

Thin film models for an active gel

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Abstract

In this study we present a free-boundary problem for an active liquid crystal based on the Beris-Edwards theory that uses a tensorial order parameter and includes active contributions to the stress tensor to analyse the rich defect structure observed in applications such as the Adenosinetriphosphate (ATP) driven motion of a thin film of an actin filament network. The small aspect ratio of the film geometry allows for an asymptotic approximation of the free-boundary problem in the limit of weak elasticity of the network and strong active terms. The new thin film model captures the defect dynamics in the bulk as well as wall defects and thus presents a significant extension of previous models based on the Leslie-Erickson-Parodi theory. Analytic expressions are derived that reveal the interplay of anchoring conditions, film thickness and active terms and their control of transitions of flow structure.

1 Introduction

Since the works by Simha and Ramaswamy[1] and Kruse et al. [2] active liquid crystals have been used extensively as a hydrodynamic theory to describe the ordered motion of large numbers of self-propelled particles, such as bacterial suspensions, fibroblast monolayers, or the ATP driven actin network that underlies the movement of the lamellopodium of a crawling cell. The different levels of description, from the microscopic to the continuum hydrodynamic theory of this rapidly expanding research field has been reviewed in Marchetti et al. [3].

In many studies active matter extensions are based on the Leslie-Ericksen-Parodi (LEP) theory [4–6] such as in [7, 8], where active polar gels were derived from thermodynamic principles. As in passive liquid crystals, defects are a common phenomenon and their dynamics is strongly influenced by the fact that the system is out-of-equilibrium due to the energy source from the active terms. Observations in in-vitro experiments [9] show that they may directly depend on strength of the activity, where it was demonstrated that the observed defects tend to disappear again for sufficiently high levels of activity [10].

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Based on the LEP theory, point defects such as asters, vortices and spirals were described [2, 7]. Furthermore, phase diagrams of unbounded two-dimensional states [11] as well as flow transitions in confined films [12] were investigated. In particular, it was found that spontaneous flow arises in a confined active polar gel (with no-slip or free-slip conditions at the domain walls) above a critical layer thickness. This transition was also described within a thin-film model with a free, capillary surface [13].

However, there are some inherent deficiencies to describe the complete defect structure of passive liquid crystals based on the Leslie-Ericksen-Parodi theory, which is connected to the discontinuity of the director field and the infinite associated local elastic energy at the defect points. This problem becomes even more critical for the description of wall and line defects along which the elastic energy in the Leslie-Ericksen-Parodi theory is essentially discontinuous and, in particular, standard energy renormalization techniques can not be applied. Moreover, when modelling the evolution of thin nematic films with moving contact lines using LEP theory, related problems occur due to singularity of the director field at the contact line [14–21]. Therefore, more general approaches such as the Beris-Edwards theory [22, 23] of liquid crystal hydrodynamics, that use a tensorial order parameter, the so-called Q -tensor, instead of a director field, have been devised. Extensions of this theory by active terms go back to Marenduzzo et al. [24, 25] and have been extended in two- and three dimensions to various problems involving different geometries, such as spherical shells [26, 27], and have been investigated in a number of directions [28–33]. But even for the passive Beris-Edwards theory, the conditions at boundaries and in particular, stress and anchoring conditions at free interfaces are less well studied within this model. Important contributions to these issues can be found in [17, 34, 35]. In particular, it was conjectured [36] that a Q -tensor based approach might facilitate the resolution of nematic point defects in the vicinity of moving film contact lines [37].

The derivation of the corresponding thin-film model is the goal of this article. We begin by formulating the active Beris-Edwards model (section 2) including all the boundary conditions for a two-dimensional cross section of a thin film. We emphasize that basic features of the two-dimensional Beris-Edwards model resemble those of its three-dimensional version, but that it also has independent interesting two-dimensional applications in biology [29, 38], also on curved surfaces for thin shells of active matter [26, 27]. In this case, we are able to represent the Q -tensor through a scalar order parameter q and the director field n and reduce the active Beris-Edwards model to the corresponding active Ericksen model [39] that describes the coupled evolution of q and n . Making use of the scale separation of the thin-film geometry, a leading order approximation is derived (section 3) in the limit of weak elasticity and strong active terms to arrive at a new thin-film model, both for the passive and active cases. We also show that our model formally reduces to the one based on Leslie-Ericksen-Parodi theory, when the scalar order parameter q is homogeneous, and coincides with one of [17] in the passive case.

Finally, in section 4 we derive explicit solutions for special cases of flat constant films and small angle mismatch between the anchoring conditions. They show that in the passive case solutions with nonlinear nematic fields exist when certain compatibility relations between film thickness and nematic boundary conditions are satisfied. In particular, in paragraph 4.2 we construct solutions with the director field being discontinuous across the special isotropic line along which $q = 0$. These solutions can be viewed as the limiting profiles as the elastic constant tends to zero of the antisymmetric nematic field in the channel observed numerically in [40], cf. in particular with the approximate formula (29) there, see also [41]. In the presence of active terms, some of the found passive solutions continue to exist and exhibit nonzero flow that can be spontaneously initiated from zero, for example by increasing the film thickness, similar to the effect observed in [11, 12].

A discussion of further extensions and applications concludes the paper (section 5). In ap-

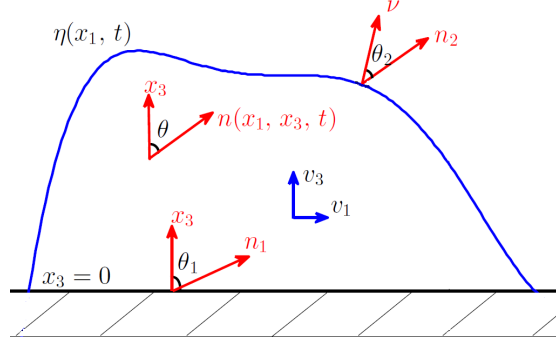


Figure 1: Sketch of the geometry of a thin film together with variables involved in the Q -tensor system (2.4)-(2.6).

pendix A we present the rescaled Ericksen model under the thin-film approximation. In appendix B we derive the polar thin-film model based on the Leslie-Ericksen-Parodi system with active terms.

2 Formulations of active liquid crystals

2.1 Beris-Edwards model for an active gel

The model in [7] and the simplified version in [11] can be viewed as based on the framework of LEP theory for liquid crystals augmented by sources of energy due to ATP hydrolysis that drives the system and makes the bulk of the cell an *active* (polar) gel. The bulk liquid i.e. the gel is characterized mainly by the velocity and the director field, which describes the averaged orientation of the actin filaments at a given point in space and time. The driving force is provided in their models via the chemical potential difference of ATP and its hydrolysis products. This hydrolysis of ATP fuels the molecular motors (and is also used for the polymerization and depolymerization of the actin filaments). Instead of treating the chemical potential difference between ATP and its hydrolysis products. This hydrolysis of ATP fuels the molecular motors to generate forces along the actin network, and is also used for the polymerization and depolymerization of the network filaments (which we will not include in the model here).

Instead of treating the active gel through a theory based on the LEP formulation for liquid crystals [4–6], we include the corresponding terms into the Beris-Edwards theory that uses Q -tensors to describe liquid crystals and is a popular field of research across the theoretical literature [23, 42–45], see also the recent overviews [46, 47], as a more general alternative theory for liquid crystals. In a subsequent step, we express the two-dimensional Q -tensor in terms of the director field and an additional scalar order parameter to obtain the Ericksen type model, for which we then derive the thin film model in section 3. An active gel model in terms of Q -tensors and its subsequent reformulation is also given in [25], but we additionally need to include appropriate conditions at the free interface, which we base on [34, 48].

