

# Existence of Solutions to Boundary Value Problems for Smectic Liquid Crystals

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## Abstract

We prove lower semicontinuity and lower bounds for a Chen-Lubensky energy describing nematic/smectic liquid crystals with physically realistic boundary conditions. The Chen-Lubensky energy captures stable phases of the liquid crystal material, ranging from purely nematic or smectic states to coexisting nematic/smectic states. By including appropriate additional terms, the model includes the effects of applied electric or magnetic fields, and/or electrical self-interactions in the case of polarized liquid crystals. As a consequence of our results, we establish existence of minimizers with weak or strong anchoring of the director field (describing molecular orientation) at the boundary, and Dirichlet or Neumann boundary conditions on the smectic order parameter for the liquid crystal material.

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## 1 Introduction

### 1.1 Background on Liquid Crystals

Liquid crystals are intermediate states between liquid and solid (crystal) states that occur in a certain class of anisotropic materials, and are typically made up of elongated "rod-like" molecules. In the nematic phase for a liquid crystal, which occurs when the temperature is lowered from that of the (isotropic) liquid state, the molecules tend to be aligned along their long axes, but with no positional order in their center of masses. Further lowering of the temperature yields the smectic A phase, in which the molecules tend to align in layers with the long axes parallel to the layer normals. At a lower temperature, the molecules still tend to align in layers but their long axes have a preferred (nonzero) tilt angle with the layer normal; this is called the smectic C phase. (See Figure 1.) Stable states of liquid crystals need not be uniform. A smectic phase can locally melt into a different smectic phase or a less ordered phase. This can occur if the liquid crystal is subjected to external stresses thereby introducing defects into the layer structure or locally altering the tilt angle. Applications of electric or magnetic fields, temperature fluctuations, or external influences at the boundary can cause phase transitions in the liquid crystal between nematic and smectic phases, including mixed (coexisting) states with nonempty nematic/smectic subregions within the liquid crystal. (See [8, 12, 20, 25, 30].)

A variational model for which local minimizers represent stable states of a liquid crystal material at a constant temperature (allowing pure and mixed nematic/smectic states) was formulated by Chen and Lubensky [8] in 1976. (See also Renn and Lubensky [20] for a modification of the energy to include chiral nematic/smectic C liquid crystals.) The energy developed by Chen and Lubensky accounts for phase transitions between nematic and smectic A or smectic C phases. It is an extension of an earlier formulation due to de Gennes [10] which modeled nematic-to-smectic A phase transitions only.

The de Gennes energy for nematic/smectic A liquid crystals combined an Oseen-Frank energy term for a unit vector field,  $\mathbf{n}(\mathbf{x})$ , representing the average local orientation of the liquid crystal molecule, and a Ginzburg-Landau term involving the covariant derivative of a complex-valued order parameter,  $\psi(\mathbf{x})$ , related to the local smectic layers. It was shown in [2] by Bauman, Calderer, Liu, and Phillips that de Gennes' energy is coercive and lower semicontinuous among admissible families of functions in an ap-

appropriate Sobolev space with physically realistic boundary conditions. In addition, it was shown that nematic versus smectic phases correspond to different temperature regimes, which can be described by conditions on the coefficients and material parameters, related to a "critical temperature" separating purely nematic and nematic/smectic states.

For the Chen-Lubensky energy accounting for nematic/smectic C liquid crystals, not even existence of minimizers (with appropriate boundary conditions) has been shown. The difficulty is a lack of apparent coercivity and weak lower semicontinuity, since second-order derivatives of the order parameter in the energy involve covariant second derivatives that do not control second derivatives of the order parameter in the direction of the director field. To overcome this, Luk'yanchuk modified the second-order term in the Chen-Lubensky energy (see [21]) by making the second-order gradient term isotropic. Existence of minimizers and an analysis of nematic/smectic C phase transitions for this energy was proved by Joo and Phillips in [17], assuming that the order parameter  $\psi$  is zero on the boundary. Subsequently, Calderer and Park in [24] proved existence of minimizers for the Luk'yanchuk energy among restricted classes of boundary values for domains that are "vortex tubes" with boundary conditions related to the domain structure.

In this paper we prove existence of minimizers, as well as weak lower semicontinuity and coercivity, for the Chen-Lubensky energy (in divergence-form) among admissible functions in a general class of physically realistic boundary conditions. The boundary conditions include weak or strong anchoring at the boundary, and boundary values that naturally result in mixed-state nematic/smectic minimizers.

## 1.2 The Chen-Lubensky Energy

Before stating our results in more detail, let us first describe the divergence-form of the Chen-Lubensky energy and some observations about its structure. Let  $\Omega \subset \mathbb{R}^n$  be a connected bounded Lipschitz domain in  $\mathbb{R}^3$  which represents the region occupied by the liquid crystal. The domain  $\Omega$  represents the liquid crystal body. The energy is a sum of two terms,

$$\int_{\Omega} (f_{CL}(\psi, \mathbf{n}) + f_N(\mathbf{n})),$$

Here,  $\psi : \Omega \rightarrow \mathbb{C}$  and  $\mathbf{n} : \Omega \rightarrow \mathbb{S}^2$ . The vector,  $\mathbf{n}(\mathbf{x})$ , is the director, which is a unit vector representing the direction of the local average of the principal molecular axes near  $\mathbf{x}$ . The function,  $\psi$ , is a complex-valued

order parameter; formally writing  $\psi(\mathbf{x}) = \rho(\mathbf{x})e^{i\omega(\mathbf{x})}$ ,  $\rho(\mathbf{x})$  is an amplitude of smectic layering and measures how well the smectic phase has developed near  $\mathbf{x}$ . In particular, the material is in the nematic phase at  $\mathbf{x}$  if  $\psi(\mathbf{x}) = 0$ . Smectic layers near  $\mathbf{x}$  are contained in level sets of  $\omega$  near  $\mathbf{x}$ .

In the case of uniform layers as in Figure 1, the layer spacing is equal to  $d_0$  and the layer spacing in the corresponding untilted phase would be  $\bar{d} = \frac{d_0}{\cos \theta_0}$ .

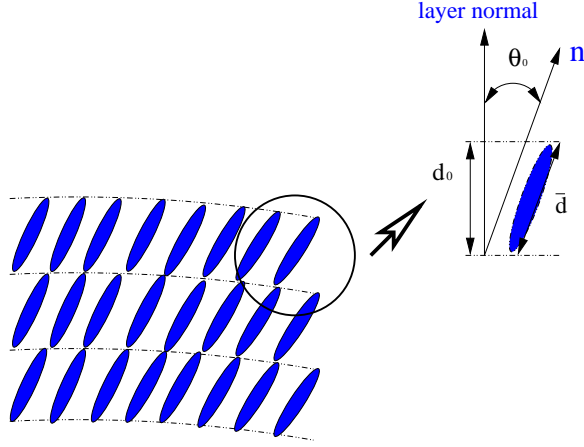


Figure 1: Layer spacing and tilt angle in uniform layer structure

Wave numbers are defined as  $q_0 = \frac{2\pi}{d_0}$  and  $\bar{q} = \frac{2\pi}{\bar{d}}$  respectively. The energy is expressed in terms of the covariant derivative  $D\psi = \nabla\psi - i\bar{q}\mathbf{n}\psi$ , where components parallel and perpendicular to  $\mathbf{n}(\mathbf{x})$  are  $D_{\parallel}\psi = (\mathbf{n} \cdot \nabla\psi - i\bar{q}\psi)\mathbf{n}$  and  $D_{\perp}\psi = D\psi - D_{\parallel}\psi$ . The C-L energy density is then

