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Configuration of a Smectic A Liquid Crystal Due to an Isolated Edge Dislocation

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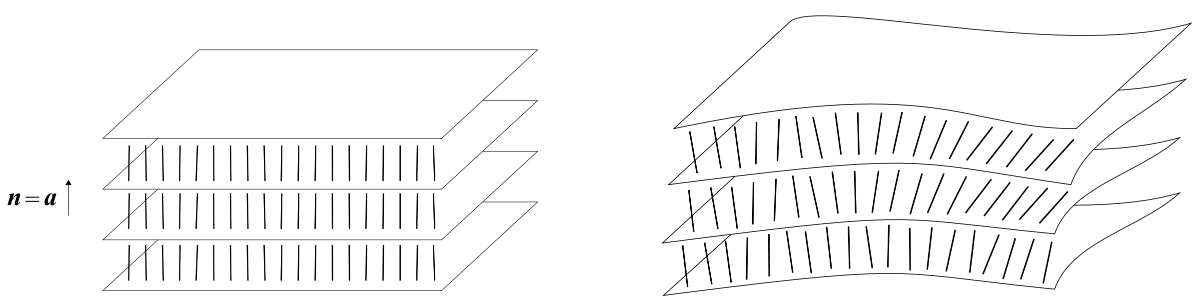
Abstract

We discuss the static configuration of a smectic A liquid crystal subject to an edge dislocation under the assumption that the director and layer normal fields ($\boldsymbol{n}$ and $\boldsymbol{a}$, respectively) defining the smectic arrangement are not, in general, equivalent. After constructing the free energy for the smectic, we obtain exact solutions to the equilibrium equations which result from its minimisation at quadratic order in the variables which describe the distortion, and hence a complete description of the smectic configuration across the domain of the sample. We also examine the effect of relaxing the constraint $\boldsymbol{n} \equiv \boldsymbol{a}$ for different values of the constants which characterise the response of the material to distortions, and compare these results with the "classical" case considered by previous authors, in which equivalence of $\boldsymbol{n}$ and $\boldsymbol{a}$ is enforced.

1 Smectic A Liquid Crystals

Liquid crystals (LCs) are mesomorphic phases of matter which are exhibited by materials consisting of anisotropic rod- or disc-like molecules. The LCs exist in temperature ranges between those of the material's isotropic liquid and crystalline solid phases, and display physical properties reminiscent of both. General information on the physical properties of various LCs may be found, for instance, in the book of de Gennes and Prost [9]; more mathematical introductions are to be found in the works of Stewart [20] and Virga [24]. We will be concerned with the smectic A (SmA) phase [21], in which the constituent rod-like molecules align themselves along an axis of anisotropy, as found in the well-studied nematic phase, in addition to arranging themselves into layers such that, in an unstrained configuration, the anisotropic axis lies perpendicular to the local layer alignment; see Fig. 1(a). As such, it proves convenient to describe SmA by means of two unit vectors: the director, $\boldsymbol{n}$, defining the local molecular orientation, and the unit layer normal, $\boldsymbol{a}$, which describes the local layer structure.



(a) Relaxed planar configuration of SmA.

(b) Distorted configuration induced by an applied stress.

Figure 1: **(a)** In the absence of external stresses, a SmA sample with no defects will tend to align in a relaxed configuration such that $\boldsymbol{n} \equiv \boldsymbol{a}$. **(b)** Applying a stress leads to a distortion in which $\boldsymbol{n}$ and $\boldsymbol{a}$ may separate.

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Motivated by the observations of Auernhammer *et al.* [1–3], Elston [7], and Soddemann *et al.* [19], we allow for the possibility that $\boldsymbol{n}$ and $\boldsymbol{a}$ may separate under the imposed distortion, as depicted in Fig. 1(b). We assume that the free energy associated with any departure of the SmA from its unstrained configuration is of the form set forth by De Vita & Stewart [6]:

$$\begin{aligned} w_{\mathrm{DS}} &= \tfrac{1}{2}K_1^a(\nabla\cdot\boldsymbol{a})^2 + \tfrac{1}{2}K_1^n(\nabla\cdot\boldsymbol{n}-s_0)^2 + \tfrac{1}{2}K_2\nabla\cdot\{(\boldsymbol{n}\cdot\nabla)\boldsymbol{n}-(\nabla\cdot\boldsymbol{n})\boldsymbol{n}\} \\ &\quad + \tfrac{1}{2}B_0|\nabla\Phi|^{-2}\left(1-|\nabla\Phi|\right)^2 + \tfrac{1}{2}B_1\left\{1-(\boldsymbol{n}\cdot\boldsymbol{a})^2\right\} + B_2(\nabla\cdot\boldsymbol{n})\left(1-|\nabla\Phi|^{-1}\right), \end{aligned} \tag{1.1}$$

where the scalar function Φ defines the layer normal $\boldsymbol{a}$ via

$$\boldsymbol{a} = \frac{\nabla\Phi}{|\nabla\Phi|}. \tag{1.2}$$

In equation (1.1), K_1^a, K_1^n, and K_2 are elastic constants and B_0, B_1, and B_2 are constant energy densities. The first term on the right-hand side is the energy associated with bending of the smectic layers; the second term is the splay energy, with s_0 denoting the spontaneous splay; the third term is the saddle-splay energy; the fourth is the energy associated with layer compression/expansion; the fifth is the energy attributed to coupling between $\boldsymbol{n}$ and $\boldsymbol{a}$; the sixth and final term is the energy due to coupling between splay and compression of the layers. Equation (1.1) provides a general description of the energy associated with deformations of a lipid bilayer. Note that we will be concerned only with SmA LCs with no polarisability or spontaneous splay, and thus the free energy we require is given by [6]

$$\begin{aligned} w_{\mathrm{A}} &= \tfrac{1}{2}K_1^a(\nabla\cdot\boldsymbol{a})^2 + \tfrac{1}{2}K_1^n(\nabla\cdot\boldsymbol{n})^2 + \tfrac{1}{2}K_2\nabla\cdot\{(\boldsymbol{n}\cdot\nabla)\boldsymbol{n}-(\nabla\cdot\boldsymbol{n})\boldsymbol{n}\} \\ &\quad + \tfrac{1}{2}B_0|\nabla\Phi|^{-2}\left(1-|\nabla\Phi|\right)^2 + \tfrac{1}{2}B_1\left\{1-(\boldsymbol{n}\cdot\boldsymbol{a})^2\right\}. \end{aligned} \tag{1.3}$$

A comprehensive account of the manner in which Φ defines the layer structure, as well as the physical properties of the energy in equation (1.1) and a range of applications to problems concerning the behaviour of lipid bilayers, may be found in the paper of De Vita and Stewart [6].

Background material on the theory of edge dislocations in crystalline solid media may be found in references [10, 12, 13]; for information regarding dislocations in smectics, the reader may consult the latter two of these references or the book of de Gennes and Prost [9, Section 9.2].