We only consider two-dimensional models here and introduce a spatial domain Ω with coordinates (x_1, x_3) , while t represents time, (see Fig. 1 for a schematic sketch of the geometry and variables involved). The Beris-Edwards model is associated with the standard Landau-de

Gennes energy in the form [49]

$$\mathcal{F}_{LG}[Q; \Omega] = \int_{\Omega} (f_e(Q) + f_b(Q)) dx, \quad (2.1)$$

where $Q \in H^1(\Omega, \mathcal{L}_0)$ takes on values in the space of the symmetric and traceless matrices, or Q -tensors,

$$\mathcal{L}_0 := \{Q \in \mathbb{R}^{2 \times 2}, Q = Q^T, \text{tr}(Q) = 0\}.$$

In (2.1), the bulk contribution is given by

$$f_b(Q) = -\frac{a^2}{2} \text{tr}(Q^2) + \frac{c^2}{4} (\text{tr}(Q^2))^2 \quad (2.2)$$

with $c > 0$ and

$$f_e(Q) = \frac{L_1}{2} Q_{ij,k} Q_{ij,k} \quad (2.3)$$

is the elastic contribution, with an elastic constant $L_1 > 0$. (We deliberately avoid further complications by consider a model with only one elastic constant.) Here, and elsewhere, we use the usual convention that duplicate indices are summed over and indices with commas indicate spatial derivatives, e.g. $Q_{ij,k}$ is used for the derivative of Q_{ij} with respect to x_k for $i, j, k = 1, 2, 3$.

In the most general form, the active Beris-Edwards model can be written as (see e.g. [23, 27, 43, 44] and references therein):

$$0 = \partial_i v_i, \quad (2.4)$$

$$0 = -\partial_i p + \mu \partial_j^2 v_i + \partial_j (\tau_{ij} + \sigma_{ij} - \zeta \Delta \chi Q_{ij}) \quad (2.5)$$

$$Q_t + (v \cdot \nabla) Q = \Gamma H + S(\nabla v, Q) + \lambda_1 \Delta \chi Q, \quad (2.6)$$

where v_i and p are the velocity components and the pressure, and μ the isotropic viscosity. The term

$$S(\nabla v, Q) = (\xi e + \omega)(Q + I/2) + (Q + I/2)(\xi e - \omega) - 2\xi(Q + I/2)\text{tr}(Q\nabla u), \quad (2.7)$$

with

$$e_{ij} = \frac{1}{2} (\partial_j v_i + \partial_i v_j), \quad \omega_{ij} = \frac{1}{2} (\partial_j v_i - \partial_i v_j), \quad I_{ij} = \delta_{ij}, \quad (2.8)$$

describes how the flow gradient rotates and stretches the order-parameter. The scalar parameter ξ appearing both in equations (2.5) and (2.6) depends on the molecular details of a given liquid crystal and measures the ratio between the tumbling and the aligning effect that a shear flow exert over the liquid crystal directors. The active terms are associated with the activity parameters ζ and λ_1 and have been introduced in (2.5) and (2.6) as in [25, 27]. As in [25], we have an active term in the linear momentum equation (2.5) and another one contributing to the director field dynamics (2.6). The former captures the stresses that are induced by the molecular motors and propel fluid either inwards or outwards along the filaments if they are either contractile ($\zeta < 0$) or extensile stresses ($\zeta > 0$), respectively, though experiments and microscopic approaches suggest that actomyosin gels are typically contractile [50–53]. The contribution to the director field dynamics either relaxes ($\lambda_1 < 0$) or increases orientation ($\lambda_1 > 0$) over time, the latter having been observed for concentrated actomyosin gels, which show self-alignment effects [12, 54]. Both activity contributions depend on the difference $\Delta \chi$ in chemical potential between ATP and its hydrolysis products ADP and inorganic phosphate, as this provides the energy for the molecular motors that induce the motion. These activity terms were introduced by [7] based on symmetry principles, and derived microscopically in [50–53] for active filaments. Similar considerations for active suspensions of self-propelled particles can be found in [1, 55].

The molecular field H in (2.6) is the first variation of the Landau-de Gennes energy (2.1) with respect to Q ,

$$H_{ij} = -\frac{\delta \mathcal{F}_{LG}}{\delta Q_{ij}} = a^2 Q_{ij} - c^2 Q_{ij} \text{tr}(Q^2) + \lambda(x) \delta_{ij} + L_1 \partial_k^2 Q_{ij}. \quad (2.9)$$

The Lagrange multiplier $\lambda(x)$ arises from the constraint $\text{tr } Q = 0$. We note that this constraint is equivalent to the normalisation condition of the director field, as can be seen by taking the trace of the representation (2.19) for Q . However, taking the trace of equation (2.6), gives, after some algebra, that $\lambda(x) = -2(\xi + 1)Q_{il}\omega_{li} = 0$, where the last equality follows from $Q_{il} = Q_{li}$. We will therefore drop the $\lambda(x)I$ term from (2.9). The symmetric and antisymmetric parts of the stress tensor σ_{ij} and τ_{ij} that appear in (2.5) are due to the director-flow interaction and have the form

$$\begin{aligned} \tau_{ij} = & -\xi(Q_{ik} + \delta_{ik}/2)H_{kj} - \xi H_{ik}(Q_{kj} + \delta_{kj}/2) \\ & + 2\xi(Q_{ij} + \delta_{ij}/2)H_{km}Q_{km} - L_1 \partial_j Q_{km} \partial_i Q_{km} \end{aligned} \quad (2.10)$$

and

$$\sigma_{ij} = Q_{ik}H_{kj} - H_{ik}Q_{kj}. \quad (2.11)$$

For future reference, we also introduce the total stress tensor T , which includes all contributions, including those from the active term, that is

$$T_{ij} = -p\delta_{ij} + 2\mu e_{ij} + \tau_{ij} + \sigma_{ij} - \zeta \Delta \chi Q_{ij}. \quad (2.12)$$

Boundary conditions at the substrate. We assume that the substrate is impermeable and that the no-slip condition holds for the liquid, hence both components of the liquid vanish at $x_3 = 0$,

$$v = 0. \quad (2.13a)$$

We also impose strong anchoring, so that at $x_3 = 0$, we have

$$Q = Q_1 = q_1(n_1 \otimes n_1 - \frac{1}{2}I), \quad (2.13b)$$

with a given constant $q_1 \in \mathbb{R}$ and $n_1 = [\sin(\theta_1), \cos(\theta_1)] \in \mathbb{R}^2$ (see also [56]).

Boundary conditions at the free interface. We use the isotropic surface energy from [48] (retaining only the first constant term),

$$F_s(Q, \nu) = g_0, \quad (2.14)$$

with $\nu(x_1, t)$ denoting the unit normal to the free surface $\eta(x_1, t)$, which leads to the surface stress (with $I_s \equiv I - \nu \otimes \nu$)

$$T^s = F_s I_s \quad (2.15)$$

that appears in the right hand side of stress condition at the interface $x_3 = \eta(x_1, t)$

$$\nu_i T_{ij} = (\delta_{ik} - \nu_i \nu_k) \partial_k T_{ij}^s. \quad (2.16)$$

In addition, we have the kinematic condition

$$\eta_t = v_3 - v_1 \eta_{,1} \quad (2.17)$$

at $x_3 = \eta(x_1, t)$ and we impose the conical anchoring condition on Q , see also [47, 57, 58],

$$Q = q_2 \left(R(\theta_2) \nu \otimes R(\theta_2) \nu - \frac{1}{2} I \right), \quad (2.18)$$

with a given constant $q_2 \in \mathbb{R}$ and $\theta_2 \in [0, \pi)$, where

$$R(\theta) = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}$$

is the rotation by angle θ_2 . We note, however, that in the thin film limit derived below in section 3, the normal to the free boundary is, to leading order, equal to the canonical unit vector e_3 , hence this boundary condition reduces to a strong anchoring condition with a fixed angle θ_2 with respect to the x_3 coordinate direction.

2.2 Reduction to an active Ericksen model

The reduction of the model (2.4)–(2.6) proceeds as follows: By definition the two eigenvalues of Q are $\pm q/2$ for some scalar order parameter $q \in \mathbb{R}$. Moreover, one can show that for each $Q \in \mathcal{L}_0$ there exists a unit vector $n \in S^1$ (called director) such that representation

$$Q = q[n \otimes n - I/2] \quad (2.19)$$

holds. From this it also follows that each two-dimensional Q-tensor on a plane is completely characterized by two degrees of freedom: the order parameter q and the director n . The representation (2.19) does not distinguish between $+n$ and $-n$. For definiteness, we fix the sign at the free interface, and hence by continuity everywhere in the film, by requiring that n points out of the liquid and the director field is continuous everywhere in the film bulk. In section 5 we will describe situations when the reduction presented in this section can be extended without changes to the case of singular director fields n having defects.

