Covariant elasticity and dislocations in smectic-C liquid crystals

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We derive a rotationally invariant form for the elastic energy of a smectic-C liquid crystal. The magnitude of the **c** director, but not its direction, can screen layer strain just as two independent components of the director screen strain in smectic-A liquid crystals. Type I and type II smectic-C liquid crystals can be classified according to whether the **c**-director penetration depth λ_c is less than or greater than the smectic coherence length ξ. We calculate the energies of isolated dislocations and the interaction energies of parallel dislocations as a function of direction. We find an attractive interaction at large distances between like-sign screw dislocations and a repulsive interaction at short distances, leading to a minimum energy separation.

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I. INTRODUCTION

Smectic liquid crystals are layered structures. Their energy is invariant with respect to simultaneous rigid uniform rotations of both the layers and molecular orientation specified by the Frank director **n**. In the de Gennes free energy [1] for the smectic-A phase, covariant derivatives enforce this invariance. This free energy establishes an analogy between the nematic–to–smectic-A transition in liquid crystal and the normal-to-superconducting transition in metals and a one-to-one correspondence between many properties of superconductors and smectic-A liquid crystals. In particular, it classifies smectic-A liquid crystals as type I or type II depending on whether their twist (or bend) penetration depth λ is less than or greater than their coherence length ξ, and it leads to the prediction [2] of the existence of the twist-grain-boundary (TGB) phase [3] as the analog of the Abrikosov vortex phase [4]. The two independent components of the Frank director screen elastic layer distortions in liquid crystals just as the vector potential screens phase distortions in superconductors. In type I systems, the director relaxes quickly to an equilibrium value determined by layer strains, and the Landau-Peierls elastic energy [5,6] expressed in terms of layer strain alone provides an adequate description of elastic properties, including energies of dislocations. In type II systems, the full covariant energy is needed for a complete description of elastic distortions, particularly those associated with dislocations [7].

Smectic-C liquid crystals are also layered structures, but the Frank director, rather than pointing normal to the layers, has a nonvanishing component, called the **c** director, in the plane of the layers. The energies of smectic-C liquid crystals, like that of smectic-A liquid crystals must be invariant under simultaneous rotation of layers and director. It should, therefore, be a function of covariant derivatives enforcing rotational invariance. Though the type I elasticity of smectic-C liquid crystals has been extensively discussed [8,6,9], a covariant elastic theory for smectic-C liquid crystals has not, to our knowledge, been introduced. However, rotationally invariant free energies [10,11] to describe the smectic-A–to–smectic-C and the nematic–to–smectic-C transition have been introduced. In this paper, we will derive the covariant elastic energy for a smectic-C liquid crystal and use it to calculate energies of isolated and interacting dislocations. This energy shows that the magnitude, but not the direction, of the **c** director can relax to relieve layer strain. From this we can define a **c**-director penetration depth λ_c and distinguish type I and type II smectics according to whether λ_c/ξ is less than or greater than unity. An appealing feature of the simplified free energy we use to calculate dislocation energies is that the conventional singular strain [proportional to $\tan^{-1}(x_1/x_2)$, where x_1 and x_2 are orthogonal coordinates] associated with a dislocation uniquely determines the total strain and director distortion and thus the dislocations energies. This is in contrast to type I elastic theories [9] for which there can be two distinct dislocation solutions and no obvious criterion other than energetics to specify which solution is the correct solution.

The most important results of this paper are summarized in Figs. 1 and 2. Figure 1 shows the energy per unit length of a linear dislocation in the plane defined by the layer normal (z direction) and the **c** director (x direction) as a function of angle γ of the core relative to the z axis. A pure screw dislocation ($\gamma = 0$) has the lowest energy, but the energy does not increase rapidly with γ. Figure 2 show the interaction energy between two parallel like-sign dislocations whose cores lie in planes, separated by a distance y, parallel to the xz plane and make an angle $\pi/10$ with respect to the z axis. At distances y much greater than λ_c, the interaction is *attractive*, falling off as $-1/y^2$. At distances of order λ_c the interaction becomes repulsive, and there is a negative minimum energy at a distance somewhat larger that λ_c. The magnitude of the energy minimum is greater that the energy increase in core energy produced by aligning cores along $\gamma = \pi/10$ rather than $\gamma = 0$. As we shall see in the companion article, this fact plays an important role in stabilizing the experimentally observed TGB_C phase [12–14].

This paper is divided into five sections, of which this is the first. Section II presents a general derivation of

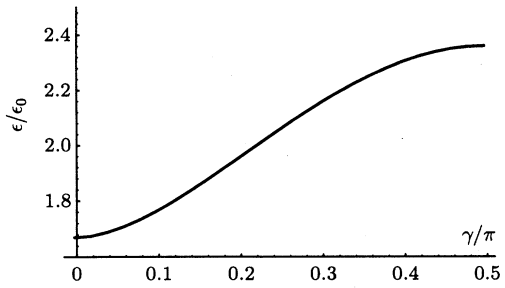

FIG. 1. The energy per unit length [measured in units of $\epsilon_0 = Dd^2/(8\pi)$] of a dislocation as a function of angle γ its core makes with the z axis. The tilt angle A_0 [Fig. (3)] is $\pi/10$, the parameter β [Eq. (4.6)] is equal to 3, and $\lambda_c/\xi = 10$.

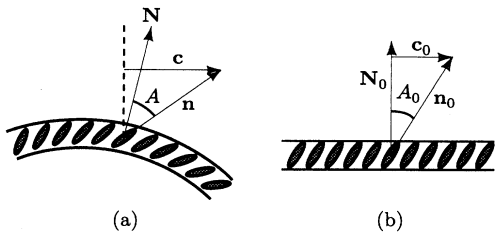

FIG. 3. (a) Schematic representation of the layer normal vector $\mathbf{N}$, the Frank director $\mathbf{n}$, and the $\mathbf{c}$ director for an arbitrary layer distortion. (b) The equilibrium vectors $\mathbf{N}_0$, $\mathbf{n}_0$, and $\mathbf{c}_0$ in the smectic-C phase.

covariant elastic energies valid for both smectic-A and smectic-C liquid crystals and discusses both type I and type II smectic-C elasticity. Section III derives general expressions for the energies of dislocations for type II systems. The energies of dislocations in type I systems can be obtained as a limit from the results for type II systems. Section IV calculates the energies of individual dislocations as a function of the angle the core makes with the layer normal and the $\mathbf{c}$ director. Section V calculates the interaction energies between parallel dislocations as a function of distance and angle. Finally, the Appendix discusses the origin of the differences between our results and those of Ref. [9].

II. COVARIANT ELASTICITY

Smectic liquid crystals are layered structures with a mass density that is periodic in one direction and translationally invariant in the other two orthogonal directions. They are characterized by an equilibrium layer spacing d and a complex mass-density-wave amplitude $\psi = |\psi|e^{-iq_0u}$, where $q_0 = 2\pi/d$ and u is the layer displacement variable. In addition, there are two distinct directions in smectics: the layer normal specified by the unit vector $\mathbf{N}$ and the direction of average molecular alignment specified by the Frank director $\mathbf{n}$, as shown in Fig. 3. We will denote the angle between $\mathbf{n}$ and $\mathbf{N}$ by A so that $\mathbf{n}\cdot\mathbf{N} = \cos A$. Deep in the smectic phase, one can regard the magnitude $|\psi|$ of the mass-density wave as fixed because its deviations from local equilibrium are energetically costly. Variations δd in the layer spacing, which we can parametrize by a wave number $q_s = q_0 + \delta q = 2\pi/(d+\delta d)$, and in $\mathbf{n}$ and $\mathbf{N}$ can lead to low-energy distortions. In this section, we will present a general derivation of the covariant elastic energy for both smectic-A and smectic-C phases. Though this derivation for the smectic-A phase is not really new, it is enlightening. The free energy we obtain for a smectic-C liquid crystal has not, to our knowledge, appeared before.

