Fluctuations in the nematic-isotropic phase transition

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We study the fluctuations in a lattice model of the nematic-isotropic phase transition, whose mean-field approximation follows the Maier-Saupe theory. We show that fluctuations significantly change the order parameter, the transition entropy, and the precocity of the phase transition $(T_c-T^*)/T_c$. A comparison with Monte Carlo simulation data shows that the fluctuation corrections remove most of the deficiencies of Maier-Saupe approximation.

I. INTRODUCTION

There exist two simple approaches to the nematic-isotropic phase transition. One is the mean-field theory of Maier and Saupe[1] and the other the Landau–de Gennes[2] expansion of the free energy in powers of a symmetric traceless field which serves as an order parameter for the nematic phase. Both approaches describe the qualitative features of the transition.

The Maier-Saupe approach, however, fails to account for a number of important quantitative details. Some of these discrepancies are as follows.

(i) The jump of the order parameter $S=\langle P_2(\cos\theta)\rangle$ across the transition is calculated to be 0.43 (see Fig. 1) whereas experimentally it is quite often significantly smaller (~ 0.3).[3]

(ii) The temperature dependencies of the order parameter and of the elastic constants are much stronger experimentally[4] than the mean-field results.[5]

(iii) The latent heat L of the transition is too large in the mean-field calculation by a factor of 2 to 3.[6]

(iv) The precocity of the phase transition defined as the relative difference between the actual transition temperature T_c and the temperature of instability T^* (=superconducting temperature=would be second-order transition temperature) $p\equiv(T_c-T^*)/T_c\approx 2\times 10^{-3}$ is grossly overestimated by a factor ~ 45 (Ref. 7). (See Table I.) The common feature of (i)–(iv) is an exaggeration of the strength of the first-order transition. This is not significantly improved if Gaussian fluctuation corrections are taken into account.

In the Landau–de Gennes treatment, these problems except for (ii) can be cured since the coefficients of the energy [Q is a second-rank tensor of director $\mathbf{n}(\theta,\varphi)$, see Eq. (1b)]

$$f=a_2\tau\,\mathrm{Tr}Q^2+\varepsilon\,\mathrm{Tr}Q^3+\tfrac{1}{2}a_4\,\mathrm{Tr}Q^4$$

are *arbitrary* parameters [$\tau\equiv(T-T^*)/T^*$] and the strength of the first-order jumps can be adjusted to experiments by a suitable choice of ε relative to a_2,a_4.

As far as point (ii) is concerned, the situation is not yet certain. While the older work[8] claimed to see a temperature behavior of S, $S=S_0+S_1\tau^{\beta}$, being consistent with the Landau–de Gennes mean-field exponent $\beta=\frac{1}{2}$, in the later phenomenological analysis the same data[8] was used to suggest a tricritical nature of the transition with the value of $\beta=\frac{1}{4}$.[9] The same tricritical value of β has been supported by the latest experiments.[10]

This parallels the discussion of the temperature dependence of the ratio of the first and second Cotton-Mouton

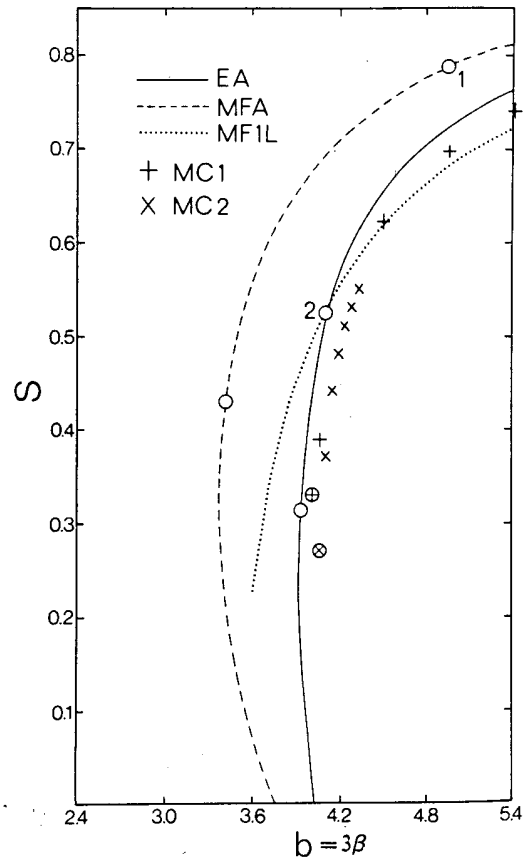


FIG. 1. Order parameter as a function of $b=3\beta$. Curves in Figs. 1–3 and 5 are obtained by using mean-field theory (MFA); mean-field plus one-loop correction (MF1L); high-temperature expansion of Eq. (12) (HTE); effective action in hopping expansion (EA). The crosses are the Monte Carlo data of Lebwohl and Lasher (MC1) (Ref. 16), and the symbols × are those of Meirovitch (MC2) (Ref 17). For MF1L the curves in Figs. 1, 3, 5 are truncated halfway before the one-loop corrections become unnaturally large. The transition point in each case is surrounded by a circle. The circle 1 is located by the combined use of MFA + HTE, while the circle 2 by MF1L + HTE.

TABLE I. Values of some quantities characteristic to the phase transition given by different approximations, and compared with the Monte Carlo data.

	MFA[a]	MFA + HTE	MF1L + HTE	EA	MC1	MC2
β_c	1.135	1.65	1.37	1.31	1.34	1.35
S_c	0.429	0.79	0.69 0.53[b]	0.32	0.33	0.27
$(T_c-T^*)/T_c$	0.092	negative	c	0.027		
L	0.368	0.449	0.37	0.14	0.073	0.08

[a]For abbreviations see Fig. 1.
[b]One-loop correction to S being included.
[c]β^* cannot be defined (see Fig. 2).

coefficients, which regulate the dependence of S on the magnetic field as $S\sim c_1H^2+c_2H^4$. From Landau–de Gennes mean-field theory one would have $c_1\sim\tau^{-1}$ and $c_2\sim\tau^{-3}$ and so $c_2/c_1\sim\tau^{-\Delta}$ with $\Delta=2$. The analysis of experimental data in Ref. 11 seemed to deduce also here a tricritical exponent $\Delta\sim\frac{5}{4}$. However, another recent experiment and a careful analysis of it claims[12] that for the present no definite conclusion for Δ can be drawn. So, the Landau–de Gennes mean-field value $\Delta=2$ is not yet excluded from being correct. This point of view seems to have been accepted also by the other authors.[13]

In any case the observation of a small precocity (iv) shows that the cubic term of the Landau–de Gennes theory is so small that the transition is almost of second order. This implies that, if the gradient terms of Q are included,[14] the director fluctuations are rather violent and become almost critical. Hence, simple one-loop corrections are expected to be insufficient to account for the experimental facts.

With fluctuations being so important the question arises whether the disagreements of the Maier-Saupe results with experiment are really due to insufficiences in the physical description or are consequences of the mean-field nature of the approximation.[15] In fact, the Monte Carlo simulations[16] and the numerical calculation[17] suggest that the latter option is closer to the truth than the former. We therefore decided that there is a need for an improved theoretical treatment of fluctuations. Only if these are properly taken into account will it make sense to build detailed models and seek for an accurate agreement with experimental data.

Methods for treating fluctuations in lattice models have recently been developed by Matsui, Kleinert, and Ami[18] (MKA) in the context of spin models. Since there the transition is of second order and the results are nevertheless rather satisfactory, we concluded that the same methods should be quite reliable in the case of the weakly first-order nematic-isotropic transition. It is the purpose of this paper to show that this is, indeed, the case. We consider the lattice model[19] studied by Monte Carlo simulation and a numerical calculation in Refs. 16 and 17 and treat it with the techniques of MKA.[18]

II. MOTIVATION FOR THE LATTICE MODEL

The partition function of the lattice model can be written down in the following form:

$$Z=\left[\prod_{\mathbf{x}}\int\frac{d^2n(\mathbf{x})}{4\pi}\right]\times\exp\left[\beta\sum_{\mathbf{x},\mathbf{i}}\sum_{k,l}Q_{kl}(\mathbf{x})Q_{kl}(\mathbf{x}+\mathbf{i})\right]. \tag{1a}$$

Here $\mathbf{x}$ are the sites of a simple cubic lattice and $\mathbf{i}$ the oriented links pointing to the nearest neighbors in the ith direction ($i=1,2,3$). The matrices $Q_{kl}(\mathbf{x})$ are traceless uniaxial matrices composed of the director $n_k(\mathbf{x})$ ($k=1,2,3$) of rodlike molecules at $\mathbf{x}$ as follows:

$$Q_{kl}(\mathbf{x})=n_k(\mathbf{x})n_l(\mathbf{x})-\tfrac{1}{3}\delta_{kl},\quad \mathbf{n}^2(\mathbf{x})=1\,. \tag{1b}$$

The d^2n is the solid angle element over a unit sphere. The quantity β is the inverse temperature in natural units.

The mean-field approximation (MFA) to this model is identical to the standard Maier-Saupe result. When studying the fluctuations in this model via Monte Carlo techniques[16] and a numerical method[17] one finds that the results are much closer to experiment than to the mean-field approximation.

