ANALYTIC DESCRIPTION OF LAYER UNDULATIONS IN SMECTIC A LIQUID CRYSTALS

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Abstract. *We investigate layer undulations of smectic A liquid crystals when a magnetic field is applied in the direction parallel to smectic layers. In a prior work [10], we characterized the critical field using the Landau-de Gennes model of smectic A liquid crystals. In this paper, we obtain the asymptotic expression of unstable modes using the* Γ*-convergence theory and the sharper estimate of the critical field. Under the assumption that the layers are fixed at the boundaries, the maximum undulation occurs in the middle of the cell and the displacement amplitude decreases as approaching the boundaries. We also obtain the estimate of the critical field, which is consistent with Helfrich-Hurault theory. With the natural boundary condition, however, the displacement amplitude does not diminish near the boundary and the critical field is reduced compared to the one calculated in the classic theory. This is consistent with the experiment done by Laverentovich et al. [14]. Numerical simulations confirm the predictions of the analysis.*

1. Introduction. We consider smectic A liquid crystals confined in two flat plates and uniformly aligned in a way that the smectic layers are parallel to the bounding plates. If a magnetic field is applied in a direction parallel to the smectic layers, the instability occurs above the threshold magnetic field. When the magnetic field reaches the critical threshold, one can see periodic perturbation of the layers. This phenomenon is called the Helfrich-Hurault effect (See [12] and [13].) We show this phenomenon analytically by studying the minimizer of the second variation of Landau-de Gennes free energy ([6]) at the undeformed state. We also perform numerical simulations to illustrate layer undulations.

Liquid crystal phases form when a material has a degree of positional or orientational ordering yet stays in a liquid state. In the nematic state, molecules tend to align themselves along a preferred direction with no positional order of centers of mass. The unit vector field $\mathbf{n}$, nematic director, represents the average direction of molecular alignment. Moreover, if the liquid crystal is chiral, $\mathbf{n}$ follows a helical pattern, with temperature dependent pitch. Upon lowering the temperature, or increasing concentration, according to whether the liquid crystal is thermotropic or lyotropic, the nematic liquid crystal experiences a transition to the smectic A phase with molecules arranged along equally spaced layers. The molecules tend to align themselves along the direction perpendicular to the layers.

The Helfrich-Hurault effect in a lamellar system can be caused by magnetic/electric field [7, 10, 14, 17, 19, 21] or by mechanical tension [7, 18]. In this paper, we study the magnetic field driven instabilities in smectic A liquid crystals. Helfrich and Hurault proposed the model that can explain the periodic perturbations in cholesteric liquid crystals under a magnetic field or an electric field applied parallel to the helical axis ([12], [13]) in an infinite sample. They equated the director and the layer normal and assumed that the layers are fixed at the cell boundaries, i.e., the undulations vanish at the boundaries. Still with these assumptions, Stewart extended the classic Helfrich-Hurault theory to three dimensional finite samples of smectic A liquid crystals in [19]. More recently, he performed the analysis with the model where the director and the smectic layer normal may differ [21].

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The notion of Γ-convergence has been introduced by De Giorgi (See [3], [5]) in the 70s. As the small parameter ε tends 0, the solution of variational problem is reduced to that of limiting problem. In [4], the authors used the Γ-convergence theory to study the switching process in elongated thin film elements by micromagnetic model. They identified four qualitatively different regimes with the choice of material parameters and verified the periodic oscillation in the direction of long axis in one of the regimes.

Experimental studies of undulations of two dimensional and three dimensional systems were performed in [14] and [17], respectively. They used cholesteric liquid crystals with a pitch $5\mu m$ and $50-70\mu m$ cell thickness for the optical study. Since the layer thickness of smectic A liquid crystals is in the nanometer range (nm), it is too small to visualize the layer distortions. Their experiments show that there are layer undulations on the boundary of the sample. Motivated by the experimental result, Lavrentovich *et al.* proposed the model with weak anchoring condition so that the undulations are allowed to appear on the boundaries. By making an ansatz of periodic undulations, they show that their model explains the experiment better than the classic Helfrich-Hurault theory. The model presented in this paper with the natural boundary condition on the layer function also agrees with the experiment.

In sections 2 and 3, we present the model and the geometry for our problem and state the stability of the undeformed state of smectic A liquid crystals. Also see [10]. We define the critical field H_c above which the undeformed state is unstable and below which the undeformed state is stable. In [10], we derived the estimate of the threshold in terms of the cell thickness. More precisely, we proved that there exist universal constants $0 < c_1 < c_2$, such that, if $2d$ is the cell thickness, then the critical field H_c satisfies

$$\left(\frac{c_1 K}{\chi_a d\lambda}\right)^{\frac{1}{2}} \le H_c \le \left(\frac{c_2 K}{\chi_a d\lambda}\right)^{\frac{1}{2}}, \tag{1.1}$$

where K, χ_a, λ are material constants, which will be discussed below. This estimate is consistent with the result found in the classic Helfrich-Hurault theory (see p.363 of [7] and [13]). We should mention that the scaling of the critical field in this case is different from the threshold for Fredericks transition of nematic liquid crystals, where the critical field is proportional to $1/d$ [23].

In section 4, we study the Γ-convergence of the energy when the layers are fixed at the boundary. In order to study the limiting problem with the help of Γ-convergence theory, we take the small parameter $\varepsilon = h^{-1}$ where h is the ratio of the layer thickness to the cell thickness. In [7], the parameter h is taken by 0.5×10^6. If we assume that there are no layer perturbations at the boundary, we see that the minimizer of the Γ-limit is the periodic oscillation. We recover from Γ-convergence the sharper estimate of the critical field,

$$H_c \approx \left(\frac{\pi K}{\chi_a d\lambda}\right)^{\frac{1}{2}}. \tag{1.2}$$

Furthermore, we prove that the maximum undulation occurs in the middle of the cell and the displacement amplitude decreases as approaching the boundary by a cosine function. These are consistent with the result found in classic Helfrich-Hurault theory.

In section 5, we allow layer undulations at the boundaries by eliminating the Dirichlet boundary condition for the layer function. The formulation of Γ-limit has been motivated from the work in [16] where they studied the Allen-Cahn functional with a Dirichlet boundary condition. Instead of the periodic profile as in section 4, the director has boundary layers at both end points ($y = \pm d$). The frequency of the oscillation is no longer proportional to $d^{-1/2}$, in fact, it can be shown that the frequency is of smaller order than $d^{-1/2}$. Also, the Γ-convergence theory gives the sharper estimate of the critical field,

$$H_c \approx \left(\frac{K}{\chi_a d\lambda} \right)^{\frac{1}{2}}. \tag{1.3}$$

One can see that the natural boundary condition reduces the critical field compared to the classical threshold field (1.2).

In section 6, we show layer undulation patterns numerically by solving the gradient flow equations with two different boundary conditions discussed in sections 4 and 5. The simulations show that if the natural boundary condition is imposed on the layer function, the threshold field and the frequency of the undulation pattern are lower than in the classic theory, which is a good agreement with the predictions of the analysis. Furthermore the layer perturbation does not vanish at the boundaries as expected from the experiment and also from our analysis.

2. The formulation of the problem.

2.1. The free energy and the geometry. The total free energy density of smectic A liquid crystals consists of the nematic f_n and smectic f_s part. The Oseen-Frank energy density for a nematic is given by

$$\begin{aligned} f_n &= K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2 \\ &\quad + (K_2 + K_4)(tr(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2), \end{aligned}$$

where K_1, K_2 and K_3 are the splay, twist, and bend elastic constants, respectively. The last term in f_n is a null-Lagrangian since its integral only depends on the boundary values of $\mathbf{n}$. We consider the energy with one constant approximation case, $K_1 = K_2 = K_3 = \frac{K}{2} > 0$ and $K_4 = 0$. Then the nematic energy density becomes

$$\frac{K}{2}|\nabla \mathbf{n}|^2.$$

In order to associate smectic and nematic structure with a state $(\mathbf{n}, \Psi)$ we write

$$\Psi(\mathbf{x}) = \rho(\mathbf{x})e^{iq\varphi(\mathbf{x})}.$$

Then the molecular mass density is defined by

$$\delta(\mathbf{x}) = \rho_0(\mathbf{x}) + \frac{1}{2}(\Psi(\mathbf{x}) + \Psi^*(\mathbf{x})) = \rho_0(\mathbf{x}) + \rho(\mathbf{x}) \cos q\varphi(\mathbf{x}),$$

where ρ_0 is a locally uniform mass density, $\rho(\mathbf{x})$ is the mass density of the smectic layers, and φ parametrizes the layers so that $\nabla\varphi$ is the direction of the layer normal. Also, q is the wave number and $2\pi/q$ is the layer thickness.