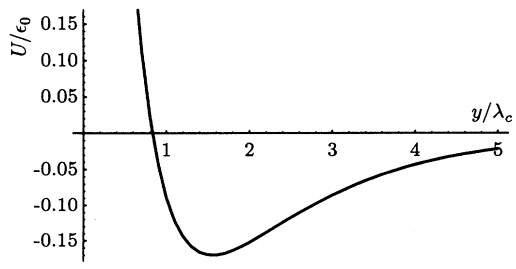

FIG. 2. The interaction energy per unit length (in units of ϵ_0) as a function of separation for two parallel dislocations whose cores lie in planes, separated by a distance y, parallel to the xz plane and make an angle $\gamma = \pi/10$ with the z axis. This calculation was done with $A_0 = \pi/10$ and $\beta = 3$.

A. Definition of variables

In smectic-A liquid crystals, the equilibrium director $\mathbf{n}_0$ is spatially uniform and parallel to the layer normal $\mathbf{N}_0$ so that $\mathbf{n}_0\cdot\mathbf{N}_0 = 1$. We will take $\mathbf{N}_0 = \mathbf{e}_z$ to be along the z axis. In smectic-C liquid crystals, $\mathbf{n}_0$ tilts relative to $\mathbf{N}_0$, and $\mathbf{n}_0\cdot\mathbf{N}_0 = \cos A_0$, where A_0 is the equilibrium tilt angle [Fig. 3(b)]. Equilibrium tilt order is characterized by the equilibrium $\mathbf{c}$ director $\mathbf{c}_0$, with $\mathbf{c}_0\cdot\mathbf{N}_0 = 0$ and

$$c_0 = \sin A_0 \tag{2.1}$$

such that

$$\mathbf{n}_0 = \mathbf{c}_0 + \cos A_0\mathbf{N}_0. \tag{2.2}$$

Distortions of $\mathbf{N}$ from equilibrium can be parametrized in terms of $\boldsymbol{\nabla}u$:

$$\begin{aligned}\mathbf{N} &= \frac{(-\boldsymbol{\nabla}_\perp u, 1-\partial_z u)}{[(1-\partial_z u)^2 + (\boldsymbol{\nabla}_\perp u)^2]^{1/2}} \\ &\approx (\boldsymbol{\nabla}_\perp u, 1 - \tfrac{1}{2}(\boldsymbol{\nabla}_\perp u)^2) \\ &= \mathbf{N}_0 + \delta\mathbf{N}\ .\end{aligned} \tag{2.3}$$

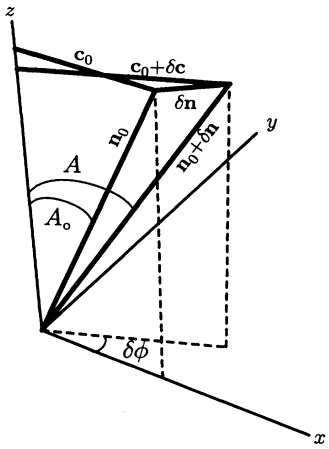

FIG. 4. This figure shows the vectors $\mathbf{n}_0$, $\mathbf{n}_0+\delta\mathbf{n}_0$, $\mathbf{c}_0$, and $\mathbf{c}=\mathbf{c}_0+\delta\mathbf{c}$.

In the smectic-A phase, distortions of $\mathbf{n}$ can be parametrized by $\delta\mathbf{n}$, the component of $\mathbf{n}$ in the xy plane:

$$\mathbf{n}=(\delta\mathbf{n},\sqrt{1-(\delta n)^2})\approx(\delta\mathbf{n},1-\tfrac{1}{2}(\delta n)^2)\ . \tag{2.4}$$

In the smectic-C phase, $\mathbf{n}$ can be parametrized as

$$\mathbf{n}=(\mathbf{c},\sqrt{1-c^2}), \tag{2.5}$$

where

$$\mathbf{c}=(c_0+\delta c)(\cos\phi,\sin\phi,0) \tag{2.6}$$

is the $\mathbf{c}$ director (see Fig. 4). The linear deviations of $\mathbf{c}$ from $\mathbf{c}_0=c_0(1,0,0)$ is

$$\delta\mathbf{c}=\delta c\mathbf{e}_x+c_0\delta\phi\mathbf{e}_y=(\delta c,c_0\delta\phi,0), \tag{2.7}$$

and

$$\delta\mathbf{n}=(\delta c,c_0\delta\phi,-\cos A_0c_0\delta c). \tag{2.8}$$

Thus deviations in $\mathbf{n}$ from equilibrium are specified by changes δc in the magnitude of the $\mathbf{c}$ director (i.e., in the projection of $\mathbf{n}$ onto the plane perpendicular to $\mathbf{N}_0$) and by changes $\delta\phi$ in the direction of the $\mathbf{c}$ director relative to the x axis (the direction of equilibrium order).

B. Rotationally invariant free energy

The free energy density f of both smectic phases must be invariant with respect to simultaneous spatially uniform rotations of $\mathbf{n}$ and $\mathbf{N}$ but not of $\mathbf{n}$ and $\mathbf{N}$ separately. It, therefore, can only be a function of

$$\mathbf{n}\cdot\mathbf{N}=\cos A, \tag{2.9}$$

gradients of $\mathbf{n}$, the inverse layer spacing q_s, and rotationally invariant gradients of u. In addition, f must reduce to the Frank free energy density of a nematic,

$$f_n=\tfrac{1}{2}K_1(\nabla\cdot\mathbf{n})^2+\tfrac{1}{2}K_2[\mathbf{n}\cdot(\nabla\times\mathbf{n})]^2+\tfrac{1}{2}K_3[\mathbf{n}\times(\nabla\times\mathbf{n})]^2 \tag{2.10}$$

when smectic order vanishes. Thus we can write

$$f=f_n+f_{\rm sm}(\mathbf{n}\cdot\mathbf{N},q_s)+f_u. \tag{2.11}$$

The energy f_u measures energy of layer bending *not* associated with director splay. We will consider it in more detail shortly. The equilibrium smectic wave number $q_0(\cos A)$ as a function of $\cos A$ is determined by minimizing $f_{\rm sm}(\cos A,q_s)$ with respect to q_s. For q_s near $q_0(\cos A)$, $F_{\rm sm}$ can be expanded to second order in $\delta q=q_s-q_0(\cos A)$:

$$f_{\rm sm}(\cos A)=f_s(\cos A)+\tfrac{1}{2}\tilde{B}[q_s-q_0(\cos A)]^2, \tag{2.12}$$

where $f_s(\cos A)=f_{\rm sm}(\cos A,q_0(\cos A))$. The final equilibrium value of the tilt angle A (or equivalently the magnitude of the $\mathbf{c}$ director) is obtained by minimizing $f_{\rm sm}(\cos A)$ over A. To carry out this procedure, it is useful, but not essential, to introduce an explicit phenomenological form for f_s that has both smectic-A ($A_0=0$) and smectic-C ($A_0\neq0$) minima:

$$f_s(\mathbf{n}\cdot\mathbf{N})=\tfrac{1}{2}\tilde{D}(\mathbf{n}\cdot\mathbf{N})^2+\tfrac{1}{4}E(\mathbf{n}\cdot\mathbf{N})^4. \tag{2.13}$$

The second term in Eq. (2.12) does not contribute to the determination of A because $q_s-q_0(\cos A_0)=0$ in equilibrium with $A=A_0$. Therefore minimization of $f_{\rm sm}$ over A produces

$$\frac{\partial f_s}{\partial A}=-f_s'\sin A=0, \tag{2.14}$$

where $f_s'=df_s/d(\cos A)$. This equation has solutions $A_0=0$ (smectic A) and $f_s'=0$ (smectic C). If f_s is given by Eq. (2.13), then $A_0=0$ for $\tilde{D}>E$ or $\tilde{D}<0$ and $\cos^2A_0=\tilde{D}/E$ for $0<\tilde{D}<E$. Thus

$$f_s=f_s^0+\frac{1}{2}\frac{\partial^2f_s}{\partial A^2}(\delta A)^2 \tag{2.15}$$

to second order in deviations $\delta A=A-A_0$ of A from equilibrium where

$$\frac{\partial^2f_s}{\partial A^2}=\begin{cases}-f_s'(0) & \text{(smectic } A)\\ f_s''(\cos A_0)\sin^2A_0 & \text{(smectic } C),\end{cases} \tag{2.16}$$

and f_s^0 is the equilibrium value of f_s.

