measured in kelvin and k the Boltzmann constant) $T = 1.1232 \pm 0.0001$ [31] ($T = 1.1232 \pm 0.0006$ [32]). From the Monte Carlo results, as reported in [26,33], the biaxial model ($\lambda = 0.2$) is found to exhibit a second-order biaxial-uniaxial phase transition at low temperature ($T \approx 0.2$) and a uniaxial-isotropic transition at a higher temperature ($T \approx 1.1$).

The interaction of a uniform external magnetic field $\boldsymbol{B}$ chosen along the laboratory Z axis (unit vector z) with the ith molecule resulting from its coupling with the longest molecular symmetry axis $\boldsymbol{w}_i$ is taken as

$$U_{i}^{\text{field}} = -\epsilon\xi\big[\tfrac{3}{2}(\boldsymbol{w}_i\cdot z)^{2} - \tfrac{1}{2}\big], \tag{6}$$

where ξ is a dimensionless quantity that determines the strength of coupling of the molecular symmetry axis with the magnetic field and is given by

$$\xi = \frac{(\Delta\kappa)B^{2}}{3\mu_0\epsilon}. \tag{7}$$

Here $\Delta\kappa = \kappa_{\parallel} - \kappa_{\perp}$ is the anisotropy of the molecular magnetic polarizability and μ_0 is the permeability of the free space.

In the simulations we take $\Delta\kappa > 0$ and hence ξ to be a positive quantity so that the molecules tend to get their long axes aligned along the magnetic field. The total energy $\mathcal{E}$ of the system is therefore given by

$$\mathcal{E} = \sum_{\langle i,j \rangle} U_{ij}^{\text{disp}} + \sum_{i} U_{i}^{\text{field}}, \qquad (8)$$

where the angular bracket represents the nearest neighbors.

III. COMPUTATIONAL ASPECTS

A series of MC simulations using the conventional Metropolis algorithm on a periodically repeated simple cubic lattice for five system sizes $L = 18, 22, 26, 30$, and 40 has been performed. An orientational move was attempted following the Barker-Watts method [34]. For a given set of values of λ, L, and ξ, the simulation at the lowest temperature studied was started from the perfectly ordered state with the molecular longest symmetry axis $\boldsymbol{w}$ parallel to the space-fixed field (chosen along the laboratory Z axis). The simulations at the other temperatures for the same set were run in cascade starting from an equilibrium configuration at the nearest lower temperature.

In each simulation histograms of energy $h(E)$ were accumulated. For this we divided the continuous energy range (from $-3.0L^3$ to 0) with a sufficiently small bin width ($\Delta E = 1.0$). In our simulations 10^6 sweeps or Monte Carlo steps per site (MCS) for the equilibration and (4–6) $\times$ 10^6 MCS for the production run were used for every set of values of λ, ξ, and T. For the largest lattice size ($L = 40$), the total run length is more than 10 000 times the correlation time. The total run was divided into several (100) blocks by performing independent simulations so that we could compute the jackknife errors [35].

In order to analyze the orientational order we have calculated the second-rank order parameters $\langle R_{mn}^2 \rangle$ following the procedure described by Vieillard-Baron [36]. According to this, a $\boldsymbol{Q}$ tensor is defined for the molecular axes associated with a reference molecule. For an arbitrary unit vector $\boldsymbol{w}$, the elements of the $\boldsymbol{Q}$ tensor are defined as $Q_{\alpha\beta}(\boldsymbol{w}) = \langle (3w_\alpha w_\beta - \delta_{\alpha\beta})/2 \rangle$, where the average is taken over the configurations and the subscripts α and β label Cartesian components of $\boldsymbol{w}$ with respective to an arbitrary laboratory frame. By diagonalizing the matrix one obtains nine eigenvalues and nine eigenvectors, which are then recombined to give the four order parameters $\langle R_{00}^2 \rangle$, $\langle R_{02}^2 \rangle$, $\langle R_{20}^2 \rangle$, and $\langle R_{22}^2 \rangle$ with respect to the director frame [37]. Out of these four second-rank order parameters the usual uniaxial order parameter $\langle R_{00}^2 \rangle$ (or S) that measures the alignment of the longest molecular symmetry axis with the primary director $\boldsymbol{n}$ is involved in our study because we have simulated a very short temperature range (1.110–1.140) around T_{NI} within which no biaxial phase occurs.