(i) The calculated order-parameter jump is $S_c=0.27$ (Ref. 16); 0.33 (Ref. 17) (Table I).

(ii) The temperature dependence of the order parameter is much more pronounced than in the mean-field approximation.

(iii) The true latent heat is $L=0.073$ (Ref. 16); 0.08 (Ref. 17) whereas the mean-field value is 0.368 (in arbitrary units) (Table I).

We therefore expect that also the precocity will be very small, although this has not been investigated by Refs. 16 and 17. The gross features of the fluctuation corrections will not be changed if one passes from Eq. (1) to more realistic models (inclusion of splay, bend, and twist elastic energies, continuum formulation, introduction of steric effects, chain flexibility, etc.).

It is, therefore, reasonable to expect that a more accurate evaluation of the lattice model can give a satisfactory description of the behavior of nematic-liquid crystals. The simple model [Eq. (1)] will therefore be used as a testing ground for the importance of fluctuations and our ability to calculate them.

In order to approach the problem step by step, we shall first employ conventional methods of dealing with the

system [high-temperatures expansion (HTE) in Sec. III, mean-field approximation in Sec. IV, and mean-field plus one-loop correction (MF1L) in Sec. V]. These will serve to establish the nature of the needed corrections, in particular the intertwining of low- and high-temperature corrections, and to report some new results.

The high-temperature expansion, which is presented in the next section, allows for an efficient summation of the free energy which agrees well with its Monte Carlo estimation in the isotropic phase.[16,17]

In order to locate the transition temperature and to calculate the corrected specific heat, we first employ the combined use of the mean-field approximation for the nematic phase and high-temperature expansion for the isotropic phase (MFA + HTE). This approximation is rephrased in Sec. IV in a language which is appropriate for the subsequent development in Secs. V and VI. The resulting transition temperature (see Fig. 1, Table I) is in striking disagreement with the Monte Carlo result: If the latter is identified as the true transition point, the clearing point calculated from the MFA + HTE is located at a temperature at which most pure nematogens are frozen. Correspondingly, the order parameter jumps to $S_c = 0.79$ at this point.

Thus such an improvement of the isotropic phase alone is not sufficient: The mean-field free energy is much too large to properly locate the takeover of the ordered state. As a next step, the Gaussian correction, presented in Sec. V, is used together with the HTE to relocate the transition temperature at a value which compares well to the Monte Carlo results (see Fig. 2, Table I). Unfortunately, there is still a much too large order-parameter jump $S_c = 0.69$. We therefore calculate the one-loop correction to the order parameter itself (see Fig. 1). Although this gives an improvement to $S_c = 0.53$, this value is still too large to be acceptable. The results obtained so far indicate that the mean-field approximation owes its semiquantitative success mainly to a balance among its equally poor descriptions of both the nematic and isotropic phases.

It is clearly desirable to have an approximation in which the fluctuations in both phases are treated in the same way and with the same degree of accuracy. Such an approximation is well known in the context of field theory. It employs the framework of effective actions.[20] Instead of selecting the extremum of the classical energy to approximate the free energy (as in the mean-field treatment), it approximates the free energy by the extremum of a fluctuation-corrected "semiclassical" action. In continuum field theory the fluctuation corrections are organized by the number of loops in Feynman diagrams. In this way the effective action sums an infinite subset of conventional loop diagrams. It also respects the Ward identities of the theory. In MKA (Ref. 18) this framework was adapted to lattice theories, replacing the loop expansion of the effective action by a hopping expansion which converges like $1/D^n$, with D being the dimensionality of the system. In Sec. VI it will be applied to the liquid-crystal model (1). When comparing the results with the Monte Carlo data, we find an excellent improvement over the mean-field (plus Gaussian-correction) results (see Figs. 1–3, Table I). For $(T_c - T^*)/T_c$, we obtain 0.027, reducing the mean-field value by a factor of 3.4. This is still far from the experimental values but it is hard to judge this result, as the value of $(T_c - T^*)/T_c$ in the model is unknown. Monte Carlo simulations of the correlation functions should yield this information.

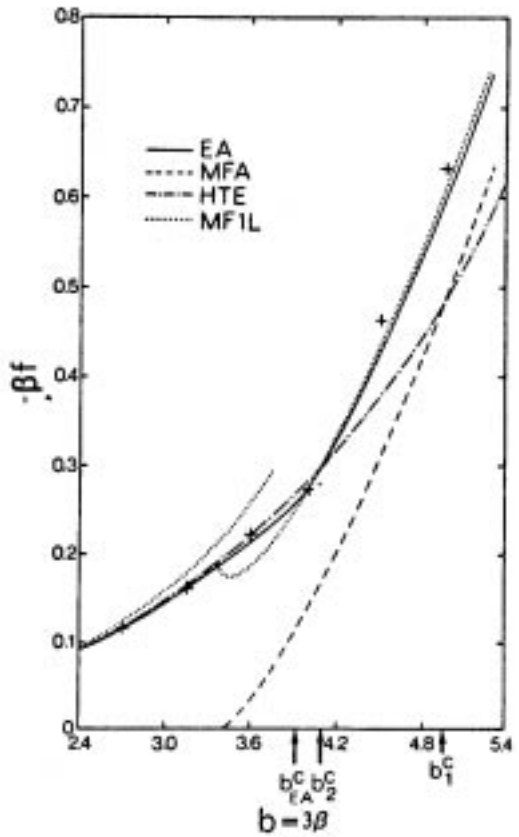


FIG. 2. Free-energy density as a function of $b = 3\beta$. For MF1L there is a region, $3.37 \lesssim b \lesssim 3.75$ in which $\mu_0^2 < 0$.

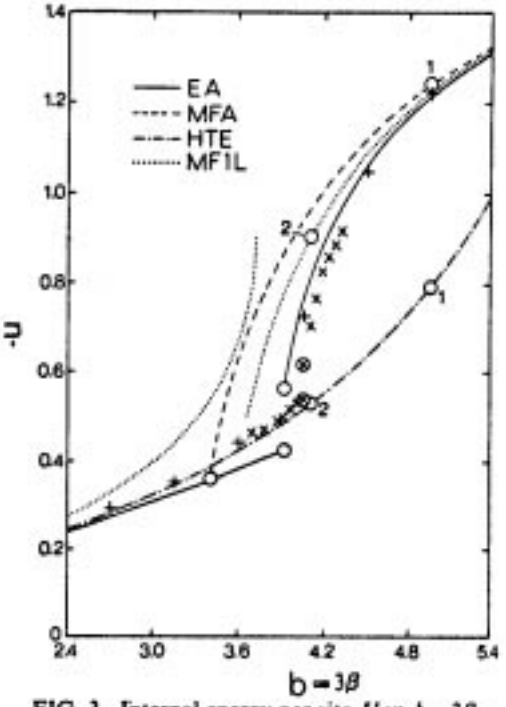


FIG. 3. Internal energy per site U vs $b = 3\beta$.

III. THE HIGH-TEMPERATURE EXPANSION (HTE)

A convenient method to evaluate the thermodynamic quantities in the disordered phase is the high-temperature (small-β) expansion. In its simplest version one expands the exponential in (1) into a power series in β. This has been done to $O(\beta^3)$ in Ref. 16. The calculational effort rapidly increases with the power of β.

For a more efficient evaluation of the free energy it is convenient to employ the so-called "character expansion" well known in lattice-spin and -gauge models. Here one first splits the exponential in (1) into a product of link factors and expands each of them into a set of functions which is complete and orthogonal under the integration measure for the field variables. For (1) these functions are the even Legendre polynomials

$$\exp\left[\beta\sum_{k,l} Q_{kl}(\mathbf{x})Q_{kl}(\mathbf{x}+\mathbf{i})\right]=\exp[\tfrac{2}{3}\beta P_2(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}+i))]=\sum_{l=0}^{\infty}\tilde{C}_l(\beta)P_{2l}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}+\mathbf{i})) \tag{2}$$

with coefficients

$$\tilde{C}_l(\beta)=(4l+1)\int_0^1 dz\, P_{2l}(z)\exp[\tfrac{2}{3}\beta P_2(z)]\,. \tag{3}$$

Extracting the $l=0$ contribution as an overall factor, the partition function (1) reads

$$Z=[\tilde{C}_0(\beta)]^{3N}\left[\prod_{\mathbf{x},i}\sum_{l_i(\mathbf{x})=0}^{\infty}C_{l_i(\mathbf{x})}(\beta)\right]\left[\prod_{\mathbf{x}}\int\frac{d^2\mathbf{n}(\mathbf{x})}{4\pi}\right]\prod_{\mathbf{x},i}[4l_i(\mathbf{x})+1]P_{2l_i(\mathbf{x})}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}+\mathbf{i}))\,,$$
$$C_l(\beta)=\frac{1}{4l+1}\frac{\tilde{C}_l(\beta)}{\tilde{C}_0(\beta)}\,, \tag{4}$$

where N is the total number of lattice sites.

