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Phase ordering in bulk uniaxial nematic liquid crystals

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The phase-ordering kinetics of a bulk uniaxial nematic liquid crystal is addressed using techniques that have been successfully applied to describe ordering in the O(n) model. The method involves constructing an appropriate mapping between the order-parameter tensor and a Gaussian auxiliary field. The mapping accounts for both the geometry of the director about the dominant charge 1/2 string defects and biaxiality near the string cores. At late times t following a quench, there exists a scaling regime where the bulk nematic liquid crystal and the three-dimensional O(2) model are found to be isomorphic, within the Gaussian approximation. As a consequence, the scaling function for order-parameter correlations in the nematic liquid crystal is *exactly* that of the O(2) model and the length characteristic of the strings grows as $t^{1/2}$. These results are in accord with experiment and simulation. Related models dealing with thin films and monopole defects in the bulk are presented and discussed. [S1063-651X(97)06612-9]

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I. INTRODUCTION

ost phase-ordering systems studied to date support only one type of topologically stable defect species [1–3]. One example is the O(n) model with an n-component vector order parameter. In three spatial dimensions, the defects formed at the quench are linelike strings for $n=2$ and pointlike monopoles for $n=3$. Phase ordering in bulk uniaxial nematic liquid crystals (nematics) provides the simplest scenario in which two defect species, monopoles and strings, are topologically stable. The stability of monopoles derives from the O(3) symmetry of the nematic director $\hat{n}(\vec{r},t)$. The additional invariance under the local inversion $\hat{n}(\vec{r},t)\rightarrow-\hat{n}(\vec{r},t)$ allows the nematic to support stable charge 1/2 disclination lines (strings) [4]. The issue of which defect species dominates the dynamics in bulk nematics at late times t following a quench has recently been settled. Cell-dynamical simulations using spin models of bulk nematics [5,6] have computed the order-parameter correlation function and found it to be indistinguishable from that of the O(2) model and consistent with a string-dominated late-time scaling regime. Experiments by Chuang *et al.* [7] directly imaged the bulk nematic, revealing an intricate, evolving defect tangle. While both types of defect were observed, the strings dominated at late times. The length scale L_s characterizing the typical separation of the strings was seen to grow as $L_s\sim t^{1/2}$, while the average line density of string $\langle\eta\rangle$ decayed like $\langle\eta\rangle\sim L_s^{-2}\sim t^{-1}$. The study of ordering in nematics is also of interest to cosmologists [8,9] since similar processes involving cosmic string and monopole evolution, thought to occur in the early universe, may be responsible for structure formation.

In this paper a theory is presented that describes the dominant scaling behavior of the bulk nematic in terms of a string-dominated late-time regime. Generalizing a successful method used to treat the ordering kinetics of the O(n) model, the nematic order-parameter tensor is mapped onto a two-component Gaussian auxiliary field [2]. The string defects explicitly appear in the construction of the mapping. As discussed below, this approach has several advantages over an earlier, seminumerical theory by Bray *et al.* [10].

The auxiliary field approach is first applied to the straightforward case of phase ordering in nematic films containing charge 1/2 vortices, which have been studied in simulations [5] and experiments [11]. As in the bulk nematic, the mapping is constructed to account for the rotation of the director by only π about the core of the defect. Once this is done the theory reveals that phase ordering in the nematic film is equivalent to phase ordering in the two-dimensional O(2) model examined previously [2]. This is not surprising since the two systems are known to be isomorphic [5,12]. Constructing a theory for the bulk nematic is more challenging since the order-parameter tensor must include a biaxial piece near the core of the string. In the earlier theory of Bray *et al.* [10] this point was not addressed since there they used a ''hard-spin'' approximation for the dynamics of the nematic. However, the necessity of having a biaxial core region when treating the full equations has been noted in the numerical work of Schopohl and Sluckin [13] on bulk nematic string defects in equilibrium. The present theory successfully incorporates biaxiality and clarifies the role that it plays in the coarsening of the bulk nematic. The theory recovers the growing length $L_s\sim t^{1/2}$ seen in simulations [5,6] and experiments [7]. In the scaling regime, the order-parameter correlation function for the bulk nematic is found to be *exactly* that of the three-dimensional O(2) model [2], in excellent agreement with simulations [5] (Fig. 1). Although the theoretical results of Bray *et al.* [10] suggested agreement between the correlation function for the bulk nematic and the O(2) model, they were unable to demonstrate an exact equivalence since their theory was not based on a mapping that explicitly contained strings. The major accomplishment of this work is to analytically demonstrate the isomorphism between the dynamics of the bulk nematic and the dynamics of the three-dimensional O(2) model, within the Gaussian

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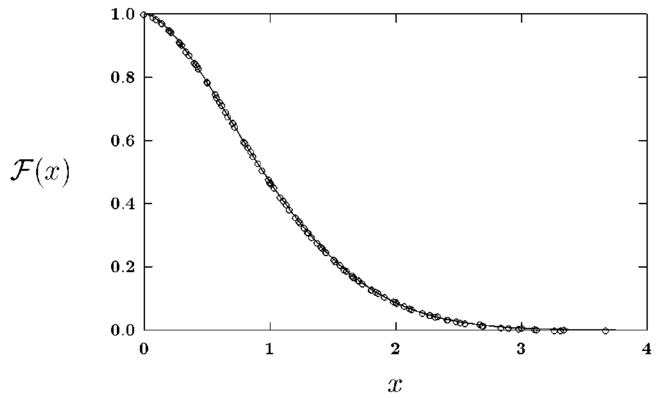

FIG. 1. The scaling function $\mathcal{F}(x)$ for order-parameter correlations as a function of the scaled length $x = r/L_s(t)$ for the three-dimensional O(2) model [2] is represented by the solid line. As shown in Sec. III B, this function exactly describes order-parameter correlations in bulk nematics. The cell-dynamical simulation data of Blundell and Bray [5] for this quantity in a bulk nematic are also shown, as circles. The abscissa of the simulation data is scaled so as to give the best fit to the theory.

approximation. Through this isomorphism, the well-developed theory for the O(2) model [2,14,15] can be applied directly to the nematic. In particular, this theory predicts that the average line density of string decays as $\langle \eta \rangle \sim L_s^{-2} \sim t^{-1}$ [14,16], in accord with the experiments of Chuang *et al.* [7].