We have calculated the reduced specific heat per particle C and the ordering susceptibility χ from fluctuations in the scaled total energy E ($E = \mathcal{E}/\epsilon$) and the order parameter, respectively. In order to determine the order parameter and the ordering susceptibility we have determined the constant-energy averages (corresponding to each energy bin) of the order parameter and its square from the simulation data [38] and the reweighting method was employed.

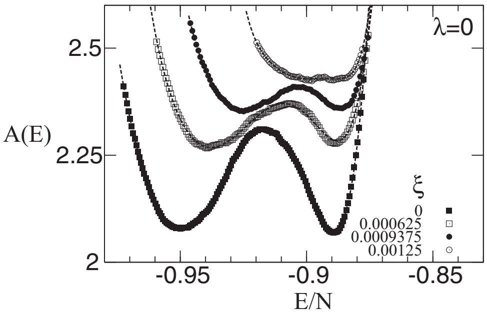

FIG. 1. Free energy A as a function of energy per molecule with and without an external magnetic field for the uniaxial system for $L = 40$. An eighth-order polynomial fit to the data is also presented.

IV. RESULTS

Monte Carlo simulations were performed for different values of the external field parameter ξ at five or six different temperatures within the said temperature range to generate histograms for both the uniaxial and biaxial models for all system sizes. For the uniaxial molecules simulations have been performed for five different values of ξ ranging from 0 to 0.001 25 with an increment of 0.000 312 5 for each lattice size, while for the biaxial model four different values of ξ from 0 to 0.000 75 with an increment of 0.000 25 have been used. (Such low values of ξ have been chosen so that the thermodynamic state remains below the critical end point.) A total of about 200 simulations were thus performed for different values of λ, L, ξ, and T.

The temperature dependence of the internal energy $\langle E \rangle$, the order parameter $\langle R_{00}^2 \rangle$, and the corresponding response functions, i.e., the specific heat C and the order parameter susceptibility χ, were obtained after performing the MHR to the data obtained in the simulations. We have derived the relevant part of the free-energy-like functions $A(E)$ from the energy distribution functions [27,28] $P(E)$ for both $\lambda = 0$ and 0.2 using the relation $A(E) = -\ln P(E)$, where the normalized histogram count $P(E) = h(E)/\sum_E h(E)$. For the uniaxial molecules an energy barrier separating the two minima in A is observed for all the lattice sizes except the smallest one having $L = 18$. The mesogenic molecules having biaxiality $\lambda = 0.2$, however, does not show any noticeable energy barrier, even in the absence of the external magnetic field, up to the system size $L = 30$. The double-well structure of the free-energy-like quantity for the biaxial system is observed only for the largest system size simulated ($L = 40$).

For the uniaxial case we have shown (Fig. 1) the field dependence of the free energy A at the transition temperature for the largest system size ($L = 40$) for which the free-energy barrier between the two minima is well pronounced and the effect of the external field on ΔF is clearly visible. Here the bulk free-energy barrier ΔF is given by $\Delta F(\xi,L) = A(E_m;T,\xi,L) - A(E_1;T,\xi,L)$, where E_1 is the energy at which the two minima of A of equal depth appear and E_m gives the position of the maximum of the free energy A [27,28]. The temperatures in all the above cases were adjusted to obtain two minima of equal depth. We observe that the double well becomes shallower as ξ increases. The external

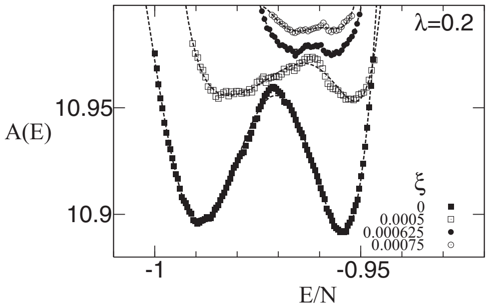

FIG. 2. Free energy A as a function of energy per molecule with and without an external field for the biaxial system for $L = 40$.

field thus reduces the strength of the first-order transition and this suggests that for a particular value of the field $\xi_c(L)$ the barrier between the two minima of $A(E)$ is likely to vanish, which would correspond to the end point where the first-order phase transition turns into a crossover [39].