$$f_{CL} = a_{\perp}|D \cdot D_{\perp}\psi|^2 + a_{\parallel}|D \cdot D_{\parallel}\psi|^2 - c_{\perp}|D_{\perp}\psi|^2 + c_{\parallel}|D_{\parallel}\psi|^2 - r'|\psi|^2 + g|\psi|^4, \quad (1)$$

where  $a_{\perp}, a_{\parallel}, c_{\parallel}, g > 0$ , such that  $c_{\perp} > 0$  for the *SmC* phase and  $c_{\perp} \leq 0$  for *SmA*. The energy density measures the cost of distortions in the smectic layer structure as well as variations in the angle between  $\mathbf{n}$  and the layer normal relative to the bulk tilt angle  $\theta_0$ . Letting  $\psi = \rho e^{i\omega}$ , we have

$$f_{CL} = a_{\perp} \left[ \left( \text{div} \nabla_{\perp} \rho - \rho |\nabla_{\perp} \omega|^2 \right)^2 + \left( \nabla_{\perp} \omega \cdot \nabla_{\perp} \rho + \text{div}(\rho \nabla_{\perp} \omega) \right)^2 \right] + a_{\parallel} \left[ \left( \text{div} \nabla_{\parallel} \rho - \rho (\nabla \omega \cdot \mathbf{n} - \bar{q}) \right)^2 + \left( (\nabla_{\parallel} \omega - \bar{q} \mathbf{n}) \cdot \nabla_{\parallel} \rho + \text{div}[\rho (\nabla_{\parallel} \omega - \bar{q} \mathbf{n})] \right)^2 \right] - c_{\perp} \left[ |\nabla_{\perp} \rho|^2 + \rho^2 |\nabla_{\perp} \omega|^2 \right] + c_{\parallel} \left[ |\nabla_{\parallel} \rho|^2 + \rho^2 |\nabla_{\parallel} \omega - \bar{q} \mathbf{n}|^2 \right] - r' \rho^2 + g \rho^4,$$

where  $\nabla_{\parallel}h = (\nabla h \cdot \mathbf{n})\mathbf{n}$  and  $\nabla_{\perp}h = \nabla h - \nabla_{\parallel}h$  for a function  $h$ .

Away from defects or near the boundary, the amplitude  $\rho$  should vary slowly relative to the layer structure given by  $\omega$ . Thus if we examine states with constant  $\rho$  it follows that

$$f_{CL} = a_{\perp}\rho^2 \left( \text{div}(\nabla_{\perp}\omega) \right)^2 + a_{\parallel}\rho^2 \left( \text{div}((\nabla\omega \cdot \mathbf{n} - \bar{q})\mathbf{n}) \right)^2 + a_{\parallel}\rho^2 (\nabla\omega \cdot \mathbf{n} - \bar{q})^4 \\ + a_{\perp}\rho^2 \left( |\nabla_{\perp}\omega|^2 - \frac{c_{\perp}}{2a_{\perp}} \right)^2 + c_{\parallel}(\nabla\omega \cdot \mathbf{n} - \bar{q})^2 - \left( r' + \frac{c_{\perp}^2}{4a_{\perp}} \right) \rho^2 + g\rho^4.$$

The first two terms are elastic energy densities for layer bending, which we note vanish for pure *SmA* configurations, i.e. if  $\bar{q}\mathbf{n} = \nabla\omega$ . The next three terms measure variations in layer thickness and deviation in the tilt angle relative to bulk values. In order to see this we consider uniform states with  $\nabla\omega$  and  $\mathbf{n}$  constant. If  $c_{\perp} \geq 0$  then a pair  $(\rho e^{i\omega}, \mathbf{n})$  minimizes these four terms provided  $\nabla\omega \cdot \mathbf{n} = \bar{q}$  and  $|\nabla_{\perp}\omega|^2 = \frac{c_{\perp}}{2a_{\perp}}$ . This corresponds to the *SmC* phase with  $\tan^2 \theta_0 = \frac{c_{\perp}}{2a_{\perp}\bar{q}^2}$ . If  $c_{\perp} < 0$ , then  $(\rho e^{i\omega}, \mathbf{n})$  minimizes the four terms provided  $|\nabla_{\perp}\omega| = 0$ , corresponding to  $\theta_0 = 0$ , characterizing the *SmA* phase. We next consider the amplitude  $\rho$ . A bulk state is either nematic or smectic if and only if  $\rho = 0$  or  $\rho > 0$  respectively. Set  $r = r' + \frac{c_{\perp}^2}{4a_{\perp}}$  if  $c_{\perp} \geq 0$ , and  $r = r'$  if  $c_{\perp} < 0$ . It follows that minimizing bulk states for  $f_{CL}$  satisfy  $\rho = 0$  or  $\rho > 0$  if and only if  $r \leq 0$  or  $r > 0$  respectively. Moreover if  $r > 0$  then  $\rho = \frac{r}{2g}$ .

In the classic model  $r$  and  $c_{\perp}$  are taken to be temperature dependent such that for critical temperatures  $T_{AC} < T_{NA}$ , we have  $r(T) < 0$  if  $T_{NA} < T$ ,  $0 < r(T)$  if  $T < T_{NA}$ ,  $c_{\perp}(T) < 0$  if  $T_{AC} < T$ , and  $0 < c_{\perp}(T)$  if  $T < T_{AC}$ . Then as  $T$  decreases, the minimizing uniform bulk states (ground states) progress from  $N \rightarrow SmA \rightarrow SmC$ . The first and second terms in (1) are modifications of the energy from [8] where  $D_{\perp} \cdot (D_{\perp}\psi)$  and  $D_{\parallel} \cdot (D_{\parallel}\psi)$  are used in place of  $D \cdot (D_{\perp}\psi)$  and  $D \cdot (D_{\parallel}\psi)$  respectively. The energies measure smectic layer distortion in similar ways. The Oseen-Frank energy density is

$$f_N = K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + \tau)^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n}) + \mathbf{b}|^2 \\ + (K_2 + K_4)(\text{tr}(\nabla\mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2) \quad (2)$$

where the elastic constants satisfy

$$0 < c_0 \leq K_2 + K_4 \leq c_1, K_2 + K_4 \leq \min(K_1, K_3), K_4 \leq 0, \quad (3)$$

with  $\tau \in \mathbb{R}$ ,  $\mathbf{b} \in L^2(\Omega)$ . The energy density  $f_N$  measure the cost per unit volume of variations in  $\mathbf{n}$ .

We consider two types of domains  $\Omega \subset \mathbb{R}^3$ .