We note also that under representation (2.19) the bulk energy (2.2) reduces to

$$f_b(Q) = f_b(q) = -\frac{a^2 q^2}{4} + \frac{c^2 q^4}{16}, \quad (2.20)$$

which attains its global minima at $q_{min} = \pm \sqrt{2}a/c$.

Substituting (2.19) into (2.9) (and taking into account that $\lambda = 0$) one obtains

$$\begin{aligned} H_{ij} = & \left(a^2 q - \frac{c^2 q^3}{2} \right) \left[n_i n_j - \frac{\delta_{ij}}{2} \right] + L_1 q_{,kk} \left[n_i n_j - \frac{\delta_{ij}}{2} \right] \\ & + 2L_1 q_{,k} n_{i,k} n_j + 2L_1 q_{,k} n_i n_{j,k} + L_1 q [2n_{i,k} n_{j,k} + n_{i,kk} n_j + n_i n_{j,kk}] \end{aligned}$$

On the other hand, expressing of H from (2.6) gives

$$\Gamma H_{ij} = q(n_j N_i + n_i N_j) + (q_t + v_k q_{,k}) \left[n_i n_j - \frac{\delta_{ij}}{2} \right] - S(\nabla v, Q) - \lambda_1 \Delta \chi q (n_i n_j - \delta_{ij}/2) \quad (2.21)$$

where we denote the rate of change of the director with respect to the background fluid

$$N_i = \dot{n}_i - \omega_{ij} n_j, \quad \dot{n}_i = \partial_t n_i + v_j \partial_j n_i, \quad (2.22)$$

and \dot{n}_i denotes the material derivative.

Calculating the variational quantity $\Gamma(H_{ij}n_j + n_i H_{ij})$ for both of the last two representations for H and subsequently equating them one obtains the following equation:

$$\begin{aligned} & L_1 \Gamma[2qn_{i,kk} - 2q|n_{i,k}|^2 n_i + q_{,kk} n_i + 4q_{,k} n_{i,k}] + \Gamma(a^2 q - \frac{c^2 q^3}{2}) n_i \\ &= 2qN_i + (q_t + v_k q_{,k}) n_i - \frac{2}{3}(q+2)\xi e_{ji} n_j - \lambda_1 \Delta \chi q n_i. \end{aligned} \quad (2.23)$$

Multiplying the last equation by n_i and using relations $N_i n_i = n_i^2 - 1 = 0$ one obtains an Allen-Cahn type equation for the scalar order parameter

$$q_t + v_k q_{,k} - \frac{2}{3}(q+2)\xi e_{ji} n_j n_i = L_1 \Gamma q_{,kk} - 4q L_1 \Gamma |n_{j,k}|^2 + \Gamma \left(a^2 q - \frac{c^2 q^3}{2} \right) + \lambda_1 \Delta \chi q, \quad (2.24)$$

Using (2.24) one can simplify (2.23) to a parabolic equation for the director field $n(x)$:

$$L_1 \Gamma[2qn_{i,kk} + 4q_{,k} n_{i,k}] = 2qN_i - 2q L_1 \Gamma |n_{j,k}|^2 n_i - \frac{2}{3}(q+2)\xi[e_{ji} n_j - e_{ik} n_i n_k n_j]. \quad (2.25)$$

Finally, the expressions (2.11) and (2.10) for the symmetric and antisymmetric stresses become

$$\Gamma \sigma_{ij} = q^2(n_i N_j - N_i n_j) - \frac{\xi q(q+2)}{3}(n_i n_k e_{kj} - e_{ik} n_k n_j)$$

and

$$\begin{aligned} \Gamma \tau_{ij} = & -\frac{q\xi}{3}(q+2)(n_j N_i + n_i N_j) + \frac{q\xi^2}{3}(4-q)(e_{ik} n_k n_j + n_i n_k e_{kj}) \\ & + \frac{2\xi^2}{3}(q-1)^2 e_{ij} - \frac{8q^2 \xi^2}{3} \left(\frac{3}{4} + q - q^2 \right) \xi n_i n_j e_{ik} n_l n_k \\ & + \frac{\xi q}{2} n_i n_j (q_t + v_k q_{,k}) - \Gamma L_1 \left(\frac{3}{4} q_{,i} q_{,j} + 2q^2 n_{k,i} n_{k,j} \right) \\ & + \xi \lambda_1 \Delta \chi (1 - q^2) q (n_i n_j - \delta_{ij}/2), \end{aligned}$$

where the last term appears upon inserting the expression (2.21) for H_{ij} into (2.10). Finally, we also have the explicit appearance of the active stress in (2.5),

$$-\zeta \Delta \chi Q_{ij} = -\zeta \Delta \chi q (n_i n_j - \delta_{ij}/2),$$

so that the total stress tensor (2.12) becomes

$$T_{ij} = -p\delta_{ij} + T_{ij}^E + \tilde{T}_{ij}, \quad (2.26)$$

with

$$T_{ij}^E = -L_1 \left(\frac{3}{4} q_{,i} q_{,j} + 2q^2 n_{k,i} n_{k,j} \right), \quad (2.27)$$

$$\begin{aligned} \tilde{T}_{ij} = & \alpha_1 n_k n_p e_{kp} n_i n_j + \alpha_2 N_i n_j + \alpha_3 N_j n_i \\ & + \alpha_4 e_{ij} + \alpha_5 e_{ik} n_k n_j + \alpha_6 e_{jk} n_k n_i + \frac{\xi q}{2\Gamma} n_i n_j (q_t + v_k q_{,k}) \\ & + [\xi \lambda_1 (1 - q^2)/\Gamma - \zeta] \Delta \chi q (n_i n_j - \delta_{ij}/2). \end{aligned} \quad (2.28)$$

The Leslie constants α_i and the parameters of Beris-Edwards model are related by (see (2.10)–(2.15) in [43])

$$\alpha_1(q) = -\frac{2}{3}q^2(3 + 4q - 4q^2)\xi^2/\Gamma, \quad (2.29a)$$

$$\alpha_2(q) = \left\{ -\frac{1}{3}q(2 + q)\xi - q^2 \right\} / \Gamma, \quad (2.29b)$$

$$\alpha_3(q) = \left\{ -\frac{1}{3}q(2 + q)\xi + q^2 \right\} / \Gamma, \quad (2.29c)$$

$$\alpha_4(q) = \frac{4}{9}(1 - q)^2\xi^2/\Gamma + 2\mu, \quad (2.29d)$$

$$\alpha_5(q) = \left\{ \frac{1}{3}q(4 - q)\xi^2 + \frac{1}{3}q(2 + q)\xi \right\} / \Gamma, \quad (2.29e)$$

$$\alpha_6(q) = \left\{ \frac{1}{3}q(4 - q)\xi^2 - \frac{1}{3}q(2 + q)\xi \right\} / \Gamma. \quad (2.29f)$$

We conclude that under representation (2.19) the model (2.4)–(2.6) turns into four equations

$$0 = \partial_i v_i, \quad (2.30a)$$

$$0 = -\partial_i p - L_1 \partial_j \left(\frac{3}{4} q_{,i} q_{,j} + 2q^2 n_{k,i} n_{k,j} \right) + \partial_j \tilde{T}_{ij}, \quad (2.30b)$$

$$\begin{aligned} L_1 \Gamma [2q n_{i,kk} + 4q_{,k} n_{i,k}] &= 2q N_i - 2q L_1 \Gamma |n_{j,k}|^2 n_i \\ &\quad - \frac{2}{3} (q + 2) \xi [e_{ji} n_j - e_{ik} n_l n_k n_i], \end{aligned} \quad (2.30c)$$

$$\begin{aligned} q_t + v_k q_{,k} &= \frac{2}{3} (q + 2) \xi e_{ji} n_j n_i + L_1 \Gamma q_{,kk} - 4q L_1 \Gamma |n_{j,k}|^2 \\ &\quad + \Gamma \left(a^2 q - \frac{c^2 q^3}{2} \right) + \lambda_1 \Delta \chi q, \end{aligned} \quad (2.30d)$$

where \tilde{T}_{ij} is given by (2.28).