The article is organised as follows. In Section 2, we present the free energy at quadratic order in the director deflection and layer displacement, from which we derive the equilibrium equations and obtain an exact solution for the latter at that order. The derivation of the free energy, which we have constructed to fourth order, is deferred until Appendix A since the resulting expressions are unwieldy; in addition to enabling the computation of the results contained in the main body of the paper, this allows us to recover a known higher-order solution, details of which are presented in Appendix B. In Section 3, the solution for the layer displacement at quadratic order is compared graphically with the "classical" two-constant case, in which the director and layer normal are constrained to be identical throughout the sample, by means of rewriting both solutions as suitable integrals over a finite domain and numerically integrating the resultant expressions. In Section 4, we use the results obtained to arrive at expressions for both the director profile and the layer normal, thus providing a complete description of the static configuration of the SmA in the presence of the dislocation. Section 5 closes with a summary of the results obtained and suggestions for further work.

2 Separation of Director and Layer Normal at Quadratic Order

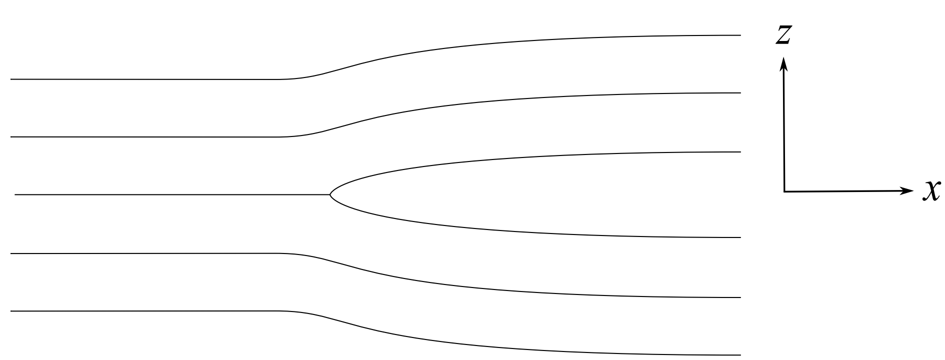


Figure 2: Schematic representation of the arrangement of the smectic layers in the presence of an edge dislocation. The Burgers vector in this case is $\boldsymbol{b} = d\boldsymbol{e}_z$, where d denotes the smectic interlayer distance.

Consider a sample of SmA subject to an edge dislocation such that the Burgers vector of the dislocation [9, Section 9.2], which will be taken to have magnitude $b = d$, with d denoting the interlayer spacing of the SmA, is parallel to the z-axis; the dislocation axis is parallel to the y-axis. We wish to measure the deviation of the configuration of the SmA away from that of the reference configuration, described by

$$\boldsymbol{n} = \boldsymbol{n}_0 \equiv (0, 0, 1), \qquad \Phi = \Phi_0 \equiv z. \tag{2.1}$$

The imposed dislocation will lead to a director profile of the general form

$$\boldsymbol{n} = (\sin\theta(x, z),\ 0,\ \cos\theta(x, z)), \tag{2.2}$$

while the function Φ is modified to read

$$\Phi = z - u(x, z). \tag{2.3}$$

From the latter of these equations, it readily follows that $\nabla\Phi = (-u_x,\ 0,\ 1 - u_z)$, and thus

$$\boldsymbol{a} = \frac{(-u_x,\ 0,\ 1 - u_z)}{\sqrt{1 - 2u_z + u_x^2 + u_z^2}}, \tag{2.4}$$

where, for ease of notation, we employ the convention that a variable appearing as a subscript denotes partial differentiation with respect to that variable. Given the somewhat unwieldy form of equation (2.4), it makes sense to follow previous work [4, 13] and anticipate only small deviations away from the reference configuration, and that such deformations occur over distances such that we need only take into account terms to quadratic order in a Taylor series of the pertinent variables when computing the free energy.

A derivation of the free energy to quartic order is contained in Appendix A. In spite of the lengthiness of some of the resultant expressions, all results in aforementioned previous works are readily obtained by truncation at the appropriate lower order.

2.1 Equilibrium Equations

We depart from the precedent set forth in previous work and allow $\boldsymbol{n}$ and $\boldsymbol{a}$ to separate. By only retaining quadratic terms in u, θ, and their spatial derivatives, we obtain analytical expressions, exact up to this order of approximation, for both u and θ. According to equation (A.14), the free energy w_{A} may be written to second order as

$$w_{\mathrm{A}} = \tfrac{1}{2}\left\{K_1^a u_{xx}^2 + K_1^n \theta_x^2 + B_0 u_z^2 + B_1(\theta + u_x)^2\right\}. \tag{2.5}$$

We seek minimisers u and θ of the total energy per unit length in y, given by

$$W = \int_D w_{\mathrm{A}}\, dA, \tag{2.6}$$

where D denotes the two-dimensional domain occupied by the SmA sample; here $D = \mathbb{R}^2$. We require the first variation of the total energy, δW, to be zero. It is readily shown [5] that this requirement is expressed by the following two PDEs:

$$\frac{\partial^2}{\partial x^2}\left(\frac{\partial w_{\mathrm{A}}}{\partial u_{xx}}\right) = \frac{\partial}{\partial x}\left(\frac{\partial w_{\mathrm{A}}}{\partial u_x}\right) + \frac{\partial}{\partial z}\left(\frac{\partial w_{\mathrm{A}}}{\partial u_z}\right), \tag{2.7}$$

$$\frac{\partial}{\partial x}\left(\frac{\partial w_{\mathrm{A}}}{\partial \theta_x}\right) = \frac{\partial w_{\mathrm{A}}}{\partial \theta}. \tag{2.8}$$

Carrying out the required partial differentiation shows that these are equivalent to

$$K_1^a u_{xxxx} = B_0 u_{zz} + B_1(\theta_x + u_{xx}), \tag{2.9}$$

$$K_1^n \theta_{xx} = B_1(\theta + u_x), \tag{2.10}$$

respectively. Note that requiring $\boldsymbol{n} = \boldsymbol{a}$ to second order gives $\theta + u_x = 0$, allowing for the recovery of the classical case; we proceed with the general case $\boldsymbol{n} \neq \boldsymbol{a}$.

The boundary conditions imposed are motivated by the anticipated dislocation structure. Choosing the origin $(x, z) = (0, 0)$ of our coordinate frame to lie at the core of the dislocation, we will solve the equations (2.9) and (2.10) in the half-space $z > 0$; we require (see Fig. 2)

$$u(x, 0) = \frac{b}{4}(1 + \operatorname{sgn}(x)), \qquad \operatorname{sgn}(x) = \begin{cases} -1 & x < 0, \\ 1 & x > 0. \end{cases} \tag{2.11}$$

Further, we assume the distortion tends to zero in the far-field, so that

$$u_x(x, z) \to 0, \qquad u_z(x, z) \to 0, \qquad \theta(x, z) \to 0 \qquad \text{as } |x| \to \infty \qquad \text{for all } z > 0, \tag{2.12}$$

and that the distortions are finite for all z in the upper half-plane:

$$|u(x, z)| < \infty, \qquad |\theta(x, z)| < \infty \qquad \text{for all } z > 0. \tag{2.13}$$

2.2 Solution for the Layer Displacement

Differentiating (2.9) twice with respect to x and rearranging gives

$$\theta_{xxx} = \frac{K_1^a}{B_1} u_{xxxxxx} - \frac{B_0}{B_1} u_{zzxx} - u_{xxxx},$$

so that, on substitution into the derivative of (2.10) with respect to x, it follows that

$$B_1(\theta_x + u_{xx}) = K_1^n \left(\frac{K_1^a}{B_1} u_{xxxxxx} - \frac{B_0}{B_1} u_{zzxx} - u_{xxxx} \right).$$