The equilibrium smectic wave number is $q_0=q_0(\cos A_0)$. As usual we can express $\delta q=q_s-q_0$ as $q_0\partial_zu$ and

$$f_{\rm sm}=f_s^0+\frac{1}{2}\frac{\partial^2f}{\partial A^2}(\delta A)^2+\frac{1}{2}B(\partial_zu)^2-L\partial_zu\delta A, \tag{2.17}$$

where $B=\tilde{B}(\cos A_0)q_0^2$ and $L=q_0(\partial q_0/\partial A)\tilde{B}$.

We now return to f_u. The energy associated with layer

compression has been included in $F_{\rm sm}$ via the last term in Eq. (2.12) arising from $(\delta q)^2$. There is an energy cost associated with layer bending independent of director splay. In the smectic-A phase, it is simply

$$f_u^A = \tfrac{1}{2}K_u(\nabla_\perp^2 u)^2. \tag{2.18}$$

The constant K_u has the same units (force) as the Frank elastic constant in f_n. It exists, however, only in the smectic phase and tends to zero with $|\psi|$. Thus, in most materials, $K_u \ll K_1$, and K_u is generally ignored in the smectic-A phase. In the smectic-C phase, f_u can be anisotropic:

$$f_u^C = \tfrac{1}{2}K_u^x(\partial_x u)^2 + \tfrac{1}{2}K_u^y(\partial_y u)^2 + K_u^{xy}(\partial_x\partial_y u)^2. \tag{2.19}$$

The last term in this expression could also be expressed as $K_u^{xy}\partial_x^2 u\partial_y^2 u$ with the addition of a Gaussian curvature term $\frac{1}{2}K_u^{xy}\epsilon_{ik}\epsilon_{jl}\partial_i(\partial_j u\partial_k\partial_l u)$, which integrates to the surface. In what follows, we will find that f_u cannot be ignored in the smectic-C phase. We will, however, ignore its anisotropy and use the smectic-A form [Eq. (2.18)]. This, as we shall see, will allow us to employ standard procedures to calculate dislocation energies that do not require us to keep track of what happens at interior surfaces (i.e., at the surface of dislocation cores).

C. The smectic-A elastic energy

To obtain a final expression for covariant elastic energies, we need to express $\delta\mathbf{N}$ in terms of the variables parametrizing δA and $\delta\mathbf{n}$ [Eqs. (2.3) and (2.8)]. In the smectic-A phase, $A_0 = 0$, and

$$\cos\delta A = \mathbf{n}\cdot\mathbf{N} = 1 - \tfrac{1}{2}(\boldsymbol{\nabla}_\perp u + \delta\mathbf{n})^2 \approx 1 - \tfrac{1}{2}(\delta A)^2, \tag{2.20}$$

or

$$(\delta A)^2 = (\boldsymbol{\nabla}_\perp u + \delta\mathbf{n})^2. \tag{2.21}$$

Thus

$$f_{\rm sm}^A = \tfrac{1}{2}B(\partial_z u)^2 + \tfrac{1}{2}D(\boldsymbol{\nabla}_\perp u + \delta\mathbf{n})^2 + \tfrac{1}{2}K_u(\nabla_\perp^2 u)^2 + f_n(\mathbf{n}), \tag{2.22}$$

where $D = -f_s'(0)$. There is no $\delta A\partial_z u$ cross term because $\partial q_0/\partial A = -(\partial q_0/\partial\cos A)\sin A = 0$. This is the familiar covariant low-temperature form of the de Gennes free energy [1,7]. It shows that the two independent components (δn_x and δn_y) of the director relax locally to screen layer distortions and thereby minimize $(\boldsymbol{\nabla}_\perp u + \delta\mathbf{n})^2$. Penetration depths λ_2 and λ_3 for twist and bend can be obtained from Eq. (2.22) by comparing the coefficients of $[\mathbf{n}\cdot(\boldsymbol{\nabla}\times\mathbf{n})]^2$ and $[\mathbf{n}\times(\boldsymbol{\nabla}\times\mathbf{n})]^2$ with $(\delta\mathbf{n})^2$:

$$\lambda_2 = (K_2/D)^{1/2}, \qquad \lambda_3 = (K_3/D)^{1/2}. \tag{2.23}$$

In type II smectic-A liquid crystals, these penetration depths are larger than the smectic coherence length ξ, whereas in type I systems they are smaller than ξ.

The usual smectic elastic energy expressed as a function of u only is obtained by minimizing $f_{\rm sm}^A$ over $\delta\mathbf{n}$. To lowest order, $\delta\mathbf{n} = -\boldsymbol{\nabla}_\perp u$, and

$$f_{\rm el}^A = \tfrac{1}{2}B(\partial_z u)^2 + \tfrac{1}{2}(K_1 + K_u)(\nabla_\perp^2 u)^2. \tag{2.24}$$

If $K_u \ll K_1$, then $K_1 + K_u$ can be replaced by K_1. In this case, all layer bending energy is produced by director splay. Equation (2.24) can be used to obtain dislocation energies in type I smectics [15,16] where the core energy comes predominantly from the destruction of smectic order. In type II smectics, $\delta\mathbf{n}$ differs from $-\boldsymbol{\nabla}_\perp u$ in a region of radius $\lambda_{2,3} > \xi$ from the core and Eq. (2.22) should be used.

D. Type II smectic-C elastic energy

In the smectic-C phase,

$$\begin{aligned}\delta(\mathbf{n}\cdot\mathbf{N}) &= -\sin A_0\,\delta A = \mathbf{n}_0\cdot\delta\mathbf{N} + \delta\mathbf{n}\cdot\mathbf{N}_0 \\ &= -\tan A_0\,\delta c - \mathbf{c}_0\cdot\boldsymbol{\nabla}u\end{aligned} \tag{2.25}$$

so that $\delta A = (\delta c/\cos A_0) + \partial_x u$. Using this expression and Eq. (2.8) for $\delta\mathbf{n}$ in f with $K_2 = K_3$, we obtain

$$\begin{aligned}f = {}& \tfrac{1}{2}D(\delta c + \alpha\partial_x u)^2 + \tfrac{1}{2}(\partial_z u)^2 - \tilde{L}\partial_z u(\delta c + \alpha\partial_x u) \\ & + \tfrac{1}{2}c_0^2 K_1\left[\partial_y\delta\phi + \left(\partial_x - \alpha^{-1}\partial_z\right)\delta c\right]^2 + \tfrac{1}{2}K_u(\nabla_\perp^2 u)^2 \\ & + \tfrac{1}{2}c_0^2 K_2\left[(\mathbf{e}_y\times\boldsymbol{\nabla})\delta\phi + \left\{\left(\mathbf{e}_x - \alpha^{-1}\mathbf{e}_z\right)\times\boldsymbol{\nabla}\right\}\delta c\right]^2,\end{aligned} \tag{2.26}$$

where $\tilde{L} = L/\cos A_0$, $D = f_s''\tan^2 A_0$ [$= 2E\sin^2 A_0$ for Eq. (2.13)] and where we introduced