In Fig. 2 the free energy for $\lambda = 0.2$ and its dependence on the magnetic field is shown for $L = 40$. It is found that at zero field ($\xi = 0$) the free-energy barrier ΔF is much smaller for the biaxial molecules compared to the uniaxial molecules and with increasing ξ the barrier ΔF reduces to zero at a faster rate. This therefore indicates that the N-I transition for the biaxial molecules is more weakly first order and also the critical magnetic field of this system is smaller than that of its uniaxial counterpart. For finite systems the peak height of the order parameter susceptibility χ (or the specific heat C) increases with increasing system size and the scaling relation for $\chi^{\max}$ (or $C^{\max}$) in a first-order phase transition obeys $\chi^{\max} \sim L^d$ (or $C^{\max} \sim L^d$) [27,28], d being the dimensionality of the system. We have verified that this scaling relation holds for both the uniaxial and the biaxial systems. It is observed that with increasing ξ the heights of the maxima $C^{\max}(L)$ and $\chi^{\max}(L)$ are reduced. This observation is noticeable, particularly for the higher lattice sizes $L = 26$, 30, and 40, which shows that the presence of a magnetic field weakens the first-order nature of the N-I transition.

Determining the finite-size transition temperature $T_{NI}(L)$ from the location of the maximum of the specific heat and the susceptibility curves we have used the scaling relation $T_{NI}(L) - T_{NI} \sim L^{-d}$ and performed a linear extrapolation for $L \rightarrow \infty$ to obtain the transition temperature T_{NI} in the thermodynamic limit for both values of λ. These are listed in Table I, where we find the expected increase in T_{NI} with an increase in ξ for both $\lambda = 0$ and 0.2.

The shift δT_{NI} [$= T_{NI}(\xi) - T_{NI}(0)$] in transition temperature is plotted against ξ ($\propto B^2$) in Fig. 3. We obtain good quadratic fits to the data in both cases, unlike the linear behavior predicted by the LdG theory. The quadratic functions used for the fits are $f(\xi) = -5.7 \times 10^{-6} + 0.64\xi + 1097.1\xi^2$ for $\lambda = 0$ and $g(\xi) = -2.0 \times 10^{-6} + 0.93\xi + 1520.0\xi^2$ for $\lambda = 0.2$. The results therefore show that the rise in T_{NI} over its zero-field value with increasing field is steeper for the biaxial molecules than that for the uniaxial ones.

The finite-size stability limit $T_-(L)$ of the isotropic phase for the uniaxial molecules is estimated as the temperature where the second local minimum (at higher energy) of A just vanishes as T is gradually lowered below T_{NI}. From extrapolation to the thermodynamic limit we estimate T_- for different field strengths. We observe in Fig. 4 that the width of the stability limit of the I phase for the uniaxial molecules $T_{NI}(\xi) - T_-(\xi)$ decreases with an increase in magnetic field (Fig. 4). From the fit to the data (as shown in Fig. 4) we find that this temperature difference is linear in ξ (i.e., quadratic in B). It is therefore possible to obtain an estimate of the critical magnetic field by performing a linear extrapolation (Fig. 4) up to the field strength ξ_C at which $T_{NI}(\xi) - T_-(\xi)$ becomes zero. For the uniaxial case we get $\xi_C = 0.001\,32$. The N-I transition for the case of biaxial molecules is so weak that the determination of $T_-(\xi)$ at the thermodynamic limit and hence the critical field following the above approach is beyond our scope as it is likely to involve simulations in much bigger systems.