This may then be substituted into (2.9) to yield

$$\lambda_n^2 \left(u_{zzxx} - \lambda_a^2 u_{xxxxxx} \right) + \beta \left\{ \left(\lambda_a^2 + \lambda_n^2 \right) u_{xxxx} - u_{zz} \right\} = 0, \tag{2.14}$$

where we have introduced the length scales

$$\lambda_a = \sqrt{K_1^a / B_0}, \qquad \lambda_n = \sqrt{K_1^n / B_0}, \tag{2.15}$$

in order to facilitate later comparison with previously-established results, along with the dimensionless parameter β, given by

$$\beta = B_1 / B_0. \tag{2.16}$$

We note here that, based on the work of Ribotta and Durand [16], we anticipate on physical grounds that $\beta \lesssim 1$ for any given sample of SmA. Nevertheless, we will have cause to refer to the limit as $\beta \to \infty$ in what follows; we stress that this limit is unphysical and purely for mathematical convenience and the elucidation of features of the more general free energies in equations (1.1) and (1.3).

Following the observation by Kleman and Lavrentovich [12] for the classical case, let us assume that the general solution to the PDE (2.14) in the region $z > 0$ may be expressed in the form

$$u(x, z) = \frac{b}{4} \left(1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{g(z) e^{i\sigma x}}{i\sigma} \, d\sigma \right). \tag{2.17}$$

Substitution into (2.14) readily yields the following ODE for $g(z)$ in terms of the combination of parameters $\Gamma(\sigma)$:

$$g''(z) = \frac{\sigma^4 \left\{ \lambda_a^2 \lambda_n^2 \sigma^2 + \beta \left(\lambda_a^2 + \lambda_n^2 \right) \right\}}{\lambda_n^2 \sigma^2 + \beta} g(z) \equiv \Gamma^2(\sigma) g(z), \tag{2.18}$$

whose general solution is

$$g(z) = A(\sigma) e^{-\Gamma(\sigma) z} + B(\sigma) e^{\Gamma(\sigma) z}.$$

Based on $(2.13)_1$, we require $g(z)$ to be finite for all $z > 0$, and so it immediately follows that $B(\sigma) = 0$. Further, the boundary condition (2.11) leads to the requirement

$$\int_{-\infty}^{\infty} \frac{A(\sigma) e^{i\sigma x}}{i\sigma} \, d\sigma = \pi \, \mathrm{sgn}(x). \tag{2.19}$$

Now, it may readily be shown by expanding $e^{i\sigma x} = \cos(\sigma x) + i \sin(\sigma x)$, substituting $\sigma x \to \tau$ and integrating along an appropriate contour in the complex plane that

$$\int_{-\infty}^{\infty} \frac{e^{i\sigma x}}{i\sigma} \, d\sigma = 2 \, \mathrm{sgn}(x) \int_0^{\infty} \frac{\sin \tau}{\tau} \, d\tau = \pi \, \mathrm{sgn}(x),$$

from which it is evident that we may choose $A(\sigma) \equiv 1$, and thus

$$\begin{aligned} u(x, z) &= \frac{b}{4} \left(1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{i\sigma x - \Gamma(\sigma) z}}{i\sigma} \, d\sigma \right) \\ &= \frac{b}{4} + \frac{b}{2\pi} \int_0^{\infty} \frac{e^{-\Gamma(\sigma) z} \sin(\sigma x)}{\sigma} \, d\sigma. \end{aligned} \tag{2.20}$$

In Section 4 below we will go on to compute exact solutions for the director and the layer normal, thereby obtaining a complete description of the SmA configuration due to the dislocation. First, however, we compare the behaviour of the displacement u with its counterpart in the two-constant case, as outlined by multiple authors [9, 12, 13], for typical values of the constants appearing in the free energy.

3 Comparison with the Two-Constant Case

Let us denote the layer displacement in the classical case by $\upsilon(x,z)$. This may be written in the form [12]

$$\upsilon(x,z) = \frac{b}{4}\left(1 + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{e^{i\sigma x - \lambda\sigma^2 z}}{i\sigma}\, d\sigma\right)$$

$$= \frac{b}{4} + \frac{b}{2\pi}\int_{0}^{\infty} \frac{e^{-\lambda\sigma^2 z}\sin(\sigma x)}{\sigma}\, d\sigma, \tag{3.1}$$

where $\lambda^2 = \lambda_a^2 + \lambda_n^2$. To facilitate graphical comparison of this displacement with that given above by equation (2.20), it proves convenient to write each of the expressions υ and u above in terms of integrals over a finite domain. This is achieved by appeal to the substitution

$$\zeta = \frac{1}{1+\lambda\sigma} \implies d\sigma = -\frac{d\zeta}{\lambda\zeta^2}, \tag{3.2}$$

so that equation (2.20) may, after appropriate substitution and rearrangement, be written in the form

$$u(x,z) = \frac{b}{4} + \frac{b}{2\pi}\int_0^1 f(\zeta)\, d\zeta, \tag{3.3}$$

where

$$f(\zeta) = \frac{\exp\left\{-\Delta(\zeta)z\right\}\sin\left\{\left(\zeta^{-1}-1\right)x/\lambda\right\}}{\zeta-\zeta^2}, \tag{3.4}$$

with

$$\Delta(\zeta) = \frac{(1-\zeta)^2}{\lambda^2}\sqrt{\frac{\lambda_a^2\lambda_n^2\left(\zeta^{-1}-1\right)^2+\beta\lambda^4}{\lambda_n^2\left(\zeta-\zeta^2\right)^2+\beta\lambda^2\zeta^4}}. \tag{3.5}$$

One readily deduces that

$$\Delta(\zeta)\to\infty \quad \text{as} \quad \zeta\to 0^+, \qquad\qquad \Delta(\zeta)\to 0 \quad \text{as} \quad \zeta\to 1^-,$$

from which

$$f(\zeta)\to 0 \quad \text{as} \quad \zeta\to 0^+, \qquad\qquad f(\zeta)\to\frac{x}{\lambda} \quad \text{as} \quad \zeta\to 1^-, \tag{3.6}$$

which ensure that the integral does not diverge. Utilising (3.2) in (3.1) yields

$$\upsilon(x,z) = \frac{b}{4} + \frac{b}{2\pi}\int_0^1 k(\zeta)\, d\zeta, \tag{3.7}$$

where

$$k(\zeta) = \frac{\exp\left\{-\left(\zeta^{-1}-1\right)^2 z/\lambda\right\}\sin\left\{\left(\zeta^{-1}-1\right)x/\lambda\right\}}{\zeta-\zeta^2}, \tag{3.8}$$

which is readily obtained as $f(\zeta)$ in the (unphysical) limit as $\beta\to\infty$. It is therefore evident that the two displacements agree at the endpoints of integration by virtue of the limits of f in equation (3.6) being independent of β. We note that the diffusion-like property of the spatial derivatives of υ

$$\partial_z\upsilon = \lambda\partial_x^2\upsilon, \tag{3.9}$$

does not hold for u; instead, we have the relationship

$$\lambda\partial_x^2 u - \partial_z u = \frac{b}{2\pi}\int_0^\infty \left\{\frac{\Gamma(\sigma)}{\sigma} - \lambda\sigma\right\} e^{-\Gamma(\sigma)z}\sin(\sigma x)\, d\sigma. \tag{3.10}$$

The properties stated in equations (3.6) allow for numerical integration of the expressions for υ and u outlined in equations (3.3)–(3.5) and (3.7), (3.8), respectively, by defining the function $f(\zeta)$ in a piecewise manner over the interval $[0,1]$ and appealing to the *ApproximateInt* command in Maple [14]. From this, a range of plots has been generated for typical SmA parameter values [22].

