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Landau–de Gennes theory of isotropic-nematic-smectic liquid crystal transitions

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We propose a Landau–de Gennes variational theory fit to simultaneously describe isotropic, nematic, smectic-*A*, and smectic-*C* phases of a liquid crystal. The unified description allows us to deal with systems in which one, or all, of the order parameters develop because of the influence of defects, external fields and/or boundary conditions. We derive the complete phase diagram of the system, that is, we characterize how the homogeneous minimizers depend on the value of the constitutive parameters. The coupling between the nematic order tensor and the complex smectic order parameter generates an elastic potential which is a nonconvex function of the gradient of the smectic order parameter. This lack of convexity yields in turn a loss of regularity of the free-energy minimizers. We then consider the effect on an infinitesimal second-order regularization term in the free-energy functional, which fixes the optimal number of defects in the singular configurations.

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I. INTRODUCTION

The liquid crystalline state of matter has been described and studied in deep detail over the past century. The pioneering works of Oseen [1], Zocher [2], and Frank [3] gave birth to the first theory of the nematic liquid crystal phase. In it, the microscopic configuration is described through a unit vector $\mathbf{n}$, the *director*, parallel to the molecular orientation. A step forward was accomplished by de Gennes [4], who generalized the notion of director and introduced the *nematic order tensor*, which provides information on both the molecular orientations and the degree of ordering. The order-tensor theory succeeded in describing not only the nematic distortions but also the isotropic-nematic (*I*-*N*) phase transitions and cores of singular defects.

The onset of a smectic-*A* (Sm-*A*) phase in a nematic liquid crystal is described by a rise of a periodic modulation in the mass density of molecules in the liquid, along the director direction [5,6]. By exploiting an analogy between smectic liquid crystals and superconductors, de Gennes [7] proposed an independent, complex order parameter that allows for the description of nematic-smectic phase transitions. In a smectic-*C* (Sm-*C*) phase, the axis of this translational symmetry breaking is not parallel to the director, so that a 2-director theory was originally proposed to identify such phases [8].

Depending on the choice of the order parameters, different free energy functionals have been proposed over the years. All possible elastic terms depending on the nematic order tensor have been analyzed by Longa and co-workers [9]. The interaction between the nematic director and the complex smectic order parameter was first described by Chen and Lubensky [10–12]. These interaction terms have found many applications [13–16]. On the other hand, the 2-director variational theory has been put forward by Leslie and co-workers [17,18], and proven useful in several applications as well [19–21].

Direct *I*–Sm-*A* transitions have been reported [22,23]. Tricritical points exist both in the *N*–Sm-*A*–Sm-*C* [24,25] and in the *I*–Sm-*A*–Sm-*C* transitions [26]. Even direct *I*–Sm-*C* transitions have been detected [27]. This abundant experimental evidence of the existence of all possible transitions between isotropic, nematic, and smectic phases pushes towards a unified theory, in terms of a free energy functional constructed on the nematic order tensor and the complex smectic order parameter.

The need to construct a nematic-smectic theory based on the order tensor arises also from symmetry reasons. Indeed, the free-energy potentials which couple the nematic director and the complex smectic order parameter are not separately invariant under the reflection of the director and the smectic layers, but only under the simultaneous reflection of both degrees of freedom. The correct symmetry is automatically restored when the order tensor is used as a building block for the free-energy potential. The first attempt to couple the nematic order tensor with the complex smectic order parameter was carried out by Lelidis and Durand [28], that restricted their analysis to uniaxial order tensors with constant eigenvectors, and planar smectic layers, orthogonal to one of the eigenvectors. A more complete phenomenological theory, which covers the transitions between the isotropic, nematic, and smectic-*A* phases, has been proposed by Brand and co-workers [29,30].

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More recent studies accomplish the task of including smectic-C phases in the Landau theory [31,32]. Such theories include finite terms which depend on the second derivatives of the smectic order parameter in order to account for the additional biaxial symmetry. However, the presence of second-order gradient terms has nontrivial implications on the nature of the equilibrium differential equations, which consequently become fourth order. From the physical point of view, second-gradient terms directly penalize the curvature of the layers, and are widely used in shell theories [33,34]. Inserting them in the free-energy density would be necessary if the smectic layers were replaced by real vesicles hosting the liquid crystal molecules [35]. Second-gradient terms modify the boundary conditions to be applied on the smectic degrees of freedom as well. For example, a free-energy functional depending only on the first gradient of the smectic order parameter allows fixing the boundary layers to be parallel to the external surface. To include second-order derivatives in the free energy amounts to accepting also the mathematical possibility of fixing the boundary layer spacing at will.

In this paper we show that it is possible to develop a consistent phenomenological Landau theory, based only on the first gradients of the order parameters. Isotropic, nematic, smectic-A, and smectic-C phases may be reached as the temperature is lowered even in the absence of any second-order term in the free-energy functional. Quadratic terms depending on the second derivatives may be replaced by quartic terms depending on the first derivatives of the smectic order parameters. This choice is supported by the observation that the two-component vector order parameter $\boldsymbol{\chi}$ [36], which announces the onset of the smectic-C phase, is indeed quadratic in the gradient of the complex smectic-A order parameter. Thus, terms quadratic in $\boldsymbol{\chi}$ give rise to terms depending on the fourth power of the smectic order parameter. The first part of this paper is devoted to the careful analysis of the phase portrait associated to the proposed free-energy functional.

The other side of the first-order elastic potential we propose in this work is that it may yield to a lack of convexity of the elastic potential as a function of the gradient of the smectic order parameter. In turn, such loss of convexity may give rise to singular minimizers, or even to the nonexistence of minimizers [37,38]. This, however, is not a shortcoming of the model but an added benefit. Indeed, *edge* and *chevron* singular structures in smectic liquid crystals have been both observed experimentally [39–42], and studied theoretically within the nematic-director theory [13,14,43–46].

We show that the catastrophic replication of defects can be avoided with the insertion of an infinitesimal curvature penalty in the free-energy functional. Examples of problems with nonconvex potentials and higher-order regularizing terms include martensitic phase transformations [47], micromagnetics [48], and the Ginzburg-Landau model of nucleation [49]. Two well-known prototype models for a scalar order parameter u are the Ginzburg-Landau energy [50]

$$\int_\Omega (u^2-1)^2+\nu^2|\nabla u|^2, \tag{1}$$

and the Aviles-Giga energy [51]

$$\int_\Omega (|\nabla u|^2-1)^2+\nu^2|\nabla^2 u|^2. \tag{2}$$

The former is a model of vortex nucleation. The latter describes convective pattern formation and thin films. In particular, it is a special case of the more general potential we propose in the present paper. One observed trend in such problems is that energy minimizers may develop increasingly involved microstructures as $\nu \to 0^+$. This fact arises in our calculations as well.

Order parameters. Nematic and smectic phases reflect symmetry breaking related to different degrees of freedom. Nematic ordering refers to the local probability distribution of molecular orientations $f_{\mathbf{x}}(\ell)$, with ℓ the unit vector along the molecular axis. More precisely, the isotropic-nematic transition is defined as the point at which the symmetric, traceless *nematic order tensor* [52]

$$\mathbf{Q}(\mathbf{x}) := \int_{\mathbb{S}^2} \ell \otimes \ell f_{\mathbf{x}}(\ell) da - \frac{1}{3}\mathbf{I} \tag{3}$$

becomes non-null ($\mathbf{I}$ is the identity tensor). The nematic order tensor $\mathbf{Q}$ is, respectively, labeled as *isotropic*, *uniaxial*, or *biaxial*, when its eigenvalues are all equal, two equal but different from the third, or all three different. Frequently, the thermodynamic Landau–de Gennes potential σ_{LdG}, that we shall introduce below, forces the nematic order tensor to be uniaxial. When this is the case, the general form it may assume is

$$\mathbf{Q}_{\mathrm{uni}}(\mathbf{x}) := s(\mathbf{x})\left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{1}{3}\mathbf{I}\right), \tag{4}$$

where $s \in \left[-\frac{1}{2},1\right]$ is the *nematic order parameter* and $\mathbf{n}$ is the *director*. If the liquid crystal is made up of elongated molecules, σ_{LdG} is minimized when the degree of orientation assumes a positive value s_0. In this case, $\mathbf{n}$ coincides with the eigenvector of $\mathbf{Q}$ associated with the higher eigenvalue.