Although strings are generically present in bulk nematics, certain choices of experimental setup and sample material will produce copious amounts of monopoles at the quench [17]. The theory of Bray *et al.* [10] is unable to address these experiments since in that theory there is no signature for monopoles. However, within the framework presented below it is relatively straightforward to develop a theory of nematics in which monopoles appear. In this theory the order-parameter correlation function is found to be similar to (but not exactly) that for the three-dimensional O(3) model [2] (Fig. 2). The characteristic monopole spacing L_m grows as $L_m \sim t^{1/2}$ and leads to a decaying average monopole density $\langle n \rangle \sim L_m^{-3} \sim t^{-3/2}$. Experiments [17] that examine monopole-antimonopole annihilation in isolation from strings suggest that these growth laws should hold. However, experiments [7] also reveal that the average monopole density decays more rapidly in the presence of strings, with $\langle n \rangle \sim t^{-3}$. It appears that in order to account for this observation the theory presented here should be extended to consider the interactions between strings and monopoles [16].

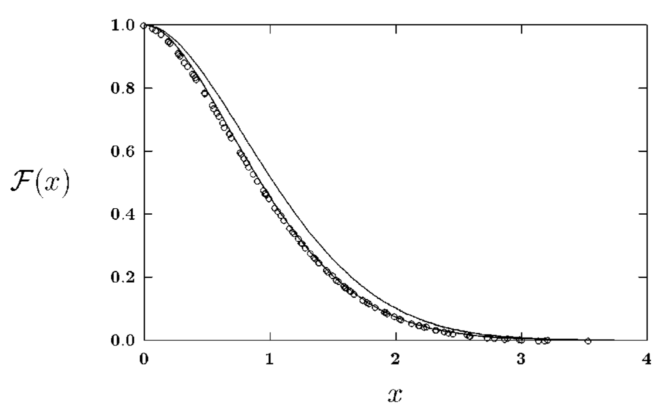

FIG. 2. The scaling function $\mathcal{F}(x)$ as a function of the scaled length $x = r/L_m(t)$ for order-parameter correlations in the theory for monopoles in bulk nematics, discussed in Sec. IV, is represented by the lower curve. The upper curve is the scaling function for order-parameter correlations in the three-dimensional O(3) model from [2]. The circles are the cell-dynamical simulation data of Blundell and Bray [5] for $\mathcal{F}$ in a bulk nematic. The abscissa of the simulation data is scaled so as to give the best fit to the theory for monopoles in bulk nematics.

II. MODELS

In this section the O(n) model and the Landau–de Gennes model of nematics are discussed. Since the former model is used as a guide in the treatment of the latter, the theory for ordering kinetics in the O(n) model is also reviewed. Initially, the structural features common to both models are emphasized. In later sections, the technical details specific to the ordering of nematics will be discussed.

A. The O(n) model

In the O(n) model the evolution of the nonconserved, n-component order-parameter field $\vec{\psi}$ is governed by the time-dependent Ginzburg-Landau (TDGL) equation

$$\frac{\partial \vec{\psi}}{\partial t} = -\frac{\delta F[\vec{\psi}]}{\delta \vec{\psi}}. \tag{2.1}$$

The free energy $F[\vec{\psi}]$ has the form

$$F[\vec{\psi}] = \int d^d r \left[\tfrac{1}{2} (\nabla \vec{\psi})^2 + V(\psi) \right], \tag{2.2}$$

where the potential $V(\psi)$, expressed in terms of $\psi \equiv |\vec{\psi}|$, is O(n) symmetric with a degenerate ground state at nonzero $\psi = \psi_0$. In this model, as with the nematic liquid crystal, the disordered high-temperature initial state is rendered unstable by a quench to a low temperature where the usual noise term on the right-hand side of Eq. (2.1) can be ignored. Substitution of Eq. (2.2) into Eq. (2.1) produces the explicit equation of motion

$$\frac{\partial \vec{\psi}}{\partial t} = \nabla^2 \vec{\psi} - \frac{\partial V(\psi)}{\partial \vec{\psi}}. \tag{2.3}$$

The evolution induced by Eq. (2.3) causes $\vec{\psi}$ to order and assume a distribution that is far from Gaussian. To make analytic progress it is by now standard [1] to introduce a mapping

$$\vec{\psi} = \vec{\sigma}(\vec{m}) \tag{2.4}$$

between the physical field $\vec{\psi}$ and an n-component auxiliary field $\vec{m}$ with analytically tractable statistics. The mapping $\vec{\sigma}$ is chosen to reflect the defect structure in the system and satisfies the Euler-Lagrange equation for a defect in equilibrium

$$\nabla_m^2 \vec{\sigma} = \frac{\partial V(\vec{\sigma})}{\partial \vec{\sigma}}. \tag{2.5}$$

As shown below, Eq. (2.5) is also instrumental in treating the nonlinear potential term in Eq. (2.3). Defects correspond to the nonuniform solutions of Eq. (2.5) that map onto the uniform solution far from the defect core. Since only the lowest-energy defects, those with unit topological charge, will survive until late times, the relevant solutions to Eq. (2.5) will be of the form [2]

$$\vec{\sigma}(\vec{m}) = A(m)\hat{m}, \tag{2.6}$$

where $m = |\vec{m}|$ and $\hat{m} = \vec{m}/m$. Thus the magnitude of $\vec{m}$ represents the distance away from a defect core and its orientation corresponds to the orientation of the order parameter field at that point. This geometrical interpretation will later be exploited when the generalization of Eq. (2.5) is used to choose the appropriate mapping, analogous to Eq. (2.6), for string defects in the nematic liquid crystal. The magnitude of $\vec{m}$ grows as the characteristic defect separation $L(t)$, becoming large in the late-time scaling regime. Inserting Eq. (2.6) into Eq. (2.5) gives an equation for A, the order-parameter profile around a defect [2],

$$\nabla_m^2 A - \frac{n-1}{m^2} A - \frac{\partial V}{\partial A}(A) = 0. \tag{2.7}$$

For small m an analysis of Eq. (2.7) yields the linear dependence $A(m) \sim m$, characteristic of a unit charge defect [18]. For large m the amplitude A approaches its ordered value $A = \psi_0$ algebraically, which is a feature common to both the O(n) model and the nematic.