1. Let  $\Omega$  be a bounded open connected set with the boundary  $\partial\Omega$  of class  $C^1$ .
2. Let  $\Omega$  be the cell

$$\Omega = \{(x, y, z) \mid -h < z < h, -l < x < l, -m < y < m\}.$$

In the first case, we can view the liquid crystal as a droplet surrounded by another material. For the second case we imagine the liquid crystal filling the cell between two plates  $z = \pm h$ . For case 2, throughout this paper we assume that the functions  $\psi$ ,  $\nabla\psi$ , and  $\mathbf{n}$  are  $2l$ -periodic in  $x$  and  $2m$ -periodic in  $y$ . Thus from the standpoint of PDE estimates, we can treat  $\partial\Omega$  as of class  $C^1$  and compact. The original motivation for introducing the energy

$$F(\psi, \mathbf{n}) = \int_{\Omega} (f_{CL} + f_N)$$

was to study nematic-smectic transitions [8, 20, 25]. In these papers,  $\Omega = \mathbb{R}^3$  and the analyses addressed eigenfunctions and the spectrum for  $D^2F(0, \mathbf{n})$  at a given nematic state  $(0, \mathbf{n})$ . Questions related to the existence of equilibria or minimizers in an appropriate space were not considered. The energy was subsequently used in a series of papers as a basis from which to construct models incorporating the energetic effects of boundary conditions, polarizations, and electromagnetic fields on smectic layer structures [18, 27, 28, 30, 31]. Here we focus on the problem of introducing boundary conditions. In practice it is observed that as a liquid crystal is slowly cooled from one phase to another the layer structure at the boundary is either retained or has to overcome an energy barrier in order to change [6, 27]. These situations can be modeled with strong or weak anchoring boundary conditions respectively. The mismatch between the bulk smectic structures in the new phase and the smectic structures retained at the boundary leads to defects in the otherwise near-uniform smectic layers of solutions.

From a purely variational perspective, some form of anchoring condition is needed since the energy (1) with  $c_{\perp} > 0$  is not bounded below on classes of functions for which  $|\psi|$  is allowed to vary. To illustrate this we consider the case of the cell

$$\Omega = \{(x, y, z) : |z| < 1, |x| < \pi, |y| < \pi\}, \quad (4)$$

and the sequence  $\{(\psi_m, \mathbf{n}_m); m = 1, 2, \dots\}$  such that

$$\begin{cases} \psi_m(x, y, z) = \frac{\cosh(mz)e^{imx}}{\cosh(m)}, \\ \mathbf{n}_m = \mathbf{e}_2 \end{cases} \quad (5)$$

In this case, we obtain

$$\begin{aligned} D_{\parallel}\psi_m &= (0, -i\bar{q}\psi_m, 0), D_{\perp}\psi_m = (\partial_x\psi_m, 0, \partial_z\psi_m), \\ D \cdot (D_{\perp}\psi_m) &= \partial_x^2\psi_m + \partial_z^2\psi_m = 0, D \cdot (D_{\parallel}\psi_m) = -\bar{q}^2\psi_m. \end{aligned}$$

It follows that

$$F(\psi_m, \mathbf{n}_m) = -8c_{\perp}m\pi^2 + O\left(\frac{1}{m}\right) \text{ as } m \rightarrow \infty.$$

Here the smectic structure diminishes within  $\Omega$  in favor of energy concentration near  $\partial\Omega$ .

We next rewrite the bulk energy in a way that illustrates how anchoring conditions can prevent energy diverging by concentrating near  $\partial\Omega$ . Let

$$\mathcal{A} = \{(\psi, \mathbf{n}) \in H^1(\Omega; \mathbb{C}) \times H^1(\Omega; \mathbb{S}^2) : D_{\perp}\psi, D_{\parallel}\psi \in H(\text{div}; \Omega)\}.$$

where

$$H(\text{div}; \Omega) = \{\mathbf{v} \in L^2(\Omega; \mathbb{C}^3) : \text{div } \mathbf{v} \in L^2(\Omega)\}.$$

We say that  $\{(\psi_j, \mathbf{n}_j)\} \subset \mathcal{A}$  converges weakly to  $(\psi, \mathbf{n}) \in \mathcal{A}$  if  $(\psi_j, \mathbf{n}_j) \rightharpoonup (\psi, \mathbf{n})$  in  $H^1(\Omega)$  and  $(D_{\perp}\psi_j, D_{\parallel}\psi_j) \rightharpoonup (D_{\perp}\psi, D_{\parallel}\psi)$  in  $H(\text{div}; \Omega)$ .

Recall that if  $\mathbf{v} \in H(\text{div}; \Omega)$ , then its trace  $\mathbf{v} \cdot \nu \in H^{-\frac{1}{2}}(\partial\Omega)$  where  $\nu$  is the outward normal to  $\partial\Omega$  [14]. We then write for  $w \in H^1(\Omega)$

$$\langle \mathbf{v} \cdot \nu, w \rangle = \int_{\Omega} w \text{div } \mathbf{v} + \int_{\Omega} \mathbf{v} \cdot \nabla w$$

where  $\langle u, v \rangle = \langle u, v \rangle_{H^{-\frac{1}{2}}(\partial\Omega), H^{\frac{1}{2}}(\partial\Omega)}$  for  $u \in H^{-\frac{1}{2}}(\partial\Omega)$  and  $v \in H^{\frac{1}{2}}(\partial\Omega)$ . Note that  $D_{\perp}\psi = \nabla_{\perp}\psi$  and  $D \cdot \nabla_{\perp}\psi = \text{div}(\nabla_{\perp}\psi)$ . Setting  $\mathbf{v} = \nabla_{\perp}\psi$  and  $w = \psi^*$

$$\begin{aligned} \int_{\Omega} \nabla_{\perp}\psi \cdot \nabla_{\perp}\psi^* &= \int_{\Omega} \nabla_{\perp}\psi \cdot \nabla\psi^* \\ &= \langle \nabla_{\perp}\psi \cdot \nu, \psi^* \rangle - \int_{\Omega} \psi^* \text{div}(\nabla_{\perp}\psi). \end{aligned}$$

We can write

$$\begin{aligned} \int_{\Omega} f_{CL} &= \int_{\Omega} \left( a_{\perp} \left| D \cdot D_{\perp}\psi + \frac{(c_{\parallel} + c_{\perp})}{2a_{\perp}} \psi \right|^2 + a_{\parallel} |D \cdot D_{\parallel}\psi|^2 \right. \\ &\quad \left. + c_{\parallel} |D\psi|^2 - \left( r' + \frac{(c_{\parallel} + c_{\perp})^2}{4a_{\perp}} \right) |\psi|^2 + g|\psi|^4 \right) \\ &\quad - (c_{\perp} + c_{\parallel}) \mathcal{R}e \langle \nabla_{\perp}\psi \cdot \nu, \psi^* \rangle, \end{aligned} \quad (6)$$

where  $\mathcal{R}e(z)$  denotes the real part of a complex number  $z$ . Since  $g > 0$ , the integral over  $\Omega$  is bounded below. We next consider

$$\mathcal{F}(\psi, \mathbf{n}) = \int_{\Omega} (f_{CL} + f_N) + \int_{\partial\Omega} f_S(\mathbf{n}),$$

where  $f_S$  is given by the Rapini-Papoular energy density

$$f_S = \beta (1 - \alpha_0(\mathbf{n} \cdot \nu)^2), \beta \geq 0, 1 > \alpha_0 > 0 \quad (7)$$

and seek minimizers for  $\mathcal{F}$  in several settings.

From the assumption (3), there exist constants  $C, \mathcal{M} > 0$  so that

$$C\|\mathbf{n}\|_{H^1(\Omega)}^2 \leq \int_{\Omega} f_N(\mathbf{n}) + \mathcal{M} \quad (8)$$

for all  $\mathbf{n} \in H^1(\Omega; \mathbb{S}^2)$ . Moreover if  $\{\mathbf{n}_j\} \subset H^1(\Omega; \mathbb{S}^2)$ ,  $\mathbf{n}_j \rightharpoonup \mathbf{n}_0$ , then

$$\int_{\Omega} f_N(\mathbf{n}_0) + \int_{\partial\Omega} f_S(\mathbf{n}_0) \leq \liminf_{j \rightarrow \infty} \left\{ \int_{\Omega} f_N(\mathbf{n}_j) + \int_{\partial\Omega} f_S(\mathbf{n}_j) \right\}.$$

(See [2].) Thus the total energy is bounded below if we can rule out energy concentrating at  $\partial\Omega$  as in (5), and it suffices then to examine coercivity and lower semicontinuity properties for  $\int_{\Omega} f_{CL}$ .