Smectic ordering deals with the distribution in space of the molecular mass centers. In a smectic phase, the molecules tend to organize themselves in a layered structure, whose skeleton need not necessarily be a family of parallel planes. The complex *smectic order parameter* $\psi=\rho e^{i\omega}$ measures the inhomogeneity of the spatial molecular density. The non-negative modulus ρ yields the amplitude of density modulation. The level sets of the real function ω complete the description by identifying the position of smectic layers. Thus, $\nabla\omega$ is everywhere parallel to the layer normal, while $|\nabla\omega|$ is proportional to the inverse of the layer spacing.

The character of a smectic phase depends on the mutual arrangements of nematic and smectic variables. When the nematic order tensor is uniaxial, and a director can be defined, a smectic phase is labeled as Sm-A or Sm-C, depending on whether the director is parallel to the layer normal, or not. However, in the general biaxial case a unique director is not available, and a more general phase definition is required. This is not a scholastic objection, since Sm-C phases are intrinsically biaxial due to the tilt of layer normal breaking the symmetry among the directions orthogonal to $\mathbf{n}$. To overcome this obstacle, we can resort to the earlier remark in which we linked the director with one of the eigenvectors of the nematic order tensor. In terms of $\mathbf{Q}$ and ψ, the order parameter that recognizes whether the layer normal is an eigenvector of $\mathbf{Q}$ is given by $\boldsymbol{\chi} := \mathbf{Q}\nabla\psi \wedge \nabla\psi$. Thus, to construct a phenomenological Landau theory that may enforce Sm-A–Sm-C transitions we must include in the free-energy functional an interaction term

$$\sigma_{AC} = f\ \boldsymbol{\chi}\cdot\boldsymbol{\chi} = f\ |\mathbf{Q}\nabla\psi \wedge \nabla\psi|^2. \qquad (5)$$

Negative values of the coupling constant f enforce Sm-C phases. The potential (5) requires the presence in the elastic free energy of a new term proportional to $|\nabla\psi|^4$, to ensure that the complete functional remains bounded from below. In Sec. II we describe all terms entering the free-energy functional, while Sec. III is devoted to the analysis of the variety of phase transitions predicted by this model. We then move to the analysis of the singular configurations allowed by the nonconvexity of the free-energy density. Sections IV and V address the onset of chevron and edge dislocations, respectively. In these sections we discuss the key role played by the infinitesimal regularizing second-order term.

II. FREE-ENERGY FUNCTIONAL

We consider a liquid crystal confined in a three-dimensional domain Ω. The order parameters $\mathbf{Q}:\Omega\to\mathcal{A}$, and $\psi:\Omega\to\mathbb{C}$ describe the microscopic state of the material. The codomain $\mathcal{A}$ of the nematic order tensor is the set of all traceless, symmetric tensors $\mathbf{Q}$, with spectrum $\mathrm{sp}\,\mathbf{Q} \subset [-\frac{1}{3},\frac{2}{3}]$. Given a point $P_o\in\Omega$, we let

$$\boldsymbol{\chi}(P_o) := \mathbf{Q}(P_o)\nabla\psi(P_o) \wedge \nabla\psi(P_o), \qquad (6)$$

and we label the liquid crystal as

$$\begin{aligned} &\text{isotropic} && \text{if } \mathbf{Q}=\mathbf{0} \text{ and } \psi=0,\\ &\text{nematic} && \text{if } \mathbf{Q}\neq\mathbf{0} \text{ and } \psi=0,\\ &\text{smectic-}A && \text{if } \mathbf{Q},\psi\neq 0 \text{ and } \boldsymbol{\chi}=\mathbf{0},\\ &\text{smectic-}C && \text{if } \mathbf{Q},\psi\neq 0 \text{ and } \boldsymbol{\chi}\neq\mathbf{0}. \end{aligned} \qquad (7)$$

For the sake of brevity, we limit our analysis to achiral, and nonpolarized liquid crystals, and we define the following free-energy functional:

$$\mathcal{F}[\mathbf{Q},\psi] := \int_\Omega [\sigma_{\mathrm{el},n}(\nabla\mathbf{Q},\mathbf{Q}) + \sigma_{\mathrm{LdG}}(\mathbf{Q}) + \sigma_{\mathrm{el,sm}}(\nabla\psi) + \sigma_{\mathrm{sm}}(|\psi|) + \sigma^{(1)}_{n,\mathrm{sm}}(\mathbf{Q},|\psi|) + \sigma^{(2)}_{n,\mathrm{sm}}(\mathbf{Q},\nabla\psi)]dv. \qquad (8)$$

The complete free-energy functional contains the following terms.

(i) The nematic elastic energy $\sigma_{\mathrm{el},n}$ has been analyzed in detail elsewhere [9]. It is quadratic in $\nabla\mathbf{Q}$, and for our purposes we only need to recall that it is minimized when $\mathbf{Q}$ is uniform, so that $\nabla\mathbf{Q}=\mathbf{0}$.

The Landau–de Gennes potential is given by [52]

$$\sigma_{\mathrm{LdG}}(\mathbf{Q}) := a\ \mathrm{tr}\,\mathbf{Q}^2 - b\ \mathrm{tr}\,\mathbf{Q}^3 + c\ \mathrm{tr}\,\mathbf{Q}^4. \qquad (9)$$

The material parameter c is positive to keep the functional bounded from below. The constant b is positive in all liquid crystals made up of rodlike molecules, while a changes sign when the isotropic configuration $\mathbf{Q}=\mathbf{0}$ becomes unstable. With the choices above, the minimum of the potential (9) is attained when the nematic is *uniaxial*, i.e., when two of the eigenvalues of $\mathbf{Q}$ coincide. However, uniaxiality may be destroyed by means of suitable external fields or boundary conditions [53–55].

(ii) The elastic contribution arising from $\nabla\psi$ must contain a fourth-power term in order to balance the term $\sigma^{(2)}_{n,\mathrm{sm}}$ we introduce below. Thus,

$$\sigma_{\mathrm{el,sm}}(\nabla\psi) := b_1|\nabla\psi|^2 + b_2|\nabla\psi|^4, \qquad (10)$$

where at least the elastic constant b_2 must be positive.

The smectic potential σ_{sm} drives the onset of the smectic phases,

$$\sigma_{\mathrm{sm}}(|\psi|) := \tilde{a}|\psi|^2 + \tilde{c}|\psi|^4. \qquad (11)$$

The material parameter $\tilde{c}$ is forced to be positive, while $\tilde{a}$ may change sign close to the smectic transitions.