The Landau-de Gennes energy density for smectic A is given by

$$f_s = \frac{C}{2}|\nabla\Psi - iq\mathbf{n}\Psi|^2,$$

where C is a positive constant. The energy density $f_n + f_s$ with $r|\Psi|^2 + \frac{g}{2}|\Psi|^4$ was used in [1] to study a phase transition and stability analysis of equilibrium states.

Since we investigate smectic structure far from the nematic–smectic transition, we may assume that the magnitude of the smectic order parameter is a constant, i.e., ρ is a constant. Then f_s becomes

$$f_s = \frac{Cq^2\rho^2}{2}|\nabla\varphi - \mathbf{n}|^2.$$

This energy density vanishes when $\nabla\varphi = \mathbf{n}$, which describes the configuration of smectic A liquid crystals.

The magnetic free energy density is given by [7], [20]

$$f_m = -\frac{\chi_a}{2}(\mathbf{n}\cdot\mathbf{H})^2 = -\frac{\chi_a}{2}\sigma^2(\mathbf{n}\cdot\mathbf{h})^2,$$

where χ_a is the magnetic anisotropy, $\mathbf{H} = \sigma\mathbf{h}$, and $\sigma = |\mathbf{H}|$. We assume that $\chi_a > 0$. Then the director prefers to be parallel to the direction of the applied magnetic field.

Collecting all contributions to the free energy, the free energy density for the one-constant approximation model becomes

$$f = \frac{K}{2}|\nabla\mathbf{n}|^2 + \frac{B}{2}|\nabla\varphi - \mathbf{n}|^2 - \frac{\chi_a}{2}\sigma^2(\mathbf{h}\cdot\mathbf{n})^2, \tag{2.1}$$

where $B = Cq^2\rho^2$ is called the de Gennes compressibility constant.

In this paper, we consider a two dimensional domain

$$\Omega = (-L, L) \times (-d, d),$$

where $L = cd$ for some constant $c > 0$. We also assume that $\mathbf{h} = (1, 0)$ so that the magnetic field tends to make the director orient along the x direction. We impose the periodic boundary conditions for ϕ and $\mathbf{n}$ in the x direction so that we can minimize the unnecessary boundary effect, while we assume strong anchoring condition for $\mathbf{n}$ on the boundary plates, i.e., simply

$$\mathbf{n}(x, \pm d) = (0, 1) \qquad \text{for all } x \in [-L, L]. \tag{2.2}$$

3. Stability of undeformed states. We make the problem dimensionless by introducing new variables

$$(\widetilde{x}, \widetilde{y}) = (\frac{x}{\lambda}, \frac{y}{\lambda}) \qquad \text{and} \qquad \varphi = \lambda\,\phi,$$

where $\lambda = \sqrt{\frac{K}{B}}$ is of the order of the smectic layer thickness. Then the free energy (2.1) becomes

$$\frac{B\lambda^2}{2}\int_{\widetilde{\Omega}}\left(|\widetilde{\nabla}\mathbf{n}|^2 + (\widetilde{\nabla}\phi - \mathbf{n})^2 - \kappa(\mathbf{n}\cdot\mathbf{h})^2\right)d\widetilde{\mathbf{x}}, \tag{3.1}$$

where the dimensionless parameters are given by

$$\kappa = \frac{\chi_a\sigma^2}{B}, \quad \widetilde{\Omega} = (-\widetilde{L}, \widetilde{L}) \times (-h, h), \quad h = \frac{d}{\lambda}, \quad \widetilde{L} = \frac{L}{\lambda}$$

Since h is the ratio of the cell thickness to the layer thickness, we may assume that $h \gg 1$. In fact, the values $d = 1mm$ and $\lambda = 20\mathring{A}$ are employed in [7]. Then $h = 5 \times 10^5$.

From the fact $|\mathbf{n}| = 1$, we can introduce the scalar variable θ, with $0 \le \theta < 2\pi$, such that

$$\mathbf{n} = (\sin\theta, \cos\theta).$$

Then the free energy (3.1) becomes

$$\mathfrak{F} = \int_{\widetilde{\Omega}} (\phi_{\widetilde{x}} - \sin\theta)^2 + (\phi_{\widetilde{y}} - \cos\theta)^2 + |\widetilde{\nabla}\theta|^2 - \kappa \sin^2\theta)\, d\widetilde{x}\, d\widetilde{y} \tag{3.2}$$

and the corresponding boundary condition on θ is the homogeneous Dirichlet boundary condition on the top and the bottom of the plate. This energy (3.2) has a trivial critical point, $\theta = 0, \phi = \widetilde{y}$, which describes the undeformed state where the layers are parallel to the bounding plates and the directors are aligned in the $\widetilde{y}$ direction. The second variation of the energy at the undeformed state, $\phi_0 = \widetilde{y}$, and $\theta_0 = 0$, gives

$$\begin{aligned} \frac{1}{2} D^2 \mathfrak{F}(\theta_0 + t\theta, \phi_0 + t\phi) &:= \frac{1}{2}\frac{d^2}{dt^2}\Big|_{t=0} \mathfrak{F}(\theta_0 + t\theta, \phi_0 + t\phi) \\ &= \int_{\widetilde{\Omega}} ((\phi_{\widetilde{x}} - \theta)^2 + \phi_{\widetilde{y}}^2 + |\widetilde{\nabla}\theta|^2 - \kappa|\theta|^2)\, d\widetilde{x} d\widetilde{y}. \end{aligned} \tag{3.3}$$

The undeformed state, (θ_0, ϕ_0), is stable if the second variation is nonnegative at (θ_0, ϕ_0).

Here, the admissible sets $\mathcal{A}$ is given by

$$\begin{aligned} \mathcal{A} = \{(\theta, \phi) \in H^1(\widetilde{\Omega}) \times H^1(\widetilde{\Omega}) : \|\theta\|_2 = 1, \theta(\widetilde{x}, \pm h) = 0 \text{ for all } \widetilde{x}, \\ \theta \text{ and } \phi \text{ satisfy the periodic boundary condition in the } \widetilde{x} \text{ direction}\}. \end{aligned}$$

Setting

$$\mathcal{G}(\theta, \phi) := \int_{\widetilde{\Omega}} ((\phi_{\widetilde{x}} - \theta)^2 + \phi_{\widetilde{y}}^2 + |\widetilde{\nabla}\theta|^2)\, d\widetilde{x} d\widetilde{y}, \tag{3.4}$$

one can see from (3.3) that the critical field κ_c is defined by

$$\kappa_c = \inf_{(\theta,\phi)\in\mathcal{A}} \mathcal{G}(\theta, \phi). \tag{3.5}$$

Thus, the undeformed state, (θ_0, ϕ_0), is stable if $\kappa \le \kappa_c$ and unstable if $\kappa > \kappa_c$. In particular, when $\kappa = \kappa_c$, the stable bifurcation is possible. In the section 3 of [15], they proved that the critical field κ_c is achieved when Dirichlet boundary condition is imposed on $\partial\Omega$.