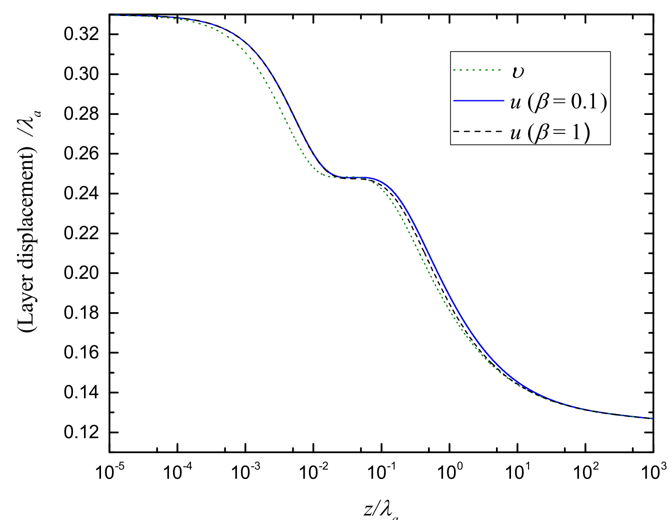
Displayed in Figs. 3(a),(b) below, we see the displacements u and υ due to the dislocation plotted as functions of z, selecting $\beta = 0.1$ and $\beta = 1$ for the former. Also shown is the difference between the two quantities for these values of β. Note that we have set $x = \lambda_a = \lambda_n$, and the value $b = \lambda_a/2$ has been chosen to ensure the validity of the quadratic free energy and the resultant linear equilibrium equations. We observe a difference of roughly 3.5% close to the dislocation core and close to 6% in the "far-field" between the displacements due to the dislocation in the classical case and $\beta = 0.1$, with similar non-negligible differences found when comparing the classical solution with the case $\beta = 1$.

Next, Figs. 4(a), (b) show the effects of varying the constant K_1^n in the case $x = \lambda_a$ as before; plots are shown for $\lambda_n = \lambda_a/10$, λ_a, and $10\lambda_a$ with values of β as indicated in the relevant captions. This variation has an even more pronounced influence on the predicted values of u, particularly for z close to the core of the dislocation.

It follows from the results presented here that the more general free energy proposed by De Vita and Stewart constitutes a significantly refined model for the energetics of SmA, furnishing us with predictions for a wider range of SmA samples in which the experimentally observed phenomenon of director/layer normal decoupling is non-negligible.

Figure 3: Effect of variation of β upon the layer displacement, plotted as a function of z for $x = \lambda_a = \lambda_n$.

(a) The normalised layer displacements for values of β within its physically allowable range.



(b) The difference between the solution u as seen in equation (2.20) and the classical solution υ stated in equation (3.1).

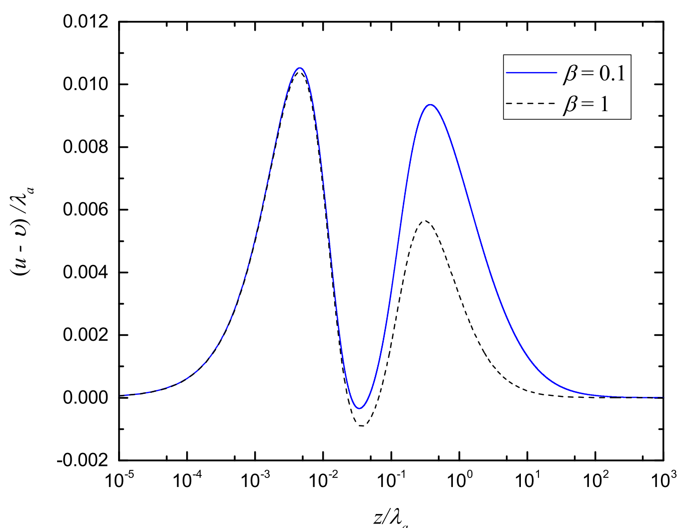
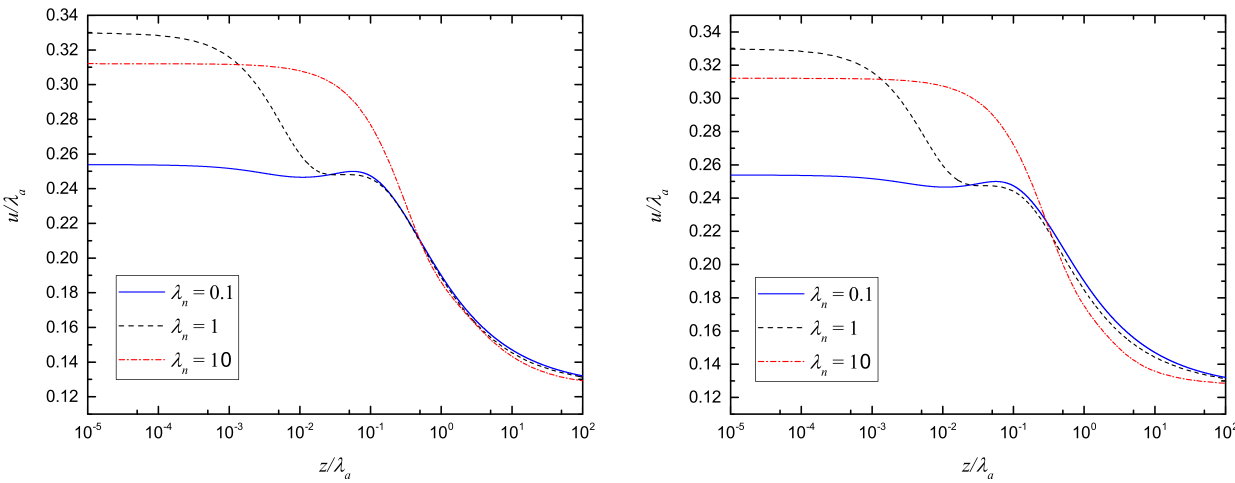


Figure 4: The normalised layer displacements for various values of the parameters λ_n and β.

(a) $\beta = 1/10$. **(b)** $\beta = 1$.