The coefficients $C_l(\beta)$ have the threshold behavior $\sim\beta^l$ for small β. Hence any configuration $\{l_i(\mathbf{x})\}$ has the threshold behavior β^L with $L=\sum_{\mathbf{x},i}l_i(\mathbf{x})$ and the high-temperature expansion is obtained as

$$Z=[\tilde{C}_0(\beta)]^{3N}\sum_{L=0}^{\infty}Z_L\,,$$
$$Z_L=\left[\prod_{\mathbf{x},i}\sum_{l_i(\mathbf{x})=0}^{\infty}C_{l_i(\mathbf{x})}(\beta)\right]\delta_{\sum_{\mathbf{x},i}l_i(\mathbf{x}),L}\left[\prod_{\mathbf{x}}\int\frac{d^2\mathbf{n}(\mathbf{x})}{4\pi}\right]\prod_{\mathbf{x},i}[4l_i(\mathbf{x})+1]P_{2l_i(\mathbf{x})}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}+\mathbf{i}))\,. \tag{5}$$

Introducing polar coordinates $\mathbf{n}=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$ and using the addition theorem for spherical harmonics

$$P_{2l}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{y}))=\frac{4\pi}{4l+1}\sum_{m=-2l}^{2l}Y^*_{2l,m}(\theta(\mathbf{x}),\phi(\mathbf{x}))Y_{2l,m}(\theta(\mathbf{y}),\phi(\mathbf{y}))\,, \tag{6}$$

as well as the orthogonality relation

$$\int\frac{d^2\mathbf{n}}{4\pi}Y^*_{l_1,m_1}(\theta,\phi)Y_{l_2,m_2}(\theta,\phi)=\frac{1}{4\pi}\delta_{l_1,l_2}\delta_{m_1,m_2}\,, \tag{7}$$

where $d^2n=\sin\theta\,d\theta\,d\phi$, one easily verifies the following graphical rules for calculating Z_L.

(i) Only networks of closed chains contribute.

(ii) Along each connected set of links without branch points, l is conserved (and will, therefore, be referred to as a flux).

(iii) A connected chain of k links without branch points contributes the following (after integration over the $k-1$ internal variables):

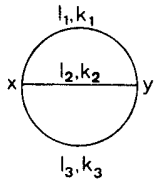
$$C_l^k(\beta)(4l+1)P_{2l}(\mathbf{n}(\mathbf{a})\cdot\mathbf{n}(\mathbf{b}))\,, \tag{8}$$

where l is the flux of the chain and $\mathbf{a},\mathbf{b}$ are the end points of the chain.

(iv) Identifying the end points $\mathbf{a}=\mathbf{b}$ and integrating over $\mathbf{n}(\mathbf{a})$ one has for a simple (self-avoiding) closed chain of k links and flux l the contribution

$$C_l^k(\beta)(4l+1)\,. \tag{9}$$

(v) For three self-avoiding chains of k_1,k_2,k_3 links with flux l_1,l_2,l_3 which are merged at two common endpoints $\mathbf{x}$ and $\mathbf{y}$ one has the contribution



$$= C_{l_1}^{k_1}(\beta) C_{l_2}^{k_2}(\beta) C_{l_3}^{k_3}(\beta)(4l_1+1)(4l_2+1)(4l_3+1)$$

$$\times \int \frac{d^2n(\mathbf{x})}{4\pi} \int \frac{d^2n(\mathbf{y})}{4\pi} P_{2l_1}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{y})) P_{2l_2}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{y})) P_{2l_3}(\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{y}))$$

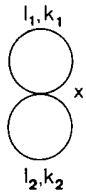
$$= \begin{bmatrix} 2l_1 & 2l_2 & 2l_3 \\ 0 & 0 & 0 \end{bmatrix}^2 \prod_{i=1}^{3} C_{l_i}^{k_i}(\beta)(4l_i+1) \tag{10}$$

with

$$\begin{bmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{bmatrix}$$

being a $3j$ symbol.

(vi) A figure-eight loop with k_1, k_2 links of flux l_1, l_2 on its simple loops and the central site $\mathbf{x}$ contributes as



$$= \int \frac{d^2n(\mathbf{x})}{4\pi} C_{l_1}^{k_1}(\beta) C_{l_2}^{k_2}(\beta)(4l_1+1)(4l_2+1) P_{2l_1}(\mathbf{n}^2(\mathbf{x})) P_{2l_2}(\mathbf{n}^2(\mathbf{x}))$$

$$= C_{l_1}^{k_1}(\beta) C_{l_2}^{k_2}(\beta)(4l_1+1)(4l_2+1)\,. \tag{11}$$

These rules are sufficient to evaluate the Z_L up to $L=8$. It remains to count the number of configurations which contribute to a given order. These numbers are well known from the three-dimensional Ising model and one has for Z_L, $L=0,1,\ldots,8$ (see Fig. 4 for the graphs corresponding to these expressions) the following:

$$Z_0=1,\quad Z_1=Z_2=Z_3=Z_5=0\,,$$

$$Z_4=3N\times 5C_1^4(\beta)\,,$$

$$Z_6=22N\times 5C_1^6(\beta)\,,$$

$$Z_7=18N\times 5^3 C_1^7(\beta)\begin{bmatrix} 2 & 2 & 2 \\ 0 & 0 & 0 \end{bmatrix}^2 = N\times\tfrac{900}{7}C_1^7(\beta)\,,$$

$$Z_8=Z_{8,a}+Z_{8,b}+Z_{8,c}+Z_{8,d}+Z_{8,e}\,,$$

$$Z_{8,a}=3N\times 9C_2^4(\beta)\,, \tag{12}$$

$$Z_{8,b}=\tfrac{3}{2}N(3N-13)5^2C_1^8(\beta)=N(3N-13)\tfrac{75}{2}C_1^8(\beta)\,,$$

$$Z_{8,c}=18NC_1^6(\beta)C_2(\beta)5^2\times 9\begin{bmatrix} 2 & 2 & 4 \\ 0 & 0 & 0 \end{bmatrix}^2$$

$$=N\times\tfrac{1620}{7}C_1^6(\beta)C_2(\beta)\,,$$

$$Z_{8,d}=24NC_1^8(\beta)5^3\begin{bmatrix} 2 & 2 & 2 \\ 0 & 0 & 0 \end{bmatrix}^2 = N\times\tfrac{1200}{7}C_1^8(\beta)\,,$$

$$Z_{8,e}=207N\times 5C_1^8(\beta)=N\times 1035C_1^8(\beta)\,,$$

$$Z_8=N[27C_2^4(\beta)+\tfrac{1620}{7}C_1^6(\beta)C_2(\beta)$$

$$+\tfrac{10065}{14}C_1^8(\beta)]+\tfrac{225}{2}C_1^8(\beta)N^2\,.$$

Notice that the lowest nontrivial contribution Z_4 starts out with β^4. The terms given to $O(\beta^3)$ in Ref. 16 are therefore all contained in the trivial prefactor $[\tilde{C}_0(\beta)]^{3N}$ in (5).

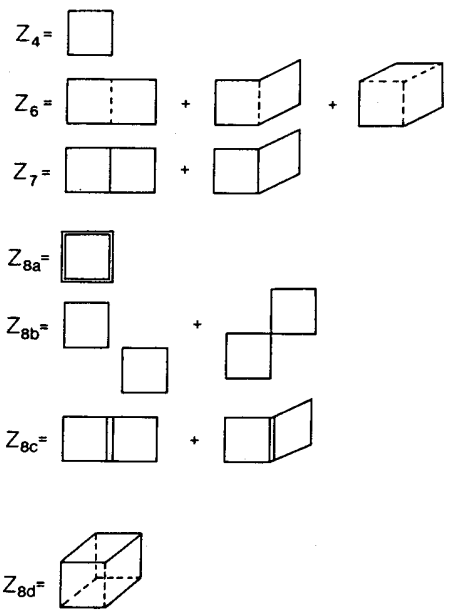


FIG. 4. Graphs contributing to Z_L up to $L=8$. Solid lines of multiplicity 1 denote links carrying flux l. Dotted lines are there to guide the eye. $Z_{8,e}$ consists of all possible self-avoiding closed loops of 8 links with flux l and is not drawn here.

To evaluate the $C_l(\beta)$ it is convenient to express $\tilde{C}_0(\beta)$ as

$$\tilde{C}_0(\beta)=\int_0^1 dz \exp[\tfrac{2}{3}\beta P_2(z)]=\frac{e^{-\beta/3}}{\sqrt{\beta}}D(\sqrt{\beta})=e^{\omega(\beta)}\,, \tag{13a}$$

where

$$D(x)=\int_0^x dy\, e^{y^2} \tag{13b}$$

is Dawson's integral and $w(\beta)$ is a characteristic function which will occur frequently in the following sections. The $C_l(\beta)$ occurring in (12) are

$$\begin{aligned} C_1(\beta)&=e^{-w(\beta)}\tfrac{3}{2}\int_0^1 dz(z^2-\tfrac{1}{3})e^{\beta(z^2-1/3)} \\ &=\tfrac{3}{2}w'(\beta)\,, \\ C_2(\beta)&=e^{-w(\beta)}\left[\frac{35}{8}\frac{d^2}{d\beta^2}-\frac{5}{6}\frac{d}{d\beta}-\frac{7}{18}\right]e^{w(\beta)} \\ &=\tfrac{35}{8}\{w''(\beta)+[w'(\beta)]^2\}-\tfrac{5}{6}w'(\beta)-\tfrac{7}{18}\,. \end{aligned} \tag{14}$$

To facilitate numerical calculations one may perform an integration by parts to relate $w'(\beta)$ to $w(\beta)$

$$\begin{aligned} w'(\beta)&=e^{-w(\beta)}\int_0^1 dz(z^2-\tfrac{1}{3})e^{\beta(z^2-1/3)} \\ &=-\frac{1}{3}-\frac{1}{2\beta}+\frac{1}{2\beta}e^{2\beta/3-w(\beta)}\,. \end{aligned} \tag{15}$$

This may be used to express all higher derivatives in terms of $w(\beta)$ as well. In particular, the identity

$$w''(\beta)+[w'(\beta)]^2=\left[\frac{1}{3}-\frac{3}{2\beta}\right]w'(\beta)+\tfrac{2}{9} \tag{16}$$

allows us to express $C_2(\beta)$ as

$$C_2(\beta)=\frac{7}{12}+\frac{5}{8}\left[1-\frac{21}{2\beta}\right]w'(\beta)\,. \tag{17}$$

The thermodynamic quantities which may be derived from (12) will be discussed in the following sections. The critical temperature itself cannot be inferred from the series (12) but requires an independent evaluation of the free energy in the nematic phase. One may, however, calculate the supercooling temperature T^* as the would-be second-order transition point by using Padé approximants. We do not present this here since a numerically useful result requires the evaluation of higher orders than Z_8.