Another admissible set we consider is

$$\mathcal{A}_0 = \{(\theta, \phi) \in \mathcal{A} : \phi(\widetilde{x}, \pm h) = 0 \text{ for all } \widetilde{x}\}.$$

Since ϕ is the layer perturbation, the set $\mathcal{A}_0$ corresponds to the setting in the classic Helfrich-Hurault theory, where the layers are fixed at the cell boundaries. Then, as above, the critical field κ_0 is defined by

$$\kappa_c^0 = \inf_{(\theta,\phi)\in\mathcal{A}_0} \mathcal{G}(\theta, \phi). \tag{3.6}$$

3.1. Factorization. The periodic boundary conditions allow us to use the Fourier series representation.

$$\theta(\widetilde{x},\widetilde{y}) = \sum_{n=-\infty}^{\infty} \theta_n(\widetilde{y}) e^{i\mu_n \widetilde{x}} \quad \text{and} \quad \phi(\widetilde{x},\widetilde{y}) = \sum_{n=-\infty}^{\infty} \phi_n(\widetilde{y}) e^{i\mu_n \widetilde{x}}$$

where $\mu_n = 2\pi n/\widetilde{L}$. Then (3.4) becomes

$$\mathcal{G}(\theta,\phi) = 2\widetilde{L}\int_{-h}^{h} \left(\sum_{n=-\infty}^{\infty} (|\theta_n'|^2 + \mu_n^2|\theta_n|^2 + |\theta_n - i\mu_n\phi_n|^2 + |\phi_n'|^2) \right) d\widetilde{y} \tag{3.7}$$

where $'$ denotes the differentiation with respect to $\widetilde{y}$. Setting $\psi = i\phi$, we define

$$\begin{aligned} \kappa_n &= \inf_{(\theta,\psi)\in\mathcal{B}} \int_{-h}^{h} (|\theta'|^2 + \mu_n^2|\theta|^2 + |\theta - \mu_n\psi|^2 + |\psi'|^2)\, d\widetilde{y} \\ &:= \inf_{(\theta,\psi)\in\mathcal{B}} E(\theta,\psi,n), \end{aligned} \tag{3.8}$$

where

$$\mathcal{B} = \{(\theta,\psi) \in W_0^{1,2}(-h,h) \times W^{1,2}(-h,h) : \int_{-h}^{h} |\theta(\widetilde{y})|^2\, d\widetilde{y} = 1\}.$$

Then, as in [2] and in [10], we have

$$\kappa_c = \inf_n \kappa_n. \tag{3.9}$$

Using (3.9), we showed in [10] that if $L \geq h \geq 1$, then there exist universal constants c_1 and c_2 such that

$$\frac{c_1}{h} \leq \kappa_c \leq \frac{c_2}{h}, \tag{3.10}$$

which is equivalent to (1.1), where the estimate is expressed in terms of the real parameters.

Similarly, we define the critical field κ_n^0 by

$$\kappa_n^0 = \inf_{(\theta,\psi)\in\mathcal{B}_0} E(\theta,\psi,n),$$

where

$$\mathcal{B}_0 = \{(\theta,\psi) \in \mathcal{B} : \psi \in W_0^{1,2}(-h,h)\},$$

and it follows

$$\kappa_c^0 = \inf_n \kappa_n^0. \tag{3.11}$$

Note that the critical field κ_c^0 has the same scaling (3.10) as κ_c, since the construction (θ,ψ) for the upper bound from [10] belongs to $\mathcal{B}_0$.

Lemma 3.1. *For each integer n, the infimum of (3.8) in $\mathcal{B}$ or $\mathcal{B}_0$ is taken by real valued functions (θ_n,ψ_n), which satisfy the system*

$$-\theta_n^{''} + (\mu_n^2+1)\theta_n - \mu_n\psi_n = \kappa_n\theta_n \tag{3.12}$$

$$-\psi_n^{''} + \mu_n^2\psi_n - \mu_n\theta_n = 0 \tag{3.13}$$

with the boundary condition

$$\theta_n(\pm h) = 0 \tag{3.14}$$

$$\psi_n'(\pm h) = 0 \quad or \quad \psi_n(\pm h) = 0. \tag{3.15}$$

Any solution to (3.12) and (3.13) with the condition (3.14) and (3.15) is of the form $(c\theta_n, c\psi_n)$ *with some constant* $c \in \mathbb{C}$ *such that* $|c| = 1$.

Proof. We only need to prove that κ_n is simple. We consider ψ as a function of θ, which is the solution to the boundary value problem (3.13) and (3.15). Fix n and suppose θ_1 and θ_2 are two eigenfunctions with κ_n and write $\psi_j = \psi(\theta_j)$ for $j = 1, 2$. Setting, for $j = 1, 2$,

$$L(\theta_j) = \theta_j'' - (1 + \mu_n^2)\theta_j + \mu_n \psi_j,$$

we have from (3.12)

$$L(\theta_j) = -\kappa_n \theta_j.$$

Computing $L(\theta_1)\theta_2 - L(\theta_2)\theta_1$ gives

$$-W'(\theta_1, \theta_2) + \mu_n(\psi_1\theta_2 - \psi_2\theta_1) = 0 \tag{3.16}$$

where $W(\theta_1, \theta_2)$ denotes the Wronskian of θ_1 and θ_2. Using (3.13) for the second term of (3.16), we have

$$-W'(\theta_1, \theta_2) - W'(\psi_1, \psi_2) = 0.$$

Then, by the boundary conditions (3.14) and (3.15), we get

$$W(\theta_1, \theta_2) + W(\psi_1, \psi_2) = 0.$$

Then one can deduce that $\theta_1 + \psi_1$ and $\theta_2 + \psi_2$ are linearly dependent. There is a nonzero constant c such that $\theta_2 + \psi_2 = c(\theta_1 + \psi_1)$. Note that $\psi_j = \psi(\theta_j)$ and $\psi(\theta)$ is a linear function in θ. Thus we have

$$\theta_2 - c\theta_1 = -\psi(\theta_2 - c\theta_1). \tag{3.17}$$

If $\psi'(\pm h) = 0$, by (3.17) and the definition of $\psi(\theta_2 - c\theta_1)$, setting $f = \theta_2 - c\theta_1$, we have

$$\begin{aligned} &f'' - (\mu_n^2 + \mu_n)f = 0 \text{ in } (-h, h) \\ &f(\pm h) = f'(\pm h) = 0. \end{aligned}$$

Then $f \equiv 0$ and therefore $\theta_2 = c\theta_1$.

If $\psi(\pm h) = 0$, from (3.12), (3.13) and (3.17), we have

$$f = \kappa_n f.$$

Then $f \equiv 0$ since $\kappa_n < \frac{c_2}{h} \ll 1$ from (3.10). (See [10]). We proved that κ_n is simple. Thus, as in the Sturm-Liouville theory, one can see that (θ_n, ψ_n) is the unique real solution up to the multiplicative constant $c \in \mathbb{C}$ with $|c| = 1$. ∎

REMARK 3.1. *As observed in Lemma 2.3 in [2], since* $\lim_{|n|\to\infty}\kappa_n = \infty$, *we can have* $\kappa = \kappa_n$ *for finitely many* n *and thus the set of minimizers of* $\mathcal{G}$ *spans a finite dimensional subspace with a basis given by*

$$\{(\theta_{n_j}(\widetilde{y})e^{i\mu_{n_j}\widetilde{x}}, \psi_{n_j}(\widetilde{y})e^{i\mu_{n_j}\widetilde{x}})\}_{j=1}^{j=k},$$

where $(\theta_{n_j}, \psi_{n_j})$ *are the minimizer of* $E(\theta_{n_j}, \psi_{n_j}, n_j)$ *with the property described in Lemma 3.1 and* $\kappa_c = \kappa_{n_j}$ *for* $j = 1, 2, \cdots, k$.