4 Solutions for Director Profile and Layer Normal

It still remains for us to derive an expression for θ. To this end, equation (2.9) is easily rearranged to yield

$$\theta_x = \frac{\lambda_a^2}{\beta} u_{xxxx} - \frac{1}{\beta} u_{zz} - u_{xx}. \tag{4.1}$$

Carrying out the required differentiation leads to

$$\theta_x = \frac{b}{2\pi} \int_0^\infty \left\{ \frac{\lambda_a^2 \sigma^3}{\beta} + \sigma - \frac{\Gamma^2(\sigma)}{\beta\sigma} \right\} e^{-\Gamma(\sigma) z} \sin(\sigma x)\, d\sigma. \tag{4.2}$$

Integration of equation (4.2) with respect to x gives the general solution

$$\theta = \frac{b}{2\pi} \int_0^\infty \chi(\sigma) \left\{ \cos(\sigma x) + \tau(z) \right\} \, d\sigma, \tag{4.3}$$

where

$$\chi(\sigma) = \left\{ \frac{\Gamma^2(\sigma)}{\beta\sigma^2} - \frac{\lambda_a^2\sigma^2}{\beta} - 1 \right\} e^{-\Gamma(\sigma) z}, \tag{4.4}$$

and $\tau(z)$ is an arbitrary function of z arising from the integration. On physical grounds, we must have $\theta(x, z) \to 0$ as $|x| \to \infty \ \forall \ z > 0$, as per $(2.12)_3$; then, since $\chi(\sigma)$ has only a finite number of maxima and minima and no discontinuities for $\sigma \in [0, \infty)$, we may utilise [18, Section 3, Theorem 4] to determine that

$$\lim_{x\to\infty} \theta(x, z) = \frac{b}{2} \left\{ \lim_{x\to\infty} \int_0^\infty \chi(\sigma)\cos(\sigma x)\, d\sigma + \lim_{x\to\infty} \int_0^\infty \chi(\sigma)\tau(z)\, d\sigma \right\}$$

$$\Longrightarrow \int_0^\infty \chi(\sigma)\tau(z)\, d\sigma = 0. \tag{4.5}$$

Hence, rewriting $\Gamma^2(\sigma)$ in the form

$$\Gamma^2(\sigma) = \lambda_a^2 \sigma^4 \left\{ 1 + \frac{\beta \lambda_n^2}{\lambda_a^2(\lambda_n^2\sigma^2 + \beta)} \right\},$$

we readily arrive at

$$\theta(x, z) = \frac{b}{2\pi} \int_0^\infty \chi(\sigma)\cos(\sigma x)\, d\sigma = \frac{b}{2\pi} \int_0^\infty \left\{ \frac{\lambda_n^2\sigma^2}{\lambda_n^2\sigma^2 + \beta} - 1 \right\} e^{-\Gamma(\sigma) z} \cos(\sigma x)\, d\sigma. \tag{4.6}$$

We have thus computed exact expressions for both the director profile and layer normal in the presence of an isolated edge dislocation for sufficiently low values of b.

Note that, in the limit as $\beta \to 0$, it is straightforward to deduce

$$\lim_{\beta\to 0} \chi(\sigma) = (1-1)e^{-\lambda_a \sigma^2 z} = 0 \implies \lim_{\beta\to 0} \theta(x,z) = 0, \tag{4.7}$$

and hence $\beta = 0$ corresponds to no director distortion. Based on our definition of β in equation (2.16), it is straightforward to see that this is the limit in which there is no energetic cost associated with separation between $\boldsymbol{n}$ and $\boldsymbol{a}$. It follows that any layer compression in this limit must be negligible, so that the constituent molecules may remain aligned along the z-axis as in the relaxed configuration. (Note that this does not rule out layer expansion, however.)

Rewriting $\Gamma^2(\sigma)$ in the form

$$\Gamma^2(\sigma) = \lambda^2\sigma^4 \left\{ \frac{1 + (\lambda_a^2\lambda_n^2\sigma^2/\beta\lambda^2)}{1+(\lambda_n^2\sigma^2/\beta)} \right\}$$

and continuing to increase β leads to

$$\lim_{\beta\to\infty} \Gamma^2(\sigma) = \lambda^2\sigma^4, \qquad\qquad \lim_{\beta\to\infty} \chi(\sigma) = -e^{-\lambda\sigma^2 z}, \tag{4.8}$$

and thus

$$\lim_{\beta\to\infty} \theta = -\lim_{\beta\to\infty} u_x = -\frac{b}{2\pi}\int_0^\infty e^{-\lambda^2\sigma z}\cos(\sigma x)\,d\sigma, \tag{4.9}$$

appearing to recover the result of the classical case $\boldsymbol{n} = \boldsymbol{a}$; see equations (3.9), (3.10). However, as noted in Section 2.2 after equation (2.16), this corresponds to a purely formal limit with no physical relevance since $\beta \lesssim 1$ [16], and hence the classical solution cannot be derived from the more general case for physically realisable values of the parameters characterising the SmA. Since the results for the classical case show significant deviation from those arising from (2.20), we propose that the more general free energy presented in Section 1 is more suitable for modelling the energetics of static phenomena in SmA samples where the difference between director and layer normal is significant.

Following the approach of the preceding section, let us write the expression (4.6) as an integral over the finite interval $[0,1]$. Employing the substitution (3.2) once more, it follows that θ may be expressed in the equivalent form

$$\theta(x,z) = \frac{b}{2\pi\lambda}\int_0^1 h(\zeta)\,d\zeta, \tag{4.10}$$

where

$$h(\zeta) = \left\{ \frac{\lambda_n^2(\zeta^{-1}-1)^2}{\lambda_n^2(1-\zeta)^2+\beta\lambda^2} - \frac{1}{\zeta^2} \right\} e^{-\Delta(\zeta)z} \cos\left\{ \left(\zeta^{-1}-1\right) x/\lambda \right\}. \tag{4.11}$$

It is readily deduced that, as $\zeta \to 0^+$,

$$|h(\zeta)| = \mathcal{O}\left(\frac{1}{\zeta^4} e^{-1/\zeta^3} \right),$$

and thus

$$h(\zeta) \to 0 \text{ as } \zeta \to 0^+, \qquad h(\zeta) \to -1 \text{ as } \zeta \to 1^-, \tag{4.12}$$

from which it is evident that the integral will not diverge. Let δ be the angle between $\boldsymbol{a}$ and the positive z-axis; the layer normal may be expressed in the form

$$\boldsymbol{a} = (\sin\delta,\, 0,\, \cos\delta) \approx \left(-u_x(1+u_z),\, 0,\, 1+u_z+u_z^2-\tfrac{1}{2}u_x^2\right),$$

from which it is evident that, to quadratic order,

$$\delta = \arcsin\left\{-u_x(1+u_z)\right\}. \tag{4.13}$$

Recalling equation (3.3), it is straightforward to conclude that

$$u_x = \frac{b}{2\pi\lambda}\int_0^1 \mu(\zeta)\,d\zeta, \tag{4.14}$$

$$u_z = \frac{b}{2\pi}\int_0^1 \nu(\zeta)\,d\zeta, \tag{4.15}$$

where we have defined

$$\mu(\zeta) = \frac{e^{-\Delta(\zeta)z}\cos\left\{\left(\zeta^{-1}-1\right)x/\lambda\right\}}{\zeta^2}, \tag{4.16}$$

$$\nu(\zeta) = \frac{\Delta(\zeta)e^{-\Delta(\zeta)z}\sin\left\{\left(\zeta^{-1}-1\right)x/\lambda\right\}}{\zeta^2-\zeta}. \tag{4.17}$$

We record that

$$\mu(\zeta) \to 0 \text{ as } \zeta \to 0^+, \qquad \mu(\zeta) \to 1 \text{ as } \zeta \to 1^-, \tag{4.18}$$

$$\nu(\zeta) \to 0 \text{ as } \zeta \to 0^+, \qquad \nu(\zeta) \to 0 \text{ as } \zeta \to 1^-. \tag{4.19}$$

Taken together, the expressions obtained for u in (3.3)–(3.5) and for θ in (4.10), (4.11) allow us to determine expressions for the director $\boldsymbol{n}$ and the layer normal $\boldsymbol{a}$, and hence the alignment of the SmA, across the entire sample to quadratic order in the variables characterising the distortions induced by the edge dislocation.