$$\alpha = \cos A_0 = \sqrt{1 - c_0^2}. \tag{2.27}$$

This free energy shows that the director can screen layer distortions, but only in one direction rather than two as in the smectic-A phase. The magnitude of the $\mathbf{c}$ director can adjust to minimize $\frac{1}{2}(\delta c + \alpha\partial_x u)^2 - \tilde{L}\partial_z u(\delta c + \alpha\partial_x u)$. In what follows, we will use a simplified form of Eq. (2.26) in which we set $K_1 = K_2 = K$ and $\tilde{L} = 0$. Setting $K_1 = K_2$ decouples $\delta\phi$ and δc, and setting $\tilde{L} = 0$ decouples $\partial_z u$ and $(\delta c + \alpha\partial_x u)$. We will also replace $K_u(\nabla_\perp^2 u)^2$ by $K_u(\nabla^2 u)^2$. We do not expect these simplifications to lead to any qualitative modifications of our results for dislocations in smectic-C liquid crystals. Our free energy is thus

$$\begin{aligned}f = {}& \tfrac{1}{2}D(\delta c + \alpha\partial_x u)^2 + \tfrac{1}{2}B(\partial_x u)^2 \\ & + \tfrac{1}{2}K_c(\boldsymbol{\nabla}\delta c)^2 + \tfrac{1}{2}K_\phi(\boldsymbol{\nabla}\phi)^2 + \tfrac{1}{2}K_u(\nabla^2 u)^2,\end{aligned} \tag{2.28}$$

where $K_c = c_0^2 K(1 + \cos^2 A_0)/\cos^2 A_0$ and $K_\phi = c_0^2 K$. The penetration depth λ_c for relaxation of the magnitude of the $\mathbf{c}$ director is

$$\lambda_c = (K_c/D)^{1/2}. \tag{2.29}$$

As in smectic-A liquid crystals, one can distinguish type I and type II systems: in type II smectic-C liquid crystals,

$\lambda_c > \xi$ whereas in type I smectic-C liquid crystals, $\lambda_c < \xi$. In type II systems, there is a substantial contribution to dislocation energies arising from deviations of δc from $\cos A_0 \partial_x u$ in a region with λ_c of the core.

E. Type I smectic-C elasticity

In type I systems, $\delta c \approx \cos A_0 \partial_x u$ everywhere except in the core region of radius $\xi < \lambda_c$ where ψ itself is zero. The relaxed elastic energy for type I systems is then

$$f_u^C = \tfrac{1}{2} B(\partial_z u)^2 + \tfrac{1}{2}\alpha^2 K_c[\nabla(\partial_x u)]^2 + \tfrac{1}{2} K_u(\nabla^2 u)^2. \tag{2.30}$$

Here we have written $\nabla(\partial_x u)$ rather than $\nabla \partial_x u$ to emphasize that when there are dislocations present and $\nabla \times (\nabla u) \neq 0$, interchanging ∇ and ∂_x is not permitted. We will return to this point in Sec. IV. Note that when $K_c \to 0$, we regain the elastic energy of a type I smectic-A liquid crystal. This will be a useful limit for checking calculations to follow. If we assume there are no dislocations, we can write Eq. (2.30) as

$$\begin{aligned} f_u^C = {} & \tfrac{1}{2} B(\partial_z u)^2 + \tfrac{1}{2} K_x(\partial_x^2 u)^2 + \tfrac{1}{2} K_y(\partial_y^2 u)^2 \\ & + K_{xy}(\partial_x \partial_y u)^2 + K_u(\partial_x^2 u)(\partial_y^2 u) + \tfrac{1}{2} K_\phi(\nabla\phi)^2, \end{aligned} \tag{2.31}$$

where we ignored terms in $(\partial_z^2 u)^2$ and where

$$\begin{aligned} K_x &= \alpha^2 K_c + K_u, \; K_y = K_u, \\ K_{xy} &= \tfrac{1}{2}\alpha^2 K_c + K_u. \end{aligned} \tag{2.32}$$

Normally, we are interested in bulk properties in systems in which $\partial_i \partial_j u$ has no spatially uniform part. In this case, the terms in $(\partial_x \partial_y u)^2$ and $\partial_x^2 u \partial_y^2 u$ can be combined via integration by parts, or equivalently by the introduction of a Gaussian curvature term that integrates to the surface. Thus, we can write the free energy in terms an integral over Fourier modes as

$$\begin{aligned} F_u^C = {} & \frac{1}{2}\int \frac{d^2q}{(2\pi)^3}[B q_z^2 + K_x q_x^4 \\ & + 2K_{xy} q_x^2 q_y^2 + K_y q_y^4]|u(\mathbf{q})|^2. \end{aligned} \tag{2.33}$$

Both Eqs. (2.31) and (2.33) must be positive definite for thermodynamic stability. The quantities $\partial_x^2 u$, $\partial_y^2 u$, and $\partial_x \partial_y u$ are all independent. Thus K_x, K_y, and $K_{xy} - K_u = \frac{1}{2}\alpha^2 K_c$, and the determinant $K_x K_y - K_u^2$ must be positive. The determinant $K_x K_y - K_u^2 = \alpha^2 K_c K_u$ is positive provided K_c and K_u are positive, as they must be. The finite wave-number free energy of Eq. (2.33) is positive provided B, K_x, K_y, and K_{xy} are positive. There is no requirement that the determinant $K_x K_y = K_{xy}^2$ be positive because q_x^2 and q_y^2 are positive. In fact, in the present case, $K_x K_y - K_{xy}^2 = -\frac{1}{4}\alpha^2 K_c$ is negative. References [8] and [9] erroneously imposed the constraint $K_x K_y - K_{xy}^2 > 0$. We will discuss the consequences of this assumption in the Appendix.

Note that the $(\nabla^2 u)^2$ terms in this free energy are anisotropic even though we assumed that the part $K_u(\nabla_\perp^2 u)^2$ arising from layer bending was isotropic. Note also that the coefficient of $(\partial_y^2 u)^2$ is K_u whereas the other two terms in $(\nabla_\perp^2 u)^2$ have coefficients including $\alpha^2 K_c$. As we have already discussed, $K_u \ll K_c$. This implies that the bending of layers in the yz plane cost much less energy than bending them in the xz plane because the latter involves director bend and splay whereas the former does not. See Fig. 5.

FIG. 5. Schematic representation of layer bend (a) in the yz plane and (b) in the xz plane. Bend in the xz plane involves both director bend and splay and cost more energy than bend in the yz plane, which does not.

III. DISLOCATIONS: FORMAL DEVELOPMENT

Dislocations are topological line defects with a one-dimensional core along which the smectic order parameter ψ goes to zero. The line integral around a closed loop Γ enclosing a single dislocation core is $kd = b$, where k is the integer-valued strength of the dislocation:

$$\oint_\Gamma du = \int_\Gamma \nabla u \cdot d\mathbf{l} = \int_S \nabla \times (\nabla u) \cdot d\mathbf{S} = kd, \tag{3.1}$$

where S is any covering surface of Γ. Thus dislocations give rise to singular contributions to ∇u with a nonvanishing curl, and u can be divided into an analytic part $u^{(a)}$ and a singular part $u^{(s)}$: $u = u^{(a)} + u^{(s)}$. Then, defining $\mathbf{v} = \nabla u^{(s)}$, we have

$$\nabla u = \nabla u^{(a)} + \mathbf{v}, \tag{3.2}$$

with

$$\nabla \times \mathbf{v} = \mathbf{b}(\mathbf{x}), \tag{3.3}$$

where

$$\mathbf{b}(\mathbf{x}) = \sum_\mu k_\mu d \int ds \delta(\mathbf{x} - \mathbf{R}_\mu(s)) \tag{3.4}$$

is the dislocation density, where $\mathbf{R}_\mu(s)$ is the position of dislocation μ with strength k_μ as a function of its arc-length s. We can always choose $\mathbf{v}$ to be divergenceless. In this case $\mathbf{v}(\mathbf{x})$ or equivalently its Fourier transform,

$$\mathbf{v}(\mathbf{q}) = i\frac{\mathbf{q} \times \mathbf{b}(\mathbf{q})}{q^2}, \tag{3.5}$$

is uniquely determined by $\mathbf{b}$.