(iii) The nematic-smectic interaction consists in two terms, since the nematic order is coupled both with the smectic degree of order $|\psi|$ and with the gradient $\nabla\psi$, which keeps information on layer direction and spacing. More precisely, we choose

$$\sigma^{(1)}_{n,\mathrm{sm}}(\mathbf{Q},|\psi|) = -\tilde{b}|\psi|^2\ \mathrm{tr}\,\mathbf{Q}^2. \qquad (12)$$

The coupling constant $\tilde{b}$ may be positive or negative. A positive choice implies that the onset of any order (either nematic or smectic) is favored when one of the two order parameters is already non-null. Finally, we include two terms in $\sigma^{(2)}_{n,\mathrm{sm}}$:

$$\sigma^{(2)}_{n,\mathrm{sm}}(\mathbf{Q},\nabla\psi) = e\mathbf{Q}\nabla\psi\cdot\nabla\psi + f\boldsymbol{\chi}\cdot\boldsymbol{\chi}, \qquad (13)$$

where $\boldsymbol{\chi}$ is defined as in (6). If $e\leqslant 0$ the first term is minimized when $\nabla\psi$ is parallel to the eigenvector of $\mathbf{Q}$ corresponding to the higher eigenvalue, that is in a Sm-A phase. Similarly, negative values of f promote Sm-C phases.

Remark. The potential (10) is invariant under rotations of the nematic layers, while it should be invariant under simultaneous rotations of both the smectic layers and the nematic molecules. Indeed, when ψ and the nematic director $\mathbf{n}$ are chosen as order parameters [10], only the covariant gradient $\mathbb{D}_n = (\nabla - iq\mathbf{n})$ may enter the elastic terms depending on the smectic order parameter. This important symmetry feature is naturally contained in our present description, as one can see by replacing $\nabla\psi$ in (10) by $\mathbb{D}_Q\psi = (\mathbf{I}-\mathbf{Q})\nabla\psi$. Terms resulting from such replacement are already represented in (13). Indeed, let us consider

$$|\mathbb{D}_Q\psi|^2 = (\nabla\psi - \mathbf{Q}\nabla\psi)^2 = |\nabla\psi|^2 - 2\mathbf{Q}\nabla\psi\cdot\nabla\psi + |\mathbf{Q}\nabla\psi|^2. \tag{14}$$

The first term is the b_1 term in (10), while the second is the e term in (13). The final term in (14) is contained within the f term in (13), since

$$\begin{aligned}\boldsymbol{\chi}\cdot\boldsymbol{\chi} &= (\mathbf{Q}\nabla\psi\wedge\nabla\psi)\cdot(\mathbf{Q}\nabla\psi\wedge\nabla\psi)\\ &= |\nabla\psi|^2|\mathbf{Q}\nabla\psi|^2 - (\mathbf{Q}\nabla\psi\cdot\nabla\psi)^2.\end{aligned} \tag{15}$$

Finally, the coefficients in front of the interaction terms can be varied independently, since it is the very presence of an interaction term that ensures that the global potential will be invariant only with respect to contemporary rotations of the involved order parameters. Therefore, even at this early stage, we may conclude that the free-energy functional (8) reflects the necessary symmetries in a more general way.

III. PHASE TRANSITIONS

In this section we analyze the uniform minimizers of the free-energy functional (8). In order to shorten our presentation, we focus on two particular problems. First, we focus on the transitions from the isotropic phase (either I-N, I–Sm-A, or I–Sm-C). Then, we consider the situation in which uniaxial nematic order is already established, and determine the critical values of the material parameters that give rise to the onset of smectic phases. In both cases, we consider uniform configurations in which

$$\mathbf{Q}(\mathbf{x}) \equiv \mathbf{Q}_0 \quad\text{and}\quad \psi(\mathbf{x}) = \rho_0 e^{i\mathbf{q}_0\cdot\mathbf{x}}. \tag{16}$$

When we replace (16) in (8), the result is

$$\mathcal{F}(\mathbf{Q}_0,\rho_0,\mathbf{q}_0) = V\sigma_0(\mathbf{Q}_0,\rho_0,\mathbf{q}_0), \tag{17}$$

where $V=\mathrm{Vol}(\Omega)$ and

$$\begin{aligned}\sigma_0(\mathbf{Q}_0,\rho_0,\mathbf{q}_0) &= a\,\mathrm{tr}\,\mathbf{Q}_0^2 - b\,\mathrm{tr}\,\mathbf{Q}_0^3 + c\,\mathrm{tr}\,\mathbf{Q}_0^4 + b_1\rho_0^2 q_0^2 + b_2\rho_0^4 q_0^4\\ &\quad + \tilde{a}\rho_0^2 + \tilde{c}\rho_0^4 - \tilde{b}\rho_0^2\,\mathrm{tr}\,\mathbf{Q}_0^2 + e\rho_0^2\mathbf{Q}_0\mathbf{q}_0\cdot\mathbf{q}_0\\ &\quad + f\rho_0^4|\mathbf{Q}_0\mathbf{q}_0\wedge\mathbf{q}_0|^2.\end{aligned} \tag{18}$$

A. Isotropic transitions

Let us assume that the system is close to the isotropic phase. In this case, both ρ_0 and $|\mathbf{Q}_0|$ are small, and the following transitions may arise.

1. Isotropic-nematic transitions

If $\rho_0=0$, Eq. (18) yields

$$\sigma_0|_{\rho_0=0} = a\,\mathrm{tr}\,\mathbf{Q}_0^2 - b\,\mathrm{tr}\,\mathbf{Q}_0^3 + c\,\mathrm{tr}\,\mathbf{Q}_0^4, \tag{19}$$

which is the standard Landau–de Gennes potential for the phenomenological first-order nematic transition. If $a > \frac{3}{32}\frac{b^2}{c}$, it possesses a unique stationarity configuration, the isotropic state. When $a \leqslant \frac{3}{32}\frac{b^2}{c}$ two new stationary configurations appear, characterized by

$$s = s_{\pm} = \frac{3b \pm \sqrt{3(3b^2 - 32ac)}}{8c}. \tag{20}$$

Since $b \geqslant 0$ for rodlike materials, the higher value s_+ becomes the absolute minimizer when $a \leqslant \frac{1}{12}\frac{b^2}{c}$, while the isotropic state becomes unstable below the *super-cooling* temperature T_{SC}, that is, when $a \leqslant 0$. One usually defines the *nematic-isotropic* temperature T_{NI} as the temperature at which $a^* = \frac{1}{12}\frac{b^2}{c}$, while the width of the transition hysteresis is, obviously, in the range $0 \leqslant a \leqslant \frac{3}{32}\frac{b^2}{c}$.

2. Isotropic–smectic-A transitions

If $\mathbf{Q}_0=0$, the potential (18) reads as

$$\sigma_0|_{\mathbf{Q}_0=0} = b_1\rho_0^2 q_0^2 + b_2\rho_0^4 q_0^4 + \tilde{a}\rho_0^2 + \tilde{c}\rho_0^4. \tag{21}$$

The nontrivial stationary points of (21) are given by

$$\rho_0^2 = -\frac{\tilde{a}}{2\tilde{c}} \quad\text{and}\quad q_0^2 = \frac{b_1}{\tilde{a}}\frac{\tilde{c}}{b_2}. \tag{22}$$

Since b_2 and $\tilde{c}$ are positive, a smectic phase may arise only provided both b_1 and $\tilde{a}$ are negative. In particular, both b_1 and $\tilde{a}$ must vanish at the transition, in order to keep inverse layer spacing q_0 finite. Thus, the smectic phase may arise directly from the isotropic one if both b_1 and $\tilde{a}$ vanish at the temperature T_{NI} defined above.