IV. THE MEAN-FIELD APPROXIMATION (MFA)

We will formulate the mean-field approximation as a saddle-point approximation to the partition-function integral (1). This is convenient both for the calculation of loop corrections in Sec. V and to introduce some of the notations which will be used in the effective-action calculation of Sec. VI. To employ a saddle-point approximation one has to change from the restricted fields $\mathbf{n}(\mathbf{x})$ in (1) which obey $\mathbf{n}^2(\mathbf{x})=1$ to unconstrained field variables. This may be done by a decomposition of the matrices $Q(\mathbf{x})$ into $l=2$, $m=0,\pm1,\pm2$ helicity components

$$Q=\begin{bmatrix} -\frac{Y_0}{\sqrt{6}}+\frac{Y_2}{\sqrt{2}} & \frac{Y_{-2}}{\sqrt{2}} & -\frac{Y_1}{\sqrt{2}} \\ \frac{Y_{-2}}{\sqrt{2}} & -\frac{Y_0}{\sqrt{6}}-\frac{Y_2}{\sqrt{2}} & -\frac{Y_{-1}}{\sqrt{2}} \\ -\frac{Y_1}{\sqrt{2}} & -\frac{Y_{-1}}{\sqrt{2}} & \frac{2Y_0}{\sqrt{6}} \end{bmatrix}, \tag{18}$$

where the Y_m are the following functions of θ and ϕ:

$$\begin{aligned} Y_0&=\left[\frac{3}{2}\right]^{1/2}(\cos^2\theta-\tfrac{1}{3})=\left[\frac{8\pi}{15}\right]^{1/2}Y_{2,0}(\theta,\phi)\,, \\ Y_1&=-\sqrt{2}\sin\theta\cos\theta\cos\phi=\left[\frac{16\pi}{15}\right]^{1/2}\mathrm{Re}Y_{2,1}(\theta,\phi)\,, \\ Y_{-1}&=-\sqrt{2}\sin\theta\cos\theta\sin\phi=\left[\frac{16\pi}{15}\right]^{1/2}\mathrm{Im}Y_{2,1}(\theta,\phi)\,, \\ Y_2&=\frac{1}{\sqrt{2}}\sin^2\theta\cos(2\phi)=\left[\frac{16\pi}{15}\right]^{1/2}\mathrm{Re}Y_{2,2}(\theta,\phi)\,, \\ Y_{-2}&=\frac{1}{\sqrt{2}}\sin^2\theta\sin(2\phi)=\left[\frac{16\pi}{15}\right]^{1/2}\mathrm{Im}Y_{2,2}(\theta,\phi)\,, \end{aligned} \tag{19}$$

and the $Y_{2,m}(\theta,\phi)$ are the spherical harmonics normalized as in (7).

Introducing a suffix $m=0,\pm1,\pm2$, one has for the action in (1)

$$\sum_{k,l}Q_{kl}(\mathbf{x})Q_{kl}(\mathbf{x}+\mathbf{i}) =\sum_m Y_m(\theta(\mathbf{x}),\phi(\mathbf{x}))Y_m(\theta(\mathbf{x}+\mathbf{i}),\phi(\mathbf{x}+\mathbf{i}))\,. \tag{20}$$

One may introduce unrestricted field variables by inserting into (1) the trivial factor

$$1=\prod_{\mathbf{x},m}\int_{-\infty}^{\infty}dQ_m(\mathbf{x})\int_{-i\infty}^{i\infty}\frac{dA_m(\mathbf{x})}{2\pi i}\exp\left[-\sum_{\mathbf{x},m}A_m(\mathbf{x})[Q_m(\mathbf{x})-Y_m(\mathbf{x})]\right].$$

The integrals over the original director variables $\mathbf{n}(\mathbf{x})$ can now be done as they factorize into independent integrals at each site. This gives

$$Z=\prod_{\mathbf{x},m}\int_{-\infty}^{\infty}\frac{dQ_m(\mathbf{x})}{\sqrt{2\pi}}\int_{-i\infty}^{i\infty}\frac{dA_m(\mathbf{x})}{\sqrt{2\pi}}\exp\left[\beta\sum_{\mathbf{x},i,m}Q_m(\mathbf{x})Q_m(\mathbf{x}+\mathbf{i})-\sum_{\mathbf{x},m}A_m(\mathbf{x})Q_m(\mathbf{x})+\sum_{\mathbf{x}}V[A(\mathbf{x})]\right], \tag{21}$$

where $V(A)$ is given by the single-site integral

$$e^{V(A)}=\int \frac{d^2n}{4\pi}\exp\left[\sum_m A_m Y_m\right]$$
$$=\frac{1}{4\pi}\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\exp\left[\sum_m A_m Y_m(\theta,\phi)\right]. \tag{22}$$

In a saddle-point approximation to (21), Q_m and A_m are solutions of

$$A_m=6\beta Q_m,\quad Q_m=\frac{\partial V(A)}{\partial A_m}. \tag{23}$$

One easily verifies that $A_m=Q_m=0$ (all m) are a solution of (23) for any β. For $\beta>1.122$ there also exists another nonzero solution. Choosing the bulk orientation for the uniaxial nematic phase to be in the third direction, one has $A_m=Q_m=0$ for $m=\pm1,\pm2$ and

$$A_0\equiv\left[\frac{2}{3}\right]^{1/2}\alpha,\quad Q_0\equiv\left[\frac{2}{3}\right]^{1/2}S,$$
$$\alpha=6\beta S,\quad S=\tfrac{3}{2}w'(\alpha),\quad w(\alpha)=V(A)\,|_{A_{\pm1}=A_{\pm2}=0}. \tag{24}$$

S is the usual order parameter $\langle P_2(\cos\theta)\rangle$ and $w(\alpha)=V(A)\,|_{A_{\pm1}=A_{\pm2}=0}$ is the characteristic function which was defined in Sec. III [Eq. (13)].

In this approximation, the free-energy density is

$$-f_{\rm MF}\equiv\frac{1}{\beta}\frac{\ln Z_{\rm MF}}{N}=-2S^2+\frac{w(\alpha)}{\beta}. \tag{25}$$

The $\alpha,S\neq0$ solution dominates over the $\alpha=S=0$ solution in free energy for $\beta>\beta_{c,\rm MF}=1.135$ (see Figs. 1 and 2). The jump of the order parameter, the latent heat per site, and the supercooling value for β are (Table I)

$$S(\beta_{c,\rm MF})=S_{c,\rm MF}=0.429,$$
$$L_{\rm MF}=\Delta\left[\frac{d}{d\beta}\beta f_{\rm MF}\right]=2S_{c,\rm MF}^2=0.368, \tag{26}$$
$$\beta^*_{\rm MF}=1.25,\quad 1-\frac{T^*_{\rm MF}}{T_{c,\rm MF}}=0.092.$$

Let us now try to improve these results by using the free energy calculated by the high-temperature expansion in Sec. III. It intersects the mean-field free energy at $\beta_c=1.65$ (see Fig. 2) which is much larger than the Monte Carlo values. The associated value of the order parameter is $S_c=0.79$, and the latent heat per site is $L=0.366$ (Table I).

So the improvement in the isotropic phase alone which is provided by the high-temperature expansion is not sufficient to improve the phase-transition picture. Corrections in the nematic phase are needed as well in order to obtain a reasonable value even just for the critical temperature.