A. Type II systems

The elastic energy [Eq. (2.28)] depends on the total displacement field u and can be written as

$$f_u = \tfrac{1}{2}B(\partial_z u^{(a)} + v_z)^2 + \tfrac{1}{2}D[\delta c + \alpha(\partial_x u^{(a)} + v_x)]^2 + \tfrac{1}{2}K_u(\nabla^2 u^{(a)})^2 + \tfrac{1}{2}K_c(\boldsymbol{\nabla}\delta c)^2. \quad (3.6)$$

Note that this energy is a unique and well-defined function of $\mathbf{v}$ because it can be written as an unambiguous function of $\boldsymbol{\nabla}u$. This would not be the case had we allowed K_u to be anisotropic with an energy proportional to $(\partial_x\partial_y u)^2$. Note also that $\mathbf{v}$ does not appear in the K_u terms because we chose it to be proportional to $(\nabla^2 u)^2$ rather than $(\nabla_\perp u)^2$. This will simplify future analysis.

Using Eqs. (3.5) and (3.6), we can find u and δc for any given dislocation density $\mathbf{b}(\mathbf{x})$. We merely minimize the free energy derived from f_u over u and δc for a given $\mathbf{v}$ determined by $\mathbf{b}$. To carry out this procedure, it is convenient to recast f in a more compact form. Let $\phi_1 = u^{(a)}$ and $\phi_2 = \delta c$. Then

$$F = \tfrac{1}{2}\int d^2x[\phi_a(\mathbf{x})G^{-1}_{ab}(\boldsymbol{\nabla})\phi_b(\mathbf{x}) + 2\lambda_a(\mathbf{x})\phi_a(\mathbf{x}) + Bv_z^2(\mathbf{x}) + \alpha^2 Dv_x^2(\mathbf{x})], \quad (3.7)$$

where

$$G^{-1}(\nabla) = \begin{pmatrix} -B\nabla_z^2 - \alpha^2 D\nabla_x^2 + K_u\nabla^4 & -\alpha D\nabla_x \\ \alpha D\nabla_x & D - K_c\nabla^2 \end{pmatrix}, \quad (3.8)$$

and

$$\lambda_1(\mathbf{x}) = B\nabla_z v_z + \alpha^2 D\nabla_x v_x, \quad (3.9)$$

$$\lambda_2(\mathbf{x}) = \alpha D v_x. \quad (3.10)$$

Minimization over ϕ_a leads to the Fourier-space expression

$$\phi_a(\mathbf{q}) = -G_{ab}(\mathbf{q})\lambda_b(\mathbf{q}) \quad (3.11)$$

so that F can be expressed as a function of $\mathbf{v}$ alone. The result is

$$F = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}[-\lambda_a(-\mathbf{q})G_{ab}(\mathbf{q})\lambda_b(\mathbf{q}) + B|v_z(\mathbf{q})|^2 + \alpha^2 D|v_x(\mathbf{q})|^2], \quad (3.12)$$

where

$$\lambda_1(\mathbf{q}) = -iBq_z v_z(\mathbf{q}) - i\alpha^2 Dq_x v_x(\mathbf{q}),$$
$$\lambda_2(\mathbf{q}) = \alpha D v_x(\mathbf{q}), \quad (3.13)$$

and

$$G_{ab}(\mathbf{q}) = \frac{1}{\Delta(\mathbf{q})}\begin{pmatrix} D(\mathbf{q}) & i\alpha Dq_x \\ -i\alpha Dq_x & B(\mathbf{q}) \end{pmatrix} \quad (3.14)$$

with

$$D(\mathbf{q}) = D + K_c q^2, \quad (3.15)$$
$$B(\mathbf{q}) = Bq_z^2 + \alpha^2 Dq_x^2 + K_u q^4, \quad (3.16)$$
$$\Delta(\mathbf{q}) = B(\mathbf{q})D(\mathbf{q}) - \alpha^2 D^2 q_x^2. \quad (3.17)$$

Finally, expressing $\mathbf{v}$ in terms of $\mathbf{b}$ via Eq. (3.5), we obtain

$$F = \frac{1}{2}\int \frac{d^3q}{(2\pi)^2} b_i^*(\mathbf{q})U_{ij}(\mathbf{q})b_j(\mathbf{q}), \quad (3.18)$$

where

$$U_{ij}(\mathbf{q}) = \frac{1}{q^2\Delta(\mathbf{q})}\tilde{U}_{ij}(\mathbf{q}), \quad (3.19)$$

with

$$\tilde{U}_{xx}(\mathbf{q}) = B[\alpha^2 DK_c q_x^2 + DK_u q^2 + K_u K_c q^4]q_y^2, \quad (3.20)$$
$$\tilde{U}_{yy}(\mathbf{q}) = \alpha^2 BDK_c(q_x^2 + q_z^2)^2 + BDK_u q^2 q_x^2 + K_c K_u q^4(Bq_x^2 + \alpha^2 Dq_z^2), \quad (3.21)$$
$$\tilde{U}_{zz}(\mathbf{q}) = \alpha^2 DK_c[Bq_z^2 + K_u q^4]q_y^2, \quad (3.22)$$
$$\tilde{U}_{xy}(\mathbf{q}) = -B[\alpha^2 DK_c(q_x^2 + q_z^2) + K_u(Dq^2 + K_c q^4)]q_x q_y, \quad (3.23)$$
$$\tilde{U}_{yz}(\mathbf{q}) = -\alpha^2 DK_c[B(q_x^2 + q_z^2) + K_u q^4]q_y q_z\ , \quad (3.24)$$
$$\tilde{U}_{xz}(\mathbf{q}) = \alpha^2 BDK_c q_x q_y^2 q_z. \quad (3.25)$$

The expressions derived in this section will permit us to calculate the energy and strain field of individual dislocations and the interaction energy of dislocation pairs and arrays. They are valid at all length scales larger than the coherence length ξ. In particular, they apply to type I systems at length scales between the ξ and the penetration depth λ.

B. Type I systems

In type I systems, where the ξ and the core size are larger that λ, we calculate dislocation energies using the type I free energy of Eq. (2.30). Replacing $\boldsymbol{\nabla}u$ by $\boldsymbol{\nabla}u^{(a)} + \mathbf{v}$, we obtain an equation for $u^{(a)}$ in terms of $\mathbf{v}$ by minimizing Eq. (2.30) with respect to $u^{(a)}$:

$$-B\partial_z(\partial_z u^{(a)} + v_z) + \nabla^2[K_u\nabla^2 u^{(a)} + \alpha^2 K_c(\partial_x^2 u^{(a)} + \partial_x v_x)] = 0\ . \quad (3.26)$$

The order of gradients in this expression is important: $\nabla^2\partial_x v_x$ cannot be replaced by $\partial_x\nabla^2 v_x$. Equation (3.26) leads to

$$u^{(a)}(\mathbf{q}) = G(\mathbf{q})[iBq_z v_z + i\alpha^2 K_c q_x q^2 v_x], \quad (3.27)$$

where

$$G(\mathbf{q}) = [Bq_z^2 + k_u q^4 + \alpha^2 K_c q^2 q_x^2]^{-1}. \quad (3.28)$$

Using Eqs. (3.27) and (3.5) in the type I free energy [Eq. (2.30)], we obtain dislocation energies that are identical with the $D \to \infty$ limit of the type II energies we just calculated. In this limit $\Delta(\mathbf{q}) \to DG(\mathbf{q})$ and all of the energies $\tilde{U}_{ij}$ have terms at most linear in D so that the limit $\Delta^{-1}\tilde{U}_{ij}$ as $D \to \infty$ is well defined.