5 Conclusions and Discussion

This article has examined the effects of an isolated edge dislocation on the static configuration of a SmA liquid crystal. After deriving the relevant expression for the total SmA free energy and the resulting equilibrium equations that must be satisfied by the director deflection and layer displacement, it was shown that, in the absence of the constraint that $\boldsymbol{n}$ must always coincide with $\boldsymbol{a}$, it is possible to construct exact solutions for both the layer displacement and director deflection when the free energy is truncated at quadratic order. These expressions provide us with a complete description of the SmA sample in the presence of this dislocation in terms of its departure from the relaxed configuration of planar layers with $\boldsymbol{n} \equiv \boldsymbol{a}$. Moreover, the solution u for the layer displacement differs substantially from the classical case in which $\boldsymbol{n}$ and $\boldsymbol{a}$ always coincide, as was demonstrated by the modified identity expressed in equation (3.10), as well as the plots contained in Figs. 3–4 for various values of the relevant elasticity and energy terms.

The differences between the predictions of the more general framework of De Vita and Stewart and those of the classical case justify the use of the former as a model for SmA samples in which this separation plays a non-negligible role in determining their behaviour in equilibrium settings such as that considered here and when undergoing motion (see, for instance, reference [23]). Given that significant decoupling between $\boldsymbol{n}$ and $\boldsymbol{a}$ has been demonstrated in previous work [1–3, 7, 19], it is clear that such a model provides valuable insight which is surely necessary for those wishing to fully understand the rich and complex behaviour of the SmA phase.

Many further avenues of investigation present themselves. Having explored the isolated edge dislocation case, it may be of interest to investigate configurations of multiple dislocations and ask what sort of distortion is to be anticipated, as well as how different strengths and configurations of these defects would alter the smectic structure. It might also prove pertinent to examine the dynamics to which this would lead or, conversely, how the imposition of flow (for example by the application of a pressure gradient across the sample) might affect the configurations considered here.

Screw dislocations [9, Subsection 9.2.1.3] may be investigated along similar lines and these remain to be analysed in the context of the theory presented above; the interplay between layering structure and a more flexible director orientation relative to the layers may well lead to a more refined description and model for such structures. A consequent energy analysis may also provide fresh insight to the smectic layer structure close to the defect points.

Finally, it has been assumed throughout that the sample under consideration has infinite spatial extent: physically speaking, this corresponds to assuming that the sample boundaries are sufficiently far from the core of the defect so as to have no effect on the resultant configuration. It may prove worthwhile to examine the case of a dislocation near to a boundary under a variety of anchoring conditions. Such matters certainly warrant a great deal of further exploration.

A Calculating the Free Energy to Fourth Order

Equation (2.2) may be approximated by

$$\boldsymbol{n} = \left(\theta - \tfrac{1}{6}\theta^3,\ 0,\ 1 - \tfrac{1}{2}\theta^2 + \tfrac{1}{24}\theta^4\right), \tag{A.1}$$

from which it is readily deduced that $\boldsymbol{n} \cdot \boldsymbol{n} = 1 + \mathcal{O}(\theta^6)$. Further, on noting that, for $v \ll 1$

$$\sqrt{1+v} = 1 + \frac{1}{2}v - \frac{1}{8}v^2 + \frac{1}{16}v^3 - \frac{5}{128}v^4 + \mathcal{O}(v^5),$$

$$\frac{1}{\sqrt{1+v}} = 1 - \frac{1}{2}v + \frac{3}{8}v^2 - \frac{5}{16}v^3 + \frac{35}{128}v^4 + \mathcal{O}(v^5),$$

it is easy to show that the approximations

$$|\nabla\Phi| = 1 - u_z + \tfrac{1}{2}u_x^2 + \tfrac{1}{2}u_x^2 u_z - \tfrac{1}{8}u_x^4 + \tfrac{1}{2}u_x^2 u_z^2, \tag{A.2}$$

$$|\nabla\Phi|^{-1} = 1 + u_z - \tfrac{1}{2}u_x^2 + u_z^2 + u_z^3 - \tfrac{3}{2}u_x^2 u_z + \tfrac{3}{8}u_x^4 + u_z^4 - 3u_x^2 u_z^2 \tag{A.3}$$

hold to fourth order, and thus we may approximate $\boldsymbol{a}$ as

$$\boldsymbol{a} = \left(-u_x - u_x u_z + \tfrac{1}{2}u_x^3 - u_x u_z^2(1+u_z) + \tfrac{3}{2}u_x^3 u_z,\ 0,\ 1 - \tfrac{1}{2}u_x^2 - u_x^2 u_z + \tfrac{3}{8}u_x^4 - \tfrac{3}{2}u_x^2 u_z^2\right). \tag{A.4}$$

It readily follows that $\boldsymbol{a}$ is also a unit vector to fourth order. We may now use equations (A.1)–(A.4) to compute the terms comprising w_{DS}. Firstly, a simple calculation yields

$$(\nabla\cdot\boldsymbol{a})^2 = u_{xx}^2 + 2u_{xx}^2 u_z + 4u_x u_{xx} u_{xz} + 3u_{xx}^2 u_z^2 + 4u_x^2 u_{xz}^2 - 3u_x^2 u_{xx}^2 + 2u_x^2 u_{xx} u_{zz} + 12 u_x u_{xx} u_z u_{xz}, \tag{A.5}$$

while

$$(\nabla\cdot\boldsymbol{n} - s_0)^2 = \theta_x^2 - 2\theta\theta_x\theta_z + \theta^2(\theta_z^2 - \theta_x^2) + s_0\left(s_0 - 2\theta_x + 2\theta\theta_z + \theta^2\theta_z - \tfrac{1}{3}\theta^3\theta_z\right). \tag{A.6}$$

Tedious but straightforward calculations allow us to conclude that

$$(\boldsymbol{n}\cdot\nabla)\boldsymbol{n} - (\nabla\cdot\boldsymbol{n})\boldsymbol{n} = (\theta_z,\ 0,\ -\theta_x), \qquad \Longrightarrow\ \nabla\cdot\{(\boldsymbol{n}\cdot\nabla)\boldsymbol{n} - (\nabla\cdot\boldsymbol{n})\boldsymbol{n}\} = 0, \tag{A.7}$$

where it is assumed that partial derivatives of θ commute. Squaring both sides of equation (A.3) leads to

$$|\nabla\Phi|^{-2} = 1 + 2u_z - u_x^2 + 3u_z^2 + 4u_z^3 - 4u_x^2 u_z + u_x^4 + 5u_z^4 - 10u_x^2 u_z^2, \tag{A.8}$$

which, taken in conjunction with (A.2), allows us to conclude

$$|\nabla\Phi|^{-2}\left(1 - |\nabla\Phi|\right)^2 = u_z^2 + 2u_z^3 - u_x^2 u_z + \tfrac{1}{4}u_x^4 + 3u_z^4 - 4u_x^2 u_z^2. \tag{A.9}$$