Since the suggested value for h in [7] is $h = 0.5 \times 10^6$, we may set the small parameter $\varepsilon = 1/h$. Introducing the transformations, $x = \widetilde{x}/h, y = \widetilde{x}/h$, and $u = \phi/h$, the energy in (3.2) becomes

$$\mathfrak{F}(\theta, u) = \frac{1}{\varepsilon}\int_D \Big(\frac{(u_x - \sin\theta)^2}{\varepsilon} + \frac{(u_y - \cos\theta)^2}{\varepsilon} + \varepsilon|\nabla\theta|^2 - \sigma\sin^2\theta\Big)\,dx\,dy$$

where $D = (-c, c) \times (-1, 1)$ and $\sigma = h\kappa$. As in (3.3), one can see that the critical field σ_c is defined by

$$\sigma_c = \inf_{(\theta,u)\in\mathcal{A}} \mathcal{J}(\theta, u), \tag{3.18}$$

where

$$\mathcal{J}(\theta, u) := \int_D \Big(\frac{1}{\varepsilon}(u_x - \theta)^2 + \frac{1}{\varepsilon}u_y^2 + \varepsilon|\nabla\theta|^2\Big)\,dxdy. \tag{3.19}$$

From (3.10), there exist universal constants c_1 and c_2 such that

$$c_1 \le \sigma_c \le c_2. \tag{3.20}$$

Using notations $\delta = \delta(\varepsilon) = \varepsilon\mu^2$, $\mu = \mu_n = \frac{2\pi n}{c}$, and $I = (-1, 1)$, we have

$$\mathcal{J}(\theta, u) = 2c\int_I \Big(\frac{1}{\varepsilon}|i\mu u - \theta|^2 + \frac{1}{\varepsilon}(u')^2 + \varepsilon\mu^2\theta^2 + \varepsilon(\theta')^2\Big)\,dy. \tag{3.21}$$

Since we are interested in n such that $\sigma_c = \sigma_n$ and since $\sigma_0 \ge 1$, we may assume that $\mu_n \neq 0$ and use $\varphi = i\mu u$ to have

$$\begin{aligned}\sigma_n &= \inf_{(\theta,\varphi)\in\mathcal{B}} \int_I (\varepsilon|\theta'|^2 + \delta|\theta|^2 + \frac{1}{\varepsilon}|\theta - \varphi|^2 + \frac{1}{\delta}|\varphi'|^2)\,dy \\ &:= \inf_{(\theta,\varphi)\in\mathcal{B}} F_\varepsilon(\theta, \varphi, \delta),\end{aligned} \tag{3.22}$$

where

$$\mathcal{B} = \{(\theta, \varphi) \in W_0^{1,2}(I) \times W^{1,2}(I) : \int_{-1}^{1} |\theta(y)|^2\,dy = 1\}.$$

From (3.20), we can see that the infimum of F is of order 1. In section 4, we study the Γ-convergence theory of F_ε with $\varphi(\pm 1) = 0$ for the configuration of the minimizer. This corresponds to the assumption that the layers are fixed at the boundary cell. In section 5, we use natural boundary conditions to allow the perturbation of the layers at the boundary.

4. Fixed layers on the boundary. In this section, we impose the homogeneous Dirichlet boundary condition for φ on the parallel plates so that the layers are fixed at the boundary of the cell. This is the case in classic Helfrich-Hurault theory.

Let

$$F_\varepsilon(\theta,\varphi,\delta) := \begin{cases} \int_I (\varepsilon\theta'^2 + \frac{1}{\delta}\varphi'^2 + \delta\theta^2 + \frac{1}{\varepsilon}(\theta-\varphi)^2)\,dz & \text{if } (\theta,\varphi,\delta) \in [W_0^{1,2}(I)]^2 \times \mathbb{R}^+, \\ +\infty & \text{else,} \end{cases} \tag{4.1}$$

and

$$F_0(\theta,\varphi,\delta) := \begin{cases} \int_I (\delta\theta^2 + \frac{1}{\delta}\theta'^2)\,dz & \text{if } \theta = \varphi \in W_0^{1,2}(I), \\ +\infty & \text{else.} \end{cases} \tag{4.2}$$

We look for a minimizer of F_ε with the constraint

$$\int_I |\theta(z)|^2\,dz = 1. \tag{4.3}$$

PROPOSITION 4.1. *(Compactness) Let the sequences* $\{\varepsilon_j\}_{j\uparrow\infty} \subset (0,\infty)$, $\{\theta_j\}_{j\uparrow\infty} \subset W_0^{1,2}(I)$, $\{\varphi_j\}_{j\uparrow\infty} \subset W_0^{1,2}(I)$ *and* $\{\delta_j\}_{j\uparrow\infty} \subset (0,\infty)$ *be such that*

$$\varepsilon_j \to 0, \qquad \int_I |\theta_j|^2\,dy = 1, \text{ and } \qquad \{F_{\varepsilon_j}(\theta_j,\varphi_j,\delta_j)\}_{j\to\infty} \qquad \text{is bounded.}$$

Then

$$\{\theta_j,\varphi_j,\delta_j\}_{j\uparrow\infty} \quad \text{is relatively compact in } L^2(I)\times L^2(I)\times\mathbb{R}.$$

Moreover, the limit $(\theta,\varphi) \in W_0^{1,2}(I) \times W_0^{1,2}(I)$.

Proof. Let $F_{\varepsilon_j}(\theta_j,\varphi_j,\delta_j) \le C$ where C is denoted by a universal positive constant which may differ from line to line.. Then $\delta_j \le C$ and thus $\{\delta_j\}_{j\uparrow\infty}$ is relatively compact in $\mathbb{R}$. Since we have $\int_I |\theta_j|^2\,dz = 1$, it follows, for a subsequence, still labeled $\{\theta_j\}$ that

$$\theta_j \rightharpoonup \theta \quad \text{in } L^2(I).$$

Note that we have $\|\varphi_j\|_{W^{1,2}(I)} \le C$ from

$$\int_I |\varphi_j|^2\,dz \le 2\int_I ((\varphi_j-\theta_j)^2 + \theta_j^2)\,dz \le C\varepsilon_j + 1 \le C$$

and

$$\int_I |\varphi_j'|^2\,dz \le C\delta_j < C.$$

Thus we have

$$\varphi_j \rightharpoonup \varphi \quad \text{in } W^{1,2}(I) \qquad \text{and} \qquad \varphi_j \to \varphi \quad \text{in } L^2(I).$$

The lower semicontinuity of the norm gives

$$\int_I (\theta-\varphi)^2\,dy \le \liminf_{j\to\infty} \int_I (\theta_j-\varphi_j)^2\,dz \le \lim_{j\to\infty}(C\varepsilon_j) = 0$$

so that $\theta = \varphi$ and $\theta \in W^{1,2}(I)$. Now we prove that $\lim_{j\to\infty} \int_I |\varphi_j|^2\, dz = 1$:

$$\begin{aligned}\left|\int_I \varphi_j^2\, dz - 1\right| &= \left|\int_I |\varphi_j|^2\, dz - \int_I |\theta_j|^2\, dz\right| \le \int_I |\varphi_j^2 - \theta_j^2|\, dz \\ &\le \|\varphi_j - \theta_j\|_{L^2(I)} \|\varphi_j + \theta_j\|_{L^2(I)} \le C\|\varphi_j - \theta_j\|_{L^2(I)} \\ &\le C\varepsilon_j^{\frac{1}{2}}.\end{aligned}$$

Thus we have $\int_I \varphi^2\, dz = 1$ and hence $\int_I \theta^2\, dz = 1$. Since the weak convergence and the norm convergence imply the strong convergence, we have

$$\theta_j \to \theta \quad \text{ in } L^2(I).$$

Finally, in order to show that $(\theta, \varphi) \in W_0^{1,2}(I) \times W_0^{1,2}(I)$, we use the following estimate for $\varphi_j - \varphi$, from the proof of Theorem 1.5.1.10 in [11],

$$\int_{\partial\Omega} |u|^2\, d\sigma \le C(\Omega)\{\|u\|_{L^2(\Omega)} \|\nabla u\|_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)}\} \tag{4.4}$$

for all $u \in W^{1,2}(\Omega)$. □

Proposition 4.2. *The variational problem in $(\theta, \varphi, \delta) \in [W_0^{1,2}(I)]^2 \times \mathbb{R}$ of minimizing*

$$F_\varepsilon(\theta, \varphi, \delta) \quad \textit{constrained by} \quad (4.3),$$

Γ-converges in $[L^2(I)]^2 \times \mathbb{R}$ as $\varepsilon \to 0$, to the variational problem in $(\theta, \varphi, \delta) \in W_0^{1,2}(I) \times W_0^{1,2}(I) \times \mathbb{R}$ of minimizing

$$F_0(\theta, \varphi, \delta) \quad \textit{constrained by} \quad (4.3)$$

where F_0 is defined in (4.2).