3. Isotropic–smectic-C transitions

Let us assume that $a = \frac{1}{12}\frac{b^2}{c}$, $\tilde{a}=0$, and $b_1=0$, so to guarantee that we directly pass from the isotropic to a smectic phase. We represent the resulting smectic wave vector $\mathbf{q}_0$ in the principal basis of $\mathbf{Q}$ as $\mathbf{q}_0 = q_0(\cos\theta\mathbf{e}_1 + \sin\theta\cos\varphi\mathbf{e}_2 + \sin\theta\sin\varphi\mathbf{e}_3)$, and denote the corresponding eigenvalues of $\mathbf{Q}$ as

$$\lambda_1 = \frac{2}{3}s_0, \quad \lambda_2 = -\frac{1}{3}s_0 + \beta, \quad \lambda_3 = -\frac{1}{3}s_0 - \beta, \tag{23}$$

with $0 \leqslant \beta \leqslant s_0$, so that the eigenvalues are numbered in decreasing order. The potential (18) now becomes

$$\begin{aligned}\sigma_0 &= \frac{1}{12}\frac{b^2}{c}\,\mathrm{tr}\,\mathbf{Q}_0^2 - b\,\mathrm{tr}\,\mathbf{Q}_0^3 + c\,\mathrm{tr}\,\mathbf{Q}_0^4 + b_2\rho_0^4 q_0^4 + \tilde{c}\rho_0^4\\ &\quad - \tilde{b}\rho_0^2\,\mathrm{tr}\,\mathbf{Q}_0^2 + e\rho_0^2\mathbf{Q}_0\mathbf{q}_0\cdot\mathbf{q}_0 + f\rho_0^4|\mathbf{Q}_0\mathbf{q}_0\wedge\mathbf{q}_0|^2\\ &= \frac{1}{18c}s^2(b-2cs)^2 + \frac{1}{6c}\beta^2(b^2 + 12bcs + 8c^2s^2)\\ &\quad + 2\beta^4 c + b_2\rho_0^4 q_0^4 + \tilde{c}\rho_0^4 - \frac{2}{3}\tilde{b}\rho_0^2(s^2 + 3\beta^2)\\ &\quad + e\rho_0^2 q_0^2\left(s_0\cos^2\theta - \frac{1}{3}s_0 + \beta\sin^2\theta\cos 2\varphi\right)\\ &\quad + f\rho_0^4 q_0^4\sin^2\theta[\cos^2\theta\sin^2\varphi(s_0+\beta)^2\\ &\quad + \cos^2\theta\cos^2\varphi(s_0-\beta)^2 + \beta^2\sin^2\theta\sin^2 2\varphi].\end{aligned} \tag{24}$$

The uniaxial Sm-A solution $\theta=0$, with $\beta=0$, $s=s_+=b/(2c)$, and ρ_0, q_0 as in (22), is always a stationarity point of (24). However, it becomes unstable if

$$f < \frac{e}{\rho_0^2 q_0^2 s_+} =: f_{\mathrm{cr}}. \tag{25}$$

If the coupling constant f lies below the threshold f_{cr}, the I–Sm-A transition becomes a direct I–Sm-C phase transition. The presence of the vanishing quantity $\rho_0^2 q_0^2$ in the denominator of (25) implies that $f_{\mathrm{cr}} \to -\infty$, if the material parameter e is strictly negative. This implies that no direct I–Sm-C transition may arise if the e term is explicitly promoting the Sm-A phase.

To summarize the results we can state the following:

(i) The isotropic phase becomes unstable against nematic configurations at the temperature T_{SC} at which a vanishes. We have also identified the temperature $T_{NI} > T_{SC}$ at which the isotropic and the nematic phases possess the same free energy.

(ii) A smectic phase may be directly reached from the complete disorder if also both b_1 and $\tilde{a}$ vanish at T_{NI} (that becomes then T_{SI}).

(iii) The smectic phase thus obtained is indeed a tilted Sm-C phase if any of the following two cases arises at the transition temperature: either $e > 0$ (any f), or $e = 0$ and $f < f_{\mathrm{cr}}$.

B. Nematic transitions

Let us now focus on a physically different situation. Imagine that the nematic liquid crystal order is well established, with $s = s_+$ and $\beta = 0$. If we again denote by θ the angle that $\mathbf{q}_0$ determines with the director $\mathbf{e}_1$, the potential (18) can be written as

$$\sigma_0 = \sigma_{\mathrm{LdG}}(s_+) + \tilde{a}\rho_0^2 - \frac{2}{3}\tilde{b}\rho_0^2 s_+^2 + \tilde{c}\rho_0^4 + b_1\rho_0^2 q_0^2 + b_2\rho_0^4 q_0^4 + \frac{1}{3}e\rho_0^2 q_0^2 s_+(3\cos^2\theta - 1) + f\rho_0^4 q_0^4 s_+^2 \cos^2\theta(1 - \cos^2\theta). \tag{26}$$

Just as above, the onset of Sm-A order is characterized by the simultaneous vanishing of the coefficients of ρ_0^2 and $\rho_0^2 q_0^2$, when $\theta = 0$. Consistently, we define the critical temperature T_{NA} such that $\tilde{a} - \frac{2}{3}\tilde{b}s_+^2 = \hat{a}(T - T_{NA})$ and $b_1 + \frac{2}{3}es_+ = \hat{b}(T - T_{NA})$, where $\hat{a}$ and $\hat{b}$ are positive. In other words, we are assuming that only $\tilde{a}$ and b_1 are temperature dependent, while all the other constitutive parameters entering the smectic part of the free-energy density do not vary significantly with the temperature in the vicinity of T_{NA}. In reality, this probably means that the physical parameters $\tilde{a}$ and b_1 are not independent—but this is not a relevant point for us presently. In particular, we assume that the parameters e, f are both negative. In this way the free-energy term $\sigma_{n,\mathrm{sm}}^{(2)}$ in (13) is given by the sum of two competing terms. The former pushes towards a Sm-A phase, while the latter is minimized in the Sm-C phase.

To better interpret how the optimal values of the order parameters ρ_0, q_0, θ depend on the material constants, we further introduce the following notations:

$$q_{\mathrm{sm}}^2 := \frac{\hat{b}\tilde{c}}{\hat{a}b_2}, \quad \rho_M^2 = \frac{\hat{a}T_{NA}}{2\tilde{c}},$$

$$T_{AC} = T_{NA}\left(1 - \frac{e}{fs_+ q_{\mathrm{sm}}^2 \rho_M^2}\right). \tag{27}$$

We remark that T_{AC} which, as we show below, is the temperature of the Sm-A–Sm-C transition, is lower than T_{NA} as long as both e and f are negative. Furthermore, $T_{AC} > 0$ provided $f < e/(s_+ q_{\mathrm{sm}}^2 \rho_M^2)$. Thus, the material parameter f must be sufficiently negative in order to be able to promote a Sm-C phase at a finite temperature. We finally define the dimensionless parameter

$$\mu := -\frac{4b_2}{fs_+^2}. \tag{28}$$

The coefficient of the terms depending on the fourth power of $\boldsymbol{\nabla}\psi$, that is on $\rho_0^4 q_0^4$, must be positive whatever the degree of nematic order and the tilt angle θ. A little algebra shows that this is certainly the case if $\mu > 1$. With the choices above it is straightforward to prove that the minimizers of (26) are the following.

(N) If $T \geqslant T_{NA}$, the optimal value is $\psi = 0$, so that no smectic order arises.

(Sm-A) If $T_{AC} \leqslant T \leqslant T_{NA}$ the free-energy minimizers are the following:

$$\rho_0 = \rho_M\sqrt{1 - \frac{T}{T_{NA}}}, \quad q_0 = q_{\mathrm{sm}}, \quad \theta = 0. \tag{29}$$

The Sm-A phase arises with a second-order transition with the layer spacing given by the first of Eqs. (27).