Equations (A.1) and (A.4) may be combined to yield

$$\boldsymbol{n}\cdot\boldsymbol{a} = 1 - \theta u_x - \tfrac{1}{2}\theta^2 - u_x^2 u_z + \tfrac{1}{2}\theta u_x^3 - \theta u_x u_z^2 + \tfrac{1}{6}\theta^3 u_x + \tfrac{3}{8}u_x^4 - \tfrac{3}{2}u_x^2 u_z^2 + \tfrac{1}{24}\theta^4 + \tfrac{1}{4}\theta^2 u_x^2, \tag{A.10}$$

from which

$$\begin{aligned}1 - (\boldsymbol{n}\cdot\boldsymbol{a})^2 = {} & \theta^2 + u_x^2 + 2\theta u_x + 2u_x^2 u_z + 2\theta u_x u_z - \tfrac{1}{3}\theta^4 - u_x^4 - 2\theta u_x^3 \\ & - \tfrac{4}{3}\theta^3 u_x - 2\theta^2 u_x^2 + 2\theta u_x u_z^2 + 3u_x^2 u_z^2.\end{aligned} \tag{A.11}$$

Finally, since

$$\nabla\cdot\boldsymbol{n} = \theta_x - \theta\theta_z - \tfrac{1}{2}\theta^2\theta_x - \tfrac{1}{6}\theta^3\theta_z, \tag{A.12}$$

it may be deduced by further appeal to equation (A.3) that

$$\begin{aligned}(\nabla\cdot\boldsymbol{n})\left(1 - |\nabla\Phi|^{-1}\right) = {} & -\theta_x u_z + \tfrac{1}{2}\theta_x u_x^2 - \theta_x u_z^2 + \theta\theta_z u_z - \theta_x u_z^3 \\ & + \tfrac{3}{2}\theta_x u_x^2 u_z - \tfrac{1}{2}\theta\theta_z u_x^2 + \theta\theta_z u_z^2 + \tfrac{1}{2}\theta^2\theta_x u_z.\end{aligned} \tag{A.13}$$

Putting all this together, the free energy w_{DS} may be expressed to fourth order in the form

$$\begin{aligned}w_{\mathrm{DS}} = {} & \tfrac{1}{2}K_1^a(u_{xx}^2 + 2u_{xx}^2 u_z + 4u_x u_{xx} u_{xz} + 3u_{xx}^2 u_z^2 + 4u_x^2 u_{xz}^2 - 3u_x^2 u_{xx}^2 \\ & + 2u_x^2 u_{xx} u_{zz} + 12u_x u_{xx} u_z u_{xz}) + \tfrac{1}{2}K_1^n\left\{\theta_x^2 - 2\theta\theta_x\theta_z + \theta^2(\theta_z^2 - \theta_x^2)\right. \\ & \left. + s_0\left(s_0 - 2\theta_x + 2\theta\theta_z + \theta^2\theta_z - \tfrac{1}{3}\theta^3\theta_z\right)\right\} + \tfrac{1}{2}B_0\left(u_z^2 + 2u_z^3 - u_x^2 u_z + \tfrac{1}{4}u_x^4\right. \\ & \left. + 3u_z^4 - 4u_x^2 u_z^2\right) + \tfrac{1}{2}B_1\left(\theta^2 + u_x^2 + 2\theta u_x + 2u_x^2 u_z + 2\theta u_x u_z - \tfrac{1}{3}\theta^4 - u_x^4\right. \\ & \left. - 2\theta u_x^3 - \tfrac{4}{3}\theta^3 u_x - 2\theta^2 u_x^2 + 2\theta u_x u_z^2 + 3u_x^2 u_z^2\right) + B_2\left(-\theta_x u_z + \tfrac{1}{2}\theta_x u_x^2\right. \\ & \left. - \theta_x u_z^2 + \theta\theta_z u_z - \theta_x u_z^3 + \tfrac{3}{2}\theta_x u_x^2 u_z - \tfrac{1}{2}\theta\theta_z u_x^2 + \theta\theta_z u_z^2 + \tfrac{1}{2}\theta^2\theta_x u_z\right).\end{aligned} \tag{A.14}$$

As stated in Section 1, the free energy w_{A} for samples of SmA consisting of non-polarisable molecules is recovered when $s_0 = K_2 = B_0 = 0$.

B Director and Layer Normal Coincident: Recovering the Brener and Marchenko Solution

In the case where $\boldsymbol{n} \equiv \boldsymbol{a}$, the free energy simplifies to read

$$\begin{aligned}w_{\mathrm{A}} &= \tfrac{1}{2}(K_1^a + K_1^n)(\nabla\cdot\boldsymbol{a})^2 + \tfrac{1}{2}B_0|\nabla\Phi|^{-2}\left(1 - \nabla|\Phi|\right)^2 \\ &\equiv \tfrac{1}{2}\left(B_0 w_0 + K_1 w_1\right),\end{aligned} \tag{B.1}$$

where $K_1 = K_1^a + K_1^n$, and

$$w_0 = \left(u_z - \tfrac{1}{2}u_x^2\right)^2 + u_z^3(2+3u_z) - 4u_x^2u_z^2, \tag{B.2}$$

$$w_1 = u_{xx}^2 + 2u_{xx}^2u_z + 4u_xu_{xx}u_{xz} + 3u_{xx}^2u_z^2 + 4u_x^2u_{xz}^2 - 3u_x^2u_{xx}^2 + 2u_x^2u_{xx}u_{zz} + 12u_xu_{xx}u_zu_{xz}. \tag{B.3}$$

Let us calculate the first variation of the energy δW, defined for admissible variations h [8,17] by

$$\delta W = \frac{d}{dt}\iint_{\mathbb{R}^2} \eta\, dxdz\bigg|_{t=0} = \iint_{\mathbb{R}^2} \{\partial_t(\eta_0+\eta_1)\}|_{t=0}\, dxdz, \tag{B.4}$$

where

$$\eta_0 = w_0(u+th) - w_0(u), \qquad \eta_1 = w_1(u+th) - w_1(u), \tag{B.5}$$

and

$$\eta = \eta_0 + \eta_1 = w_{\mathrm{A}}(u+th) - w_{\mathrm{A}}(u). \tag{B.6}$$

It is a tedious but simple matter to compute the following:

$$\eta_0 = t\left\{h_x(u_x^3 - 2u_xu_z - 8u_xu_z^2) + h_z(2u_z + 6u_z^2 - u_x^2 + 12u_z^3 - 8u_x^2u_z)\right\} + \mathcal{O}(t^2), \tag{B.7}$$