The order-parameter correlation function is

$$C(\vec{r},t) = \langle \vec{\sigma}(\vec{r},t) \cdot \vec{\sigma}(0,t) \rangle = \psi_0^2 \langle \hat{m}(\vec{r},t) \cdot \hat{m}(0,t) \rangle, \tag{2.8}$$

where the last equality holds for late times and to leading order in $1/L$. To evaluate the last average in Eq. (2.8) we choose $\vec{m}$ to be a Gaussian field with zero mean. This Gaussian approximation forms the basis of almost all present analytical treatments of phase-ordering problems and has had much quantitative success in describing the correlations in these systems [1–3]. Theories where $\vec{m}$ is a non-Gaussian field also exist [19,20]. In the Gaussian approximation the order-parameter correlation function (2.8) can be related to the normalized auxiliary field correlation function f, defined as

$$f(\vec{r},t) \equiv \frac{\langle \vec{m}(\vec{r},t) \cdot \vec{m}(0,t) \rangle}{\langle [\vec{m}(0,t)]^2 \rangle}. \tag{2.9}$$

The relation is [2,21]

$$C(\vec{r},t) = \psi_0^2 \mathcal{F}(\vec{r},t), \tag{2.10}$$

with

$$\mathcal{F} = \frac{nf}{2\pi} B^2\left[\frac{1}{2}, \frac{n+1}{2}\right] F\left[\frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}; f^2\right], \tag{2.11}$$

where B is the beta function and F is the hypergeometric function. In the late-time scaling regime the functions $\mathcal{F}$ and f can be expressed solely in terms of the scaled length $x = r/L(t)$ so that $\mathcal{F} = \mathcal{F}(x)$. In this regime the equation of motion (2.3) can be written as a nonlinear scaling equation for $\mathcal{F}$

$$\vec{x} \cdot \vec{\nabla}_x \mathcal{F} + \nabla_x^2 \mathcal{F} + \frac{\pi}{2\mu} f \frac{\partial}{\partial f} \mathcal{F} = 0. \tag{2.12}$$

In the derivation of Eq. (2.12) the relation (2.5) is used to replace the potential term in Eq. (2.3), and then the Gaussian identity

$$\langle [\nabla_m^2 \vec{\sigma}(\vec{m}(\vec{r},t))] \cdot \vec{\sigma}(\vec{m}(0,t)) \rangle$$
$$= -\frac{nf(\vec{r},t)}{\langle [\vec{m}(0,t)]^2 \rangle} \frac{\partial}{\partial f(\vec{r},t)} \langle \vec{\sigma}(\vec{m}(\vec{r},t)) \cdot \vec{\sigma}(\vec{m}(0,t)) \rangle \tag{2.13}$$

is used to get the last term on the left-hand side of Eq. (2.12). The constant μ enters through the definition of the scaling length L:

$$L^2(t) \equiv \frac{\pi \langle [\vec{m}(0,t)]^2 \rangle}{2n\mu} = 4t. \tag{2.14}$$

This is the well-known [2,21] growth law $L \sim t^{1/2}$ for phase ordering in nonconserved vector systems.

Since the auxiliary field $\vec{m}$ is smooth [15], f is analytic for small x. This implies, through an examination of Eq. (2.12) in d spatial dimensions, that for small x, $\mathcal{F}$ behaves like

$$\mathcal{F}(x) = 1 + \frac{\pi}{4\mu d} x^2 \ln x + O(x^2) \tag{2.15}$$

for $n = 2$ and

$$\mathcal{F}(x) = 1 - \frac{\pi}{2\mu d} x^2 + \frac{4}{3\mu(d+1)} \sqrt{\frac{\pi}{2\mu d}} x^3 + O(x^4) \tag{2.16}$$

for $n = 3$, the cases relevant to this paper. The nonanalytic terms in $\mathcal{F}$ reflect the short-distance singularities in the order-parameter field produced by the defects and lead to Porod's law [22] power-law decay of the structure factor at large wave number. The $x^2 \ln x$ term in Eq. (2.15) is characteristic of string (or vortex) defects, while the x^3 term in Eq. (2.16) is due to monopole defects. For large x both $\mathcal{F}$ and f decay rapidly to zero. The eigenvalue μ is determined numerically by matching the short- and long-distance behaviors of the solution of Eq. (2.12). In this way the auxiliary field correlation function f is determined self-consistently along with $\mathcal{F}$. In contrast, there is no such self-consistency in theories based on the Ohta-Jasnow-Kawasaki approximation [10,23]. Values of μ at various n and d for the O(n) model have been determined [2]. The scaling functions $\mathcal{F}$ of this theory are in excellent agreement with the results of simulations [1,2].

B. Nematic liquid crystals

The order parameter for a bulk nematic liquid crystal is a traceless, symmetric, 3×3 tensor $Q_{\alpha\beta}$, which measures the anisotropy of physical observables in the nematic phase. The tensor $Q_{\alpha\beta}$ has the general form [24]

$$Q_{\alpha\beta}=A[\hat{n}_{\alpha}\hat{n}_{\beta}-\tfrac{1}{3}\delta_{\alpha\beta}]+\tfrac{1}{3}B[\hat{g}_{\alpha}\hat{g}_{\beta}-\hat{h}_{\alpha}\hat{h}_{\beta}]. \quad (2.17)$$

The unit three-vectors $\hat{n}$, $\hat{g}$, and $\hat{h}$ form an orthonormal triad. The amplitudes A and B are chosen to be non-negative. A is a measure of the degree of uniaxial order in the liquid crystal; it is zero in the isotropic phase and nonzero in the nematic phase. Biaxiality in the liquid crystal is measured by B. In the uniaxial nematic phase B is zero everywhere except near the string cores. The description of nematics in terms of $Q_{\alpha\beta}$ reduces to the Frank continuum theory of elasticity in terms of a director $\hat{n}(\vec{r},t)$ [25] when A is set to its ordered value and $B=0$. In the phase-ordering scenario, where defects occur, all of A, B, $\hat{n}$, $\hat{g}$, and $\hat{h}$ are space and time dependent.

In the tensor formulation the director, which measures the average local molecular orientation in the nematic, is the unit eigenvector of $Q_{\alpha\beta}$ that corresponds to the largest eigenvalue. The unit eigenvectors and associated eigenvalues of $Q_{\alpha\beta}$ are

$$\begin{aligned}\hat{n}&\leftrightarrow \tfrac{2}{3}A,\\ \hat{g}&\leftrightarrow -\tfrac{1}{3}(A-B),\\ \hat{h}&\leftrightarrow -\tfrac{1}{3}(A+B).\end{aligned} \quad (2.18)$$

Since the nematic is uniaxial, $B\leqslant 3A$ and the director can be identified with $\hat{n}$. The tensor formulation respects the full RP^2 symmetry of the uniaxial nematic since physical quantities, such as correlations, are written in terms of the $Q_{\alpha\beta}$ that are invariant under the local inversion $\hat{n}(\vec{r},t)\to-\hat{n}(\vec{r},t)$. At a string core $B=3A>0$ and the eigensubspace corresponding to the largest eigenvalue $2A/3$ is twofold degenerate. Thus, in the plane perpendicular to $\hat{h}$, the tangent to the string, the orientation of the director is ambiguous. At the isotropic core of a monopole $A=B=0$ and all three eigenvalues of $Q_{\alpha\beta}$ are degenerate so the orientation of the director is completely unspecified.