(Sm-C) When $T \leqslant T_{AC}$ the minimizers change as follows:

$$\rho_0 = \rho_M\sqrt{1 - \frac{T}{T_{NA}}},$$

$$q_0 = q_{\mathrm{sm}}\sqrt{1 + \frac{T_{AC} - T}{(T_{NA} - T)(\mu - 1)}}, \tag{30}$$

that is, the smectic layer spacing decreases, and

$$\cos 2\theta = \frac{(T_{NA} - T_{AC})(\mu - 1)}{T_{AC} - T + (T_{NA} - T)(\mu - 1)}. \tag{31}$$

Figures 1–3 illustrate the above results. Figure 1 displays both the smectic intensity ρ and the layer spacing, inversely proportional to q_0, as a function of the temperature, in both smectic phases. The amplitude of the smectic density wave, ρ_0 does not depend on the constitutive parameter μ and it is smooth across the Sm-A–Sm-C transition. In contrast, the layer spacing $d = 2\pi/q_0$ reflects the second-order character of the Sm-A–Sm-C transition at the temperature T_{AC}. Moreover, when μ is large, for instance for lower nematic order s_+, the layer spacing contraction in the Sm-C phase tends to

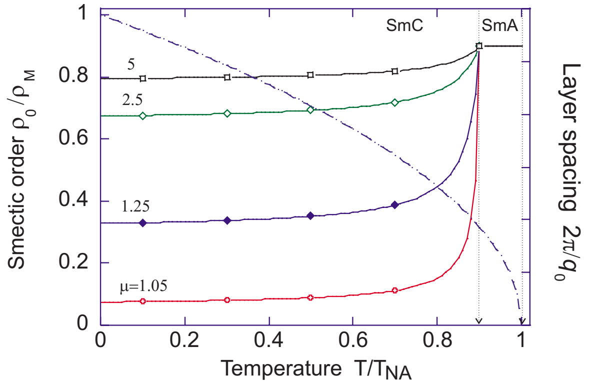

FIG. 1. (Color online) Smectic phase parameters as functions of the reduced temperature in the realistic case $T_{AC}=0.9T_{NA}$. The dashed curve represents the reduced smectic intensity ρ_0, in units of ρ_M. Continuous lines show the layer spacing, $2\pi/q_0$, in units of q_{sm}. The displayed values of μ are 1.05, 1.25, 2.5, 5.0, labeled on the plot.

disappear, which yields interesting results, as we will discuss below.

Figure 2 shows the behavior of the tilt angle θ, which emerges in the Sm-*C* phase, as a function of the temperature and μ. The tilt angle does not exhibit a very significant dependence on μ, however, the rate at which the maximum value of θ is approached is higher for smaller μ, that is when the nematic ordering is greater. In all cases, the zero-temperature limit of θ is close to (but below) $\pi/4$. This result should be expected, since the definition of the smectic-*C* order parameter shows that $\boldsymbol{\chi}$ maximizes its modulus when it is oriented at the greatest possible angle with respect to *all* the eigenvectors of the order tensor $\mathbf{Q}$. When this latter is uniaxial, the maximum value of $\boldsymbol{\chi}$ is attained when the angle between the director and the layer normal approaches $\frac{\pi}{4}$. Indeed, were θ to exceed such limiting value, the layer normal would approach one of the eigenvectors of $\mathbf{Q}$ different from the director.

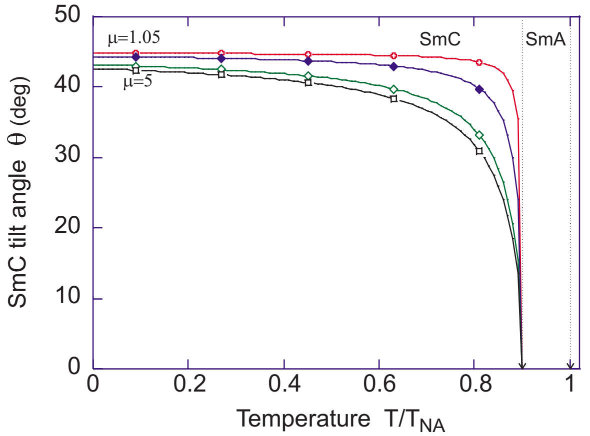

FIG. 2. (Color online) Tilt angle θ as a function of the reduced temperature for the same T_{AC} and μ values as in Fig. 1. The tilt angle depends only slightly on the constitutive parameter μ.

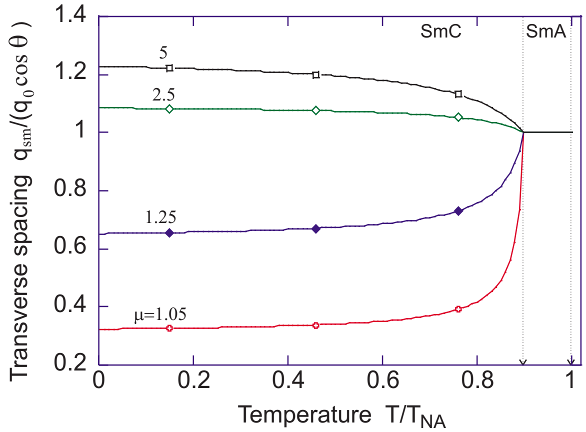

FIG. 3. (Color online) Dimensionless transverse layer spacing $\Delta=q_{\mathrm{sm}}/(q_0\cos\theta)$ for the same T_{AC} and μ values as in Fig. 1.

The layer compression on increasing tilt, shown in Fig. 1, is characteristic of most Sm-*C* materials. The typical explanation of such effect is normally given in geometrical terms as follows. Let us assume that the layer spacing $d=2\pi/q_0$ is determined by the projection of the molecular length ℓ into the layer normal direction. In particular, in the Sm-*A* phase both quantities would be expected to coincide, $d_A\approx\ell$ (and we observe the constant layer spacing above T_{AC}). In the Sm-*C* phase, the tilt angle θ would imply $d\approx\ell\cos\theta$. Thus, it is interesting to check whether the ratio $d/\cos\theta\sim1/(q_0\cos\theta)$ remains approximately constant throughout the whole smectic regime. Figure 3 displays how such transverse layer spacing depends on the temperature and the dimensionless parameter μ. It happens to remain constant only when $\mu=2$, which gives an interesting estimate of the typical value the dimensionless parameter μ should attain. When μ is greater (lower) than 2, the layer spacing is greater (lower) than its geometrical estimate. We remark that there are several experimental examples of materials that do not obey the geometrical estimate for the Sm-*C* layer contraction. In fact, there are materials for which the layer spacing remains substantially constant across the Sm-*A*–Sm-*C* transition. Figure 1 shows that this effect, named after de Vries [56,57], is to be expected in materials for which μ greatly exceeds the critical value 2 identified above. Equation (28) shows that the magnitude of μ depends essentially on the balance between the purely smectic elastic constant b_2 and the nematic-smectic coupling constant e. It is then of no surprise that the geometrical estimate that relates the layer spacing to the director length fails when the coupling between the nematic and smectic order parameters becomes negligible.