IV. SINGLE DISLOCATIONS

Equation (3.18) can be used to calculate both the strain and strain energy of isolated dislocations and the interaction energy of pairs of dislocations. We begin with isolated dislocations with a rectilinear core aligned along a unit vector $\mathbf{e}$. Then

$$\mathbf{b}(\mathbf{x}) = \mathbf{e}kd\delta_e^{(2)}(\mathbf{x}), \tag{4.1}$$

where $\delta_e^{(2)}(\mathbf{x})$ is the two-dimensional δ function in the plane perpendicular to $\mathbf{e}$ and k is the strength of the dislocation. The Fourier transform of Eq. (4.1) is

$$\mathbf{b}(\mathbf{q}) = \mathbf{e}2\pi kd\delta(\mathbf{q}\cdot\mathbf{e}) = \mathbf{e}kdL\delta_{\mathbf{q}\cdot\mathbf{e},0}. \tag{4.2}$$

The strain energy per unit length of a dislocation aligned along $\mathbf{e}$ is then

$$\epsilon_s = \frac{E}{L} = \frac{k^2d^2}{2}\int \frac{d^2q_e}{(2\pi)^2}U(\mathbf{e}), \tag{4.3}$$

where $\mathbf{q}_e = \mathbf{q} - \mathbf{e}(\mathbf{e}\cdot\mathbf{q})$ lies in the plane perpendicular to $\mathbf{e}$ and where

$$U(\mathbf{e}) = e_iU_{ij}(\mathbf{q}_e)e_j. \tag{4.4}$$

The integral in Eq. (4.3) has an upper cutoff at $\Lambda \sim \xi^{-1}$.

The total energy per unit length, $\epsilon = \epsilon_c + \epsilon_s$, of a dislocation includes a part ϵ_c, arising from the destruction of smectic order in the core in addition to the strain energy ϵ_s arising from distortions of u and δc outside the core. For strongly type II systems, ϵ_s can be much larger than ϵ_c.

A. Single screw dislocation

For a screw dislocation $\mathbf{b}$ is parallel to the z axis. Thus, for a single screw dislocation with Burgers vector of magnitude d, we have $\mathbf{e}(\mathbf{q}) = (0,0,d)$, $\mathbf{q}_e = q(\cos\theta, \sin\theta, 0)$, $U(\mathbf{e}) = U_{zz}(\mathbf{q})$, and

$$\epsilon_s^s = \frac{1}{2}\alpha^2 Dd^2\int_0^{2\pi}\frac{d\theta}{2\pi}\int_0^{\lambda_c/\xi}\frac{dp}{2\pi}\frac{p\sin^2\theta}{1+\beta^2\cos^2\theta+p^2}, \tag{4.5}$$

where we introduced the quantity

$$\beta^2 = \alpha^2K_c/K_u. \tag{4.6}$$

In the type I limit, $\lambda_c \to 0$, and, in contrast to screw dislocations in smectic-A liquid crystals, the energy

$$\epsilon_s^s = \frac{\alpha^2K_c}{8\pi}\frac{d^2}{\xi^2}\frac{\sqrt{1+\beta^2}-1}{\beta^2} \tag{4.7}$$

is nonzero. This is because there is a nonzero long distance strain in the smectic-C phase that is not present in the smectic-A phase. In type II systems, there are additional contributions to the energy arising from distortions between the core radius ξ and the penetration depth λ_c. The integral in Eq. (4.5) can be evaluated exactly. The result is

$$\epsilon_s^s = \epsilon_0\frac{\alpha^2}{\beta^2}\left[\sqrt{(1+\Lambda^2)(1+\beta^2+\Lambda^2)} - \Lambda^2 - \sqrt{1+\beta^2} + \beta^2\ln\left(\frac{\sqrt{1+\beta^2+\Lambda^2}+\sqrt{1+\Lambda^2}}{1+\sqrt{1+\beta^2}}\right)\right], \tag{4.8}$$

where $\Lambda^2 = \lambda_c^2/\xi^2$ and where we introduced

$$\epsilon_0 = \frac{Dd^2}{8\pi}. \tag{4.9}$$

In strongly type II systems, this will be the dominant contribution to the energy of a screw dislocation.

The analytic part of the displacement field can be obtained from Eq. (3.11) in type II systems or Eq. (3.27) in type I systems. The type I solution applies to both type I and type II systems at distances greater than λ_c from the core. It is

$$u_s^{(a)}(\mathbf{x}) = -\beta^2 d\int_{-\infty}^{\infty}\frac{dq_xdq_y}{(2\pi)^2}\frac{q_xq_ye^{i(q_xx+q_yy)}}{q^2(q^2+\beta^2q_x^2+\lambda_c^2q^4)} \simeq -\frac{d}{2\pi}\tan^{-1}\frac{y}{x} + \frac{d}{2\pi}\tan^{-1}\frac{y\sqrt{1+\beta^2}}{x}. \tag{4.10}$$

The first term in this equation exactly cancels the nonanalytic part arising from $\mathbf{v}$. Thus, the complete solution for u_s is

$$u_s(\mathbf{x}) = \frac{d}{2\pi}\tan^{-1}\frac{y\sqrt{1+\beta^2}}{x}. \tag{4.11}$$

This is indeed a dislocation solution that minimizes the type I free energy. From Eq. (2.30), we have

$$K_u\nabla^2[\nabla^2 + \beta^2\partial_x^2]u = 0. \tag{4.12}$$

A wide class of solutions to this equation can be expressed as linear combinations of solutions to $\nabla^2u = 0$ and $(\nabla^2 + \beta^2\partial_x^2)u = 0$. The dislocation solution to the former equation is simply the singular solutions $u^{(s)} = (d/2\pi)\tan^{-1}(y/x)$, whereas the dislocation solution to the latter equation is Eq. (4.11). Equation (4.12) is, however, misleading. Because the singular part of ∇u is not explicitly displayed, it appears that the gradient operators commute (i.e., $\nabla^2\partial_x^2u = \partial_x^2\nabla^2u$). When u is singular, however, the gradient operators do not commute. Equation (4.10) tells us that the $\nabla^2u = 0$ solution is not acceptable and the Eq. (4.11) is the only correct large-distance displacement field for our free energy.

B. Single edge dislocation

The core of an edge dislocation lies in the xy plane. Thus, for a single linear edge dislocation whose core makes an angle ω with the x axis, we have $\mathbf{e} = (\cos\omega, \sin\omega, 0) \equiv d\mathbf{e}$ and $\mathbf{q}_e = (q_1 \sin\omega, -q_1 \cos\omega, q_2)$. The energy per unit length is the given by Eq. (4.3) with

$$U(\mathbf{e}) = \cos^2\omega\, U_{xx} + 2\sin\omega\cos\omega\, U_{xy} + \sin^2\omega\, U_{yy}, \tag{4.13}$$

where U_{ij} is given in Eqs. (3.20)–(3.25). Even in the type I limit, the integral in Eq. (4.3) cannot be done analytically. An edge dislocation with $\mathbf{b}$ along y induces director splay and bend and has an energy determined by K_c, whereas one with $\mathbf{b}$ along x does not and has and energy determined by $K_u < K_c$. Thus, we expect the energy of a dislocation with $\mathbf{b}$ along the x axis to have a lower energy than one aligned along the y axis. Figure 6 shows the energy per unit length of an edge dislocation as a function of ω calculated for $A_0 = \pi/10$, $\beta = 3$, and $\lambda_c/\xi = 10$. As expected, the lowest energy is at $\omega = 0$ and the highest at $\omega = \pi/2$.