The dynamics of the nematic is governed by the TDGL equation for $Q_{\alpha\beta}$,

$$\partial_t Q_{\alpha\beta}=-\frac{\delta F[Q]}{\delta Q_{\alpha\beta}}+\lambda_{\alpha\beta}\mathrm{Tr}Q, \quad (2.19)$$

with the Lagrange multiplier $\lambda_{\alpha\beta}$ included to enforce the traceless condition. The Landau–de Gennes free energy is

$$F[Q]=\int d^3r\,[\tfrac{1}{2}(\nabla Q)^2+V(Q)], \quad (2.20)$$

with the potential

$$V(Q)=-\tfrac{1}{6}\mathrm{Tr}Q^2-\tfrac{1}{3}\mathrm{Tr}Q^3+\tfrac{1}{4}(\mathrm{Tr}Q^2)^2. \quad (2.21)$$

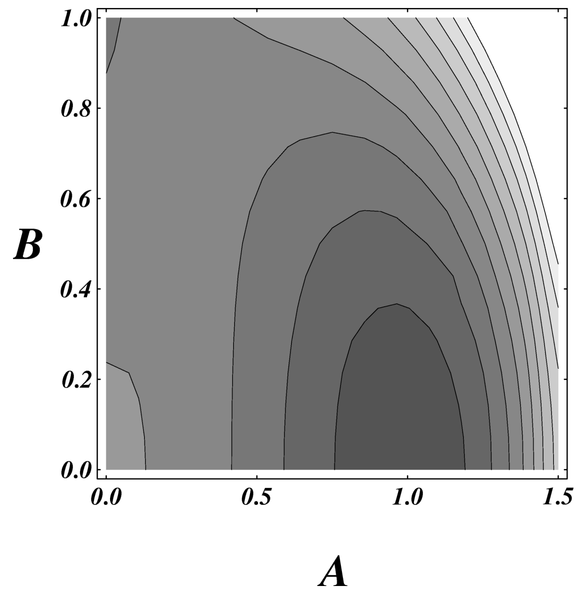

FIG. 3. Contour plot of the potential surface $V(A,B)$ [Eq. (2.22)] for the bulk nematic in the physical region $A>0$, $B>0$. A is the uniaxial amplitude and B is the biaxial amplitude. Darker shades indicate lower regions on the potential surface. The isotropic maximum at $(A,B)=(0,0)$ corresponds to a monopole core, the saddle at $(A,B)=(1/4,3/4)$ to a string core, and the minimum at $(A,B)=(1,0)$ to the bulk uniaxial state.

The coefficient of the quadratic term in Eq. (2.21) is chosen to be negative so that the bulk isotropic phase is unstable towards nematic ordering. The gradient term in Eq. (2.20) is written within the equal-constant approximation [25]. Substitution of the form (2.17) into Eq. (2.21) results in a useful expression for the potential as a function of A and B:

$$V(A,B)=-\tfrac{1}{9}A^2-\tfrac{2}{27}A^3+\tfrac{1}{9}A^4-\tfrac{1}{27}B^2+\tfrac{1}{81}B^4 + \tfrac{2}{27}[AB^2+A^2B^2]. \quad (2.22)$$

A contour plot of $V(A,B)$ for $A>0$, $B>0$ is shown in Fig. 3. There is a global isotropic maximum at $(A,B)=(0,0)$, a uniaxial minimum at $(A,B)=(1,0)$, and a saddle at $(A,B)=(1/4,3/4)$. The minimum represents the bulk nematic phase, the isotropic maximum corresponds to the monopole core, and the saddle, with $B=3A$, signifies the string core.

Substituting Eq. (2.20) into Eq. (2.19) and using $\mathrm{Tr}Q=0$ to calculate the Lagrange multiplier gives an explicit form for the equation of motion

$$\partial_t Q_{\alpha\beta}=\nabla^2 Q_{\alpha\beta}-P_{\alpha\beta}, \quad (2.23)$$

with the nonlinear piece given by

$$P_{\alpha\beta}=(\mathrm{Tr}Q^2-\tfrac{1}{3})Q_{\alpha\beta}-[Q^2]_{\alpha\beta}+\frac{\delta_{\alpha\beta}}{3}\mathrm{Tr}Q^2. \quad (2.24)$$

Static solutions to Eq. (2.23) satisfy the Euler-Lagrange equation

$$\nabla^2 Q_{\alpha\beta}=P_{\alpha\beta}. \quad (2.25)$$

The order-parameter correlation function is defined as

$$C(\vec{r},t)=\mathcal{N}\langle \mathrm{Tr}[\delta Q(\vec{r},t)\,\delta Q(0,t)]\rangle, \tag{2.26}$$

where $\mathcal{N}=\{\langle \mathrm{Tr}[\delta Q(0,t)\,\delta Q(0,t)]\rangle\}^{-1}$ is a normalization factor and $\delta Q_{\alpha\beta}=Q_{\alpha\beta}-\langle Q_{\alpha\beta}\rangle$. Both $\mathcal{N}$ and $\langle Q_{\alpha\beta}\rangle$ are constant at leading order in $1/t$. Thus, at late times, Eq. (2.23) can be written as an equation for the evolution of order-parameter correlations

$$\tfrac{1}{2}\,\partial_t C(\vec{r},t)=\nabla^2 C(\vec{r},t)-\mathcal{N}\langle \mathrm{Tr}[P(\vec{r},t)\,\delta Q(0,t)]\rangle. \tag{2.27}$$

Later, through a development that closely parallels that previously given for the O(n) model, it will be shown how Eqs. (2.25) and (2.27) lead to a scaling equation for order-parameter correlations in the nematic.

III. STRING DEFECTS IN THE NEMATIC

At late times the dominant defects in the bulk nematic are strings with topological charge 1/2. Many of the main features of phase ordering in the bulk nematic are described by the model containing strings that is presented in Sec. III B below.

A. Vortices in thin films

To begin, a model applicable to nematic thin films where the director is constrained to lie in a plane without breaking the $\hat{n}\to-\hat{n}$ symmetry is examined. By restricting the director to a plane, the intricacies of how to map the order-parameter tensor onto an auxiliary field when the director rotates by only π about the vortex can be demonstrated, without the additional complication of biaxiality that appears near the string core in bulk samples.