$$\begin{aligned}\eta_1 = t\,\{&h_{xx}(2u_{xx} + 4u_{xx}u_z + 4u_xuxz + 6u_{xx}u_z^2 - 6u_x^2u_{xx} + 2u_x^2u_{zz} + 12u_xu_zu_{xz})\\ &+ h_{xz}(4u_xu_{xx} + 8u_x^2u_{xz} + 12u_xu_{xx}u_z) + 2h_{zz}u_x^2u_{xx}\\ &+ h_x(4u_{xx}u_{xz} + 8u_xu_{xz}^2 - 6u_xu_{xx}^2 + 4u_xu_{xx}u_{zz} + 12u_{xx}u_zu_{xz})\\ &+ h_z(2u_{xx}^2 + 6u_{xx}^2u_z + 12u_zu_{xx}u_{xz})\} + \mathcal{O}(t^2),\end{aligned} \tag{B.8}$$

from which it readily follows that the integrand of δW is simply the sum of the terms enclosed in curly brackets within equations (B.7) and (B.8). Writing $\delta W = \delta W_0 + \delta W_1$, where

$$\delta W_0 = \frac{1}{2}B_0\iint_{\mathbb{R}^2} (\partial_t\eta_0)|_{t=0}\, dxdz, \qquad \delta W_1 = \frac{1}{2}K_1\iint_{\mathbb{R}^2} (\partial_t\eta_1)|_{t=0}\, dxdz,$$

it follows that we may, on integrating by parts and requiring that any admissible h and spatial derivatives thereof vanish at the limits of integration, rewrite δW_0 and δW_1 in the respective forms

$$\delta W_0 = B_0\iint_{\mathbb{R}^2} h\left\{u_{xx}\left(4u_z^2 - \tfrac{3}{2}u_x^2 + u_z\right) + u_{zz}(4u_x^2 - 18u_z^2 - 6u_z - 1) + 2u_xu_{xz}(8u_z+1)\right\} dxdz, \tag{B.9}$$

$$\begin{aligned}\delta W_1 = K_1\iint_{\mathbb{R}^2} h\,\{&u_{xxxx}(3u_z^2 - 3u_x^2 + 2u_z + 1) + 4u_xu_{xxxz}(3u_z+1) + 6u_x^2u_{xxzz}\\ &+ 6u_{xxx}(3u_zu_{xz} - 2u_xu_{xx} + u_xu_{zz} + u_{xz}) + 6u_{xxz}(3u_{xx}u_z + 5u_xu_{xz} + u_{xx})\\ &+ 12u_xu_{xx}u_{xzz} + 3u_{xx}(u_{xx}u_{zz} - u_{xx}^2 + 6u_{xz}^2)\}\, dxdz.\end{aligned} \tag{B.10}$$

The energy W is then minimised by setting $\delta W = \delta W_0 + \delta W_1 = 0$ for all admissible variations h, which yields a nonlinear and highly intractable partial differential equation for u. Progress regarding solutions u to the full equation is probably best achieved by appeal to computational means, and this will not be considered here. However, assuming small layer displacements with sufficiently small spatial derivatives, analytical progress can be made in the following manner: according to both theoretical studies [9, Subsection 9.2.1] and experimental observations [11], the distortion of the layered structure is essentially confined to parabolic regions described by $x^2 = c\lambda z$ for some constant c, where $\lambda = \sqrt{K_1/B_0}$, which tells us that this configuration relaxes back to planar layers rapidly along x but significantly less so along z. Thus, if one assumes that $u_x \sim u/\xi$ and $u_z \sim u/L$ for some characteristic length scales ξ and L of displacement in the x and z directions, respectively, with $\xi^2 = \mathcal{O}(\lambda L)$, it is apparent from equations (B.9) and (B.10) that, on regarding terms of magnitude smaller than $\sim 1/\xi^4$ as negligible, one immediately arrives at the truncated equilibrium equation

$$\lambda^2u_{xxxx} + u_{xx}\left(u_z - \tfrac{3}{2}u_x^2\right) - u_{zz} + 2u_xu_{xz} = 0 \tag{B.11}$$

for the case $z > 0$; a similar equation is obtained in the case $z < 0$. This is exactly the PDE obtained by Brener and Marchenko [4, equation (4)], which may be non-dimensionalised by means of measuring all lengths in terms of λ; the non-dimensional form reads

$$u_{xxxx} + u_{xx}\left(u_z - \tfrac{3}{2}u_x^2\right) - u_{zz} + 2u_xu_{xz} = 0. \tag{B.12}$$

It is readily checked via differentiation that a solution $u(x,z)$ of the equation

$$u_{xx} = a\,\mathrm{sgn}(z)\left(2u_z \pm u_x^2\right) \tag{B.13}$$

also solves the equation

$$u_{xxxx} = 4a^2\left(u_{zz} \pm u_{xx}u_z \pm 2u_x u_{xz} + \tfrac{3}{2}u_x^2 u_{xx}\right), \tag{B.14}$$

where a is some real number. (The case $a = 1/2$ with the lower signs chosen corresponds to equation (B.12); the case $a = 1$ with the upper signs chosen is the case considered by Nepomnyashchy and Pismen [15] for pattern-forming systems.) Further, if one introduces the similarity variable $v = x/\sqrt{z}$, the PDE (B.13) may be rewritten in the form

$$u'' = a\,\mathrm{sgn}(z)\left\{\pm(u')^2 - vu'\right\}, \tag{B.15}$$

where $' \equiv d/dv$. To simplify notation, we will provide the general solution only for the case $z > 0$. To solve equation (B.15), introduce the transformation

$$u' = \gamma(v)e^{-av^2/2}.$$

We may then express the ODE (B.15) in the form

$$\frac{d\gamma}{dv} = \pm a\gamma^2 e^{-av^2/2}, \tag{B.16}$$

a first-order separable ODE which may be integrated with respect to v to yield

$$-\gamma = \left(c_1 \pm a\int_{-\infty}^{v} e^{-at^2/2}\,dt\right)^{-1}, \tag{B.17}$$

where c_1 is a constant of integration. The general solution for u is therefore

$$u(v) = \mp\frac{1}{a}\ln\left(\mp a\int_{-\infty}^{v} e^{-at^2/2}\,dt - c_1\right) + c_2, \tag{B.18}$$

where the constants c_1 and c_2 are determined by appropriate boundary conditions on u. Thus, the solution to the PDE (B.12) may be deduced from this by setting $a = 1/2$, imposing the condition

$$\lim_{v\to\infty} u(v) - \lim_{v\to-\infty} u(v) = \frac{b}{2},$$

applying the definition of the error function

$$\mathrm{erf}(x) := \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt,$$

and returning to dimensional variables to get

$$u = 2\lambda\ln\left\{\frac{1}{2}\left[1 + e^{b/4\lambda} + (e^{b/4\lambda} - 1)\,\mathrm{erf}\left(\frac{x}{2\sqrt{\lambda z}}\right)\right]\right\}. \tag{B.19}$$

It is straightforward to apply the same approach and thereby obtain the solution for $z < 0$. Finally, we note that, in the limit where $b \ll \lambda$, one readily obtains

$$\begin{aligned} u &\sim 2\lambda\ln\left\{1 + \frac{b}{8\lambda}\left[1 + \mathrm{erf}\left(\frac{x}{2\sqrt{\lambda z}}\right)\right]\right\} \\ &\sim \frac{b}{4}\left\{1 + \mathrm{erf}\left(\frac{x}{2\sqrt{\lambda z}}\right)\right\}, \end{aligned} \tag{B.20}$$

which is equivalent to the result derived in the classical case [12, 13] as seen in equation (3.1).

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