We can evaluate $u^{(a)}$ far from the dislocation core using the type I expression of Eq. (3.27). The result is that the dominant contribution to the total u at large distances is identical in form to that of a smectic-A liquid crystal. For $\mathbf{b}$ along x, $v_x = 0$, $\partial_x u = 0$, and Eq. (3.26) reduces exactly to the equation for an edge dislocation [15,16] in a smectic-A liquid crystal. Thus for $\mathbf{b}$ along x,

$$u = \frac{d}{4}\mathrm{sgn}(z)[\mathrm{erf}(y/\sqrt{4\lambda_u|z|}) + 1], \tag{4.14}$$

where $\lambda_u^2 = K_u/B$ and $\mathrm{erf}(z) = (2/\sqrt{\pi})\int_0^\eta e^{-t^2}dt$. When $\mathbf{b}$ is along y, $v_x = -iq_x b_y/q^2$ is nonzero, and the terms following K_c in Eq. (3.26) are nonzero. Nonetheless, the large distance solution still has the same form as Eq. (4.14) with y replaced by x and λ_u^2 by $(K_u + \alpha^2 K_c)/B$. There are, however, analytic terms that contribute closer to the core even in type I systems.

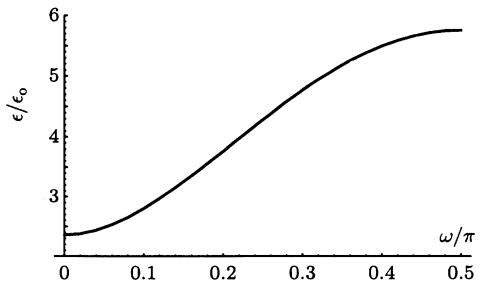

FIG. 6. Energy per unit length of an edge dislocation as a function of the angle ω $\mathbf{b}$ makes with the x axis for $B = D$, $A_0 = \pi/10$, $\beta = 3$, and $\lambda_c/\xi = 10$. The energy is lowest for $\omega = 0$ and highest for $\omega = \pi/2$.

C. Single screw-edge dislocation

Edge dislocations create more far-field distortions that do screw dislocations, and one would expect in general that screw dislocations would have lower energy that edge dislocations. A mixed edge-screw dislocation with $\mathbf{b}$ in the xz plane has $\mathbf{b} = d(\sin\gamma, 0, \cos\gamma)$ and $\mathbf{q}_e = (q_1\cos\gamma, q_2, -q_1\sin\gamma)$, and its energy ϵ_s^{se} per unit length is given by Eq. (4.3) with

$$U(\mathbf{e}) = \cos^2\gamma\, U_{zz} + 2\sin\gamma\cos\gamma\, U_{xz} + \sin^2\gamma\, U_{xx}. \tag{4.15}$$

In Fig. 1, we plot $\epsilon_s^{se}/\epsilon_0$ for $B = D$, $A_0 = \pi/10$, $\beta = 3$, and $\lambda_c/\xi = 10$. As expected, the screw dislocation with $\gamma = 0$ has the lowest energy and the pure edge dislocation with $\gamma = \pi/2$ has the highest energy.

V. INTERACTING DISLOCATIONS

In this section, we will investigate the interaction potential between parallel screw, edge, and mixed screw-edge dislocations. In the preceding section, we showed that a single screw dislocation in a smectic-C liquid crystal, unlike its smectic-A cousin, has far-field strain energy even in type I systems. This far-field strain leads to far-field interactions between dislocation, dying off as the inverse square of distance, which is anisotropic, attractive for like-sign dislocations separated along y, and repulsive for like-sign dislocations separated along x. At distances of order λ_c, the interaction becomes purely repulsive, and there is a minimum energy separation for dislocations separated along y. This is in contrast to the situation in the smectic-A liquid crystal, where the interaction between like-sign dislocations falls off exponentially with distance and is purely repulsive. As we have seen, the far-field strain of edge dislocations in smectic-C liquid crystals is similar to that of smectic-A liquid crystals. There is thus a far-field repulsive interaction between like-sign edge dislocations whose separation along z is not zero. For edge dislocations in the xy plane there is only near-field repulsion. For mixed screw-edge dislocations with cores making an angle γ with the z axis, the energy minimum that exists for pure screw ($\gamma = 0$) diminishes and moves to larger separation as γ is increased, until it disappears altogether at a critical value of γ.

The interaction potential between parallel equal strength dislocations with $\mathbf{b} = d\mathbf{e}$ separated by a vector $\mathbf{x}$ in the plane perpendicular to $\mathbf{e}$ is

$$U_{\mathrm{int}}(\mathbf{x}) = d^2 \int \frac{d^2 q_e}{(2\pi)^2} e^{i\mathbf{q}_e\cdot\mathbf{x}} U(\mathbf{e}), \tag{5.1}$$

where $U(\mathbf{e})$ is given by Eq. (4.15). For screw dislocations, $\mathbf{e} = \mathbf{e}_z$, $\mathbf{q}_e = (q_x, q_y, 0)$ and

$$U_{\mathrm{int}}^{(s)}(\mathbf{x}) = \alpha^2 d^2 K_c \int_{-\infty}^{\infty} \frac{dq_x dq_y}{(2\pi)^2} \frac{q_y^2 e^{i(q_x x + q_y y)}}{q_y^2 + (1+\beta^2)q_x^2 + \lambda_c^2 q^4}. \tag{5.2}$$

The large distance behavior ($|\mathbf{x}| \gg \lambda_c$) of this function

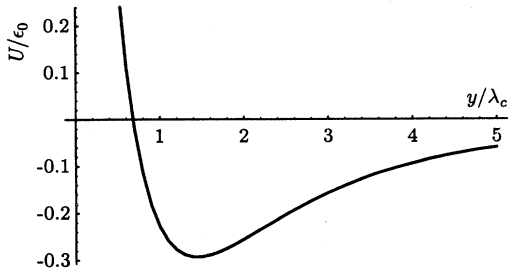

FIG. 7. Interaction energy as a function of separation y for unit strength screw dislocations. The interaction is attractive at separations large than λ_c and repulsive at short distances. It has a negative minimum energy at y or order λ_c.

can be obtained by setting $\lambda_c = 0$ (yielding the type I limit). The integral over $\mathbf{q}_e$ can now be done analytically. Performing the contour integral over q_x first, we obtain

$$U^s_{\rm int}(\mathbf{x}) = \alpha^2 K_c d^2 \int_0^\infty \frac{dq_y}{2\pi} \frac{q_y \cos q_y}{\sqrt{1+\beta^2}} e^{-q_y|x|/\sqrt{1+\beta^2}}$$
$$= \frac{\alpha^2 K_c d^2}{\sqrt{1+\beta^2}} \frac{d}{dy} \int_0^\infty \frac{dq_y}{2\pi} e^{iq_y y} e^{-q_y|x|/\sqrt{1+\beta^2}}$$
$$= \frac{\alpha^2 K_c d^2}{2\pi\sqrt{1+\beta^2}} \frac{\tilde{x}^2 - y^2}{(\tilde{x}^2+y^2)^2}, \qquad (5.3)$$

where $\tilde{x} = x/\sqrt{1+\beta^2}$. This potential is attractive for $x = 0$, repulsive for $y = 0$, and equal to zero along $x = \pm\sqrt{1+\beta^2}y$. The complete interaction potential in Eq. (5.2) can be evaluated numerically. The results for $B = D$, $\beta = 3$, and $x = 0$ is plotted as a function of y in Fig. 7. The is an energy minimum at separation $y \approx 1.4\lambda_c$.

The energy of an edge dislocation with core along the x axis is

$$U^e_{\rm int} = \frac{1}{2} d^2 K_u \int \frac{dq_y dq_z}{(2\pi)^2} \frac{q_y^2(1+\lambda_c q^2) e^{i(q_y y + q_z z)}}{q_z^2(1+\lambda_c^2 q^2) + \lambda_u^2 q^4 + \lambda_u^2 \lambda_c^2 q^6}, \qquad (5.4)$$

where $\lambda_u = K_u/B$. In the type I limit, we can set $\lambda_c = 0$, and the resulting energy is identical to that for edge dislocations in smectic-A liquid crystals:

$$U^e_{\rm int} = \frac{1}{4} d^2 B \left(\frac{\lambda_u}{\pi|z|}\right)^{1/2} e^{-y^2/(4\lambda_u|z|)}. \qquad (5.5)$$

The complete evaluation of Eq. (5.4) for $z = 0$ is shown in Fig. 8. The potential is repulsive for all separations y.