V. THE ONE-LOOP CORRECTION TO THE MEAN-FIELD RESULT (MF1L)

The loop corrections to the mean-field theory may be obtained from (21) by expanding the field around their stationary (mean-field) values

$$Q_m(\mathbf{x})=(\tfrac{2}{3})^{1/2}S\delta_{m,0}+\delta Q_m(\mathbf{x}),$$
$$A_m(\mathbf{x})=(\tfrac{2}{3})^{1/2}\alpha\delta_{m,0}+i\,\delta A_m(\mathbf{x}). \tag{27}$$

At each site one has to expand

$$V(A)=\ln\left[\int\frac{d^2n}{4\pi}\exp\left[\alpha(\cos^2\theta-\tfrac{1}{3})+i\sum_m Y_m(\theta,\phi)\delta A_m\right]\right]$$
$$=w(\alpha)+i\sum_m\langle Y_m\rangle_0\delta A_m$$
$$-\tfrac{1}{2}\sum_{m,m'}(\langle Y_m Y_{m'}\rangle_0-\langle Y_m\rangle_0\langle Y_{m'}\rangle_0)+\Delta(\delta A). \tag{28}$$

Here $\langle\ \rangle_0$ denotes the single-site expectation values,

$$\langle f(\theta,\phi)\rangle_0=\frac{\int\frac{d^2n}{4\pi}f(\theta,\phi)e^{\alpha(\cos^2\theta-1/3)}}{\int\frac{d^2n}{4\pi}e^{\alpha(\cos^2\theta-1/3)}}, \tag{29}$$

and $\Delta(\delta A)$, contains all terms which are cubic or of higher power in δA.

The $\langle\ \rangle_0$ expectation values are easily calculated to be

$$\langle Y_0\rangle_0=(\tfrac{3}{2})^{1/2}\langle\cos^2\theta-\tfrac{1}{3}\rangle_0=(\tfrac{3}{2})^{1/2}w'(\alpha),$$
$$\langle Y_0^2\rangle_0=\tfrac{3}{2}\langle(\cos^2\theta-\tfrac{1}{3})^2\rangle_0$$
$$=\tfrac{3}{2}\{w''(\alpha)+[w'(\alpha)]^2\},$$
$$\langle Y_1^2\rangle_0=\langle Y_{-1}^2\rangle_0=\langle\sin^2\theta\cos^2\theta\rangle_0 \tag{30}$$
$$=\tfrac{1}{4}-[w'(\alpha)-\tfrac{1}{6}]^2-w''(\alpha),$$
$$\langle Y_2^2\rangle_0=\langle Y_{-2}^2\rangle_0=\tfrac{1}{4}\langle\sin^4\theta\rangle_0$$
$$=\tfrac{1}{4}w''(\alpha)+\tfrac{1}{4}[w'(\alpha)-\tfrac{2}{3}]^2,$$

with all other $\langle Y_m\rangle_0$ and $\langle Y_m Y_{m'}\rangle_0$ vanishing. So one has

$$V(A)=w(\alpha)+i(\tfrac{3}{2})^{1/2}w'(\alpha)\delta A_0$$
$$-\tfrac{1}{2}\sum_m f_m(\delta A_m)^2+\Delta(\delta A),$$
$$f_0=\tfrac{3}{2}w''(\alpha),$$
$$f_1=f_{-1}=\tfrac{1}{4}-w''(\alpha)-[w'(\alpha)-\tfrac{1}{6}]^2=\frac{3w'(\alpha)}{2\alpha}, \tag{31}$$
$$f_2=f_{-2}=\tfrac{1}{4}w''(\alpha)+\tfrac{1}{4}[w'(\alpha)-\tfrac{2}{3}]^2$$
$$=\tfrac{1}{6}-\frac{w'(\alpha)}{4}\left[1+\frac{3}{2\alpha}\right].$$

For the last equations, the identity (16) has been used.

The partition function (21) is

$$Z=e^{-\beta N f_{\rm MF}}\prod_{\mathbf{x},m}\int_{-\infty}^{\infty}\frac{d\delta Q_m(\mathbf{x})}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{d\delta A_m(\mathbf{x})}{\sqrt{2\pi}}\exp\left[-S_2(\delta Q,\delta A)+\sum_{\mathbf{x}}\Delta(\delta A(\mathbf{x}))\right]. \tag{32}$$

The quadratic part of the action is

$$S_2=\tfrac{1}{2}\sum_{\mathbf{x},\mathbf{y},m}[\delta Q_m(\mathbf{x}),\delta A_m(\mathbf{x})]G_m^{-1}(\mathbf{x},\mathbf{y})\begin{bmatrix}\delta Q_m(\mathbf{y})\\ \delta A_m(\mathbf{y})\end{bmatrix} \tag{33}$$

with the propagation matrix

$$G_m^{-1}(\mathbf{x},\mathbf{y})=\begin{bmatrix}-\beta\sum_i(2+\bar\nabla_i\nabla_i) & i\\ i & f_m\end{bmatrix}\delta_{\mathbf{x},\mathbf{y}}, \tag{34}$$

where

$$\nabla_i f(\mathbf{x})=f(\mathbf{x}+\mathbf{i})-f(\mathbf{x}),\quad \bar\nabla_i f(\mathbf{x})=f(\mathbf{x})-f(\mathbf{x}-\mathbf{i})$$

are the lattice derivatives.

If one neglects the cubic and higher terms in δA, the one-loop-corrected free-energy density is obtained as

$$-f_{\rm MFIL}=-f_{\rm MF}-\frac{1}{2\beta}\sum_m \operatorname{tr}\ln G_m^{-1}, \tag{35}$$

where $f_{\rm MF}$ is given in (25). To evaluate this expression it is useful to go to momentum space and to introduce the lattice Yukawa propagator

$$\tilde v(\mu,\mathbf{p})=\frac{1}{\mu^2+2\sum_i(1-\cos p_i)}. \tag{36}$$

This gives

$$-f_{\rm MFIL}=-f_{\rm MF}-\frac{1}{2\beta}\sum_m\int_{-\pi}^{\pi}\frac{d^3p}{(2\pi)^3}\ln[\beta f_m\tilde v^{-1}(\mu_m,\mathbf{p})]. \tag{37}$$

The fluctuation masses are

$$\mu_m^2=\mu_{-m}^2=\frac{1}{\beta f_m}-6. \tag{38}$$

In the isotropic phase, all $f_m=\frac{2}{15}$ and so the degenerate masses in this phase are

$$\mu_m^2=\frac{15}{2\beta}-6\ \text{(isotropic phase)}. \tag{39}$$

They vanish at the supercooling temperature $\beta_{\rm MF}^*=1.25$. In the nematic phase, the masses associated with the $m=\pm1$ modes vanish. The $m=\pm2$ biaxial fluctuations are much more massive than the $m=0$ size fluctuations.

The one-loop corrected free energy (37) (see Fig. 2) is unphysical in the region around $\beta_{c,\rm MF}$. This is a common feature of theories which exhibit a first-order transition in the mean-field approximation and is caused by the large value of $\operatorname{tr}\ln v^{-1}$ for small masses. In the isotropic phase the negative free energy is grossly overestimated as β approaches $\beta_{\rm MF}$. This will eventually be cured if a sufficient number of loop corrections are included. In the nematic phase, further loop corrections would also improve the free energy. However, the region between $\beta_{c,\rm MF}$ and the true β_c will be expanded around the wrong ordered ground state and finite orders of the loop expansion cannot generate the singularity in the free energy at β_c.

To avoid the unphysical region of the one-loop corrected free energy, one may use the high-temperature expansion for the isotropic phase (MF1L + HTE). Its free energy crosses the loop-corrected free energy of the nematic phase in a region where the latter approximation may still be trusted (Fig. 2). The critical point is then located at $\beta=1.37$, quite close to the Monte Carlo data which gives β_c at 1.335 (Ref. 16) and 1.35 (Ref. 17). (Latent heat per site: still $L=0.37$ [see (26)].) However, the order parameter has the value $S=0.69$ on the MF curve (24), which is much too large (Fig. 1, Table I).

To improve its value, we now calculate the one-loop correction of the order parameter. Using (27) we have

$$S_{\rm MFIL}=S+(\tfrac{3}{2})^{1/2}\langle\delta Q_0(\mathbf{x})\rangle. \tag{40}$$

To calculate $\langle\delta Q_0(\mathbf{x})\rangle$ we have to invert $G_m^{-1}(\mathbf{x},\mathbf{y})$ (34)

$$G_m(\mathbf{x},\mathbf{y})=\begin{bmatrix}\frac{1}{\beta}v(\mu_m^2,\mathbf{x}-\mathbf{y}) & \frac{-i}{\beta f_m}v(\mu_m^2,\mathbf{x}-\mathbf{y})\\ \frac{-i}{\beta f_m}v(\mu_m^2,\mathbf{x}-\mathbf{y}) & \frac{1}{f_m}\left[\delta_{\mathbf{x},\mathbf{y}}-\frac{1}{\beta f_m}v(\mu_m^2,\mathbf{x}-\mathbf{y})\right]\end{bmatrix}=\begin{bmatrix}G_m^{(Q,Q)}(\mathbf{x}-\mathbf{y}) & G_m^{(Q,A)}(\mathbf{x}-\mathbf{y})\\ G_m^{(A,Q)}(\mathbf{x}-\mathbf{y}) & G_m^{(A,A)}(\mathbf{x}-\mathbf{y})\end{bmatrix}. \tag{41}$$

The matrix entries $G^{(Q,Q)}$, $G^{(Q,A)}=G^{(A,Q)}$, and $G^{(A,A)}$ propagate the $Q\to Q$, $Q\leftrightarrow A$, and $A\to A$ fields. The one-loop contribution to $\langle\delta Q_0(\mathbf{x})\rangle$ is given by a propagator $G_0^{(Q,A)}(\mathbf{x},\mathbf{y})$ which propagates the $\delta Q_0(\mathbf{x})$ field to a three-point vertex (3-vertex) contained in $\Delta(\delta A)$ of (32) and a second $G_m^{(A,A)}(\mathbf{y},\mathbf{y})$ which contracts the remaining two legs of the 3-vertex.