For a uniaxial thin-film nematic the order parameter is a 2×2 traceless symmetric tensor

$$Q_{\alpha\beta}=A[\hat{n}_\alpha\hat{n}_\beta-\tfrac{1}{2}\delta_{\alpha\beta}], \tag{3.1}$$

where $\hat{n}$ is the two-component director. In analogy to the theory of the O(2) model, the defects are incorporated through a mapping of the order-parameter tensor onto a two-component auxiliary field. The only defect species present at late times are charge 1/2 point vortices with the property that the director rotates by only π around the vortex. This property is essential in constructing the mapping. Consider a charge 1/2 vortex at the origin with the typical director configuration

$$\hat{n}=\cos\tfrac{1}{2}\,\phi\,\hat{x}+\sin\tfrac{1}{2}\,\phi\,\hat{y}, \tag{3.2}$$

where ϕ is the polar angle in the x-y plane. For future convenience we write the radial vector in the x-y plane as $\vec{s}$ and define angles in terms of $\hat{s}$ through

$$\hat{s}\equiv(\hat{s}_1,\hat{s}_2)\equiv(\cos\,\phi,\sin\,\phi). \tag{3.3}$$

With the definitions (3.2) and (3.3), the order-parameter tensor (3.1) is [26]

$$Q=\frac{A(s)}{2}\begin{bmatrix}\hat{s}_1 & \hat{s}_2\\ \hat{s}_2 & -\hat{s}_1\end{bmatrix}, \tag{3.4}$$

where $s=|\vec{s}|$. This form for $Q_{\alpha\beta}$, analogous to the mapping (2.6) for the O(n) model, is a solution to the Euler-Lagrange equation (2.25) written in terms of s

$$\nabla_s^2 Q_{\alpha\beta}=\widetilde{P}_{\alpha\beta}, \tag{3.5}$$

where $\widetilde{P}_{\alpha\beta}$ has a slightly modified definition from $P_{\alpha\beta}$ [Eq. (2.24)] because $Q_{\alpha\beta}$ is a 2×2 tensor:

$$\widetilde{P}_{\alpha\beta}=(\mathrm{Tr}Q^2-1/3)Q_{\alpha\beta}-[Q^2]_{\alpha\beta}+\frac{\delta_{\alpha\beta}}{2}\mathrm{Tr}Q^2. \tag{3.6}$$

Substituting Eq. (3.4) into Eq. (3.5) results in an equation for the amplitude A:

$$\nabla_s^2 A-\frac{A}{s^2}=2\frac{\partial U}{\partial A}(A). \tag{3.7}$$

From Eqs. (2.21) and (3.4) the potential U is given by

$$U(A)=-\frac{1}{12}A^2+\frac{1}{16}A^4. \tag{3.8}$$

An examination of Eq. (3.7) at small s has $A\sim s$, indicative of charge 1/2 vortices [18]. At large s the amplitude A algebraically approaches its ordered value $A=\sqrt{2/3}$.

To treat many such vortices in a phase-ordering context, $\vec{s}$ in Eq. (3.4) is taken to be a Gaussian field $\vec{s}(\vec{r},t)$ with zero mean. As in the O(2) model, s represents the distance to the nearest vortex, growing as the characteristic vortex spacing $L_v(t)$ at late times. However, unlike in the O(2) model, the director is not mapped directly onto $\vec{s}$: A 2π rotation of $\vec{s}$ about a vortex corresponds to a rotation of the director by π.

At late times, the amplitude A approaches its ordered value and from the definition (2.26) and Eq. (3.4) the order-parameter correlation function is seen to be

$$C(\vec{r},t)=\langle\hat{s}(\vec{r},t)\cdot\hat{s}(0,t)\rangle \tag{3.9}$$

to leading order in L_v^{-1}. This is just the O(2) correlation function (2.8) and is related to f, the correlation function for the auxiliary field $\vec{s}$ defined in analogy to Eq. (2.9), through Eqs. (2.10) and (2.11) for $n=2$. In the scaling regime the equation of motion (2.27) for $C(\vec{r},t)$ becomes Eq. (2.12) for the O(2) scaling function $\mathcal{F}$, expressed in terms of the scaled length $x=r/L_v(t)$. The length L_v has the same definition as the length L in Eq. (2.14), with $\vec{m}$ replaced by $\vec{s}$. The path from Eq. (2.27) to Eq. (2.12) is similar to that taken in the O(2) case [2]. The Euler-Lagrange equation (3.5) is used to replace $\widetilde{P}_{\alpha\beta}$ occurring in the last term in Eq. (2.27). The resulting expression is evaluated using the Gaussian identity

$$\langle \mathrm{Tr}[\nabla_s^2 Q(\vec{s}(\vec{r},t))Q(\vec{s}(0,t))]\rangle$$

$$= -\frac{2f(\vec{r},t)}{\langle[\vec{s}(0,t)]^2\rangle}\frac{\partial}{\partial f(\vec{r},t)}\langle \mathrm{Tr}Q[(\vec{s}(\vec{r},t))Q(\vec{s}(0,t))]\rangle, \tag{3.10}$$

analogous to Eq. (2.13), and produces the last term on the left-hand side of Eq. (2.12).

Thus the scaling function $\mathcal{F}$ for the order-parameter correlations and the growth law $L_v(t)\sim t^{1/2}$ for the nematic thin film are exactly those of the two-dimensional O(2) model. This correspondence, seen in simulations, can be simply understood as a consequence of the mapping of variables $\phi\rightarrow 2\phi$ between the two models [5,12]. This isomorphism is relevant to experimental efforts that use constrained nematics to study coarsening in the two-dimensional O(2) models [27] since it indicates that the existence of the local $\hat{n}\rightarrow-\hat{n}$ symmetry does not affect the leading-order dynamics in the scaling regime.