Boundary conditions at the substrate. Using (2.19) in (2.13), the boundary conditions at $x_3 = 0$ become

$$v_1 = 0, \quad v_3 = 0, \quad (2.31a)$$

$$n_3 = \cos \theta_1, \quad (2.31b)$$

$$q = q_1. \quad (2.31c)$$

Boundary conditions at the free interface. The condition (2.15) now takes the form

$$T_{ij}^s = g_0 (\delta_{ij} - \nu_i \nu_j). \quad (2.32)$$

Projecting this condition onto the normal and tangential directions at the interface gives

$$\nu_i T_{ij} \nu_j = -g_0 \partial_i \nu_i \quad (2.33a)$$

$$\nu_i T_{ij} t_j = 0. \quad (2.33b)$$

The remaining conditions at the free interface $x_3 = \eta(x_1, t)$ are

$$\eta_t = v_3 - v_1 \partial_1 \eta, \quad (2.33c)$$

$$n = R(\theta_2) \nu, \quad (2.33d)$$

$$q = q_2. \quad (2.33e)$$

3 Derivation of thin-film models

3.1 Thin-film model for active the Erickson theory

We now non-dimensionalize this model using length scales L for x_1 and εL for x_3 , where L denotes the characteristic lateral extend of the cell and εL denote its height. Hence, ε is the ratio between the two length sales and in a thin-film setting assumed to be small. We denote

$$\begin{aligned} x_3 &= \varepsilon L \bar{x}_3, & x_1 &= L \bar{x}_1, & \eta &= \varepsilon L \bar{\eta}, \\ v_1 &= U \bar{v}_1, & v_3 &= V \bar{v}_3, & t &= (L/U) \bar{t}, \\ p &= p_0 + P \bar{p}, & h &= \mathcal{E} \bar{h}, \end{aligned} \quad (3.1)$$

where \mathcal{E} and P are are defined as

$$\mathcal{E} = \frac{L_1}{\varepsilon^2 L^2}, \quad (3.2)$$

$$P = \frac{\mu U}{\varepsilon^2 L}. \quad (3.3)$$

The order parameter q and the director field n are dimensionless and do not need to be scaled. In the normal stress condition at the free surface, balancing the pressure with surface tension requires

$$P = \frac{\varepsilon g_0}{L}. \quad (3.4)$$

Together with (3.3) this means

$$\varepsilon^3 = \frac{\mu U}{g_0}. \quad (3.5)$$

Further scalings are obtained as

$$N_i = \frac{U}{\varepsilon L} \bar{N}_i, \quad (3.6a)$$

$$e_{11} = \frac{U}{L} \bar{e}_{11}, \quad e_{13} = \frac{U}{\varepsilon L} \bar{e}_{13}, \quad e_{31} = \frac{U}{\varepsilon L} \bar{e}_{31}, \quad e_{33} = \frac{U}{L} \bar{e}_{33}, \quad (3.6b)$$

$$\omega_{13} = \frac{U}{\varepsilon L} \bar{\omega}_{13}, \quad \omega_{31} = \frac{U}{\varepsilon L} \bar{\omega}_{31}, \quad (3.6c)$$

$$\alpha_i = \mu \bar{\alpha}_i, \quad \Gamma = \bar{\Gamma} / \mu, \quad a^2 = \mathcal{E} \bar{a}^2, \quad c^2 = \mathcal{E} \bar{c}^2, \quad (3.6d)$$

$$\tilde{T}_{ij} = \frac{\mu U}{\varepsilon L} \bar{\tilde{T}}_{ij}, \quad [T_{11}^E, T_{13}^E, T_{31}^E, T_{33}^E] = \frac{\mu U}{\varepsilon L} [\varepsilon^2 T_{11}^E, \varepsilon T_{13}^E, \varepsilon T_{31}^E, T_{33}^E], \quad (3.6e)$$

$$\bar{L}_1 = \frac{L_1}{\varepsilon \mu U L}, \quad \bar{\zeta} \Delta \bar{\chi} = \frac{\Gamma L}{U} \zeta \Delta \chi, \quad \bar{\lambda}_1 \Delta \bar{\chi} = \frac{L}{U} \lambda_1 \Delta \chi. \quad (3.6f)$$

Retaining only the leading order terms in ε in the rescaled system (2.30), given in appendix A, and assuming the weak elasticity limit, by which we mean that as we introduce the thin-film

approximation $\varepsilon \rightarrow 0$, we assume $\bar{L}_1 = O(1)$ and $\Delta\bar{\chi} = O(\varepsilon^{-1})$, the leading order system in the bulk becomes

$$0 = v_{1,1} + v_{3,3}, \quad (3.7a)$$

$$0 = -p_{,1} + \frac{1}{2}(v_{1,3}f_A(n_1, n_3))_{,3} + \frac{\varepsilon}{\Gamma}\Delta\chi[(\xi\lambda_1(1-q^2) - \zeta)qn_1n_3]_{,3}, \quad (3.7b)$$

$$0 = -p_{,3}, \quad (3.7c)$$

$$L_1\Gamma[2qn_{1,33} + 4q_{,3}n_{1,3}] = -2q\frac{v_{1,3}n_3}{2} - 2qL_1\Gamma(|n_{1,3}|^2 + |n_{3,3}|^2)n_1 - \frac{2v_{1,3}}{3}(q+2)\xi[n_3/2 - n_1^2n_3], \quad (3.7d)$$

$$L_1\Gamma[2qn_{3,33} + 4q_{,3}n_{3,3}] = 2q\frac{v_{1,3}n_1}{2} - 2qL_1\Gamma(|n_{1,3}|^2 + |n_{3,3}|^2)n_3 - \frac{2v_{1,3}}{3}(q+2)\xi[n_1/2 - n_1n_3^2], \quad (3.7e)$$

$$-\frac{2}{3}(q+2)\xi v_{1,3}n_1n_3 = -4qL_1\Gamma(|n_{1,3}|^2 + |n_{3,3}|^2) + L_1\Gamma q_{,33} + \Gamma\left(a^2q - \frac{c^2q^3}{2}\right) + \varepsilon\lambda_1\Delta\chi q, \quad (3.7f)$$

where here and below for convenience we have skipped the overbars everywhere and in the horizontal momentum equation we introduced the notation

$$f_A(n_1, n_3) \equiv 2\alpha_1(n_1n_3)^2 + (\alpha_5 - \alpha_2)n_3^2 + (\alpha_3 + \alpha_6)n_1^2 + \alpha_4. \quad (3.8)$$

The leading order system for the boundary conditions at $z = 0$ is given by

$$v_1 = 0, \quad v_3 = 0, \quad (3.9a)$$

$$n_3 = \cos\theta_1, \quad (3.9b)$$

$$q = q_1, \quad (3.9c)$$

and at the free surface, $x_3 = \eta(x_1, t)$ by (cf. (A.11) in Appendix A).

$$\eta_t = v_3 - v_1\partial_1\eta, \quad (3.10a)$$

$$-p = \eta_{,11}, \quad (3.10b)$$

$$\frac{1}{2}v_{1,3}f_B(n_1, n_3) = -\frac{\varepsilon}{\Gamma}\Delta\chi(\xi\lambda_1(1-q^2) - \zeta)qn_3n_1, \quad (3.10c)$$

$$n_3 = \cos\theta_2, \quad (3.10d)$$

$$q = q_2, \quad (3.10e)$$

with a given function $q_2(x, t)$, and where we define

$$f_B(n_1, n_3) \equiv 2\alpha_1(n_1n_3)^2 + (\alpha_6 - \alpha_3)n_3^2 + (\alpha_2 + \alpha_5)n_1^2 + \alpha_4. \quad (3.11)$$