The proof of Proposition 4.2 consists of the two following lemmas.

Lemma 4.3. *(Lower semi-continuity) For every $(\theta, \varphi, \delta) \in [L^2(I)]^2 \times \mathbb{R}$ and every sequence $(\theta_j, \varphi_j, \delta_j) \in [W_0^{1,2}(I)]^2 \times \mathbb{R}$ such that $(\theta_j, \varphi_j, \delta_j)$ converges to $(\theta, \varphi, \delta)$ in $[L^2(I)]^2 \times \mathbb{R}$ there holds*

$$\liminf_{j\to\infty} F_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) \ge F_0(\theta, \varphi, \delta)$$

and

$$\theta \in W_0^{1,2}(I) \qquad \textit{and} \qquad \varphi \in W_0^{1,2}(I).$$

Proof. We assume that $F_\varepsilon(\theta_j, \varphi_j, \delta_j) \le C$ for some constant C. As in the proof of Proposition 4.1, we have

$$\theta = \varphi, \qquad \varphi_j \rightharpoonup \varphi \quad \text{ in } W^{1,2}(I), \qquad \text{and} \qquad \theta \in W_0^{1,2}(I). \tag{4.5}$$

Now we claim that $\delta \neq 0$. If not, we have

$$\int_I (\varphi')^2 \le \liminf_{j\to\infty} \int_I \varphi_j^2 \le \lim_{j\to\infty} C\delta_j = 0.$$

and hence $\int_I (\theta')^2 = 0$ from (4.5). Then Poincaré inequality gives a contradiction with the constraint (4.3) and $\theta \in W_0^{1,2}(I)$.

Now that $\delta \neq 0$, we have, from the weak lower semicontinuity and (4.5),

$$\frac{1}{\delta}\int_I (\theta')^2 \leq \liminf \frac{1}{\delta_j}\int_I (\varphi_j')^2$$

and hence

$$\delta \int_I \theta^2 + \frac{1}{\delta}\int_I (\theta')^2 \leq \liminf_{j\to\infty} F_\varepsilon(\theta_j, \varphi_j, \delta_j).$$

□

LEMMA 4.4. *(Construction) For any $(\theta, \varphi, \delta) \in [W_0^{1,2}(I)]^2 \times \mathbb{R}$ with $\theta = \varphi$ and $\int_I |\theta|^2\,dz = 1$, there exists a sequence $(\theta_j, \varphi_j, \delta_j) \in [W_0^{1,2}(I)]^2 \times \mathbb{R}$ with $\int_I |\theta_j|^2\,dz = 1$, converging in $[L^2(I)]^2 \times \mathbb{R}$ as $j \to \infty$, to $(\theta, \varphi, \delta)$, and such that*

$$\limsup_{j\to\infty} F_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) = F_0(\theta, \varphi, \delta).$$

Proof. We take $\varphi_j = \varphi$, $\theta_j = \theta$, and $\delta_j = \delta$ for all $j \geq 1$.

□

LEMMA 4.5. *Let (θ, δ) be a minimizer of*

$$F_0 = \int_I (\delta\theta^2 + \frac{1}{\delta}|\theta'|^2)\,dz \quad \text{constrained by} \quad \int_I |\theta|^2\,dz = 1$$

with the boundary condition $\theta(\pm 1) = 0$. Then

$$\delta = \frac{\pi}{2} \qquad \text{and} \qquad \theta(z) = c\cos\frac{\pi}{2}z \ \text{ for some } |c| = 1. \tag{4.6}$$

The minimum value of the functional is π.

Proof. From $\theta \in W_0^{1,2}(I)$ and (4.3), we have

$$\int_I |\theta'|^2\,dz \geq \frac{\pi^2}{4}.$$

and the equality holds if and only if θ is of the form (4.6). Then we see that

$$F_0 \geq \delta + \frac{\pi^2}{4\delta} \geq \pi$$

and the equality holds if $\delta = \pi/2$.

□

From the Γ-convergence theory, if the Γ-limit F_0 has a unique minimizer, then the sequence of minimizers of F_ε converges to the minimizer of F_0 [5]. Since F_0 has a unique form of the minimizer, we have the following theorem. The proof of the similar theorem also can be found in [4].

THEOREM 4.6. *Let $(\theta, \varphi, \delta)$ be a minimizer of F_ε constrained by $\int_I |\theta|^2\,dz = 1$. For $\varepsilon = 1/h \ll 1$, we have*

$$\varepsilon\mu^2 \approx \frac{\pi}{2}, \qquad \text{and} \qquad F_\varepsilon(\theta, \varphi, \delta) \approx \pi \tag{4.7}$$

and

$$\int_I |\varphi(z) - c\cos\frac{\pi}{2}z|^2\,dz \ll 1 \tag{4.8}$$

for some constant c with $|c| = 1$.

REMARK 4.1. *One can see from (3.11) and (4.7) that the critical field is given by*

$$\kappa_c^0 \approx \frac{\pi}{h},$$

which is, in terms of real parameters,

$$H_c \approx \left(\frac{\pi K}{\chi_a d\lambda}\right)^{\frac{1}{2}}.$$

This estimate is consistent with the result found in the classic Helfrich-Hurault theory. (See p363 of [7] and [13]).

From (4.7) and (4.8) we infer that

$$\theta(\widetilde{x}, z) = \varphi(\widetilde{x}, z) = c\cos\frac{\pi}{2}z\sin\sqrt{\frac{\pi}{2h}}\widetilde{x}$$

and hence

$$\phi(x, y) = c\cos\frac{\pi}{2d}y\sin\sqrt{\frac{\pi}{2\lambda d}}x,$$

which is again the consistent result from [7].

5. Natural boundary condition on layers. In this section, we do not impose the Dirichlet boundary condition on layers. Since the compactness property in this case follows from Proposition 4.1, we need to prove the Γ-convergence of F_ε for $\varphi \in W^{1,2}(I)$. The Γ-convergence in this section is motivated from the work of [16].

PROPOSITION 5.1. *The variational problem in $(\theta, \varphi, \delta) \in W_0^{1,2}(I) \times W^{1,2}(I) \times \mathbb{R}$ of minimizing*

$$F_\varepsilon(\theta, \varphi, \delta) \quad \textit{constrained by} \quad (4.3),$$

Γ-converges in $[L^2(I)]^2 \times \mathbb{R}$ as $\varepsilon \to 0$, to the variational problem in $(\theta, \varphi, \delta) \in W^{1,2}(I) \times W^{1,2}(I) \times \mathbb{R}$ of minimizing

$$F(\theta, \varphi, \delta) \quad \textit{constrained by} \quad (4.3)$$

where

$$F(\theta, \varphi, \delta) = \begin{cases} \int_I (\delta|\theta|^2 + \frac{1}{\delta}|\theta'|^2)\,dz + \theta(1)^2 + \theta(-1)^2 & \textit{if } \delta \neq 0,\ \theta = \varphi \\ \theta(1)^2 + \theta(-1)^2 = 1 & \textit{if } \delta = 0,\ \theta = \varphi = \textit{constant} \\ \infty & \textit{else}\ . \end{cases}$$

LEMMA 5.2. *(Lower semi-continuity) For every $(\theta, \varphi, \delta) \in [L^2(I)]^2 \times \mathbb{R}$ and every sequence $(\theta_j, \varphi_j, \delta_j) \in W_0^{1,2}(I) \times W^{1,2}(I) \times \mathbb{R}$ such that $(\theta_j, \varphi_j, \delta_j)$ converges to $(\theta, \varphi, \delta)$ in $[L^2(I)]^2 \times \mathbb{R}$ there holds*

$$\liminf_{j\to\infty} F_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) \geq F(\theta, \varphi, \delta)$$

and

$$\theta \in W^{1,2}(I) \qquad \textit{and} \qquad \varphi \in W^{1,2}(I).$$

Proof. We may assume that $F_\varepsilon(\theta_j, \varphi_j, \delta_j) \le C$ for some constant C. Then we have $\theta = \varphi$ as in the proof of Proposition 4.1. We define an auxiliary function

$$\Psi(\theta_j, \varphi_j) = 2\int_0^{\theta_j} (t - \varphi_j)\, dt.$$

Evaluating the integral, we have

$$\Psi(\theta_j, \varphi_j) = 2\left(\frac{\theta_j^2}{2} - \varphi_j\theta_j\right) = (\theta_j - \varphi_j)^2 - \varphi_j^2. \tag{5.1}$$