The 3-vertex is obtained by continuing the expansion of $V(A)$ started in (28). We only need that part which contains at least one $\delta A_0(\mathbf{y})$ field. This is easily calculated to be

$$\Delta_{0,m,m}^{(3)}[\delta A(\mathbf{y})]=-\frac{i}{3!}\sum_m\delta A_0(\mathbf{y})[\delta A_m(\mathbf{y})]^2(3g_{0,m,m}-2\delta_{m,0}g_{0,0,0}),$$
$$g_{0,m,m}=\langle Y_0Y_m^2\rangle_0-\langle Y_0\rangle_0\langle Y_m^2\rangle_0-2\langle Y_0\rangle_0\{\langle Y_0^2\rangle_0-\langle Y_0\rangle_0^2\}\delta_{m,0}. \tag{42}$$

The one-loop contribution to $\langle \delta Q_0(\mathbf{x}) \rangle$ is

$$\langle \delta Q_0(\mathbf{x}) \rangle_{1\,\mathrm{loop}} = -\frac{i}{2} \sum_{\mathbf{y},m} G_0^{(Q,A)}(\mathbf{x},\mathbf{y}) G_m^{(A,A)}(\mathbf{y},\mathbf{y}) g_{0,m,m} \,. \tag{43}$$

Performing the summation over $\mathbf{y}$ and using (38) and (41), this is

$$\langle \delta Q_0(\mathbf{x}) \rangle_{1\,\mathrm{loop}} = -\frac{1}{2}\beta \frac{\mu_0^2+6}{\mu_0^2} \sum_m g_{0,m,m}(\mu_m^2+6)[1-(\mu_m^2+6)w(\mu_m^2,0)] \,. \tag{44}$$

The $g_{0,m,m}$ are

$$g_0 \equiv g_{0,0,0} = (\tfrac{3}{2})^{3/2} \langle (\cos^2\theta - \tfrac{1}{3})^3 \rangle_{0,c} = (\tfrac{3}{2})^{3/2} w'''(\alpha) \,,$$

$$g_1 = g_{-1} \equiv g_{0,1,1} = g_{0,-1,-1} = 2(\tfrac{3}{2})^{1/2} \langle (\cos^2\theta - \tfrac{1}{3}) \sin^2\theta \cos^2\theta \cos^2\phi \rangle_{0,c} = (\tfrac{3}{2})^{1/2} \frac{\partial f_1}{\partial \alpha} = (\tfrac{3}{2})^{3/2} \frac{1}{\alpha^2} [\alpha w''(\alpha) - w'(\alpha)] \,, \tag{45}$$

$$g_2 = g_{-2} \equiv g_{0,2,2} = g_{0,-2,-2} = \tfrac{1}{2}(\tfrac{3}{2})^{1/2} \langle (\cos^2\theta - \tfrac{1}{3}) \sin^4\theta \sin^2 2\phi \rangle_{0,c} = (\tfrac{3}{2})^{1/2} \frac{\partial f_2}{\partial \alpha} = (\tfrac{3}{2})^{1/2} \left[\frac{3w'(\alpha)}{8\alpha^2} - \frac{w''(\alpha)}{4} \left[1 + \frac{3}{2\alpha} \right] \right]$$

Here $\langle\ \rangle_{0,c}$ denotes the connected part of $\langle\ \rangle_0$. At the transition point of MF1L + HTE ($\beta_c = 1.37$) one obtains for the one-loop-corrected order parameter the result $S_c = 0.53$ which is still too large. Moreover, its β dependence is too weak close to the transition (see Fig. 1).

VI. EFFECTIVE ACTION IN THE HOPPING 1/D EXPANSION (EA)

From the arguments given in Secs. IV and V it is clear that we need a self-consistent method which treats the two phases on an equal footing and respects well the important fluctuations in the transition region. As mentioned in the Introduction, the formalism of effective action[20] will serve as such a method.

In Ref. 18 the effective action of $O(N)$ spin models in D dimensions was evaluated up to the two-loop level, once in a simple $1/D$ expansion and once in a hopping $1/D$ expansion.[21] The main results were as follows.

(i) Both expansions describe the thermodynamic properties and second-order transitions quite well for $D \geq 4$.

(ii) For $D=3$ and $N=1,2$ the simple $1/D$ expansion gives very good values for (the second-order) transition temperatures T_c. However, it also predicts a weak first-order transition, even though the model has a second-order transition. The $1/D$ hopping expansion, on the other hand, gives a somewhat worse value for T_c but predicts correctly a second-order transition.

Thus, the two-loop effective action with a hopping expansion appears to be a reliable tool for studying approximately second-order phase transitions. Since the nematic-isotropic transition is weakly of first order we expect the approximation to be even better than in the $O(N)$ spin models. We start by extending our three-dimensional simple cubic lattice of the model (1) to a D-dimensional hybercubic lattice while keeping the component of directors to be three such that there are five polarization states as before ($-2 \leq m \leq 2$). After rotating the contours of integrations[22] Z of (21) reads

$$Z = \prod_{\mathbf{x},m} \int_{-\infty}^{\infty} \frac{dQ_m(\mathbf{x})}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{dA_m(\mathbf{x})}{\sqrt{2\pi}} \exp\left[-\frac{\beta}{2} \sum_{\mathbf{x},\mathbf{y},m} Q_m(\mathbf{x}) \hat{H}(\mathbf{x},\mathbf{y}) Q_m(\mathbf{y}) - i \sum_{\mathbf{x},m} Q_m(\mathbf{x}) A_m(\mathbf{x}) + \sum_{\mathbf{x}} V(A_m(\mathbf{x})) \right] , \tag{46}$$

where $\hat{H}(\mathbf{x},\mathbf{y})$ is the hopping operator[23]

$$\hat{H}(\mathbf{x},\mathbf{y}) = \sum_{i=1}^{D} (\delta_{\mathbf{x},\mathbf{y}+\hat{\mathbf{i}}} + \delta_{\mathbf{x},\mathbf{y}-\hat{\mathbf{i}}}) \,. \tag{47}$$

At this stage it is convenient to integrate over $Q_m(\mathbf{x})$

$$Z = \prod_{\mathbf{x},m} \int_{-\infty}^{\infty} \frac{dA_m(\mathbf{x})}{\sqrt{2\pi}} \det{}^{1/2}\left[\frac{\pi}{\beta \hat{H}/2} \right] \exp\left[-\frac{1}{2\beta} \prod_{\mathbf{x},\mathbf{y},m} A_m(\mathbf{x}) \hat{H}^{-1}(\mathbf{x},\mathbf{y}) A_m(\mathbf{y}) + \sum_{\mathbf{x}} V(A_m(\mathbf{x})) \right] , \tag{48}$$

and to introduce new variables $\phi_m(\mathbf{x})$ which cancel the functional determinant in front of the exponential

$$A_m(\mathbf{x}) = \sum_{\mathbf{y}} \mathscr{D}^{1/2}(\mathbf{x},\mathbf{y}) \phi_m(\mathbf{y}) \equiv \hat{\phi}_m(\mathbf{x}) \,,$$
$$\mathscr{D}(\mathbf{x},\mathbf{y}) = \frac{1}{2D} \hat{H}(\mathbf{x},\mathbf{y}) \,. \tag{49}$$

Then Z becomes

$$Z = \prod_{\mathbf{x},m} \int_{-\infty}^{\infty} d\phi_m(\mathbf{x}) \exp A[\phi] \,, \tag{50a}$$

$$A[\phi] \equiv -\frac{1}{4b} \sum_{\mathbf{x},m} \phi_m(\mathbf{x}) \phi_m(\mathbf{x}) + \sum_{\mathbf{x}} V(\hat{\phi}_m(\mathbf{x})) - \frac{5}{2} N \ln(4\pi b) \,, \tag{50b}$$

Let us now evaluate each term in $\Gamma(\Phi)$ of (55) separately by expanding each propagator in the diagrams in powers of $\hat{H}(\mathbf{x},\mathbf{y})$. As one will see, this procedure gives rise to the hopping $1/D$ expansion. We start with the one-loop part Γ_1,

$$\begin{aligned}\Gamma_1/N &= -\frac{1}{2N}\sum_m \mathrm{tr}\ln\left[1-\frac{b}{D}f_m\hat{H}\right] \\ &= \tfrac{1}{2}\sum_m\sum_{k=1}^{\infty}\left[\frac{b}{D}f_m\right]^k\frac{1}{k}\frac{1}{N}\sum_{\mathbf{x}}\hat{H}^k(\mathbf{x},\mathbf{x}) \\ &= \sum_m\left[\frac{b^2}{2D}f_m^2+\frac{3}{2D^2}\left[1-\frac{1}{2D}\right]b^4f_m^4\right]+O(\hat{H}^6)\ ,\end{aligned} \tag{60}$$

where we used the formula

$$\hat{H}^2(\mathbf{x},\mathbf{x})=2D,\quad \hat{H}^4(\mathbf{x},\mathbf{x})=6D(2D-1)\ ,$$
$$\hat{H}^m(\mathbf{x},\mathbf{x})=0 \text{ for } m \text{ odd}\ . \tag{61}$$