### 1.3 Main Results

We examine the issues of coercivity and lower semicontinuity in three different physical scenarios. In Section 2 we consider the case when the material temperature is such that the liquid crystal is deep within a smectic phase. In this case it is energetically expensive to alter the smectic ordering. This is modeled by considering only states such that  $|\psi| \equiv \rho_0$  for a fixed constant  $\rho_0$ . We call these *uniformly smectic states*. (See (9).) We prove that the minimum problem for  $\mathcal{F}$  over any nonempty, weakly sequentially closed subset of such states is well posed. (See Corollary 2.3.) A central point that we expand on in this paper is the relevance of appropriate boundary conditions. The example (5) above demonstrates that when general states are allowed, the smectic structure must be imposed or restricted at the boundary in order to guarantee a minimal smectic C state. In Section 3 we prove that if  $\psi$  and (or)  $\nabla_{\perp} \psi \cdot \nu$  are fixed at  $\partial\Omega$  (strong anchoring) then minimizers for  $\mathcal{F}$  exist. (See Theorem 3.1.) One expects, however, that the smectic structure at  $\partial\Omega$  is not mechanically fixed but instead just weakly anchored.



In Section 4 we analyze the minimum problem for the energy with weak anchoring

$$\tilde{\mathcal{F}}(\psi, \mathbf{n}) = \mathcal{F}(\psi, \mathbf{n}) + \alpha_1 \int_{\partial\Omega} |\psi - g_1|^2 + \alpha_2 \int_{\partial\Omega} |\nabla_{\perp}\psi \cdot \nu - g_2|^2,$$

where  $\alpha_1 \geq 0, \alpha_2 \geq 0$ , and  $g_1, g_2 \in L^2(\partial\Omega)$ . Our main result is that the minimum problem for  $\tilde{\mathcal{F}}$  is well posed provided  $\alpha_2 > 0$ , while if  $\alpha_2 = 0$  the energy is not bounded from below in general. (See Theorem 4.1.) The motivation for posing and studying minimizers among uniformly smectic C states is the expectation that the full problem will have a minimizer near by (i.e. with  $|\psi| \approx \rho_0$ ). Our work shows that the full problem may not have a minimizer at all without taking into account appropriate boundary conditions. Finally in Section 5 we examine generalizations to include electronic interactions.

## 2 Uniformly Smectic States

We consider the set

$$\mathcal{A}_0 = \{(\psi, \mathbf{n}) \in \mathcal{A} : |\psi| = \rho_0 \text{ a.e. in } \Omega\}. \quad (9)$$

This is a family of uniformly smectic states. We show that boundary conditions are not needed for coercivity and lower semicontinuity properties within  $\mathcal{A}_0$ .

**Lemma 2.1.** *If  $(\psi, \mathbf{n}) \in \mathcal{A}_0$ , then  $\mathcal{R}e \langle \nabla_{\perp}\psi \cdot \nu, \psi^* \rangle = 0$ .*

*Proof.* Let  $\Omega_0 \Subset \Omega := \Omega_1$  be a subdomain such that  $\partial\Omega_0$  is regular and such that  $\{\Omega_t; 0 < t \leq 1\}$  is a smoothly varying, nested family of subdomains. For almost every  $t$  we have  $\nabla_{\perp}\psi \cdot \nu_t \in L^2(\partial\Omega_t)$  and

$$\mathcal{R}e \langle \nabla_{\perp}\psi \cdot \nu_t, \psi^* \rangle_{H^{-\frac{1}{2}}(\partial\Omega_t), H^{\frac{1}{2}}(\partial\Omega_t)} = \mathcal{R}e \int_{\partial\Omega_t} (\nabla_{\perp}\psi \cdot \nu_t) \psi^*. \quad (10)$$

We have  $\mathcal{R}e(\psi^* \nabla\psi) = \frac{1}{2} \nabla|\psi|^2 = 0$  almost everywhere in  $\Omega$ . Thus for almost every  $t$  satisfying (10) we have

$$\mathcal{R}e \langle \nabla_{\perp}\psi \cdot \nu_t, \psi^* \rangle_{H^{-\frac{1}{2}}(\partial\Omega_t), H^{\frac{1}{2}}(\partial\Omega_t)} = 0.$$

Since

$$\begin{aligned} & \mathcal{R}e \langle \nabla_{\perp}\psi \cdot \nu, \psi^* \rangle_{H^{-\frac{1}{2}}(\partial\Omega), H^{\frac{1}{2}}(\partial\Omega)} \\ &= \lim_{t \downarrow 0} \mathcal{R}e \langle \nabla_{\perp}\psi \cdot \nu_t, \psi^* \rangle_{H^{-\frac{1}{2}}(\partial\Omega_t), H^{\frac{1}{2}}(\partial\Omega_t)} \end{aligned}$$

the lemma is proved. □

**Theorem 2.2.** *The energy functional  $\mathcal{F}$  is coercive and weakly lower semi-continuous on  $\mathcal{A}_0$ .*

*Proof.* From (6), (8), and lemma 2.1 we see that there exist constants  $C, \mathcal{M} > 0$  such that

$$\begin{aligned} & C \left( \|D_\perp \psi\|_{H(\operatorname{div}; \Omega)}^2 + \|D_\parallel \psi\|_{H(\operatorname{div}; \Omega)}^2 + \|\psi\|_{L^4(\Omega)}^4 + \|\mathbf{n}\|_{H^1(\Omega)}^2 \right) \\ & \leq \mathcal{F}(\psi, \mathbf{n}) + \mathcal{M}, \end{aligned}$$

for all  $(\psi, \mathbf{n}) \in \mathcal{A}_0$ . Next, if  $(\psi_j, \mathbf{n}_j)$  is a sequence that satisfies, for  $j \rightarrow \infty$ ,

$$\begin{aligned} (\psi_j, \mathbf{n}_j) & \rightharpoonup (\psi, \mathbf{n}) \text{ in } H^1(\Omega), \\ D_\perp \psi_j, D_\parallel \psi_j & \rightharpoonup g_\perp, g_\parallel \text{ in } H(\operatorname{div}; \Omega), \end{aligned}$$

then using  $D_\perp \psi_j = \nabla \psi_j - (\mathbf{n} \cdot \nabla \psi_j) \mathbf{n}_j$ , it is clear that

$$D_\parallel \psi_j \rightharpoonup D_\parallel \psi \text{ and } D_\perp \psi_j \rightharpoonup D_\perp \psi \text{ in } L^2(\Omega).$$

Whence  $g_\perp = D_\perp \psi, g_\parallel = D_\parallel \psi$ , and from (6) and lemma 2.1 we see that

$$\int_\Omega f_{CL}(\psi, \mathbf{n}) \leq \liminf_{j \rightarrow \infty} \int_\Omega f_{CL}(\psi_j, \mathbf{n}_j).$$

□

A subset  $\mathcal{K}$  of a normed linear space is *weakly sequentially closed* if the weak limit of any weakly converging sequence in  $\mathcal{K}$  is also in  $\mathcal{K}$ .