Differentiating Ψ with respect to z, we have

$$\partial_z \Psi(\theta_j, \varphi_j) = 2(\theta_j - \varphi_j)(\theta_j' - \varphi_j') - 2\varphi_j\varphi_j'.$$

Then

$$\begin{aligned}\int_I (\varepsilon_j(\theta_j')^2 + \frac{1}{\varepsilon_j}(\theta_j - \varphi_j)^2)\, dz &\ge \int_I 2|\theta_j'||\theta_j - \varphi_j|\, dz \\ &= \int_I |\partial_z \Psi(\theta_j, \varphi_j) + 2\varphi_j'(\theta_j - \varphi_j) + 2\varphi_j\varphi_j'|\, dz \\ &= \int_I |\partial_z \Psi(\theta_j, \varphi_j) + (\varphi_j^2)' + 2\varphi_j'(\theta_j - \varphi_j)|\, dz.\end{aligned}$$

Using (5.1) and setting $\Phi(\theta, \varphi) = (\theta - \varphi)^2$, we have

$$\begin{aligned}\int_I (\varepsilon_j(\theta_j')^2 + \frac{1}{\varepsilon_j}(\theta_j - \varphi_j)^2)\, dz &\ge \int_I |\partial_z \Phi(\theta_j, \varphi_j)|\, dz - 2\int_I |\varphi_j'(\theta_j - \varphi_j)|\, dz \\ &\ge \int_I |\partial_z \Phi(\theta_j, \varphi_j)|\, dz - 2\|\varphi_j'\|_{L^2(I)}\|\theta_j - \varphi_j\|_{L^2(I)}.\end{aligned} \tag{5.2}$$

We extend θ_j and θ, by setting 0 outside I. Let $I_\eta = (-1-\eta, 1+\eta)$ with $0 < \eta \ll 1$ and define

$$\hat{\theta}_j = \begin{cases} \theta_j & \text{in } I \\ 0 & \text{in } I_\eta - \bar{I} \end{cases}$$

and

$$\hat{\theta} = \begin{cases} \theta & \text{in } I \\ 0 & \text{in } I_\eta - \bar{I} \end{cases}$$

We also extend φ_j and φ continuously by setting their boundary values outside of I.

$$\hat{\varphi_j} = \begin{cases} \varphi_j & \text{in } I \\ \varphi_j(-1) & \text{in } (-1-\eta, -1) \\ \varphi_j(1) & \text{in } (1, 1+\eta), \end{cases}$$

and

$$\hat{\varphi} = \begin{cases} \varphi & \text{in } I \\ \varphi(-1) & \text{in } (-1-\eta, -1) \\ \varphi(1) & \text{in } (1, 1+\eta). \end{cases}$$

Since $\hat{\theta}_j$ and $\hat{\varphi}_j$ are extended continuously and they are constants outside of I, we get

$$\int_I |\partial_z \Phi(\theta_j, \varphi_j)| = \int_{I_\eta} |\partial_z \Phi(\hat{\theta}_j, \hat{\varphi}_j)|.$$

For $\delta \neq 0$, from (5.2) and since $\Phi(\theta_j, \varphi_j) \to \Phi(\theta, \varphi)$ in $L^1(I)$, we have

$$\begin{aligned} &\liminf_{j\to\infty} F_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) \\ &\geq \liminf_{j\to\infty} \Big[\int_{I_\eta} |\partial_z \Phi(\hat{\theta}_j, \hat{\varphi}_j)|\, dz + \int_I (\delta_j \theta_j^2 + \frac{1}{\delta_j}(\varphi_j')^2)\, dz \\ &\qquad -2\|\varphi_j'\|_{L^2(I)} \|\theta_j - \varphi_j\|_{L^2(I)} \Big] \\ &\geq \int_{I_\eta} |\partial_z \Phi(\hat{\theta}, \hat{\varphi})|\, dz + \int_I (\delta\theta^2 + \frac{1}{\delta}(\varphi')^2)\, dz. \end{aligned} \tag{5.3}$$

From the construction of $\hat{\theta}$ and $\hat{\varphi}$, the definition of Φ, and $\theta = \varphi$, we have

$$\begin{aligned} \int_{I_\eta} |\partial_z \Phi(\hat{\theta}, \hat{\varphi})|\, dz &= \int_I |\partial_z \Phi(\hat{\theta}, \hat{\varphi})|\, dz + \int_{\partial I} |\Phi(\theta, \varphi) - \Phi(0, \varphi)| \\ &= (\theta(-1))^2 + (\theta(1))^2. \end{aligned} \tag{5.4}$$

Together with (5.3), we have

$$\liminf_{j\to\infty} F_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) \geq F(\theta, \varphi, \delta).$$

For $\delta = 0$, it is obvious that φ must be a constant. In fact,

$$\int_I (\varphi_j')^2 \leq C\delta_j \to 0$$

as $j \to \infty$. Therefore, $\theta = \varphi$ must be constants. The lower semicontinuity in this case follows from (5.3) and (5.4).
□

Lemma 5.3. *(Construction) For any $(\theta, \varphi, \delta) \in W^{1,2}(I) \times W^{1,2}(I) \times \mathbb{R}$ with $\int_I |\theta|^2\, dz = 1$ and $\theta = \varphi$, there exists a sequence $(\theta_j, \varphi_j, \delta_j) \in W_0^{1,2}(I) \times W^{1,2}(I) \times \mathbb{R}$ with $\int_I |\theta_j|^2\, dz = 1$, converging in $[L^2(I)]^2 \times \mathbb{R}$ as $j \to \infty$, to $(\theta, \varphi, \delta)$, and such that*

$$\limsup_{j\to\infty} F_{\varepsilon_j}(\theta_j, \varphi_j, \delta_j) = F(\theta, \varphi, \delta).$$

Proof. Given $(\theta, \varphi, \delta)$ where $\theta = \varphi$, we take $\varphi_\varepsilon = \varphi, \delta_\varepsilon = \delta$ for all ε. Then $\|\varphi\|_{L^2(I)} = 1$. We define the boundary layer construction for θ_ε by

$$\theta_\varepsilon(z) = \frac{\rho_\varepsilon(z)}{\|\rho_\varepsilon\|_{L^2(I)}}$$

where

$$\rho_\varepsilon(z) = \begin{cases} \varphi(z) - \varphi(-1)e^{-\frac{z+1}{\varepsilon}} & z \in I_1 \equiv (-1, -1+\sqrt{\varepsilon}) \\ \varphi(z) + \frac{\varphi(-1)e^{-\frac{1}{\sqrt{\varepsilon}}}}{\sqrt{\varepsilon}}(1+z-2\sqrt{\varepsilon}) & z \in I_2 \equiv (-1+\sqrt{\varepsilon}, -1+2\sqrt{\varepsilon}) \\ \varphi(z) & z \in I_3 \equiv (-1+2\sqrt{\varepsilon}, 1-2\sqrt{\varepsilon}) \\ \varphi(z) + \frac{\varphi(1)e^{-\frac{1}{\sqrt{\varepsilon}}}}{\sqrt{\varepsilon}}(1-z-2\sqrt{\varepsilon}) & z \in I_4 \equiv (1-2\sqrt{\varepsilon}, 1-\sqrt{\varepsilon}) \\ \varphi(z) - \varphi(1)e^{-\frac{1-z}{\varepsilon}} & z \in I_5 \equiv (1-\sqrt{\varepsilon}, 1). \end{cases} \tag{5.5}$$