Next, similar to [17] we rewrite equations (3.7a)–(3.7f) in the bulk in terms of the director angle θ using the representation

$$n_1 = \sin\theta, \quad n_3 = \cos\theta. \quad (3.12)$$

First, let us multiply equations (3.7d) and (3.7e) by $-n_3$ and n_1 , respectively, and then sum up them. The resulting equation has the form:

$$L_1 \Gamma [-2qn_{1,33}n_3 - 4q_{,3}n_{1,3}n_3 + 2qn_{3,33}n_1 + 4q_{,3}n_{3,3}n_1] = qv_{1,3} + \frac{v_{1,3}}{3}(q+2)\xi [n_3^2 - n_1^2]. \quad (3.13)$$

Using (3.12) and definitions

$$\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_2 + \alpha_3 = \alpha_6 - \alpha_5 \quad (3.14)$$

and (2.29) the latter equation can be reduced to (3.18) which we include with the other equations of the system (3.7a)–(3.7f), rewritten in terms of θ , giving

$$0 = v_{1,1} + v_{3,3}, \quad (3.15)$$

$$0 = -p_{,1} + \frac{1}{2}(v_{1,3}f_A(\theta))_{,3} + \frac{\varepsilon}{2\Gamma}\Delta\chi [(\xi\lambda_1(1-q^2) - \zeta)q\sin(2\theta)]_{,3}, \quad (3.16)$$

$$0 = -p_{,3}, \quad (3.17)$$

$$L_1 q [2q\theta_{,33} + 4q_{,3}\theta_{,3}] = -\frac{v_{1,3}}{2}[\gamma_1 - \gamma_2 \cos(2\theta)] \quad (3.18)$$

$$-\frac{1}{3}(q+2)\xi v_{1,3}\sin(2\theta) = -4qL_1\Gamma|\theta_{,3}|^2 + L_1\Gamma q_{,33} + \Gamma(a^2q - \frac{c^2q^3}{2}) + \varepsilon\lambda_1\Delta\chi q, \quad (3.19)$$

where we define

$$f_A(\theta) = (\alpha_1/2)\sin^2(2\theta) + (\alpha_5 - \alpha_2)\cos^2\theta + (\alpha_3 + \alpha_6)\sin^2\theta + \alpha_4. \quad (3.20)$$

The leading order system for the boundary conditions at $z = 0$ is given by

$$v_1 = 0, \quad v_3 = 0, \quad (3.21a)$$

$$\theta = \theta_1, \quad (3.21b)$$

$$q = q_1, \quad (3.21c)$$

and at the free surface, $x_3 = \eta(x_1, t)$ by

$$\eta_t = v_3 - v_1\partial_1\eta, \quad (3.22a)$$

$$-p = \eta_{,11}, \quad (3.22b)$$

$$\frac{1}{2}v_{1,3}f_B(\theta) = -\frac{\varepsilon}{2\Gamma}\Delta\chi (\xi\lambda_1(1-q^2) - \zeta)q\sin(2\theta), \quad (3.22c)$$

$$\theta = \theta_2, \quad (3.22d)$$

$$q = q_2, \quad (3.22e)$$

where we define

$$f_B(\theta) = (\alpha_1/2)\sin^2(2\theta) + (\alpha_6 - \alpha_3)\cos^2\theta + (\alpha_2 + \alpha_5)\sin^2\theta + \alpha_4. \quad (3.23)$$

We now integrate these equations. First, the combination of (3.15) and (3.22a) gives

$$\eta_t(x_1, t) = -\partial_1 \int_0^\eta v_1(x_1, x_3, t) dx_3.$$

which is in fact exact i.e. also valid for the full governing equations. From (3.17), (3.22b), (3.16), (3.22c), we get

$$p = -\eta_{,11}, \quad (3.24)$$

$$\begin{aligned} f_A(q, \theta) v_{1,3} &= 2\eta_{,111}(\eta - x_3) - \frac{\varepsilon}{\Gamma} \Delta \chi (\xi \lambda_1 (1 - q^2) - \zeta) q \sin(2\theta) \\ &\quad + \frac{\varepsilon}{\Gamma} \Delta \chi (\xi \lambda_1 (1 - q_2^2) - \zeta) q_2 \sin(2\theta_2) \\ &\quad - \frac{\varepsilon}{\Gamma} \Delta \chi \frac{f_A(q_2, \theta_2)}{f_B(q_2, \theta_2)} (\xi \lambda_1 (1 - q_2^2) - \zeta) q_2 \sin(2\theta_2) \\ &= 2\eta_{,111}(\eta - x_3) - \frac{\varepsilon}{\Gamma} \Delta \chi (\xi \lambda_1 (1 - q^2) - \zeta) q \sin(2\theta) \\ &\quad + \frac{\varepsilon}{\Gamma} \Delta \chi \frac{\gamma_1 - \gamma_2 \cos(2\theta_2)}{f_B(q_2, \theta_2)} (\xi \lambda_1 (1 - q_2^2) - \zeta) q_2 \sin(2\theta_2), \end{aligned} \quad (3.25)$$

provided $f_B(q_2, \theta_2) \neq 0$.

Therefore, the last three equations combined together result in a closed lubrication system:

$$\eta_t(x_1, t) = -\partial_1 \int_0^\eta v_1(x_1, x_3, t) dx_3, \quad (3.26a)$$

$$\begin{aligned} v_{1,3} &= \frac{2\eta_{,111}}{f_A(q, \theta)} (\eta - x_3) \\ &\quad - \frac{\varepsilon \Delta \chi}{\Gamma f_A(q, \theta)} \left[(\xi \lambda_1 (1 - q^2) - \zeta) q \sin(2\theta) \right. \\ &\quad \left. - \frac{\gamma_1 - \gamma_2 \cos(2\theta_2)}{f_B(q_2, \theta_2)} (\xi \lambda_1 (1 - q_2^2) - \zeta) q_2 \sin(2\theta_2) \right], \end{aligned} \quad (3.26b)$$

$$(q^2 \theta_{,3})_{,3} = -\frac{1}{4L_1} (\gamma_1 - \gamma_2 \cos(2\theta)) v_{1,3}, \quad (3.26c)$$

$$q_{,33} = 4q(\theta_{,3})^2 - \frac{\xi(q+2)}{3L_1\Gamma} \sin(2\theta) v_{1,3} - \frac{q}{L_1} \left(a^2 - \frac{c^2 q^2}{2} \right) - \frac{\varepsilon \lambda_1 \Delta \chi}{L_1 \Gamma} q. \quad (3.26d)$$

Notice that if $f_A(q(x_1, x_3, t), \theta(q(x_1, x_3, t))) \neq 0$ for all x_1, x_3 and t , we can substitute (3.26b) into (3.26c) and (3.26d) to eliminate $v_{1,3}$, thus decoupling the system for θ and q from the velocity field. Because of the size of the resulting equations, we have not done this here. System (3.26a)-(3.26d) is completed with the following boundary conditions:

$$v_1 = 0 \quad \text{at } x_3 = 0, \quad (3.26e)$$

$$\theta = \theta_1 \quad \text{at } x_3 = 0, \quad (3.26f)$$

$$q = q_1 \quad \text{at } x_3 = 0, \quad (3.26g)$$

$$\theta = \theta_2 \quad \text{at } x_3 = \eta, \quad (3.26h)$$

$$q = q_2 \quad \text{at } x_3 = \eta. \quad (3.26i)$$

3.2 Thin-film model for the active Leslie-Erickson-Parodi theory

If we use the Leslie-Erickson-Parodi theory with corresponding active terms as a model for the active liquid crystal [7, 8, 12, 13] and nondimensionalise as before we derive in appendix B the

following coupled system for the leading order thin-film approximation

$$\partial_t \eta = -\partial_1 \int_0^\eta v_1 dx_3, \quad (3.27a)$$

$$0 = \eta_{,111}(x_3 - \eta) + \frac{1}{2}v_{1,3}f_A(\theta) + \frac{\zeta^{ELP}\Delta\chi^{ELP}}{2}\frac{f_A(\theta_2)}{f_B(\theta_2)}\sin(2\theta_2) + \frac{\zeta^{ELP}\Delta\chi^{ELP}}{2}(\sin(2\theta) - \sin(2\theta_2)), \quad (3.27b)$$

$$2K\theta_{,33} = -(\gamma_1 - \gamma_2 \cos(2\theta))v_{1,3}, \quad (3.27c)$$

with the boundary conditions at $x_3 = 0$ given by

$$v_1 = 0, \quad (3.28a)$$

$$\theta = \theta_1, \quad (3.28b)$$

and at the free surface, $x_3 = \eta(x_1, t)$,

$$\theta = \theta_2. \quad (3.29)$$

Formal comparison of (3.27) with equations (3.26a)-(3.26c) considered with $q = q_1 = q_2 = \text{const}$ provides the following relations between the active and elastic parameters in the Eriksen-Leslie-Parodi and Ericksen thin-film models:

$$\lambda_1^{ELP} = \lambda_1, \quad \zeta^{ELP} = (\zeta - \xi\lambda_1(1 - q^2))q, \quad K = 2L_1q^2, \quad \Delta\chi^{ELP} = \frac{\varepsilon}{\Gamma}\Delta\chi. \quad (3.30)$$