B. Strings in the bulk nematic

In addition to the complication of having a director configuration with a charge 1/2 geometry, strings in a bulk nematic have a biaxial core. The form (2.17) for $Q_{\alpha\beta}$ contains the biaxiality that is required if an analytical solution to Eq. (2.25) is to be found. String defects enter the theory through the mapping of Eq. (2.17) onto a two-component auxiliary field. To motivate the form for the mapping consider the geometry of the director field around a charge 1/2 string defect oriented along the z axis. Since locally the coordinate system can always be chosen so that the string has this geometry the following development is quite general. The director $\hat{n}$ is still given by Eq. (3.2). The other members of the orthonormal triad in Eq. (2.17) are

$$\hat{g} = -\sin\tfrac{1}{2}\phi\,\hat{x} + \cos\tfrac{1}{2}\phi\,\hat{y}, \tag{3.11}$$

$$\hat{h} = \hat{z}. \tag{3.12}$$

With the notation (3.3) for the radial vector $\vec{s}$ in the x-y plane, the order-parameter tensor (2.17) becomes

$$Q = \frac{A(s)}{2}\begin{bmatrix} \frac{1}{3}+\hat{s}_1 & \hat{s}_2 & 0 \\ \hat{s}_2 & \frac{1}{3}-\hat{s}_1 & 0 \\ 0 & 0 & -\frac{2}{3} \end{bmatrix} + \frac{B(s)}{6}\begin{bmatrix} 1-\hat{s}_1 & -\hat{s}_2 & 0 \\ -\hat{s}_2 & 1+\hat{s}_1 & 0 \\ 0 & 0 & -2 \end{bmatrix}. \tag{3.13}$$

This form for $Q_{\alpha\beta}$ is a solution of Eq. (2.25) written in terms of s,

$$\nabla_s^2 Q_{\alpha\beta} = P_{\alpha\beta}, \tag{3.14}$$

provided

$$4\nabla_s^2 A - \frac{(3A-B)}{s^2} - 6\frac{\partial V}{\partial A} = 0, \tag{3.15}$$

$$\frac{4}{3}\nabla_s^2 B + \frac{1}{3}\frac{(3A-B)}{s^2} - 6\frac{\partial V}{\partial B} = 0, \tag{3.16}$$

where $V(A,B)$ is given in Eq. (2.22). Note that equations (3.15) and (3.16) would be inconsistent had a uniaxial ansatz ($B=0$) been assumed at the outset. For the potential (2.22) these equations are degenerate [28] and reduce to a single equation for A after the identification $B=1-A$:

$$4\nabla_s^2 A - \frac{(4A-1)}{s^2} - 6\frac{\partial V}{\partial A}(A,1-A) = 0. \tag{3.17}$$

At small s the solution to Eq. (3.17) is

$$A = \tfrac{1}{4} + cs, \tag{3.18}$$

$$B = \tfrac{3}{4} - cs, \tag{3.19}$$

where c is a constant, determined numerically. At large s the solution of Eq. (3.17) takes the form

$$A = 1 - \frac{3}{4s^2}, \tag{3.20}$$

$$B = \frac{3}{4s^2}. \tag{3.21}$$

As expected, the mapping (3.13) connects the biaxial saddle point on the potential surface $V(A,B)$, representing the string core, to the uniaxial nematic minimum away from the string (see Fig. 3). The linear behavior in Eqs. (3.18) and (3.19) at small s is that expected for charge 1/2 strings in the nematic. Both the linear behavior near the core and the algebraic relaxation (3.20) and (3.21) to the bulk uniaxial state are seen in the numerical results of [13].

Once again, to examine the statistical properties of the string defect tangle, $\vec{s}$ is taken to be a Gaussian auxiliary field with zero mean. The magnitude s grows as the characteristic string separation $L_s(t)$. Therefore, at late times, s is large and the biaxial piece of $Q_{\alpha\beta}$, with an amplitude B given by Eq. (3.21), is suppressed. This is physically reasonable since biaxiality occurs on length scales around the core size, while the late-time scaling properties are dominated by physics at the much larger scale of $L_s(t)$. At late times, when $A\approx 1$, the definition (2.26) and the mapping (3.13) show that the order-parameter correlation function reduces to

$$C(\vec{r},t) = \langle \hat{s}(\vec{r},t)\cdot\hat{s}(0,t)\rangle, \tag{3.22}$$

which is the O(2) correlation function (2.8). As before, $C(\vec{r},t)$ is related to $f(\vec{r},t)$, the normalized correlation function for the auxiliary field $\vec{s}$, by relations (2.10) and (2.11) with $n=2$.

The dynamical equation (2.27) for $C(\vec{r},t)$ reduces, in the scaling regime, to Eq. (2.12) for $\mathcal{F}$ from the three-dimensional O(2) model. Note that the spatial dimensionality enters through the Laplacian operator in Eq. (2.12). The scaled length in this case is $x=r/L_s(t)$ with L_s defined as L in Eq. (2.14). The derivation of this correspondence parallels the steps taken in the O(2) model that lead to Eq. (2.12). The Euler-Lagrange equation (3.14) enables the nonlinear quantity $P_{\alpha\beta}$ occurring in the last term of Eq. (2.27) to be replaced by $\nabla_s^2 Q_{\alpha\beta}$. The resulting average is then evaluated using Eq. (3.10) and produces the last term on the left-hand side of Eq. (2.12). The scaling result $L_s \sim t^{1/2}$ is recovered for the phase ordering of the bulk nematic. In Fig. 1 the theoretical results for $\mathcal{F}$ in the three-dimensional O(2) model [2] and the $\mathcal{F}$ determined in cell-dynamical simulations of the bulk nematic [5] are compared. The agreement between the two is excellent. At short-scaled distances $\mathcal{F}$ has the form (2.15), which is also seen in the simulations and is an indication that string defects are the dominant disordering agent in the bulk nematic.

The theory is now structured so that many well-established phase-ordering results for the O(2) model [2,14] can be applied to the bulk nematic. In particular, the string line density η is related to the auxiliary field $\vec{s}$, whose zeros locate the positions of the strings, through [14,16,29]

$$\eta=\delta(\vec{s})|\vec{\omega}|, \tag{3.23}$$

where the tangent to the string

$$\vec{\omega}=\nabla s_1 \times \nabla s_2 \tag{3.24}$$

points in the direction of positive winding number. The calculation performed in Appendix A shows that the average line density of string obeys $\langle \eta \rangle \sim L_s^{-2} \sim t^{-1}$ for late times, in accord with experiments [7].

IV. MONOPOLES IN THE BULK NEMATIC

To address experiments that are designed to produce copious amounts of monopoles at the quench [17], a theory for the ordering kinetics of bulk nematics is considered in which monopoles appear. The model consists of mapping the director $\hat{n}$ near a monopole directly onto a three-component Gaussian auxiliary field $\vec{m}$ *via* $\hat{n}=\hat{m}$. Thus the order parameter is

$$Q_{\alpha\beta}=A(m)[\hat{m}_\alpha \hat{m}_\beta - \tfrac{1}{3}\delta_{\alpha\beta}]. \tag{4.1}$$

Since the isotropic monopole core can be connected to the nematic minimum along the $B=0$ line on the potential surface (Fig. 3), a biaxial piece does not appear in Eq. (4.1). Equation (4.1) solves the Euler-Lagrange equation (2.25) written in terms of $\vec{m}$,

$$\nabla_m^2 Q_{\alpha\beta}=P_{\alpha\beta}, \tag{4.2}$$

if the amplitude A satisfies

$$\nabla_m^2 A - \frac{6}{m^2}A=\frac{3}{2}\frac{\partial V}{\partial A}(A,0). \tag{4.3}$$

A similar result was obtained in [30] for equilibrium. For small m, Eq. (4.3) indicates that $A \sim m^2$ while for large m the amplitude A algebraically approaches its ordered value of 1. The m^2 dependence at small m indicates that Eq. (4.1) describes charge 1 monopoles in the nematic [18]. This is also evident geometrically since $\vec{m}$ (and thus $\hat{n}$) is a radial vector field near the monopole.