Then we have $\theta_\varepsilon \in W_0^{1,2}(I)$ and $\|\theta_\varepsilon\|_{L^2(I)} = 1$. Since $\|\rho_\varepsilon\|_{L^2(I)} = 1 + O(\sqrt{\varepsilon})$, a direct computation gives

$$\begin{aligned} &\int_{I_1} [\frac{1}{\varepsilon}(\theta_\varepsilon - \varphi_\varepsilon)^2 + \varepsilon|\theta_\varepsilon'|^2]\, dz \\ &\quad = \frac{1}{\varepsilon\|\rho_\varepsilon\|_{L^2}} \int_{I_1} \Big(\varphi(z) - \varphi(-1)e^{-\frac{1+z}{\varepsilon}} - \|\rho_\varepsilon\|_2\varphi(z)\Big)^2\, dz \\ &\quad + \frac{\varepsilon}{\|\rho_\varepsilon\|^2_{L^2(I)}} \int_{I_1} \left(\varphi'(z) + \frac{\varphi(-1)}{\varepsilon} e^{-\frac{1+z}{\varepsilon}}\right)^2 dz \\ &\quad \le \frac{\varphi(-1)^2}{\varepsilon} + \frac{\varphi(-1)^2}{2} + O(\sqrt{\varepsilon}) = \varphi(-1)^2 + O(\sqrt{\varepsilon}). \end{aligned}$$

Also, we get

$$\int_{I_2} [\frac{1}{\varepsilon}(\theta_\varepsilon - \varphi_\varepsilon)^2 + \varepsilon|\theta_\varepsilon'|^2]\, dz \le O(\sqrt{\varepsilon}).$$

Similarly, we have

$$\begin{aligned} &\int_{I_4} [\frac{1}{\varepsilon}(\theta_\varepsilon - \varphi_\varepsilon)^2 + \varepsilon|\theta_\varepsilon'|^2]\, dz \le O(\sqrt{\varepsilon}) \\ &\int_{I_5} [\frac{1}{\varepsilon}(\theta_\varepsilon - \varphi_\varepsilon)^2 + \varepsilon|\theta_\varepsilon'|^2]\, dz \le \varphi(1)^2 + O(\sqrt{\varepsilon}). \end{aligned}$$

Hence, we have

$$\limsup_{\varepsilon\to 0} \int_I [\frac{1}{\varepsilon}(\theta_\varepsilon - \varphi_\varepsilon)^2 + \varepsilon|\theta_\varepsilon'|^2]\, d\widetilde{y} = \varphi(1)^2 + \varphi(-1)^2.$$

Since $\theta = \varphi$, we have

$$\limsup_{\varepsilon\to 0} F_\varepsilon(\theta_\varepsilon, \varphi_\varepsilon, \delta_\varepsilon) = \theta(1)^2 + \theta(-1)^2 + \delta + \frac{1}{\delta}\int_I |\varphi'|^2\, dz.$$

For the case $\delta = 0$, since φ is constant, the same construction gives the desired upper bound.

□

In figure 5 we depict the minimizer $(\theta_\varepsilon, \varphi_\varepsilon)$ of F_ε when $\delta = \varepsilon = 0.01$. It suggests that θ_ε has a boundary layer and φ_ε tends to a constant for small ε. Also, the computation of the energy suggests that the minimum value of F_ε is close to 1 for $\varepsilon \ll 1$. In fact, the following theorem shows that the minimum value of the Γ-limit F is 1.

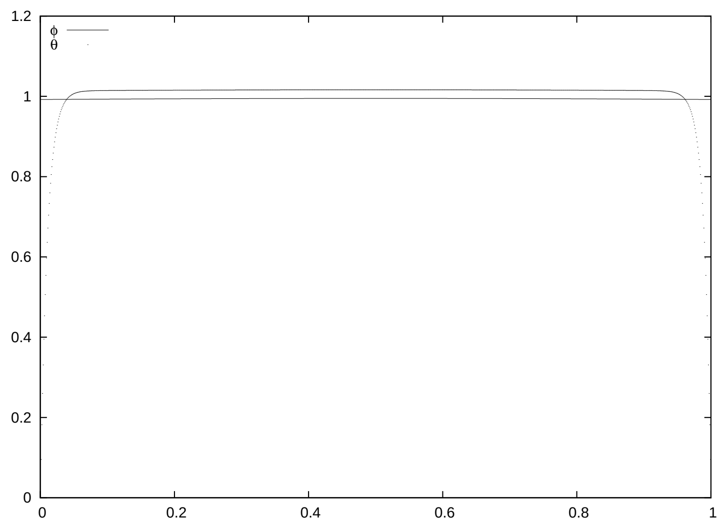

FIG. 5.1. *configurations of minimizer of* F_ε *with* $\varepsilon = 0.01, \delta = 0.01$

LEMMA 5.4. *Let* (θ, δ) *be a minimizer of* F *constrained by* $\int_I |\theta|^2\, dz = 1$. *Then*

$$\delta = 0 \qquad \textit{and} \qquad \theta(z) = \frac{c}{\sqrt{2}} \ \textit{for some}\ |c| = 1.$$

The minimum value of the functional is 1.

Proof. If $\delta = 0$, then θ must be a constant and hence $F = \theta(1)^2 + \theta(-1)^2$. From (4.3), we can see that $F = 1$. Assume that $\delta \neq 0$ and consider the corresponding Euler-Lagrange equation

$$\begin{aligned} &\frac{1}{\delta}\theta'' + \lambda\theta = 0 && \text{in } I \\ &\frac{1}{\delta}\frac{\partial\theta}{\partial\nu} + \theta = 0 && \text{on } \partial I. \end{aligned} \tag{5.6}$$

The solution to (5.6) can be given by

$$\theta = c_1 \cos\sqrt{\delta\lambda} z + c_2 \sin\sqrt{\delta\lambda} z.$$

By adding and subtracting equations at the boundaries give

$$\begin{aligned} &c_1\left(-\sqrt{\lambda}\sin\sqrt{\lambda\delta} + \sqrt{\delta}\cos\sqrt{\lambda\delta}\right) = 0, \\ &c_2\left(\sqrt{\lambda}\cos\sqrt{\lambda\delta} + \sqrt{\delta}\sin\sqrt{\lambda\delta}\right) = 0. \end{aligned}$$

This implies

$$c_1 = 0 \quad \text{and} \quad \tan\sqrt{\delta\lambda} = -\sqrt{\frac{\lambda}{\delta}} \tag{5.7}$$

$$\text{or} \quad c_2 = 0 \quad \text{and} \quad \tan\sqrt{\delta\lambda} = \sqrt{\frac{\delta}{\lambda}}. \tag{5.8}$$

Multiplying the first equation of (5.6) by θ and integrating over I, we have $F(\theta, \delta) = \delta + \lambda$. By considering F and λ as functions of δ, one can see that F is minimized when $\frac{\partial \lambda(\delta)}{\partial \delta} = -1$. We consider the first case (5.7). Using this and differentiating (5.7) with respect to δ, we get

$$(\lambda - \delta - 1)\left(\frac{1}{\sqrt{\lambda}}\cos\sqrt{\lambda\delta} - \frac{1}{\sqrt{\delta}}\sin\sqrt{\lambda\delta}\right) = 0,$$

which leads to

$$\lambda = \delta + 1 \qquad \text{or} \qquad \tan\sqrt{\lambda\delta} = \sqrt{\frac{\delta}{\lambda}}.$$

From (5.7), however, the latter is not possible. Similarly, in the second case (5.8), we have

$$\lambda = \delta + 1 \qquad \text{or} \qquad \tan\sqrt{\lambda\delta} = -\sqrt{\frac{\lambda}{\delta}}.$$

It follows that $\lambda = \delta + 1$ from (5.8). Thus

$$F = \delta + \lambda \geq 1 + 2\delta > 1$$

and hence the minimum occurs when $\delta = 0$. □

The same proof of Theorem 4.6 gives the following theorem.

THEOREM 5.5. *Let $(\theta, \varphi, \delta)$ be a minimizer of F_ε constrained by $\int_I |\theta|^2\,dz = 1$. For $\varepsilon = 1/h \ll 1$, we have*

$$\varepsilon\mu^2 \approx 0, \qquad \textit{and} \qquad F_\varepsilon \approx 1. \tag{5.9}$$

and

$$\int_I |\varphi(z) - \frac{c}{\sqrt{2}}|^2\,dz \ll 1 \tag{5.10}$$

for some constant c with $|c| = 1$.