The above results are summarized qualitatively in Fig. 4. Several phase diagrams have been reported in the literature by varying the external temperature and the composition of liquid crystal mixtures. For the sake of simplicity we have indicated $-f$ in the horizontal axis of Fig. 4. Nevertheless, we must imagine that moving along the horizontal axis corresponds to varying the molecular structure of the system, thus varying all constitutive parameters, and in particular the transition temperatures T_{NI}, T_{NA}, and the smectic parameters e, f. In all cases, no Sm-*C* phase can be identified if f is not sufficiently negative [see Eq. (27) and discussion below]. A tricritical point *N*–Sm-*A*–Sm-*C* arises if $T_{NA}<T_{NI}$ when e vanishes (see Fig. 4, left-hand side). Indeed, the vanishing of the parameter e implies $T_{AC}=T_{NA}$ [see again Eq. (27)]. This

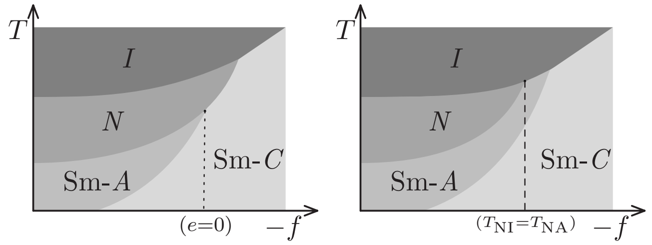

FIG. 4. Qualitative phase diagram of a liquid crystal undergoing several transitions. High values of the smectic parameter f hinder the onset of the Sm-C phase. When f becomes sufficiently negative a Sm-C phase arises at low temperatures. Eventually, the tilted phase may be reached directly from the nematic or from the isotropic state. See the text for a more detailed description of the different tricritical points that may exist.

is the case reported in [24,25], where the horizontal axis represents the concentrations in a mixture of $\bar{7}S5$ and $\bar{8}S5$. On the contrary, a tricritical point I-N–Sm-A occurs if $T_{NA}=T_{NI}$ when the parameter e is still negative (see Fig. 4, right-hand side). Such a tricritical point has been observed by plotting phase diagrams for 7CB–10CB systems [58]. Clearly, in real systems there is no guarantee that we are allowed to push the smectic parameter f below the critical value (25) that allows for direct I–Sm-C transitions.

IV. CHEVRON STRUCTURES IN SMECTIC-C PHASES

The aim of describing Sm-C phases has led us in Sec. II to defining the order parameter $\boldsymbol{\chi}$, which depends quadratically on $\nabla\psi$, and thus to construct a free-energy density which depends on $|\nabla\psi|^4$. In Sec. III we have shown that in smectic phases the coefficient b_1 multiplying $|\nabla\psi|^2$ turns negative. This fact induces a lack of convexity in the overall free-energy density as a function of $\nabla\psi$. However, we stress that this aspect is not to be related to our aim of constructing a nematic-smectic theory based on the order tensor. Indeed, similar problems are already found within the $\mathbf{n}$-ψ description [59].

One of the most interesting and well-studied patterns that originate from the lack of convexity of the free-energy density are the chevron structures in Sm-C materials. Smectic chevrons have been experimentally detected [40], and analyzed theoretically within the $\mathbf{n}$-ψ model [13,14]. To better understand these singularities we consider the simple bookshelf geometry illustrated in Fig. 5. It represents the Sm-C cell $y\in[0,d]$, in which homeotropic anchoring is enforced at the surfaces. In the left-hand panel, the anchoring is obeyed, but wall defects locally break the smectic ordering. To be more precise, if we let θ_0 be the angle Sm-C tilt angle, the induced wall defects will be separated by a distance $d/\tan\theta_0$ along the x direction. On the contrary, the right-hand panel shows a situation in which the homeotropic anchoring has been broken, but the normal to the smectic layers does not exhibit any jump discontinuity.

If we were to compare the energies of the configurations represented in Fig. 5, the chevron structure would always win, since the homogeneous nematic pays no anchoring energy, and the discontinuities in the smectic normal are energetically free as well. However, it would be impossible to identify uniquely the energy minimizer, since the chevrons could replicate at will, thus inducing any number of discontinuities in the layer normal.

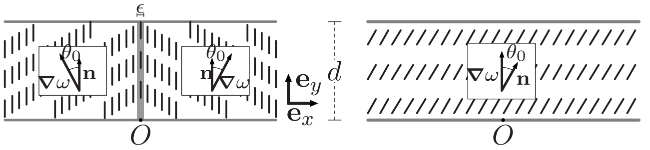

FIG. 5. Left-hand side: Snapshot of a chevron disclination in a bookshelf Sm-C liquid crystal. The chevron occupies the gray region, where the layer normal performs a $2\theta_0$ turn. Right-hand side: The chevron disclination can be avoided by breaking the homeotropic anchoring at the surface. In both cases the angle the nematic molecules determine with the layer normal is $\theta_0=\frac{\pi}{6}$.

There are several ways to overcome the degeneracy induced by the lack of convexity of the free-energy density [60]. The most physically convincing remedy consists in introducing a small energy penalty depending on the layers' curvature, and thus on the second derivatives of the smectic order parameter ψ. The simplest choice is given by

$$\sigma_{\mathrm{reg}}=D|\mathbb{D}_Q\mathbb{D}_Q\psi|^2=D|(\nabla-\mathbf{Q}\nabla)(\nabla-\mathbf{Q}\nabla)\psi|^2, \tag{32}$$

where we have now directly replaced the gradients by covariant derivatives in order to avoid introducing further nematic-smectic interaction terms. We now show that the presence of the regularizing term (32) fixes the size of the regions in which the chevrons round their edges, and introduces a fixed energy penalty per chevron.

Let us consider the chevron structure illustrated in Fig. 5 (left-hand side), and more precisely the slab $\mathcal{A}=\{|x|\leqslant d/(2\tan\theta_0)\}$. The nematic order tensor is uniform $\mathbf{Q}=s_+\left(\mathbf{e}_y\otimes\mathbf{e}_y-\frac{1}{3}\mathbf{I}\right)$. The smectic intensity ρ is constant, and we regularize the chevron by smoothing its sharp edges in a region of characteristic size ϵ (to be determined). When this is the case, the phase gradient within the gray region is given by

$$\nabla\omega(x,y)=\begin{cases}q_0(-\sin\theta_0\mathbf{e}_x+\cos\theta_0\mathbf{e}_y) & \text{if } x\leqslant-\epsilon,\\ q_0(x/\epsilon\sin\theta_0\mathbf{e}_x+\cos\theta_0\mathbf{e}_y) & \text{if } |x|<\epsilon,\\ q_0(\sin\theta_0\mathbf{e}_x+\cos\theta_0\mathbf{e}_y) & \text{if } x\geqslant\epsilon,\end{cases} \tag{33}$$

where q_0 is the preferred layer spacing. The potential σ_{reg} vanishes outside the chevron. Within this latter, an easy calculation allows to show that it contributes to the total free energy with a factor

$$\int_{\mathcal{A}}\sigma_{\mathrm{reg}}dxdy\approx\frac{2Dd}{\epsilon}\rho_0^2q_0^2\zeta(s_+)\sin^2\theta_0, \tag{34}$$

where $\zeta(s_+):=\left(1+\frac{1}{3}s_+\right)^4$. On the other hand, the chevron possesses an energy cost due to the layer mismatch and the imperfect alignment of the smectic-C molecules. The excess free energy stored in the gray region is given by

$$\Delta\int_{\mathcal{A}}\sigma dxdy \approx \frac{16}{15}b_2 d\rho_0^4 q_0^4 \epsilon \sin^4\theta_0. \tag{35}$$

Minimizing with respect to ϵ the sum of the two preceding contributions allows to determine the optimal size of the transition region

$$\epsilon_{\text{opt}} = \sqrt{\frac{15\zeta(s_+)}{8}\frac{D}{b_2}}\frac{1}{\rho_0 q_0 \sin\theta_0}. \tag{36}$$

Equation (36) confirms that the chevron structure is related to the tilted character of the Sm-C phase, as the size of the transition region would diverge were we approaching the Sm-A phase, $\epsilon_{\text{opt}} \sim \theta_0^{-1}$ as $\theta_0 \to 0$. We remark that the power law ruling such singular behavior confirms the previous theoretical calculations performed within the nematic-director theory [14]. In view of Eq. (36) the total energy cost of a singular wall of height d turns out to be

$$\Delta\mathcal{F}_{(1\text{chvrn})} = 8\sqrt{\frac{2}{15}\zeta(s_+)}\sqrt{Db_2}d\rho_0^3 q_0^3 \sin^3\theta_0. \tag{37}$$