Notice that this *hopping* expansion is a modified $1/D$ expansion if b,Φ are counted as $O(D^0)$.[25] Next there are two two-loop diagrams, ⊗ and ⊖, contributing to $\Gamma_2(\Phi)$.[26] For the diagram ⊗ we calculate

$$\begin{aligned}\Gamma_{\otimes}/N &= \frac{1}{4!N}\sum_{\mathbf{x}}\sum_{i,j,k,l}V_{ijkl}\langle\hat{\varphi}_i(\mathbf{x})\hat{\varphi}_j(\mathbf{x})\hat{\varphi}_k(\mathbf{x})\hat{\varphi}_l(x)\rangle \\ &= \frac{1}{4!N}\sum_{\mathbf{x}}\sum_{i,j,k,l}V_{ijkl}[\hat{G}_{ij}(\mathbf{x},\mathbf{x})\hat{G}_{kl}(\mathbf{x},\mathbf{x})+2\text{ terms}]\ ,\end{aligned} \tag{62}$$

where it is convenient to define the modified correlation function of the $\hat{\varphi}$ fields [see (49)] as

$$\begin{aligned}\hat{G}_{ij}(\mathbf{x},\mathbf{y}) &= \langle\hat{\varphi}_i(\mathbf{x})\hat{\varphi}_j(\mathbf{y})\rangle \\ &= \sum_{\mathbf{z},\mathbf{t}}\mathscr{D}^{1/2}(\mathbf{x},\mathbf{z})G_{ij}(\mathbf{z},\mathbf{t})\mathscr{D}^{1/2}(\mathbf{t},\mathbf{y}) \\ &= \delta_{ij}\left[\frac{1}{\frac{1}{2b}-f_i\frac{\hat{H}}{2D}}\frac{\hat{H}}{2D}\right]_{\mathbf{x},\mathbf{y}}\ .\end{aligned} \tag{63}$$

By using the hopping expansion for $\hat{G}_{ij}(\mathbf{x},\mathbf{x})$,

$$\hat{G}_{ij}(\mathbf{x},\mathbf{x})=\delta_{ij}\frac{2}{D}b^2f_i+O(D^{-2})\ , \tag{64}$$

and the matrix element of (59), $\Gamma_{\otimes}$ becomes

$$\begin{aligned}\Gamma_{\otimes}/N &= \frac{b^4}{D^2}F_4(\alpha)+O(D^{-3})\ , \\ F_4(\alpha) &= \tfrac{1}{2}\left[h_0f_0^2+8h_{12}f_1f_2+\sum_{k=1}^{2}(4h_{0k}f_0f_k+\tfrac{8}{3}h_{kk}f_k^2)\right]\ .\end{aligned} \tag{65}$$

For the ⊖ diagram we have

$$\Gamma_{\ominus}/N=\frac{1}{N}\sum_{\substack{ijk\\lmn}}\frac{1}{2}\left[\frac{1}{3!}\right]^2V_{ijk}V_{lmn}\sum_{\mathbf{x},\mathbf{y}}\langle\hat{\varphi}_i(\mathbf{x})\hat{\varphi}_j(\mathbf{x})\hat{\varphi}_k(\mathbf{x})\hat{\varphi}_l(\mathbf{y})\hat{\varphi}_m(\mathbf{y})\hat{\varphi}_n(\mathbf{y})\rangle_{1\mathrm{PI}}\ . \tag{66}$$

By noting

$$\langle\hat{\varphi}_i(\mathbf{x})\cdots\hat{\varphi}_n(\mathbf{y})\rangle_{1\mathrm{PI}}=\hat{G}_{il}(\mathbf{x},\mathbf{y})\hat{G}_{jm}(\mathbf{x},\mathbf{y})\hat{G}_{kn}(\mathbf{x},\mathbf{y})+5\text{ terms}\ , \tag{67}$$

and performing again the hopping expansion, we find

$$\begin{aligned}\Gamma_{\ominus}/N &= \frac{1}{N}\sum_{i,j,k}3\left[\frac{1}{(3!)^2}\right](V_{ijk})^2 \\ &\quad\times\sum_{\mathbf{x},\mathbf{y}}\prod_{s=i,j,k}\left[\frac{1}{\frac{1}{2b}-\frac{f_s}{2D}\hat{H}}\frac{\hat{H}}{2D}\right]_{\mathbf{x},\mathbf{y}} \\ &= \frac{1}{2}\frac{1}{3!}\sum_{i,j,k}(V_{ijk})^2\left[\frac{b}{D}\right]^3(2D)+O(D^{-3})\ ,\end{aligned} \tag{68}$$

where we have used the formula

$$\frac{1}{N}\sum_{\mathbf{x},\mathbf{y}}[\hat{H}(\mathbf{x},\mathbf{y})]^3=\frac{1}{N}\sum_{\mathbf{x},\mathbf{y}}\hat{H}(\mathbf{x},\mathbf{y})=2D\ . \tag{69}$$

Using the quantities $g(\alpha)$ as defined in Eqs. (45) and (59) we finally obtain

$$\begin{aligned}\Gamma_{\ominus}/N &= \frac{b^3}{D^2}F_3(\alpha)+O(D^{-3})\ , \\ F_3(\alpha) &= \tfrac{1}{6}[g_0^2+6(g_1^2+g_2^2)+12g_{12}^2]\ .\end{aligned} \tag{70}$$

It is easy to see that diagrams having l loops start to contribute to $\Gamma(\Phi)$ in the order of D^{-l}. Therefore, working up to the two-loop level we have exhausted all the contributions up to $O(D^{-2})$. Actually, apart from the particular polarization dependence of interaction vertices, the general structure of propagators is the same as in the O(N) spin model[18] and gives rise to the same prefactor ($b^4/2D^2$, $b^3/6D^2$, etc.) for each corresponding diagram.

In summary, our effective potential $\Gamma(\Phi)$ in the hopping expansion up to $O(D^{-2})$ is given by

$$\Gamma(\Phi)=\Gamma_{\mathrm{tree}}(\Phi)+\Gamma_1(\Phi)+\Gamma_{\otimes}(\Phi)+\Gamma_{\ominus}(\Phi)\ , \tag{71}$$

where the first zero-loop ("tree") term $\Gamma_{\mathrm{tree}}(\Phi)$ reads simply

$$\Gamma_{\text{tree}}(\Phi)/N = A(\Phi)/N + \tfrac{5}{2}\ln(4\pi b) = -\frac{\Phi^2}{4b} + V(\Phi) . \tag{72}$$

More explicitly $\Gamma(\Phi)$ has a structure

$$\Gamma(\Phi)/N = -\frac{\alpha^2}{6b} + w + \frac{b^2}{2D}[f_0^2 + 2(f_1^2 + f_2^2)] + \frac{b^3}{D^2}F_3 + \left[\frac{3}{2}\left[1 - \frac{1}{2D}\right][f_0^4 + 2(f_1^4 + f_2^4)] + F_4\right]\frac{b^4}{D^2} , \tag{73}$$

where $\alpha = (\frac{3}{2})^{1/2}\Phi$.

VII. TEMPERATURE BEHAVIOR OF THERMODYNAMIC QUANTITIES

We now proceed to impose the stationary condition (57) to the above $\Gamma(\Phi)$ and solve for Φ as a function $\Phi(b)$ of b (and D). This $\Phi(b)$, in turn, is inserted back into $\Gamma(\Phi)$ to give the free energy F,

$$-\beta F = \Gamma(\Phi(b)) . \tag{74}$$

The calculation of $\delta\Gamma(\Phi)/\delta\Phi$ is straightforward but the expression becomes rather lengthy and is therefore not given here. In the course of the calculation it is helpful to make use of functional relations such as (16), for $w(\alpha)$. The solution $\Phi(b)$ for $D=3$ can be obtained numerically. It has the two branches, $\Phi=0$ and $\Phi\neq 0$, as expected. The order parameter S is given in terms of $\Phi(b)$ by[27]

$$S = \langle P_2(\cos\theta)\rangle = \frac{1}{2b}\left[\frac{3}{2}\right]^{1/2}\Phi(b) \equiv \frac{1}{2b}\alpha(b) . \tag{75}$$

This is due to the definition $S = (\frac{3}{2})^{1/2}\langle Q_0^{\text{old}}\rangle$, and the relations [see Ref. (22)]

$$2b\langle Q_m^{\text{old}}\rangle = \langle A_m^{\text{new}}\rangle, \quad \Phi = \langle A_0^{\text{new}}\rangle , \tag{76}$$

which hold for the system described by (46) and (48).

The resulting curve $S(b)$ is given in Fig. 1 together with those obtained by other methods (MFA,MF1L). Inserting $\Phi(b)$ back into (74) we obtain the free energy per site (times $-\beta$), $-\beta f$, which is given in Fig. 2. The take-over point of the $\Phi\neq 0$ branch over the $\Phi=0$ one in $-\beta f$ locates the first-order phase transition at $b_c = 3.93$ with $S_c = 0.32$. It is important to find that the behaviors of both S and the free energy are in a much better agreement with the Monte Carlo results (MC1,MC2) than the Maier-Saupe curves (MFA) and the combination of high-temperature expansion with one-loop-corrected mean-field approximation (MF1L + HTE).