REMARK 5.1. *One can see that the critical field is given by*

$$\kappa_c \approx \frac{1}{h},$$

which is, in terms of real parameters,

$$H_c \sim \left(\frac{K}{\chi_a d\lambda}\right)^{\frac{1}{2}}.$$

It follows from Remarks 4.1 and 5.1 that the undulation may occur at the lower critical field than in the classic Helfrich-Hurault theory. Also, from (5.9) we infer that the undulation frequency is lower than it is expected from the classic theory. The estimate (5.10) suggests that the amplitude of the undulation may not decrease as approaching the cell boundaries. Instead one may expect to have the same amplitude throughout the cell.

6. Numerical Simulations. In this section, we numerically solve the gradient flow of the energy with two different boundary conditions discussed in the previous sections. The gradient flow equations are

$$\begin{aligned}\frac{\partial\phi}{\partial t} &= \Delta\phi - \nabla\cdot\mathbf{n},\\ \frac{\partial\mathbf{n}}{\partial t} &= \Pi_{\mathbf{n}}\left(\Delta\mathbf{n} + \nabla\phi - \mathbf{n} + \kappa(\mathbf{n}\cdot\mathbf{h})\mathbf{h}\right),\end{aligned} \tag{6.1}$$

where $\Pi_n(f) = f - (\mathbf{n}, f)\mathbf{n}$ is the projection onto the plane orthogonal to $\mathbf{n}$, and $(\mathbf{n}, f)$ denotes the usual L_2 inner product. This projection appears as a result of the constraint $|\mathbf{n}| = 1$. For numerical purposes, it is more convenient to write this term as

$$\frac{\partial\mathbf{n}}{\partial t} = -\mathbf{n}\times\left(\mathbf{n}\times\left(\Delta\mathbf{n} + \nabla\phi - \mathbf{n} + \kappa(\mathbf{n}\cdot\mathbf{h})\mathbf{h}\right)\right). \tag{6.2}$$

Written in this way, the equation resembles the Landau-Lifshitz equation of micromagnetics in the high damping limit [8], and the heat-flow of harmonic maps [22].

For the initial condition, we take a small perturbation from the undeformed state. More precisely, for all $(x, y) \in \Omega$,

$$\begin{aligned}\mathbf{n}(x, y, 0) &= \frac{(\epsilon u_1, 1 + \epsilon u_2)}{|(\epsilon u_1, 1 + \epsilon u_2)|},\\ \phi(x, y, 0) &= y + \epsilon\phi_0,\end{aligned}$$

where a small number $\epsilon = 0.01$ and u_1, u_2, and ϕ_0 are arbitrarily chosen. As described in section 2, we impose strong anchoring condition for the director field, (2.2), and homogeneous Dirichlet boundary condition or natural boundary condition on ϕ at the top and the bottom plates. The natural boundary condition on ϕ is

$$\frac{\partial\phi}{\partial\nu}\Big|_{y=\pm h} = \mathbf{n}\cdot\nu\Big|_{y=\pm h}.$$

Periodic boundary conditions are imposed for both $\mathbf{n}$ and ϕ on each side of the domain.

We use a Fourier spectral discretization in the x direction, and second order finite differences in the y direction. The fast Fourier transform is computed using the FFTW libraries [9]. For temporal discretization, we use the semi-implicit finite difference method to solve the corresponding initial value problem.

We take the domain size $L = 100$ and $h = 25$. A more physically relevant value for h in smectic A liquid crystals is 5×10^5. However, the layer undulations can be observed if $h \gg 1$. In fact, the undulations in cholesteric liquid crystals occur with $h \approx 10$ ([17]). The numbers of grid points in the x and y directions are both 512.

In Fig. 6.1 we show the layer structures in response to the various magnetic field strengths κ. The pictures are contour maps of ϕ since the level sets of ϕ represent the layer. One can see that the undeformed state is stable before the magnetic field κ reaches the threshold κ_c. If κ increases and reaches κ_c, the layer undulations occur.

The homogeneous Dirichlet boundary condition and the natural boundary condition were imposed for the layer function ϕ in section 4 and section 5, respectively. The first column of Fig. 6.1 depicts the layers when the homogeneous Dirichlet boundary condition is applied while in the second column the natural boundary condition is used for the layer function. Our analysis gives estimates on the critical field (Remark

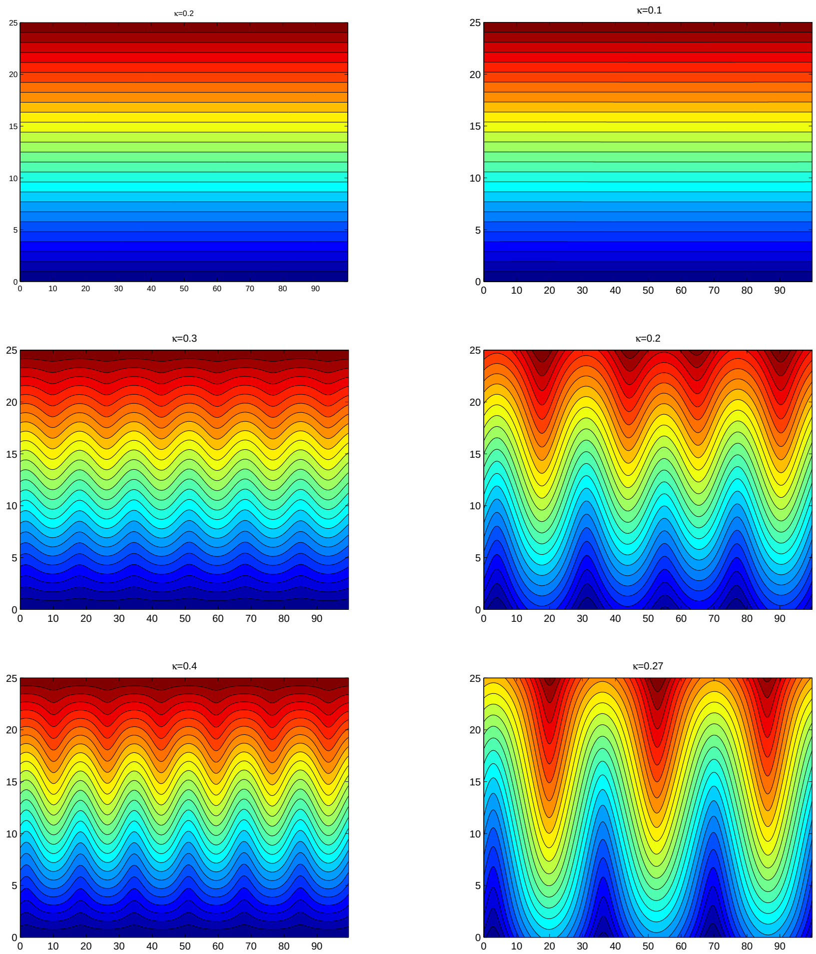

FIG. 6.1. *Contour plots of ϕ, the solution of the system (6.1). The first and the second column depict the layer when the homogeneous Dirichlet and natural boundary condition are imposed on ϕ, respectively.*

4.1 and Remark 5.1) and the wave numbers ((4.7), (5.9)). From these estimates, one can expect that the critical field and the frequency in the x direction are higher when the homogeneous Dirichlet boundary condition is applied on the layer function. In Fig. 6.1, the critical field and the frequency are higher in the first column, which confirms these results.

As κ increases beyond κ_c, the displacement amplitude increases as in the third row of Fig. 6.1. In the first column of the Fig. 6.1 the maximum undulation occurs in the middle of the cell ($y = 0$) and the displacement amplitude decreases as approaching the boundary ($y = \pm h$), which was expected from the estimate (4.8). This was the same result from the classic Helfrich-Hurault theory, the layers are fixed at the boundary, i.e., no undulations at $y = \pm h$. However, the second column of Fig. 6.1 indicates that the undulations may not vanish at the boundary even though we impose the strong anchoring condition. The displacement amplitude does not diminish as approaching the boundary and it seems that the amplitude does not depend on y. This agrees the estimate (5.10).

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