Moreover, in a region of length L_x there is a need for at least a chevron every $\Delta x = d/(2\tan\theta_0)$. Thus, a chevron structure as the one illustrated in Fig. 5, left-hand side, has an energy cost

$$\Delta\mathcal{F}_{(\text{all})} = 16\sqrt{\frac{2}{15}\zeta(s_+)}\sqrt{Db_2}L_x\rho_0^3 q_0^3 \tan\theta_0 \sin^3\theta_0. \tag{38}$$

This energy is to be compared with the energy necessary to break the homeotropic anchoring at the boundary (see Fig. 5, right-hand side). If we assume for this latter the simple Rapini-Papoular form [61]

$$\Delta\mathcal{F}_{(\text{weak})}(\theta) = WL_x s_+^2 \sin^2\theta \tag{39}$$

we arrive at the result that the chevron structure is stable whenever

$$W \geqslant W_{\text{cr}} = 16\sqrt{\frac{2\zeta(s_+)}{15 s_+^2}}\sqrt{Db_2}\rho_0^3 q_0^3 \tan\theta_0 \sin\theta_0. \tag{40}$$

V. EDGE DISLOCATIONS IN SMECTIC-*A* PHASES

As a second example to illustrate the role of the second-gradient term σ_{reg} in the energy, we now analyze the onset of edge dislocations in smectic-A bookshelf geometry. We prescribe the intensity of the Burger's vector of the configuration, and we prove that the higher order energy term controls the number of edge dislocations that combine to construct a defect of the prescribed total charge. We estimate the radius of the dislocation cores as well.

Since the regularizing term consists of second derivatives of the complex wave function ψ, it will have the most influence in configurations where ψ, and in particular its phase function ω, exhibits discontinuities. In smectic liquid crystals this is the signature of a dislocation, and the magnitude of the jump discontinuity of ω is related to the local loss or gain of layers. More precisely, the quantity measuring the *strength* of the dislocation, from the point of view of how many layers are created or lost across the core, is the Burger's vector.

In a bookshelf geometry, edge dislocations may appear due to a mismatch between two different wave numbers, one (q) related to the thickness of the undistorted smectic bookshelf bulk, and the other $(q_s \neq q)$ imprinted on the boundary [45]. In general, any source of layer frustration (such as dust particles and defects) may cause dislocations in the material.

Let us now briefly recall the definition of Burger's vector of a dislocation [62]. Let $\mathcal{C}$ be a curve surrounding a dislocation core P. Then,

$$\int_{\mathcal{C}}\mathbf{n}\cdot d\mathbf{l} = B, \quad \text{with } B = Nd. \tag{41}$$

The quantity B is called the Burger's vector of the dislocation (though it is a scalar quantity). It is invariant with respect to the path $\mathcal{C}$ that surrounds the core (see, e.g., de Gennes and Prost [52], p. 488). Furthermore, $d = 2\pi/q$ denotes the layer thickness and the integer N represents the number of layers gained or lost across P, as surrounded by $\mathcal{C}$. Note that since we are considering a smectic-A liquid crystal, the director $\mathbf{n}$ coincides with the unit normal to the layers. In general, if the curve $\mathcal{C}$ encloses several dislocations P_i, then $B = d\Sigma_i N_i$, where N_i denotes the number of layers gained or lost when circling around P_i. Imposing the smectic-A constraint $\boldsymbol{\nabla}\omega = q\mathbf{n}$, it is useful to rewrite the line integral (41) as follows:

$$\int_{\mathcal{C}}\boldsymbol{\nabla}\omega\cdot dl = 2\pi N =: [\omega] = qB, \tag{42}$$

where $[\omega]$ represents the total jump in ω across the sample.

In order to enforce the bookshelf geometry, we consider a smectic-A liquid crystal occupying the plane strip,

$$\Omega = \{(x,z): 0 < z < L, \ -d_0 < x < d_0\}, \tag{43}$$

with $L > 0$ and $d_0 > 0$ prescribed. We let the layers be parallel to the z direction. Then, the fields

$$\mathbf{n} = \mathbf{e}_x = \frac{1}{q}\boldsymbol{\nabla}\omega, \quad \rho = \rho_0 \neq 0, \quad s = s_0 \neq 0 \tag{44}$$

with $q^2 = |b_1|/(2b_2)$, and b_1, b_2 as in (10), yield a homogeneous equilibrium state. We assume that an array of $N \geqslant 1$ edge dislocations of core radius $\epsilon > 0$ sits on the z axis, $x = 0$. We require that the total magnitude of the Burger's vector is the prescribed quantity B, and let $J = qB$. We point out that $\omega = \omega(x) = qx + \text{const}$ in the bulk, whereas $\omega = \omega(x,z)$ close to the dislocation cores. We further assume that $\mathbf{n}$ and $\boldsymbol{\nabla}\omega$ are parallel wherever they are defined.

We remark that the domain Ω is a cross section of a three-dimensional domain with dislocation lines along the y axis. The dislocation cores are thus assumed to be disks of radii $\epsilon > 0$ and centers P_i, with P_i corresponding to the intersections of the dislocation lines with the xz plane.

A. Energy estimates

We now compute the total energy (8) in Ω. We are interested in the case $\epsilon \ll L$, so that the uniform bulk state prevails away from small circles of radii ϵ. We assume that the region Ω has an array of $N \geqslant 1$ dislocations of radius $\epsilon > 0$ placed along the z axis, and derive an approximation to the total energy depending on N and ϵ. Finally, the energy minimization provides us an estimate of the optimal values of the number N and the core size ϵ. In particular, we show that the presence of the regularizing energy term implies $N > 1$, provided the choice of J is such that more than one dislocation may be formed.

Since the configurations that we deal with are planar, the expression that we derive has dimensions of energy per unit length (along the y direction). We will subsequently proceed to obtain a dimensionless energy expression. For the sake of clarity, we now list the main simplifying assumptions of our derivation.

(1) We assume that all dislocations have the same strength. In other words, if we let P denote the center of the dislocation core $\mathcal{D}$ located at $(0,z)$, we assume that

$$[\omega(0,z)] := |\omega(0,z+\epsilon) - \omega(0,z-\epsilon)| = \frac{J}{N}. \tag{45}$$

(2) We assume that both the nematic and the smectic degree of orders vanish within the dislocation cores. Thus, if s_d, ρ_d, respectively, denote the isotropic and smectic order parameters in $\mathcal{D}$, we assume that $|s_d| \ll s_0$ and $|\rho_d| \ll \rho_0$.

(3) We adopt the 1-constant approximation $K|\boldsymbol{\nabla}\mathbf{Q}|^2$ for the nematic elastic energy $\sigma_{\mathrm{el},n}$.

(4) According to hypothesis (2), we take $\mathbf{Q}=\mathbf{0}$ in σ_{reg}, since this latter term must be taken into account only within the dislocation core.

(5) The dominant terms close to the dislocations are σ_{reg} and $\sigma_{\mathrm{el,sm}}$, with

$$\left|\frac{\partial^2\omega}{\partial z^2}\right| = O\left(\frac{[\omega]}{\epsilon^2}\right) \quad \text{and} \quad \left|\frac{\partial\omega}{\partial z}\right| = O\left(\frac{[\omega]}{\epsilon}\right), \tag{46}$$

for small $\epsilon > 0$, where $[\omega]$ denotes a jump in ω across the core.