**Corollary 2.3.** *If  $\mathcal{K}$  is a non-empty, weakly sequentially closed subset of  $\mathcal{A}_0$ , then there exists  $(\tilde{\psi}, \tilde{\mathbf{n}}) \in \mathcal{K}$  such that*

$$\mathcal{F}(\tilde{\psi}, \tilde{\mathbf{n}}) = \inf_{(\psi, \mathbf{n}) \in \mathcal{K}} \mathcal{F}(\psi, \mathbf{n}).$$

### 3 Strong Anchoring Boundary Conditions

We next consider the case where  $\psi$  and (or)  $\nabla_\perp \psi \cdot \nu$  are fixed in  $H^{\frac{1}{2}}(\partial\Omega)$  and  $H^{-\frac{1}{2}}(\partial\Omega)$  respectively. For simplicity we focus on the problem of minimizing  $\mathcal{F}$  in

$$\mathcal{A}_1 = \{(\psi, \mathbf{n}) \in \mathcal{A} : \psi - \psi_0 \in H_0^1(\Omega)\}.$$

**Theorem 3.1.** *There exists  $(\tilde{\psi}, \tilde{\mathbf{n}}) \in \mathcal{A}_1$  such that*

$$\mathcal{F}(\tilde{\psi}, \tilde{\mathbf{n}}) = \inf_{(\psi, \mathbf{n}) \in \mathcal{A}_1} \mathcal{F}(\psi, \mathbf{n}).$$

*Proof.* From (6) and (8), we see that there exist constants  $C_1, C_2 > 0$  such that

$$\begin{aligned} & C_1 (\|D_\perp \psi\|_{H(\text{div}; \Omega)}^2 + \|D_\parallel \psi\|_{H(\text{div}; \Omega)}^2 + \|\mathbf{n}\|_{H^1(\Omega)}^2 + \|\psi\|_{4, \Omega}^4) \\ & - (c_\perp + c_\parallel) \mathcal{R}e \langle \nabla_\perp \cdot \nu, \psi^* \rangle \leq \tilde{\mathcal{F}}(\psi, \mathbf{n}) + C_2. \end{aligned}$$

To obtain a coercivity estimate, it suffices to establish that

$$|(c_\perp + c_\parallel) \mathcal{R}e \langle \nabla_\perp \psi \cdot \nu, \psi^* \rangle| \leq \frac{C_1}{2} \|D_\perp \psi\|_{H(\text{div}; \Omega)}^2 + \mathcal{M},$$

for some constant  $\mathcal{M}$  and all  $(\psi, \mathbf{n}) \in \mathcal{A}_1$ .

For any  $(\psi, \mathbf{n}) \in \mathcal{A}_1$ , we have

$$\begin{aligned} & | \langle \nabla_\perp \psi \cdot \nu, \psi^* \rangle | = | \langle D_\perp \psi \cdot \nu, \psi_0^* \rangle | \leq \|D_\perp \psi\|_{H(\text{div}; \Omega)} \|\psi_0\|_{H^1(\Omega)} \\ & \leq \varepsilon \|D_\perp \psi\|_{H(\text{div}; \Omega)}^2 + \mathcal{M}(\varepsilon), \end{aligned}$$

for any  $\varepsilon > 0$ . It follows that if  $\{(\psi_j, \mathbf{n}_j)\}$  is a minimizing sequence for  $\mathcal{F}$  in  $\mathcal{A}_1$  it has a weakly converging subsequence with its limit in  $\mathcal{A}_1$ . In order to prove weak sequential lower semicontinuity for  $\mathcal{F}$ , it suffices to prove that

$$\mathcal{R}e \langle \nabla_\perp \psi_j \cdot \nu, \psi_j^* \rangle \rightarrow \mathcal{R}e \langle \nabla_\perp \psi \cdot \nu, \psi^* \rangle$$

whenever  $\{(\psi_j, \mathbf{n}_j)\}$  are such that

$$(\psi_j, \mathbf{n}_j) \rightharpoonup (\psi, \mathbf{n}) \text{ in } \mathcal{A}_1 \text{ as } j \rightarrow \infty.$$

In fact, for each  $j$ , we have

$$\langle \nabla_\perp \psi_j \cdot \nu, \psi_j^* \rangle = \langle \nabla_\perp \psi_j \cdot \nu, \psi_0^* \rangle$$

and that the mapping

$$g \in H(\text{div}; \Omega) \rightarrow \langle g \cdot \nu, \psi_0^* \rangle$$

is weakly continuous. Thus our assertion follows.  $\square$

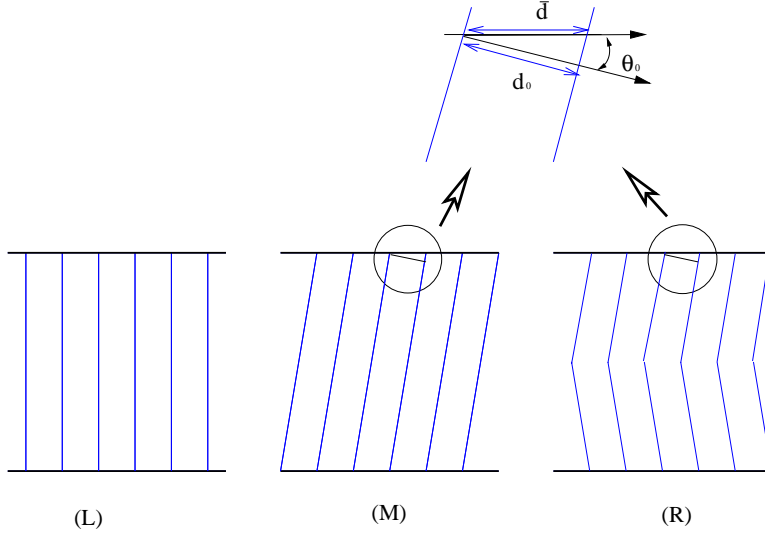


Figure 2: Layer shrinkage from  $SmA$  to  $SmC$

## 4 Weak Anchoring Conditions

We now examine weak anchoring conditions for smectic structures. As the temperature of a liquid crystal is lowered through the  $SmA$ - $SmC$  temperature transition,  $T_{AC}$ , the bulk layer thickness shrinks from  $\bar{d}$  to  $d_0 = \cos \theta_0 \bar{d}$ . In the case that  $\Omega$  is a cell, the transition from the bookshelf layering in the  $SmA$  phase (Figure 2(L)) to either the formation of tilted layers (Figure 2(M)), or chevron structures (Figure 2(R)), in the  $SmC$  phase is possible. In the first case, the layers detach at the surface and slide to the tilted equilibrium. In the second case, the boundary layer structure tends to remain intact. To reduce layer thickness then the layer tilts away from each wall so as to form a chevron within the cell. A weak anchoring energy allows either of these states to be accessible through a quasi-static evolution. (See [6, 11, 26].)

We set

$$\mathcal{A}_2 = \{(\psi, \mathbf{n}) \in \mathcal{A} : \nabla_{\perp} \psi \cdot \nu \in L^2(\partial\Omega)\}.$$

Let  $(\psi, \mathbf{n}) \in \mathcal{A}_2$  and consider

$$\tilde{\mathcal{F}}(\psi, \mathbf{n}) = \mathcal{F}(\psi, \mathbf{n}) + \alpha_1 \int_{\partial\Omega} |\psi - g_1|^2 + \alpha_2 \int_{\partial\Omega} |\nabla_{\perp} \psi \cdot \nu - g_2|^2,$$

where  $\alpha_1 \geq 0, \alpha_2 > 0$ , and  $g_1, g_2 \in L^2(\partial\Omega)$ .