However, a finite-size estimate of $\xi_C(L)$ from the field dependence of ΔF is possible [39] for both the uniaxial and the biaxial molecules as shown in Fig. 5. In the case of the uniaxial molecules we observe that as the field strength

TABLE I. Nematic-isotropic transition temperatures (at the thermodynamic limit) for different values of the external field strength parameter ξ for the uniaxial and the biaxial systems. Estimates of supercooling limits T_- (at the thermodynamic limit) are also listed for the uniaxial system. The estimated (jackknife) error in each temperature is within ±0.0001.

λ	ξ	T_{NI} (from C_V)	T_{NI} (from χ)	T_-
0	0	1.1231	1.1231	1.1221
0	0.0003125	1.1234	1.1234	1.1227
0	0.0006250	1.1239	1.1239	1.1234
0	0.0009375	1.1246	1.1247	1.1244
0	0.0012500	1.1256	1.1257	
0.2	0	1.1165	1.1165	
0.2	0.00025	1.1168	1.1168	
0.2	0.00050	1.1173	1.1174	
0.2	0.00075	1.1180	1.1181	

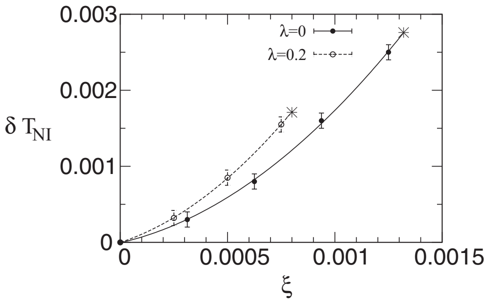

FIG. 3. Increase in the N-I phase transition temperature δT (over zero field) vs ξ for both the uniaxial ($\lambda = 0$) and biaxial ($\lambda = 0.2$) models. The extrapolation of the fitted curve for $\lambda = 0$ gives $\delta T_{NI} = 0.0027$ for the critical parameter $\xi_C = 0.001\,32$ and the asterisk represents the critical end point. For $\lambda = 0.2$ the critical estimates are $\delta T_{NI} = 0.0017$ and $\xi_C = 0.0008$.

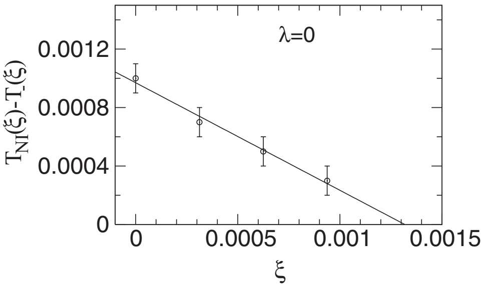

FIG. 4. Plot of $T_{NI}(\xi) - T_-(\xi)$ vs ξ. The solid line is the best linear fit. The estimated value of ξ_C is 0.001 32.

parameter ξ is increased beyond 0.000 625 the free-energy barrier decreases at a faster rate. For this case we may estimate the value of ξ_C by performing a linear extrapolation using the results of the barrier height ΔF for three higher values of ξ, i.e., 0.000 625, 0.000 937 5, and 0.001 25. This extrapolation yields the critical field parameter $\xi_C = 0.001\,31$, which is very close to the estimate obtained above at the thermodynamic limit. The corresponding critical value of the temperature can be estimated from the extrapolation of the fitted curve for $\lambda = 0$ in Fig. 3, which is $T_C = 1.1258$, δT_C being 0.0027. For the biaxial case a linear extrapolation to the data obtained for ΔF for $\xi = 0.0005, 0.000\,625$, and $\xi = 0.000\,75$ gives an estimate of ξ_C that is 0.0008 and the corresponding critical temperature $T_C = 1.1182$ ($\delta T_C = 0.0017$). Hence the critical field parameter ξ for the biaxial molecules ($\lambda = 0.2$) is only about 60% of the critical value for the uniaxial molecules.