Since $b_1 < 0$ in the smectic phase and taking into account that $q^2 = |b_1|/(2b_2)$, it is possible to rewrite $\sigma_{\mathrm{el,sm}}$ as

$$\sigma_{\mathrm{el,sm}} = b_2(|\boldsymbol{\nabla}\psi|^2 - q^2)^2 + \text{constant} \tag{47}$$

and neglect the constant term.

Let us estimate separately each term of the total energy. Note that there are bulk terms, accounting for the energy away from the dislocation, and core terms that estimate the energy in a circle of radius $\epsilon \ll q^{-1}$ (see, e.g., [63] for a detailed discussion of the free energy of the nematic core):

$$\int_\Omega \sigma_{\mathrm{el},n} \approx -KN\ln(\epsilon q),$$

$$\int_\Omega \sigma_{\mathrm{LdG}} \approx N(as_0^2 - bs_0^3 + cs_0^4)\epsilon^2,$$

$$\int_\Omega \sigma_{\mathrm{el,sm}} \approx b_2 N\left(\frac{J^2}{N^2\epsilon^2} - q^2\right)^2 \epsilon^2,$$

$$\int_\Omega \sigma_{\mathrm{sm}} \approx N(\tilde{a}\rho_0^2 + \tilde{c}\rho_0^4)\epsilon^2,$$

$$\int_\Omega \sigma_{\mathrm{reg}} \approx DN\frac{J^2}{N^2\epsilon^4}\epsilon^2 = \frac{DJ^2}{N\epsilon^2},$$

$$\int_\Omega \sigma_{n,\mathrm{sm}}^{(1)} \approx -N\tilde{b}\rho_0^2 s_0^2 \epsilon^2. \tag{48}$$

We remark that $\sigma_{n,\mathrm{sm}}^{(2)}$ does not contribute to the energy since $f=0$, and the term multiplying the parameter e vanishes as well because of the smectic-A assumption, that is, $\boldsymbol{\nabla}\omega$ is taken to be an eigenvector of $\mathbf{Q}$.

The approximation of the total energy is given by

$$\mathcal{E}_{\mathrm{tot}}^0(\epsilon,N) = \frac{DJ^2}{N\epsilon^2} + b_2 N\left(\frac{J^2}{N^2\epsilon^2} - q^2\right)^2 \epsilon^2 - KN\ln(\epsilon q) + P_B N\epsilon^2, \tag{49}$$

where $P_B = (as_0^2 - bs_0^3 + cs_0^4) + (\tilde{a}\rho_0^2 + \tilde{c}\rho_0^4) - \tilde{b}\rho_0^2 s_0^2$ denotes the total bulk energy contribution away from the dislocation cores. Since

$$\dim(b_2) = \dim(D) = \dim(KL^2) = \text{force} \times (\text{length})^2, \tag{50}$$

the following list of parameters is dimensionless:

$$\delta = \epsilon^2 q^2, \quad \beta = q^2 L^2, \quad \nu = \frac{D\beta}{b_2},$$

$$K_0 = \frac{KL^2}{b_2}, \quad P = \frac{2P_B L^2}{q^2 b_2}. \tag{51}$$

The free energy in (49) has the dimensions of an energy per unit length. Thus, to obtain a dimensionless form of the energy, we multiply Eq. (49) by L^2/b_2 and define

$$\mathcal{E}_{\mathrm{tot}}(\delta,N) = \frac{L^2\mathcal{E}_{\mathrm{tot}}^0}{b_2} = \frac{\nu J^2}{\delta N} + N\beta\left(\frac{J^2}{N^2\delta} - 1\right)^2 \delta + PN\delta - K_0 N\ln\delta. \tag{52}$$

B. Number of defects

We now fix $N \geqslant 1$, and determine the critical points of $\mathcal{E}_{\mathrm{tot}}$ with respect to δ. The stationarity equation $\partial_\delta \mathcal{E}_{\mathrm{tot}} = 0$ requires

$$N^4(\beta + P)\delta^2 - K_0 N^4\delta - J^2(\beta J^2 + \nu N^2) = 0. \tag{53}$$

Equation (53) possesses a unique positive solution $\delta(N)$, whose asymptotic behavior in the presence of many dislocations is given by

$$\delta(N) = \frac{K_0}{\beta + P} + \frac{\nu J^2}{K_0 N^2} + O\left(\frac{1}{N^4}\right) \quad \text{as } N \to \infty. \tag{54}$$

The optimal radius tends to a constant, which does not depend on the number of defects. The corresponding asymptotic expression of the total energy is given by

$$\mathcal{E}_{\text{tot}}(\delta(N),N) = K_0\left(1 - \ln \frac{K_0}{\beta + P}\right)N + O(N^{-2}) \tag{55}$$

as $N \to \infty$. Thus, the free energy avoids an unbounded number of defects provided $K_0 < e(\beta + P)$. This inequality, which is satisfied for physically realistic data as we discuss below, expresses the dominance of smectic elasticity effects over the nematic counterparts.

In order to estimate how the optimal value of N depends on J and ν, we now fix a list of physically realistic parameter values. The ratio $\lambda = (K/b_2)^{1/2}$ is the *penetration length*. It is of the same order as the layer spacing and diverges near when the system approaches the nematic-smectic transition (see Kléman and Lavrentovich [64], p. 145). The list below includes experimental values which describe the smectic-A regime, away from the transition temperature to nematic. We take $L = 10^{-3}$ m. This corresponds to the case when the length of the sample is much greater than the interlayer spacing. We then fix the following quantities:

(i) interlayer spacing $d = 2\pi q^{-1} = 1-3$ nm,
(ii) nematic elastic constant $K = 10^{-11}$ N,
(iii) smectic elastic constant $b_2 = 10^6 - 10^7$ N m^{-2},
(iv) penetration length $\lambda = 10^8 - 10^9$ m $\approx q^{-1}$.

These give the following values for the dimensionless parameter groups of the model: $\beta = q^2 L^2 \approx 10^{12}$, $K_0 = KL^2/b_2 \approx 10^{-23}$.

Since K_0 is much smaller than all the other dimensionless groups entering the free energy, we may treat it as a perturbative parameter. We define the optimal number of defects N_{opt} as the number such that

$$\left.\frac{\partial \mathcal{E}_{\text{tot}}(\delta(N),N)}{\partial N}\right|_{N=N_{\text{opt}}} = 0. \tag{56}$$

A perturbative expansion of Eq. (56) allows to prove that

$$N_{\text{opt}} = J\sqrt{\frac{P}{\nu}} + O(K_0) \quad \text{as } K_0 \to 0. \tag{57}$$

Equation (57) shows that the number of edge dislocations is proportional to the total magnitude J of the Burger's vector. Moreover, it is kept bounded by the presence of the regularizing term ν. Finally, the number of defects increases when the bulk elastic terms (represented by P) are enhanced. Indeed, it is a well-known fact that the bulk elasticity does always promote the creation of a higher number of defects, each of the lower allowed charge. We remark, however, that if the number of defects becomes too large, the smectic order itself melts and only the nematic order survives [62]. Our approximations do not allow to investigate this latter effect, since in the energy estimates (48) we have assumed that smectic ordering is perfect away from the defect cores. This assumption should be relaxed in order to determine how the bulk smectic order parameter decreases when the number of defects increases. If we finally replace the optimal number of defects (57) in Eq. (54) we derive how the dislocation core radius scales with the magnitude of the regularizing term

$$\delta_{\text{opt}} = \frac{\nu}{P} + O(K_0) \quad \text{as } K_0 \to 0. \tag{58}$$

In view of the above considerations about the possible smectic melting, the estimates (57) and (58) shall be trusted only as long as N_{opt} is not too large or, alternatively, as long as δ_{opt} is much smaller than the average defect distance.

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