**Theorem 4.1.** *There exists  $(\tilde{\psi}, \tilde{\mathbf{n}}) \in \mathcal{A}_2$  such that*

$$\tilde{\mathcal{F}}(\tilde{\psi}, \tilde{\mathbf{n}}) = \inf_{(\psi, \mathbf{n}) \in \mathcal{A}_2} \tilde{\mathcal{F}}(\psi, \mathbf{n}).$$

Note that having  $\alpha_2 > 0$  is necessary in general. Indeed, if  $\alpha_2 = 0$ , then  $\tilde{\mathcal{F}}(\psi_m, \mathbf{n}_m) \rightarrow -\infty$  as  $m \rightarrow \infty$ , where  $\{(\psi_m, \mathbf{n}_m)\}$  is defined in (5). Thus a first order weak anchoring energy barrier is required for an existence theory.

*Proof.* We first show that  $\tilde{\mathcal{F}}$  is coercive on  $\mathcal{A}_2$ . Since  $\nabla_{\perp} \psi \cdot \nu \in L^2(\partial\Omega)$ , we have

$$\langle \nabla_{\perp} \psi \cdot \nu, \psi^* \rangle = \int_{\partial\Omega} (\nabla_{\perp} \psi \cdot \nu) \psi^*. \quad (11)$$

Thus,

$$\begin{aligned} |\langle \nabla_{\perp} \psi \cdot \nu, \psi^* \rangle| &\leq \|\nabla_{\perp} \psi \cdot \nu\|_{2, \partial\Omega} \cdot \|\psi\|_{2, \partial\Omega} \\ &\leq C \|\nabla_{\perp} \psi \cdot \nu\|_{2, \partial\Omega} \cdot \|\psi\|_{H^1(\Omega)}^{\frac{1}{2}} \cdot \|\psi\|_{2, \Omega}^{\frac{1}{2}} \\ &\leq \varepsilon \left( \|\nabla_{\perp} \psi \cdot \nu\|_{2, \partial\Omega}^2 + \|\psi\|_{H^1(\Omega)}^2 \right) + C(\varepsilon) \|\psi\|_{2, \Omega}^2, \end{aligned}$$

for any  $\varepsilon > 0$ . Using (6) for  $\varepsilon$  sufficiently small, we have

$$\begin{aligned} &C_1 (\|D_{\perp} \psi\|_{H(\text{div}; \Omega)}^2 + \|D_{\parallel} \psi\|_{H(\text{div}; \Omega)}^2 + \|\mathbf{n}\|_{H^1(\Omega)}^2 + \|\psi\|_{4, \Omega}^4 + \|\nabla_{\perp} \psi \cdot \nu\|_{2, \partial\Omega}^2) \\ &\leq \tilde{\mathcal{F}}(\psi, \mathbf{n}) + \mathcal{M}, \end{aligned}$$

for fixed positive constants  $C_1, \mathcal{M}$ . If  $\{(\psi_j, \mathbf{n}_j)\}$  is a minimizing sequence for  $\tilde{\mathcal{F}}$  in  $\mathcal{A}_2$ , it must contain a subsequence  $\{(\psi_{j_m}, \mathbf{n}_{j_m})\}$  that is weakly converging in  $\mathcal{A}_2$  to some  $(\tilde{\psi}, \tilde{\mathbf{n}})$ . In order to prove that

$$\tilde{\mathcal{F}}(\tilde{\psi}, \tilde{\mathbf{n}}) \leq \liminf_{m \rightarrow \infty} \tilde{\mathcal{F}}(\psi_{j_m}, \mathbf{n}_{j_m}),$$

it suffices to establish that

$$\begin{aligned} \lim_{m \rightarrow \infty} \langle \nabla_{\perp} \psi_{j_m} \cdot \nu, \psi_{j_m}^* \rangle &= \lim_{m \rightarrow \infty} \int_{\partial\Omega} (\nabla_{\perp} \psi_{j_m} \cdot \nu) \psi_{j_m}^* \\ &= \int_{\partial\Omega} (\nabla_{\perp} \tilde{\psi} \cdot \nu) \tilde{\psi}^*. \end{aligned}$$

The first equality follows from (11) and the second one follows from the fact that

$$\begin{aligned} \nabla_{\perp} \psi_{j_m} \cdot \nu &\rightharpoonup \nabla_{\perp} \tilde{\psi} \cdot \nu \text{ in } L^2(\partial\Omega), \\ \psi_{j_m} &\rightarrow \tilde{\psi} \text{ in } L^2(\partial\Omega), \end{aligned}$$

as  $m \rightarrow \infty$ . This completes the proof.  $\square$

**Remark 4.2.** We note that if  $(\psi, \mathbf{n}) \in \mathcal{A}$  then  $\psi \in H_{loc}^2(\Omega)$ . Indeed we have  $D \cdot D\psi = D \cdot D_{\perp}\psi + D \cdot D_{\parallel}\psi \in L^2(\Omega)$ . Furthermore  $D \cdot D\psi = \Delta\psi + g$  where by Sobolev's theorem  $g \in L^{\frac{3}{2}}(\Omega)$ . Thus  $\psi \in W_{loc}^{2, \frac{3}{2}}(\Omega)$ . Applying Sobolev's theorem to  $g$  two more times gives  $\psi \in H_{loc}^2(\Omega)$ . In particular if  $\mathcal{B}$  is a bounded set in  $\mathcal{A}$  and  $\Omega' \Subset \Omega$  then there is a constant  $C(\mathcal{B}, \Omega')$  so that if  $(\psi, \mathbf{n}) \in \mathcal{B}$  then

$$\|\psi\|_{H^2(\Omega')} \leq C.$$

We have shown in the case of a  $SmC$  ground state (i.e. if  $c_{\perp} > 0$ ) that variations in  $|\psi|$  allows for energy to concentrate near  $\partial\Omega$ , that this can lead to the nonexistence of minimizers, and that the concentrations can be suppressed by anchoring the layer structure at  $\partial\Omega$ . We can then ask if it would suffice to limit  $\nabla_{\perp}|\psi|^2 \cdot \nu$  instead? Anchoring this term alone would not affect the layer structure at  $\partial\Omega$ . The answer however is that this is too weak a condition. The reason for this is that the function

$$\psi \in \mathcal{A} \rightarrow \langle \nabla_{\perp}\psi \cdot \nu, \psi^* \rangle$$

is not weakly continuous. We illustrate our point by considering the following example. Let  $\Omega$  be the cell from (4),  $K = K_1 = K_2 = K_3 > 0$ ,  $K_4 = 0$  in (3),  $r' = \frac{c_{\perp}^2}{4a_{\perp}}$  in (6), and  $\beta = 0$  in (7). Set

$$\mathcal{A}_3 = \{(\psi, \mathbf{n}) \in \mathcal{A} : \mathcal{R}e\nabla_{\perp}\psi \cdot \nu\psi^* \in L^2(\partial\Omega)\}$$

and consider the energy

$$\mathcal{F}(\psi, \mathbf{n}) + \int_{\partial\Omega} |\mathcal{R}e\nabla_{\perp}\psi \cdot \nu\psi^*|^2 \quad \text{for } (\psi, \mathbf{n}) \in \mathcal{A}_3.$$