At the same time, in absence of the active terms $\Delta\chi^{ELP} = 0$ our model (3.27) can be shown to coincide with the (passive) thin-film model derived in [17] for the weak elasticity regime, cf. system (A17)-(A20) there. Note that the special anchoring boundary conditions $\theta_1 = \pi/2$ and $\theta_2 = 0$ were considered in Lin et al. [17].

4 Impact of activity terms

At this point, further reductions of the thin-film model (3.26) or (3.27) are not, in general, possible without additional assumptions, since the remaining equations cannot be easily integrated with respect to x_3 . We will instead look at two special cases of the more general Q -tensor system (3.26): one, where the interface is flat ($\eta = 1$) and the other where the misalignment of the director at the substrate and the interface is small, $|\theta_2 - \theta_1| \ll 1$.

4.1 Flat film

Passive case We first consider the case, where $\eta = \text{const}$ is any positive constant. This yields $v_1 = 0$ and

$$q^2\theta_{,3} = c_1, \quad (4.1a)$$

$$q_{,33} = 4q(\theta_{,3})^2 - \frac{1}{L_1} \left(a^2q - \frac{c^2q^3}{2} \right) \quad (4.1b)$$

Under the additional assumption that $q_1 = q_2 \equiv q_0$ and that q remains constant we obtain the solution

$$\theta = (\theta_2 - \theta_1)\frac{x_3}{\eta} + \theta_1, \quad q = q_0 = \left[\frac{2a^2}{c^2} - \frac{8L_1}{c^2}(\theta_2 - \theta_1)^2 \right]^{1/2}. \quad (4.2)$$

We note that a similar solution for the director angle θ and for q has been found for the case of channel flow in [40].

Alternatively, one can also substitute (4.1a) into (4.1b) to obtain one ODE for q :

$$q_{,33} = \frac{4c_1^2}{q^3} - \frac{1}{L_1} \left(a^2 q - \frac{c^2 q^3}{2} \right). \quad (4.3)$$

Multiplying the last equation by $q_{,3}$ and integrating in x_3 one obtains

$$\frac{1}{2} q_{,3}^2 = -\frac{2c_1^2}{q^2} - \frac{1}{L_1} \left(\frac{a^2}{2} q^2 - \frac{c^2 q^4}{8} \right) + c_2,$$

where we have assumed that $q \neq \text{const}$ and

$$c_2 = \left(\frac{2c_1^2}{q^2} + \frac{1}{L_1} \left(\frac{a^2}{2} q_1^2 - \frac{c^2 q_1^4}{8} \right) + \frac{1}{2} q_{,3}^2 \right) \Big|_{x_3=0}. \quad (4.4)$$

The last ODE is separable and can be integrated as

$$x_3 = \int_{q_1}^q \frac{ds}{\sqrt{-\frac{4c_1^2}{s^2} - \frac{1}{L_1} \left(a^2 s^2 - \frac{c^2 s^4}{4} \right) + 2c_2}}, \quad (4.5)$$

where we have assumed that $q_2 > q_1$. Correspondingly, using (4.1a) one finds

$$\theta(x_3) - \theta_1 = \int_0^{x_3} \frac{c_1}{q^2(x_3)} dx_3 = c_1 \int_{q_1}^q \frac{ds}{s^2 \sqrt{-\frac{4c_1^2}{s^2} - \frac{1}{L_1} \left(a^2 s^2 - \frac{c^2 s^4}{4} \right) + 2c_2}}. \quad (4.6)$$

In the last expression, constants c_1 and c_2 are determined by the boundary condition for θ at $x_3 = \eta = \text{const}$:

$$\begin{aligned} \theta_2 - \theta_1 &= c_1 \int_{q_1}^{q_2} \frac{ds}{s^2 \sqrt{-\frac{4c_1^2}{s^2} - \frac{1}{L_1} \left(a^2 s^2 - \frac{c^2 s^4}{4} \right) + 2c_2}}, \\ \eta &= \int_{q_1}^{q_2} \frac{ds}{\sqrt{-\frac{4c_1^2}{s^2} - \frac{1}{L_1} \left(a^2 s^2 - \frac{c^2 s^4}{4} \right) + 2c_2}}. \end{aligned} \quad (4.7)$$

Two nonlinear compatibility conditions (4.7) may have multiple solutions or do not have ones at all depending on the given set of four parameters $q_1, q_2, \theta_1 - \theta_2$ and η . In the latter case, there exists only one trivial solution (4.2) to system (4.1). We aim to investigate existence and multiplicity parameter regions for solutions to (4.7) in a subsequent study.

Active flat film The compatibility condition of $\eta(x_1, x_3, t) = \eta = \text{const}$ with (3.26a) implies that v_1, q, θ are functions of x_3 only. By that, system (3.26b)-(3.26d) reduces to

$$\begin{aligned} v_{1,3} &= -\frac{\varepsilon \Delta \chi}{\Gamma f_A(q, \theta)} \left[\left(\xi \lambda_1 (1 - q^2) - \zeta \right) q \sin(2\theta) \right. \\ &\quad \left. - \frac{\gamma_1 - \gamma_2 \cos(2\theta_2)}{f_B(q_2, \theta_2)} \left(\xi \lambda_1 (1 - q_2^2) - \zeta \right) q_2 \sin(2\theta_2) \right] \end{aligned} \quad (4.8a)$$

$$(q^2 \theta_{,3})_{,3} = -\frac{1}{4L_1} (\gamma_1 - \gamma_2 \cos(2\theta)) v_{1,3}, \quad (4.8b)$$

$$q_{,33} = 4q(\theta_{,3})^2 - \frac{\xi(q+2)}{3L_1\Gamma} \sin(2\theta)v_{1,3} - \frac{q}{L_1} \left(a^2 - \frac{c^2 q^2}{2} \right) - \frac{\varepsilon\lambda_1\Delta\chi}{L_1\Gamma} q, \quad (4.8c)$$

which further reduce to two coupled ODEs for $\theta(x_3)$ and $q(x_3)$ by eliminating $v_{1,3}$. The latter ODEs can be effectively integrated numerically.

Note, that in the absence of the active terms ($\lambda_1 = 0$ or $\zeta = 0$) the nontrivial solution to the system (4.8) is given by (4.5)-(4.6) combined with $v_1 = 0$ and it exists only when the compatibility conditions (4.7) on the boundary data (3.26f)-(3.26i) are satisfied. Given $q_2 > q_1$, such that the square root in the denominator of (4.5) is real for all $q \in (q_1, q_2)$, by taking η and $\theta_2 - \theta_1$ sufficiently large, one can realize this passive solution. Moreover, also for small active terms with $\Delta\chi \ll 1$ this non-homogeneous solution to the system (4.8) continuously persists and by (4.8a) exhibits the non-homogeneous flow $v_1(x_3)$ with $|v_1| \ll 1$. This effect of inducing a non-zero flow in a channel geometry, when the thickness of the latter η becomes sufficiently large, has been observed in [11, 12] for the polar Leslie-Ericksen-Parodi based models.