At late times, using Eq. (4.1) with $A \approx 1$, the order-parameter correlation function (2.26) is

$$C(\vec{r},t)=\tfrac{3}{2}[\langle[\hat{m}(\vec{r},t)\cdot\hat{m}(0,t)]^2\rangle - \tfrac{1}{3}]. \tag{4.4}$$

In contrast to the string models considered earlier, the expression (4.4) for the order-parameter correlation function in the monopole model is new. The Gaussian average in Eq. (4.4) is computed in Appendix B. In the late-time scaling regime $C(\vec{r},t)$ can be written in terms of the scaled length $x=r/L_m(t)$, where $L_m(t)$ is the typical monopole separation. Thus $C(\vec{r},t)=\mathcal{F}(x)$ with

$$\mathcal{F}=1+\frac{3}{\gamma^3 f^3}(\sin^{-1}f-\gamma f) \tag{4.5}$$

and $\gamma=1/\sqrt{1-f^2}$. The auxiliary field correlation function f is defined in Eq. (2.9). The scaling function $\mathcal{F}$ satisfies the scaling equation (2.12) with $L_m(t) \sim t^{1/2}$. The development of this result closely parallels that of the string case considered earlier. The only difference between the scaling results for this model and those for the O(3) model is that the relation between $\mathcal{F}$ and f is Eq. (4.5) instead of Eq. (2.11).

Since $\vec{m}$ is smooth, f has a power series expansion that is analytic at small x. By using this expansion in Eqs. (2.12) and (4.5), the small-x behavior of $\mathcal{F}$ is found to be

$$\mathcal{F}(x)=1-\frac{3\pi}{2\mu d}x^2+\frac{3\pi^2}{4\mu(d+1)}\sqrt{\frac{\pi}{2\mu d}}x^3+O(x^4). \tag{4.6}$$

The nonanalytic x^3 term in $\mathcal{F}$, also found in the O(3) model (2.16), is due to the presence of point monopole defects. Using a fourth-order Runge-Kutta scheme, the nonlinear eigenvalue problem represented by Eqs. (2.12) and (4.5) is solved for $d=3$. The eigenvalue is $\mu=1.273\,06\ldots$, which differs from the value $\mu=0.5558\ldots$ for the O(3) model [2]. The function $\mathcal{F}$ is plotted in Fig. 2 along with the scaling function for order-parameter correlations in the three-dimensional O(3) model. Figure 2 also compares the cell-dynamical simulation data for the bulk nematic [5] to the function $\mathcal{F}$ [Eq. (4.5)]. The function $\mathcal{F}$ does not describe the simulation data as well as the string model, showing deviations at short distances. These deviations are expected since the structure of the theory at short distances (4.6) represents the wrong defects (monopoles) instead of the correct ones (strings).

Since the zeros of $\vec{m}$ locate the monopole cores, the monopole number density n can be expressed in terms of the auxiliary field $\vec{m}$ [14] as

$$n=\delta(\vec{m})\,|\det(\partial_i m_j)|, \tag{4.7}$$

where the quantity between the absolute value signs is the Jacobian for the transformation from real-space coordinates to auxiliary field variables. From the development in [14] the average monopole number density obeys $\langle n\rangle \sim L_m^{-3} \sim t^{-3/2}$. This result holds only for monopole annihilation in the absence of strings, the case considered in this section. In the experiments of Chuang *et al.* [7], where monopole annihilation occurred in the presence of strings, the average monopole density was observed to decay faster, with $\langle n\rangle \sim t^{-3}$.

V. DISCUSSION

The dominant scaling behavior observed during ordering in the bulk nematic is well described by the theory presented here in which string defects are the major disordering agents. The growth law $L_s \sim t^{1/2}$ is recovered, leading to an average string line density $\langle \eta\rangle$ that decays as $\langle \eta\rangle \sim t^{-1}$, as seen in experiments [7]. The theoretically determined scaling form for order-parameter correlations in the bulk nematic is shown analytically to be *exactly* that for the three-dimensional O(2) model [2], and this is in excellent agreement with the simulation results [5] (Fig. 1). This paper addresses the issue of biaxiality near the string cores and demonstrates that it is irrelevant to the leading-order scaling properties of the system. However, the theory is capable of being extended into the prescaling regime, where biaxiality may play a role in the dynamics.

The major accomplishment of this work is the explicit demonstration of the isomorphism between the late-stage ordering in the bulk nematic and the late-stage ordering in the three-dimensional O(2) model, within the Gaussian approximation. It is shown that, in the scaling regime, the order-parameter equations of motion for the O(2) model (2.1) and the bulk nematic (2.19) produce the same scaling equation (2.12) for the correlation function. The essential element in the present theory, which was missing in earlier theories [10], is the mapping (3.13), which explicitly includes string defects and makes a direct connection with the O(2) model. As a consequence, results for the O(2) model, such as string and vortex density correlations [14,31] or conservation laws involving string densities [32], can be directly applied to the bulk nematic.

This paper also presents a model for bulk nematics in which monopoles appear. The model is applicable to situations where monopole-antimonopole annihilations occur in isolation from string defects. Such scenarios have been realized experimentally [17], and the data are suggestive of the growth law $L_m \sim t^{1/2}$ predicted by the theory. However, to properly treat monopole dynamics in the presence of strings, theories that include interactions between string and monopole defects are required. This interesting aspect of the problem is under current investigation [16].