Up to a constant this can be rewritten as

$$\begin{aligned} \mathcal{G}(\psi, \mathbf{n}) = & \int_{\Omega} \left( a_{\perp} \left| D \cdot D_{\perp}\psi + \frac{c_{\perp}}{2a_{\perp}}\psi \right|^2 + a_{\parallel} |D \cdot D_{\parallel}\psi|^2 \right. \\ & \left. + c_{\parallel} |D_{\parallel}\psi|^2 + g|\psi|^4 + K|\nabla\mathbf{n}|^2 \right) + \int_{\partial\Omega} \left| \mathcal{R}e\nabla_{\perp}\psi \cdot \nu\psi^* - \frac{c_{\perp}}{2} \right|^2. \end{aligned}$$

Clearly  $\mathcal{G}(\psi, \mathbf{n}) \geq 0$  and  $\mathcal{G}(\psi, \mathbf{n}) = 0$  is not possible. However the sequence

$$\begin{cases} \psi_m(x, y, z) = \left( \frac{c_{\perp}}{2m \sinh(m) \cosh(m)} \right)^{1/2} \cosh(mz) e^{imx}, \\ \mathbf{n}_m = \mathbf{e}_2 \end{cases} \quad (12)$$

is such that  $(\psi_m, \mathbf{n}_m) \in \mathcal{A}_3$  and  $\mathcal{G}(\psi_m, \mathbf{n}_m) \rightarrow 0$  as  $m \rightarrow \infty$ . Thus  $\mathcal{G}$  has no minimizer in  $\mathcal{A}_3$ .

Finally we point out that by using the sequences (5) and (12) respectively, a similar argument shows that we can not weaken the Dirichlet conditions in Section 3 to those of prescribing weaker boundary conditions, such as fixing  $|\psi|$  or  $\nabla_{\perp}|\psi|^2 \cdot \nu$  at  $\partial\Omega$ .

## 5 Energy associated with ferroelectricity

In this section, we include ferroelectric effects. The special feature here is the appearance of a spontaneous or permanent polarization field. The polarization field  $\mathbf{P}$  has its orientation determined with respect to the director field and the smectic layer normal where this is a consequence of molecular packing and is influenced by the particular physical and electrostatic shapes of the liquid crystal molecules assumed in the model. To characterize this for a given  $\psi$ , we define  $\mathbf{N}_{\psi}$  by

$$\mathbf{N}_{\psi} = -\frac{i}{2} (\psi^* \nabla \psi - \psi \nabla \psi^*).$$

Note by Remark 4.2, if  $\mathcal{B}$  is a bounded set in  $\mathcal{A}$ ,  $\Omega' \Subset \Omega$ , and  $(\psi, \mathbf{n}) \in \mathcal{B}$  then  $\|\mathbf{N}_{\psi}\|_{H^1(\Omega')} \leq C(\mathcal{B}, \Omega')$ . If we set  $\psi = \rho e^{i\omega}$ , then  $\mathbf{N}_{\psi} = \rho^2 \nabla \omega$  is parallel to the smectic layer normal. The ground state orientation is depicted in Figure 3, here  $\mathbf{P}$  is orthogonal to  $\mathbf{n}$  and makes an angle  $\phi_0$  with  $\mathbf{N}_{\psi} \times \mathbf{n}$ . We enforce

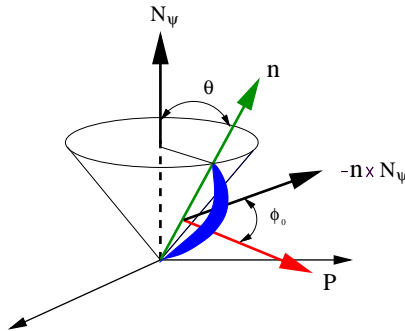


Figure 3:  $\mathbf{n} - \mathbf{N}_{\psi} - \mathbf{P}$  orientation

this orientation by adding a penalty term to the total energy that is as a generalized version of such a term from [1],

$$f_O = \frac{1}{2} K_c \left[ (\mathbf{n} \times \mathbf{N}_{\psi} \cdot \mathbf{P})^2 (\mathbf{n} \cdot \mathbf{N}_{\psi})^2 - \chi_0^2 |\mathbf{P}|^2 |\mathbf{N}_{\psi}|^4 \right]^2 \quad (13)$$

where  $\chi_0 = \cos \phi_0 \sin \theta_0 \cos \theta_0$ . Thus once the smectic tilt angle  $\theta_0$  between  $\mathbf{n}$  and  $\mathbf{N}_{\psi}$  is determined by  $f_{CL}$ , (see Section 1) it follows from (13) that the

molecules orient in such a way that the angle between  $\mathbf{P}$  and  $\mathbf{N}_\psi \times \mathbf{n}$  tend to have a fixed value  $|\cos \phi_0|$  as in Figure 3. In the case of classic chiral smectic C liquid crystals,  $SmC^*$  one has that  $\phi_0 = 0$  or  $\pi$  [19], and in the case of smectic C materials made up of bent-core molecules experiments show that  $\phi_0$  can be any fixed value [3, 16].

The reason for the interest in ferroelectric liquid crystals is that their polar fields are highly sensitive to electro-magnetic forces and thus by reorienting  $\mathbf{P}$  one can effectively reorient  $\mathbf{n}$ . The polarization vector  $\mathbf{P}$  induces a local charge density  $\nabla \cdot \mathbf{P}$  in these materials, and this generates both an electrostatic energy and an energy from electric self-interactions described by Maxwell's equations. The simplest form of the electrostatic energy is

$$f_P = B|\nabla\mathbf{P}|^2 + K_p(\nabla \cdot \mathbf{P} - \gamma)^2 + \frac{1}{\eta^2}(|\mathbf{P}|^2 - P_0^2)^2,$$

for constants  $\gamma$ ,  $K_p > 0$ ,  $B > 0$ , and  $\eta > 0$ . The first term is the polarization gradient which is a typical interfacial energy between uniform states. The  $K_p$ -term describes the energy from local dipole-dipole interactions [1, 7, 9]. In particular, these energy terms are responsible for the modulated polarization phases which exhibit stripe patterns in the  $SmC^*$  and bent-core molecules [7, 9, 15]. Deep within a ferroelectric phase one has  $|\mathbf{P}| \approx P_0$  for a fixed  $P_0 > 0$  and the third term enforces this for  $0 < \eta \ll 1$ .

The energy for electric self-interactions is

$$f_E = -\frac{1}{2} (\varepsilon_\perp |\nabla\varphi|^2 + \varepsilon_a (\mathbf{n} \cdot \nabla\varphi)^2) - \mathbf{P} \cdot \nabla\varphi,$$

subject to the Maxwell's equations

$$\begin{cases} \nabla \cdot [(\varepsilon_\perp I + \varepsilon_a \mathbf{n} \otimes \mathbf{n}) \nabla\varphi + \mathbf{P}] = 0 \text{ in } \Omega, \\ \varphi = \varphi_a \text{ on } \Gamma, \end{cases} \quad (14)$$

where  $\varepsilon_\perp > |\varepsilon_a|$ ,  $\Gamma \subset \partial\Omega$ ,  $\varphi_a \in H^{\frac{1}{2}}(\Gamma)$ , and  $\mathbf{E} = \nabla\varphi$  denotes electric field. As discussed in [24], the term  $-\mathbf{P} \cdot \nabla\varphi$  can be viewed as a charge-charge interaction.