Finally, note that when active terms are present in (4.8) there is no analogous solution to (4.2), i.e. having constant $q(x_3) = q_0$. In this case, three equations (4.8a)-(4.8b) are not compatible, unless trivial isotropic case $q_0 = 0$ holds. In contrast, the passive solution (4.2) to Leslie-Ericksen-Parodi (3.27) having the linear director profile can be continued also in the presence active terms. These solutions can be found numerically or analytically as ones to the corresponding active stationary system:

$$0 = \frac{1}{2}v_{1,3}f_A(\theta) + \frac{\zeta^{ELP}\Delta\chi^{ELP}}{2} \frac{f_A(\theta_2)}{f_B(\theta_2)} \sin(2\theta_2) + \frac{\zeta^{ELP}\Delta\chi^{ELP}}{2} (\sin(2\theta) - \sin(2\theta_2)), \quad (4.9a)$$

$$2K\theta_{,33} = -(\gamma_1 - \gamma_2 \cos(2\theta))v_{1,3}, \quad (4.9b)$$

considered with the same boundary conditions as in (3.27).

4.2 Film with small angle change in the director boundary condition

Another special case, where it is possible to discuss analytical solutions is obtained if the difference in the director angle is small.

Passive case Assuming $|\theta_2 - \theta_1| \ll 1$, then to leading order $\theta = \theta_2 = \theta_1$ is constant and (3.26c) implies $v_{1,3} = v_1 = 0$ and $\eta = \text{const}$. As a result the whole dynamics reduces to (3.26d), which can be further reduced to (4.3) with $c_1 = 0$. Then the corresponding solution is given by

$$x_3 = \int_{q_1}^q \frac{ds}{\sqrt{-\frac{1}{L_1}(a^2 s^2 - \frac{c^2 s^4}{4}) + 2c_2}} \quad \text{for } x_3 \in (0, \eta). \quad (4.10)$$

The compatibility conditions (4.7) reduce to

$$\eta = \int_{q_1}^q \frac{ds}{\sqrt{-\frac{1}{L_1}(a^2 s^2 - \frac{c^2 s^4}{4}) + 2c_2}} \quad (4.11)$$

As an important illustration of the difference between Ericksen (3.26) and Leslie-Ericksen-Parodi (3.27) models, we point out that the new solution (4.10) can be used as a building block for construction of admissible solutions with discontinuous director field $\theta(x_3)$. Namely, let us consider the particular case $q_2 = q_{\min} = \sqrt{2}a/c > q_1 = 0$, in (4.10)-(4.11). Then it is easy to

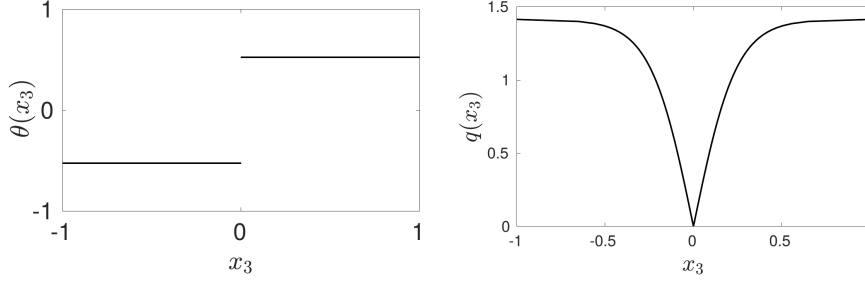


Figure 2: Director angle profile (left) and q -profile (right) for the solution (4.10), (4.12) with $\theta_1 = -\pi/6$, $\theta_2 = \pi/6$, $a = 1$, $c = 1$, $\eta = 1$, $L_1 = 0.04$ and corresponding $c_2 = 16.667$ calculated numerically.

show existence of a unique $c_2(\eta)$ satisfying (4.7). We can extend (4.10) by a reflection around $x_3 = 0$ as

$$\theta(x_3) = -\theta_1, \quad x_3 = - \int_0^q \frac{ds}{\sqrt{-\frac{1}{L_1}(a^2 s^2 - \frac{c^2 s^4}{4}) + 2c_2}} \quad \text{for } x_3 \in (-\eta, 0). \quad (4.12)$$

The resulting combined solution (4.10), (4.12) (see Fig. 2) is a suitably defined weak solution to stationary system (4.1) considered in the interval $(-\eta, \eta)$. Accordingly, the defect line $x_3 = 0$ is isotropic with $q(0) = 0$ and across it the director jumps by value $2\eta\theta_1$. Additionally, we note that the constructed solution (4.10), (4.12) corresponds to the limiting profile as the elastic constant tends to zero of the antisymmetric nematic field in the channel observed numerically in [40], cf. in particular with approximate formula (29) there. Finally, we note that the solution (4.10) with $\theta = \theta_1 = \text{const}$ to the system (3.26a)-(3.26d) does not exist in the case when active terms are present ($\lambda_1 \neq 0$ or $\zeta \neq 0$), since in that case equations (3.26a)-(3.26d) become incompatible.

Active film Another way to initiate a nontrivial dynamics in the case $\theta = \theta_2 = \theta_1 = \text{const}$ is to assume

$$\gamma_1 - \gamma_2 \cos(2\theta) = 0. \quad (4.13)$$

This would imply that (3.26c) is satisfied and $q = q_1 = q_2 = \text{const}$. Furthermore, (3.26b) can be integrated and introduced into (3.26a) yields a new modified thin-film equation

$$\eta_t = -\frac{2}{3f_A(q_1, \theta_1)} \partial_1 (\eta^3 \eta_{,111}) + C(q_1, \theta_1) \partial_1 (\eta^2). \quad (4.14)$$

Note that in this case, besides the trivial isotropic solution $q_1 = 0$, only special values of q_1 and θ_1 are allowed. These have to be compatible with both, equation (4.13) and the algebraic relation

$$0 = \left(a^2 - \frac{c^2 q^2}{2} \right) + \frac{\varepsilon \lambda_1 \Delta \chi}{\Gamma}. \quad (4.15)$$

which arises from (3.26d).

For given activity $\lambda_1 \Delta \chi \in \mathbb{R}$, solutions for q_1 and θ_1 can be obtained from (4.13) and (4.15) as

$$\cos(2\theta) = -\frac{3}{\xi} + \frac{6}{(2+q)\xi}, \quad q^2 = \frac{2a^2}{c^2} + \frac{2\varepsilon \lambda_1 \Delta \chi}{c^2 \Gamma}. \quad (4.16)$$

Finally, note that solution (4.16) to system (3.26) does not always exist. In particular, it does not exist for $\xi = 0$, i.e. when liquid crystal molecules align perfectly with the hydrodynamic flow. In absence of active terms ($\lambda_1 = 0$ or $\zeta = 0$) one has $C(q_1, \theta_1) = 0$ in (4.14), and therefore the hydrodynamic flow decouples from the nematics via the rescaling of time by $f_A(q_1, \theta_1)$.

5 Discussion and outlook

In this article, we presented a systematic asymptotic derivation of the thin-film model given by the system (3.26) from the free-boundary problem for the Beris-Edwards model (2.4)-(2.6) to describe the evolution and flow structure of an active nematic liquid crystal. We also showed that the new thin-film model formally reduces to the polar one (3.27) based on Leslie-Ericksen-Parodi theory, when the scalar order parameter q is homogeneous, which in the passive case coincides with the model derived previously in [17]. In the active case, the steady state solution to (3.26) considered in paragraph 4.1 exhibits nonzero flow that can be spontaneously initiated from the homogeneous one by increasing the film thickness, as previously observed in [11, 12].

Additionally, we were able to construct a passive steady state with discontinuous director field in section 4.2 and Fig. 2. In the Ericksen theory the defects are defined as singular points where the scalar order parameter $q = 0$ [23]. We note, that besides the singularities of the director field the solutions to (3.26) may exhibit singular lines along which $q = 0$ but n is still continuous. These lines have special physical meaning, because Q -tensor in (2.19) is zero and, therefore, the nematic field is isotropic along them. A typical example of such a line is given by the middle line of the channel at the right embedded Q -tensor plot in Fig. 2 of [40]. Our discontinuous solution can be considered as the limiting profile for that one of [40] as the elastic constant tends to zero.