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APPENDIX A

This appendix presents the calculation of the average line density for strings $\langle \eta\rangle$ for the O(n) model in $d=n+1$ spatial dimensions, defined as

$$\langle \eta\rangle = \langle \delta(\vec{s})|\vec{\omega}|\rangle, \tag{A1}$$

with

$$\omega_\alpha = \frac{1}{n!}\epsilon_{\alpha\mu_1\cdots\mu_n}\epsilon_{\nu_1\cdots\nu_n}\nabla_{\mu_1}s_{\nu_1}\cdots\nabla_{\mu_n}s_{\nu_n}. \tag{A2}$$

The form (A2), where ϵ is the fully antisymmetric tensor, generalizes the definition (3.24) for the tangent vector to a string in $d=3$. The one-point average (A1) can be written in an integral form

$$\langle \eta\rangle = \int \prod_{\mu=1,\nu=1}^{n+1,n} d\xi_\mu^\nu \, |\vec{\omega}(\xi)| G(\xi) \tag{A3}$$

in terms of

$$\omega_\alpha(\xi) = \frac{1}{n!}\epsilon_{\alpha\mu_1\cdots\mu_n}\epsilon_{\nu_1\cdots\nu_n}\xi_{\mu_1}^{\nu_1}\cdots\xi_{\mu_n}^{\nu_n} \tag{A4}$$

and the one-point reduced probability distribution $G(\xi)$, given by

$$G(\xi) = \left\langle \delta(\vec{s}) \prod_{\mu=1,\nu=1}^{n+1,n} \delta(\xi_\mu^\nu - \nabla_\mu s_\nu)\right\rangle. \tag{A5}$$

The Gaussian average in Eq. (A5) is straightforward to evaluate by first writing the δ functions in the integral representation and then performing the resulting standard Gaussian integrals. One finds

$$G(\xi) = \frac{1}{[2\pi S_0(t)]^{n/2}} \frac{1}{[2\pi S^{(2)}]^{n(n+1)/2}} \times \exp\left(-\sum_{\mu=1,\nu=1}^{n+1,n} \frac{(\xi_\mu^\nu)^2}{2S^{(2)}}\right), \tag{A6}$$

with the definitions

$$S_0(t) = \frac{1}{n}\langle [\vec{s}(0,t)]^2\rangle, \tag{A7}$$

$$S^{(2)} = \frac{1}{n(n+1)}\sum_{\mu=1,\nu=1}^{n+1,n} \langle [\nabla_\mu s_\nu]^2\rangle. \tag{A8}$$

In this theory $S^{(2)} = 1/(n+1)$ [16]. Substitution of Eq. (A6) into Eq. (A3) produces the final form for the average line density of string:

$$\langle \eta\rangle = C_n\left[\frac{S^{(2)}}{\pi S_0(t)}\right]^{n/2}, \tag{A9}$$

with the n-dependent constant C_n defined as

$$C_n = \frac{1}{\pi^{n(n+1)/2}} \int \prod_{\mu=1,\nu=1}^{n+1,n} d\xi_\mu^\nu \, |\vec{\omega}(\xi)| \times \exp\left(- \sum_{\mu=1,\nu=1}^{n+1,n} (\xi_\mu^\nu)^2 \right). \tag{A10}$$

For $n=2$ it can be shown that $C_2=1$ [16]. Since $S_0(t) \sim t$ at late times, the average line density of string scales like

$$\langle \eta \rangle \sim t^{-n/2}. \tag{A11}$$

In particular, for $n=2$, $\langle \eta \rangle \sim t^{-1}$.

APPENDIX B

This appendix outlines the evaluation of the average

$$A = \langle [\hat{m}(\vec{r},t) \cdot \hat{m}(0,t)]^2 \rangle \tag{B1}$$

appearing in the correlation function (4.4) for the monopole model. For an n-component Gaussian $\vec{m}$ field, the average A can be written in the integral form

$$A = \int d^n x_1 d^n x_2 \frac{(\vec{x}_1 \cdot \vec{x}_2)^2}{(x_1)^2 (x_2)^2} \Phi(\vec{x}_1, \vec{x}_2) \tag{B2}$$

in terms of the two-point reduced probability distribution [2]

$$\Phi(\vec{x}_1, \vec{x}_2) = \left[\frac{\gamma}{2\pi} \right]^n \exp\left(-\frac{\gamma^2}{2} (\vec{x}_1^2 + \vec{x}_2^2 - 2f \vec{x}_1 \cdot \vec{x}_2) \right), \tag{B3}$$

where the auxiliary field correlation function f is defined in Eq. (2.9) and $\gamma = 1/\sqrt{1-f^2}$. The identity

$$\frac{1}{(x_1)^2} = 2 \int_0^\infty dr_1 r_1 \exp - x_1^2 r_1^2 \tag{B4}$$

allows A to be written as a Gaussian integral

$$A = \lim_{\lambda \to 1} \int_0^\infty dr_1 r_1 \int_0^\infty dr_2 r_2 \frac{\partial^2}{\partial \lambda^2} \times \int d^n x_1 d^n x_2 \, \tilde{\Phi}_\lambda(\vec{x}_1, \vec{x}_2, r_1, r_2), \tag{B5}$$

with

$$\tilde{\Phi}_\lambda(\vec{x}_1, \vec{x}_2, r_1, r_2) = \frac{4}{f^2 \gamma^4} \left[\frac{\gamma}{2\pi} \right]^n \exp - \left(r_1^2 + \frac{\gamma^2}{2} \right) x_1^2 - \left(r_2^2 + \frac{\gamma^2}{2} \right) x_2^2 + \gamma^2 f \lambda \, \vec{x}_1 \cdot \vec{x}_2. \tag{B6}$$

The integrals over $\vec{x}_1$ and $\vec{x}_2$ in Eq. (B5) are readily done. After differentiating with respect to λ and setting $\lambda=1$, the integral over r_1 is performed. After a change of variables $y=(r_2)^2$, the following integrals remain:

$$A = 2^{-(n/2+1)} \int_0^\infty dy \left(y + \frac{\gamma^2}{2} \right)^{-1} \left(y + \frac{1}{2} \right)^{-n/2} + 2^{-(n/2+2)} n \gamma^2 f^2 \int_0^\infty dy \left(y + \frac{\gamma^2}{2} \right)^{-1} \left(y + \frac{1}{2} \right)^{-(n/2+1)}. \tag{B7}$$

These integrals can be expressed in terms of hypergeometric functions F [33], giving

$$A = 1 - \frac{\ln \gamma}{\gamma^2 - 1} \quad \text{for } n=2, \tag{B8}$$

$$A = 1 + \frac{(n-1)}{\gamma^2 (n-2)} \left[\frac{1}{\gamma^2 f^2} (F[1,1;n/2;f^2] - 1) - 1 \right] \quad \text{for } n>2. \tag{B9}$$

In particular, for $n=3$, Eq. (B9) gives

$$A = 1 + \frac{2}{\gamma^2} \left[\frac{1}{\gamma^2 f^3} (\gamma \sin^{-1} f - f) - 1 \right], \tag{B10}$$

which leads to Eq. (4.5) for $\mathcal{F}$ in the nematic with monopoles.

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