The surface energy related with the polarization is the typical Rapini-Papoular anchoring energy of polar and nonpolar effects [22] given by

$$f_R = \omega_p [|\mathbf{P}| - (\mathbf{P} \cdot \nu)] + \omega_r [|\mathbf{P}|^2 - (\mathbf{P} \cdot \nu)^2],$$

for some constants  $\omega_p > 0$  and  $\omega_r > 0$ .



Let us now discuss the vector  $\mathbf{b}$  appearing in the Oseen-Frank energy (2). It is the spontaneous bending due to the loss of mirror symmetry, i.e. the appearance of a nonzero polarization. In this section, we let  $\mathbf{b} = b_0 \mathbf{P}$  with a constant  $b_0$ . As a special case, in the  $SmC^*$  phase  $c_0 (\mathbf{n} \times \mathbf{N}_\psi)$  is often used in place of  $\mathbf{b}$  in the literature with  $c_0$  representing the tendency of spontaneous bend [11, 19]. We note that in bent-core molecules the asymmetry of the molecular shape can induce the converse of this effect which is called the flexoelectric effect [11]. Our setting is more general in the sense that the  $K_3$ -term includes a flexoelectric effect and also interacts with the electrostatic energy through Maxwell's equation (14).

The constant  $\tau$  in the  $K_2$ -term in (2) is a material parameter reflecting the spontaneous twist arising from the chirality of molecules. A combination of the spontaneous twist and bend gives rise to various physical effects in real systems of ferroelectric liquid crystals. For example, it is observed in the literature [11, pp. 384] that their equal contribution to the structure results in uniform configurations although  $\tau \neq 0$ .

For a bounded open subset  $\Omega$  in  $\mathbb{R}^3$  with a  $C^1$  boundary, let

$$\mathcal{V}_1 = \{\varphi \in H^1(\Omega) : \varphi = \varphi_a \text{ on } \partial\Omega\},$$

where  $\varphi_a$  is a given function in  $H^{\frac{1}{2}}(\partial\Omega)$ . If  $\Omega$  is the cell discussed in Section 1, we define

$$\begin{aligned} \mathcal{H}_{per}(\Omega) &= \{\varphi \in H^1(\Omega) : \varphi(-l, y, z) = \varphi(l, y, z), \varphi(x, -m, z) = \varphi(x, m, z) \\ &\quad \text{for } x \in (-l, l), y \in (-m, m), \text{ and } z \in (-h, h)\}, \\ \mathcal{V}_2 &= \{\varphi \in \mathcal{H}_{per}(\Omega) : \varphi = \varphi_a \text{ on } z = \pm h\}, \end{aligned}$$

where  $\varphi_a$  satisfies periodic conditions in  $\mathcal{H}_{per}$  for each  $z = \pm h$ . Given a domain  $\Omega$ , we take as an admissible set

$$\begin{aligned} \bar{\mathcal{A}} &= \{(\mathbf{n}, \mathbf{P}, \psi, \varphi) : (\mathbf{n}, \psi) \in \mathcal{A}, \mathbf{P} \in H^1(\Omega, \mathbb{R}^3), \mathbf{P} \cdot \nu \in H^{\frac{1}{2}}(\partial\Omega), \\ &\quad \varphi \in \mathcal{V}, \text{ and } (\mathbf{n}, \mathbf{P}, \varphi) \text{ satisfies (14)}\}, \end{aligned}$$

where  $\mathcal{A} \in \{\mathcal{A}_0, \mathcal{A}_1, \mathcal{A}_2\}$ , and  $\mathcal{V} \in \{\mathcal{V}_1, \mathcal{V}_2\}$  are chosen according to the type of the domain  $\Omega$ .

**Theorem 5.1.** *The energy functional*

$$\mathfrak{F} = \int_{\Omega} (f_{CL} + f_N + f_O + f_P + f_E) + \int_{\partial\Omega} (f_R + f_S)$$

*achieves its minimum on  $\bar{\mathcal{A}}$ .*

*Proof.* One sees that  $\mathfrak{F}$  is coercive. Since we already know that  $\int_{\Omega}(f_N + f_{CL}) + \int_{\partial\Omega} f_S$  is lower semicontinuous, it remains to show that the energy associated with the polarization is lower semicontinuous. For this, we let  $\{(\mathbf{n}_j, \mathbf{P}_j, \psi_j, \varphi_j)\}$  be a minimizing sequence. We may assume that  $\inf_{\bar{\mathcal{A}}} \mathfrak{F}$  is finite. Otherwise, lower semicontinuity is trivial.

Passing to a subsequence if necessary, we obtain a weak limit  $(\psi_{\infty}, \mathbf{n}_{\infty}, \mathbf{P}_{\infty}, \varphi_{\infty})$  so that as  $j \rightarrow \infty$

$$\begin{aligned} \mathbf{N}_{\psi_j} &\rightharpoonup \mathbf{N}_{\psi_{\infty}} \text{ in } L^2_{loc}(\Omega), \\ \nabla \mathbf{P}_j &\rightharpoonup \nabla \mathbf{P}_{\infty} \text{ in } L^2(\Omega), \\ \mathbf{P}_j &\rightarrow \mathbf{P}_{\infty} \text{ in } L^r(\Omega) (1 < r < 6), \\ \mathbf{P}_j &\rightharpoonup \mathbf{P}_{\infty} \text{ in } L^6(\Omega), \\ \mathbf{P}_j \cdot \nu &\rightarrow \mathbf{P}_{\infty} \cdot \nu \text{ in } L^2(\partial\Omega), \\ \nabla \varphi_j &\rightharpoonup \nabla \varphi_{\infty} \text{ in } L^2(\Omega), \end{aligned}$$

For each  $j$ , set

$$G_j = \left[ (\mathbf{n}_j \times \mathbf{N}_{\psi_j} \cdot \mathbf{P}_j)^2 (\mathbf{n}_j \cdot \mathbf{N}_{\psi_j})^2 - \chi_0^2 |\mathbf{P}_j|^2 |\mathbf{N}_{\psi_j}|^4 \right]^2.$$

Since  $G_j$  converges to  $G_{\infty}$  pointwise a.e., it follows from Fatou's lemma that

$$\int_{\Omega} G_{\infty} \leq \liminf_{j \rightarrow \infty} \int_{\Omega} G_j.$$

Writing  $f_E = -\frac{1}{2} \mathbf{P} \cdot \nabla \varphi$  by (14), we see that  $\int_{\Omega} (f_P + f_E) + \int_{\partial\Omega} f_R$  is lower semicontinuous. Therefore, we have

$$\mathfrak{F}(\mathbf{n}_{\infty}, \mathbf{P}_{\infty}, \psi_{\infty}, \varphi_{\infty}) \leq \liminf_{j \rightarrow \infty} \mathfrak{F}(\mathbf{n}_j, \mathbf{P}_j, \psi_j, \varphi_j).$$

Furthermore,  $(\mathbf{n}_{\infty}, \mathbf{P}_{\infty}, \varphi_{\infty})$  satisfies (14) (see theorem 3.3 in [24]) so that

$$(\mathbf{n}_{\infty}, \mathbf{P}_{\infty}, \varphi_{\infty}) \in \bar{\mathcal{A}}.$$

Therefore there exists a minimizer of  $\mathfrak{F}$  on  $\bar{\mathcal{A}}$ .  $\square$

Our result in this section is an extension of the previous work in [29] where the authors studied 2-D structures of the bent-core molecules in the polarization modulated and layer undulated phase without Maxwell's equations.

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