In order to get an estimate of ξ in real units we may use Eq. (7). The energy unit ϵ can be estimated by using the experimental and simulated nematic-isotropic transition temperatures, i.e., $\epsilon = k_B T_K(B=0)/T_{NI}(B=0)$. For a common nematic, say, 8CB, the N-I transition temperature $T_K(B = 0) = 314$ K and the anisotropy of the molecular magnetic polarizability $\Delta\kappa \approx 0.16 \times 10^{-32}$ m^3 [40]. Using these values and the simulated value of $T_{NI}(B = 0) = 1.1231$ for $\lambda = 0$ we obtain $B_C \approx 3040\sqrt{\xi_C}$ T, which is about ~110 T for common nematics. This is one order of magnitude smaller than the mean-field estimate [3,4] and is of the same order as mentioned in [10]; for $\lambda = 0.2$ using the same $\Delta\kappa$ we estimate $B_C \sim 86$ T.

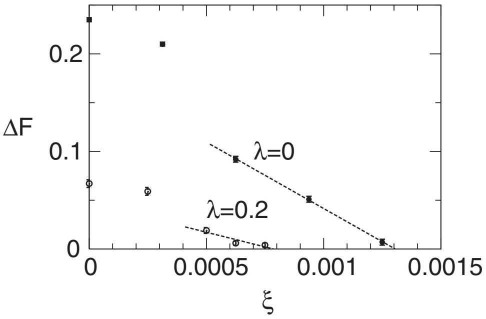

FIG. 5. Free-energy barrier height $\Delta F(L)$ vs ξ for the uniaxial model and for the lattice size $L = 40$. Linear extrapolations of three nearest points are used to estimate ξ_C, which is 0.001 31 for $\lambda = 0$ and 0.0008 for $\lambda = 0.2$.

V. CONCLUSION

Using MC simulation we have determined the entire N-I coexistence curve terminating at a field-induced critical point for two nematic systems composed of uniaxial and biaxial molecules. In disagreement with the mean-field prediction of the linear coexistence curves in the T-B^2 plane, we have obtained quadratic behavior for both $\lambda = 0$ and 0.2. The rate of change of the transition temperature with a magnetic field (or dT_{NI}/dB^2) is steeper for the system composed of biaxial molecules and the critical point occurs in such a system at a magnetic field much lower than what is necessary for a uniaxial molecular system. A comparison of our simulation results with the recent experimental findings of Ostapenko *et al.* [19] shows that the significant molecular biaxiality of the bent-core molecules has possibly played an important role in the experimental realization of the magnetic-field-induced I-N phase transition.

Our study is limited to the value of the biaxiality parameter $\lambda = 0.2$, which is smaller than the value $\lambda = 0.25$ of the bent-core molecules used in the study of Ostapenko *et al.* [19]. From the work of To *et al.* [25] it is evident that $dT_{NI}/d\lambda$ is a rapidly increasing function of λ in the neighborhood of $\lambda \sim 0.25$ and consequently the expected value of the critical field for $\lambda = 0.25$ is likely to be much lower than what we have estimated for the $\lambda = 0.2$ system. However, we are not in a position to judge whether Ostapenko *et al.* [19] have narrowly missed the critical field as is the opinion of To *et al.* [25]. For this purpose a more elaborate MC study where a range of different values of λ has been considered is necessary.

Comparing our work with the recent work of Trojanowski *et al.* [23], we point out that we have performed a more extensive and quantitatively more accurate MC study using MHR and finite-size-scaling analysis to determine the N-I coexistence curves and the critical points in the presence of an external magnetic field. The dispersion potentials in the two works are the same, but differ in the value of the biaxiality parameter λ.

We conclude by noting that in spite of what we have said, ours is a simple model system as a dispersion interaction with a lattice model has been used; we have not considered the translational degrees of freedom or the molecular flexibility. The former can be included in a MC simulation by considering an off-lattice model along with a biaxial Gay-Berne potential [41] using an isobaric-isothermal (NPT) ensemble [42], whereas the inclusion of molecular flexibility is a more formidable task [43]. Nevertheless, consideration of these features along with the variation of the molecular biaxiality would be an ideal task that would take us much closer to a real nematic. In that case, however, to make the job computationally feasible, one may have to consider fewer molecules, which in turn will make the use of finite-size scaling and determination of thermodynamic limits rather difficult.

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