As can be seen in Fig. 1 the size of the first-order transition has become quite weak due to fluctuations. Actually $(T_c - T^*)/T_c$ and ΔL are smaller than those of MFA by factor ~ 3.4 and ~ 2.6, respectively (Table I). Here T^* is the temperature of instability of the point $\Phi=0$ [see Eq. (80) below].

The free energy can be used to calculate the internal energy per site $U = -d(-\beta f)/d\beta$. This, in turn, is directly accessible to Monte Carlo simulations (MC1,MC2). We see in Fig. 3 that the agreement with those data is comparatively good. A further differentiation gives the specific heat per site $C = -\beta^2 dU/d\beta$ and the theoretical curves are shown in Fig. 5.

In the isotropic phase, the free energy is given by setting $\Phi=0$ in $\Gamma(\Phi)$ and reads

$$\Gamma(0)/N = -\beta f_{T>T_c} = \frac{2}{45}\frac{b^2}{D} + \frac{8}{2835}\frac{b^3}{D^2} + \left[\frac{8}{45\times 225} - \frac{24}{45\times 225\times 2D}\right]\frac{b^4}{D^2} . \tag{77}$$

This expression agrees with the high-temperature expansion of Sec. III (Ref. 28) except for the last term of $O(D^{-3})$, which should be compared with $(-76/45\times 225\times 7D)b^4/D^2$.

In the region of low temperature, the free energy for $D=3$ can be expanded in b^{-1} by using the asymptotic expression of $w(\alpha)$ for $\alpha \gg 1$ as follows:

$$-\beta f = \tfrac{2}{3}b - \ln b - 1.286 + O(b^{-1}) , \tag{78}$$

where the genuine $1/b$ expansion gives the same first two terms and -1.268 for the constant term. The effective action has the advantage that we can directly calculate a Landau expansion for $\Gamma(\Phi)$ for a small-order parameter Φ,

$$\Gamma(\Phi) = \Gamma(0) - \tfrac{1}{2}M^2(b)(\tfrac{3}{2}\Phi^2) + \lambda(b)\Phi^3 + g(b)\Phi^4 + O(\Phi^5) . \tag{79}$$

The point of instability b^* is located by the condition $M^2(b^*)=0$ as $b^*=4.04$. Since $M^2(b)$ is the inverse of

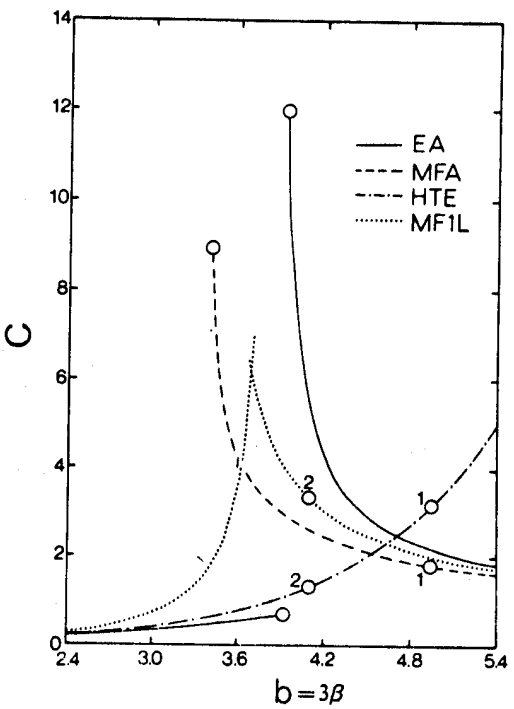


FIG. 5. Specific heat per site C vs $b=3\beta$. No data from MC1 or MC2 are available.

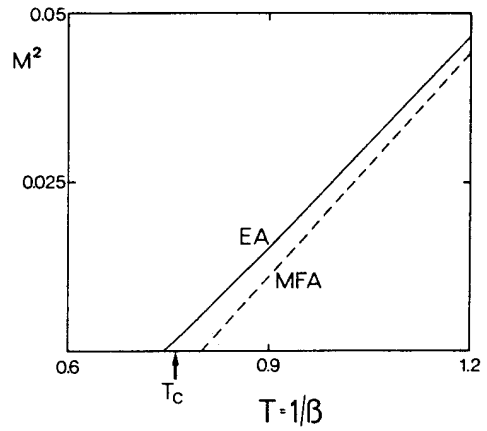


FIG. 6. Mass square of Eq. (80) vs $T=1/\beta$, together with the linear line given by MFA of Eq. (72). The arrow indicates $1/\beta_c$ in EA.

the two-point correlation at zero momentum it is inversely proportional to the total intensity of light scattering in the nematic phase. In Fig. 6, M^2 is plotted versus $T=\beta^{-1}$. It behaves approximately linearly as

$$M^2(b)\simeq A(T-T^*),\quad T^*=(\beta^*)^{-1} \tag{80}$$

and A is ~ 0.095 near T^* and approaches at $T\gg T^*$ to its mean-field value $\frac{1}{9}$. Let us end this section with the remark that the limit $D\to\infty$ of the effective action reduces to $\Gamma_{\text{tree}}(\Phi)$ of Eq. (72). This is equal to the mean field, i.e., the Maier-Saupe result, which therefore is exact for $D\to\infty$.

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APPENDIX

The interaction vertices $g(\alpha),h(\alpha)$, which were defined in Eq. (59), can be expressed in terms of the derivatives $w_n\equiv w^{(n)}(\alpha)$ [recall Eq. (15)] as follows:

$$g_{12}=\frac{1}{2\sqrt{2}}[w_3+3w_1w_2+(w_1)^3-w_2-(w_1)^2+\tfrac{4}{27}]\,, \tag{A1}$$

$$h_0=\tfrac{9}{4}w_4\,, \tag{A2}$$

$$h_{01}=\tfrac{3}{2}[-w_4-2(w_2)^2-2w_1w_3+\tfrac{1}{3}w_3]\,, \tag{A3}$$

$$h_{02}=\tfrac{3}{8}[w_4+2(w_2)^2+2w_1w_3-\tfrac{4}{3}w_3]\,, \tag{A4}$$

$$\begin{aligned}h_{11}=\tfrac{3}{2}[&w_4+(w_2)^2+4w_1w_3+2(w_1)^2w_2\\&-(w_1)^4-\tfrac{2}{3}w_3-\tfrac{2}{3}w_1w_2+\tfrac{2}{3}(w_1)^3+\tfrac{5}{9}w_2\\&+\tfrac{1}{3}(w_1)^2-\tfrac{4}{27}w_1-\tfrac{4}{81}]\,,\end{aligned} \tag{A5}$$

$$\begin{aligned}h_{22}=\tfrac{3}{32}[&w_4+(w_2)^2+4w_1w_3+2(w_1)^2w_2\\&-(w_1)^4-\tfrac{8}{3}w_3-\tfrac{8}{3}w_1w_2+\tfrac{8}{3}(w_1)^3+\tfrac{8}{9}w_2\\&-\tfrac{24}{9}(w_1)^2+\tfrac{32}{27}w_1-\tfrac{16}{81}]\,,\end{aligned} \tag{A6}$$

$$\begin{aligned}h_{12}=\tfrac{1}{4}[&-w_4-2(w_2)^2-4w_1w_3-4(w_1)^2w_2\\&+\tfrac{5}{3}w_3+\tfrac{10}{3}w_1w_2-\tfrac{4}{9}w_2]\,.\end{aligned} \tag{A7}$$

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[21]In Ref. 18 the curves for $D=3, N=2$ given by the simple $1/D$ expansion and shown in Figs. 1–3 contain a slight error. The gap equation (19) gives no solution for the range $0.22<\rho/2<0.33$. It is, however, in the unphysical region, and the remaining part of the curves needs no corrections.

[22]$Q_m^{\text{old}}=iQ_m^{\text{new}}$, $Q_m^{\text{new}}(-\infty,\infty)$; $A_m^{\text{old}}(-i\infty, i\infty)=A_m^{\text{new}}(-\infty,\infty)$.

[23]It is related to the lattice Laplacian $\bar{\nabla}\nabla$ as $\hat{H}=2D+\bar{\nabla}\nabla$. Its eigenvalues in momentum space are $2\sum_{i=1}^{D}\cos k_i$.

[24]In Eq. (56) we associated a factor $2b$ with G^{-1} in the definition of $\Gamma_0(\Phi)$, for later convenience.

[25]In a *simple* $1/D$ expansion up to $O(D^{-2})$ the factor $(1-1/2D)$ in (60) is replaced by 1, while it is kept here (see Ref. 18).

[26]The diagram O—O is one-particle reducible and can be omitted.

[27]In the spin model of Ref. 18, there holds the corresponding relation, $\langle S\rangle=\rho/2b$, $\rho^2=\sum_i \Phi_i\Phi_i$ which can be used to calculate $\langle S\rangle$ through ρ given in Fig. 3 there.

[28]The results of Sec. III can be easily generalized for general D at least up to $O(b^4)$.