For parallel mixed screw-edge dislocations in the xz plane, $\mathbf{e} = (\sin\gamma, 0, \cos\gamma)$, $\mathbf{q}_e = (q_1\cos\gamma, q_2, -q_1\sin\gamma)$. The interaction potential for $\gamma = \pi/10$ is shown in Fig. 2 and for various values of γ in Fig. 9.

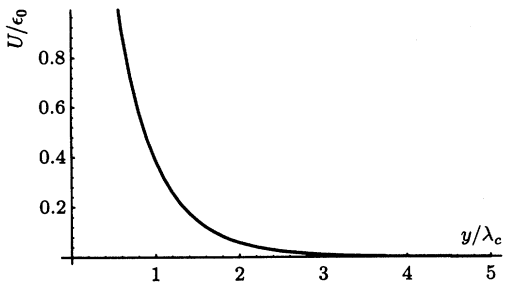

FIG. 8. The interaction energy as a function of separation y of two unit strength edge dislocations with cores along x for $B = D$, $A_0 = \pi/10$, $\beta = 3$.

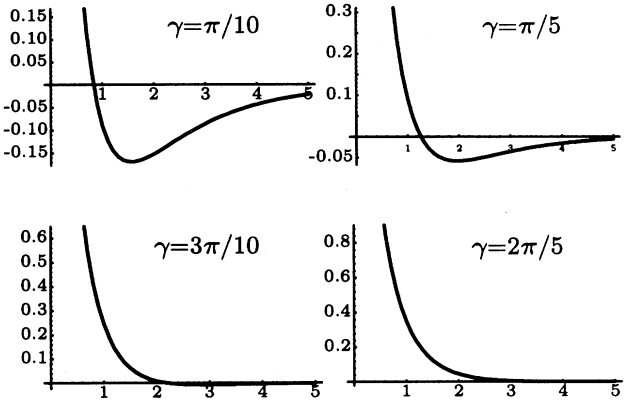

FIG. 9. Energy as a function of separation y for parallel dislocations with $\mathbf{b}$ in the xz plane for different values of γ. The energy minimum becomes less and less pronounced, moves to larger values of y, and eventually disappears as γ increases.

VI. SUMMARY AND DISCUSSION

We have introduced a covariant formulation of the elastic free energy for a smectic-C liquid crystal, which allows us to identify type I and type II smectic-C liquid crystals. We use this free energy to calculate the energies of isolated and interacting dislocations as a function of their orientation relative to the layer normal and the $\mathbf{c}$ director. Parallel dislocations with core axes in the plane of the layer normal and the $\mathbf{c}$ director (the xz plane) and separated along the normal to this plane (y direction) have an attractive interaction at large separation and a minimum energy separation of order the penetration depth λ, provided the projection of their axes along $\mathbf{c}$ is not too large. Parallel dislocation in the xz plane but separated along x rather than y have only repulsive interactions. In another paper [17], we will show how this attractive interaction can explain many of the experimentally observed properties of the TGB$_C$ phase [12–14].

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APPENDIX

In this appendix, we will discuss briefly the relation between our results and those of Ref. [9], which used an elastic energy

$$f = \tfrac{1}{2}K_x(\partial_x^2 u)^2 + \tfrac{1}{2}K_y(\partial_y^2 u)^2 + K_{xy}(\partial_x\partial_y u)^2, \quad \text{(A1)}$$

in which there was no separate $(\partial_x^2 u)(\partial_y^2 u)^2$ term. Following Ref. [8] the constraint $K_xK_y - K_{xy}^2 > 0$ was unnecessarily imposed to ensure stability. As we saw in Sec. II E, only K_x, K_y, and K_{xy} need be positive for stability. The equilibrium equation for u is

$$(K_x\partial_x^4 + 2K_{xy}\partial_x^2\partial_y^2 + K_y\partial_y^4)u = 0. \quad \text{(A2)}$$

Now consider two cases: (1) $\mu^2 = K_{xy}^2/(K_xK_y) < 1$ and (2) $\mu^2 > 1$. Case (1) corresponds to the stability constraint of Ref. [8]. Case (2) corresponds to the situation in this article. If $\mu^2 < 1$, we follow Ref. [9] and rescale x and y via $x = K_x^{1/4}\bar{x}$ and $y = K_y^{1/4}\bar{y}$. Equation (A2) becomes

$$\partial_{\bar{x}}^4 + \partial_{\bar{y}}^4 + 2\mu\partial_{\bar{x}}^2\partial_{\bar{y}}^2 = \bar{\nabla}^4 - 2a^2\partial_{\bar{x}}^2\partial_{\bar{y}}^2 \quad \text{(A3)}$$
$$= (\bar{\nabla}^2 + a\partial_{\bar{x}}\partial_{\bar{y}})(\bar{\nabla}^2 - a\partial_{\bar{x}}\partial_{\bar{y}}) = 0,$$

where $2a^2 = (1-\mu)$ and $\bar{\nabla}^2 = \partial_{\bar{x}}^2 + \partial_{\bar{y}}^2$. The restrictions of case (1), which we are considering, imply $0 \le \mu^2 < 1$ and $0 < a^2 \le 1$. Singular (i.e., dislocation) solutions to Eq. (A3) are

$$u^{\pm} = \frac{d}{2\pi}\tan^{-1}\frac{b\bar{y}}{\bar{x} \pm a\bar{y}}, \quad \text{(A4)}$$

where $b = (1-a^2)^{1/2}$. If only Eq. (A2) is given, the only criterion for choosing which linear combination of these solutions is the correct one is energetics. Reference [9] chose the combination $(u^+ + u^-)/2$, which minimized the energy. A more careful treatment of Gaussian curvature, which contributes only at boundaries, would more than likely yield some other combination.

If $\mu^2 > 1$, then we can rescale x via $x = \eta^{-1}\bar{x}$, and Eq. (A2) can be written as

$$K_y[(K_x/K_y)\eta^4\partial_{\bar{x}}^4 + \partial_y^4 + (2K_{xy}/K_y)\eta^2\partial_{\bar{x}}^2\partial_y^2]u = 0. \quad \text{(A5)}$$

Choosing $(K_x/K_y)\eta^4 = 1 + \beta^2$ and $(2K_{xy}/K_y)\eta^2 = 2 + \beta^2$, we obtain

$$K_y[\nabla^2(\nabla^2 + \beta^2\partial_{\bar{x}}^2)]u = 0 \quad \text{(A6)}$$

with $\beta^2 = 2[(\mu^2 - 1) + \mu\sqrt{\mu^2 - 1}]$. The dislocation solutions are $u = (d/2\pi)\tan^{-1}(y/x)$ and $u = (d/2\pi)\tan^{-1}(y/\sqrt{1+\beta^2}/\bar{x})$. For values of K_x, K_y, and K_{xy} in this paper, $\mu = \frac{1}{2}\alpha^2K_c/[K_u(K_u + \alpha^2K_c)]^{1/2}$, $\beta^2 = \alpha^2K_c/K_u$, and $\eta = 1$, and Eq. (4.11) is regained. As discussed in Sec. IV A, the latter solution [Eq. (4.11)] is imposed by the boundary conditions of our problem.

Thus, we see that the constraint $K_{xy}^2/(K_xK_y) < 1$ imposed by Ref. [9] leads to different dislocation solutions from those found here. This constraint is unnecessary and does not apply to the model presented here.

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