In summary, both passive and active solutions derived in section 4 for nematic (3.26) and polar (3.27) thin film models can potentially find important applications to design and development of microfluidic devices (cf. review [59]).

We now point to some further applications as well as extensions of our results. The derivation of the coupled model (3.26) starting from the Ericksen type model (2.30) considered with boundary conditions (2.31)–(2.33) has been conveyed under the assumption of continuity of the director field n in the film bulk and at the free surface. We note that these models are capable to describe solutions having point defects of integer degree k with $k \in \mathbb{Z}$. Two typical examples of defects with degree -1 in the film bulk and of degree 1 at the film contact line are presented in Fig. 3. One observes that when approaching the defect points the magnitude of the scalar order parameter q goes to zero and by that preserving the continuity of the full Q -tensor field (2.19). We should also point out that, being derived in the weak elasticity regime (cf. scaling for L_1 in (3.6f)) and under the large pressure scaling (3.3), the model (3.26a), (3.26) allows for $O(1)$ variation of the director field n along the vertical x_3 direction of the film. This is the case, for example, in the wall defect of degree -1 in a confined flat film presented in Fig. 1 (right plot), where the director angle θ changes from 0 to $\pi/2$ along the vertical film direction. Such wall defects were observed before in experiments on thin passive nematic films [60].

However, the Ericksen model may not always resolve defects of rational degree $k+1/2$, $k \in \mathbb{Z}$, because the latter exhibit special disclination curves along which n changes to $-n$ [49, 61, 62]. Nevertheless, such defects can be described by the lubrication model (3.26) if the special condition

$$\lim_{(x_1, x_3) \rightarrow (x_1^*, x_3^*)} |\sqrt{q(x_1, x_3)} \nabla n(x_1, x_3)| < \infty \quad (5.1)$$

is fulfilled, where (x_1^*, x_3^*) is an instant defect location. It is easy to check that (5.1) ensures then that the associated local Ericksen elastic energy and the corresponding terms involving director gradients in (3.26c)–(3.26d) are kept finite.

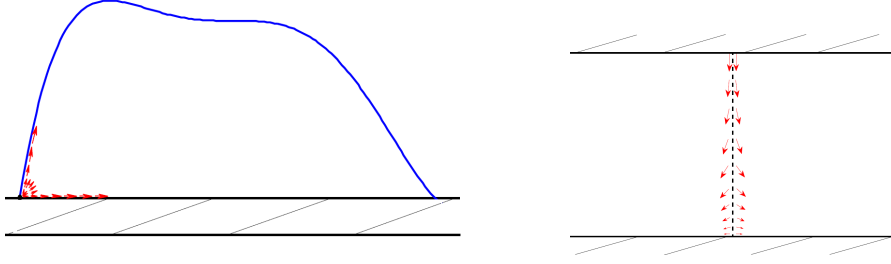


Figure 3: Examples of defects of degree 1 at the contact line (left) and a wall defect (right), which mathematically can be described by the point defect of degree -1 located at the intersection of the wall (depicted by dashed line) and the substrate. The direction of the director field in the neighborhood of the defect is shown by red arrows. The magnitude of scalar order parameter q is represented by the arrow size. The derived Q -tensor lubrication model (3.26) can smoothly resolve such integer point defects through continuous reduction of the scalar parameter field to $q = 0$ when approaching the defect.

Even a spreading of droplet of a passive liquid crystal can exhibit defects that cannot be resolved by a thin film theory based on Leslie-Ericksen theory [18], and a tensorial theory is required. This is a fortiori true for droplets of active matter [63]. Singularities occur generically at the contact-line, where the anchoring conditions usually clash, or we may have defects in the bulk of the droplet, for example horizontally aligned vortices, asters or half-defects, which may be tested against experiments with suspensions of active particles, see [63] and references therein. Notice that these defects also play an important role in the in-vitro experiments with actin filaments mentioned earlier [9, 10]. The thin film model developed here based on the Ericksen theory with an additional order parameter for the degree or anisotropy represents the basis to reliably capture these situations and the defects. It will need to be extended to three dimensions, so that horizontally aligned defects can be treated. Other parameter regimes, such as the case of moderate elasticity, where the director field decouples from the flow [17] will be of interest.

In the future, we plan to investigate system (3.26) numerically, where the nematic part of the model, equations (3.26c)-(3.26d), is given by two coupled ODEs in x_3 direction. A quasi one-dimensional numerical scheme could then be developed by solving the hydrodynamic equations (3.26a), (3.26b) and the nematic ones (3.26c)-(3.26d) separately and iteratively. We expect complicated solution patterns for (3.26) to arise with dynamical formation, mutual interaction and annihilation of point defects in the film bulk similar to ones observed recently in [27, 30]. As in the latter works, it would be important to investigate the interrelation of these patterns with the evolution of the liquid vorticity field [32].

Finally, we note that by imposing the constant scalar order parameter $q = q_2$ in (2.18) we neglected possible Marangoni effects at the free surface and, in particular, in condition (2.33b) for the tangential stress. This was motivated by the fact that under the balance (3.5), that keeps the surface tension term at leading order in (2.33a), the equation for the Marangoni force (see e.g. formula (8) in [48]) necessarily implies that q should be constant at the film free surface. Nevertheless, by relaxing condition (3.5) and neglecting surface tension one would be able to derive a model analogous to (3.26) for pure Marangoni driven active nematic thin films.

Data accessibility statement

This work has no data.

Competing interests statement

We have no competing interests.

Authors' contributions

GK, AM and BW all conceived and contributed to the development of the mathematical models and the writing of the manuscript equally.

Acknowledgements

The authors would like to thank Jonathan Robbins, Valeriy Slastikov and Arghir Zarnescu for their valuable comments on the results of this article. GK gratefully acknowledges the hospitality of the Weierstrass-Institute Berlin and OCIAM at the University of Oxford during his research visits.

Funding statement

GK would like to acknowledge support from Leverhulme grant RPG-2014-226.

A Thin-film approximation

After application of scalings (3.1)–(3.6) to Ericksen system (2.30) the non-dimensional equations for the bulk, after skipping overbars everywhere, take the form:

$$0 = v_{1,1} + v_{3,3}, \quad (\text{A.1})$$

$$0 = -p_{,1} - \varepsilon^3 T_{11,1}^E - \varepsilon T_{13,3}^E + \varepsilon \tilde{T}_{11,1} + \tilde{T}_{13,3} \quad (\text{A.2})$$

$$0 = -p_{,3} - \varepsilon^3 T_{31,1}^E - \varepsilon T_{33,3}^E + \varepsilon^2 \tilde{T}_{31,1} + \varepsilon \tilde{T}_{33,3} \quad (\text{A.3})$$

$$\begin{aligned} & L_1 \Gamma (2\varepsilon^2 q n_{1,11} + 2q n_{1,33} + 4\varepsilon^2 q_{,1} n_{1,1} + 4q_{,3} n_{1,3}) \\ &= 2q N_1 - 2q L_1 \Gamma (\varepsilon^2 |n_{1,1}|^2 + |n_{1,3}|^2 + \varepsilon^2 |n_{3,1}|^2 + |n_{3,3}|^2) n_1 \\ & - \frac{2}{3} (q+2) \xi (\varepsilon e_{11} n_1 + e_{31} n_3 - (\varepsilon e_{11} n_1 n_1 + e_{13} n_1 n_3 + e_{31} n_3 n_1 + \varepsilon e_{33} n_3 n_3) n_1); \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} & L_1 \Gamma (2\varepsilon^2 q n_{3,11} + 2q n_{3,33} + 4\varepsilon^2 q_{,1} n_{3,1} + 4q_{,3} n_{3,3}) \\ &= 2q N_3 - 2q L_1 \Gamma (\varepsilon^2 |n_{1,1}|^2 + |n_{1,3}|^2 + \varepsilon^2 |n_{3,1}|^2 + |n_{3,3}|^2) n_3 \\ & - \frac{2}{3} (q+2) \xi (e_{13} n_1 + \varepsilon e_{33} n_3 - (\varepsilon e_{11} n_1 n_1 + e_{13} n_1 n_3 + e_{31} n_3 n_1 + \varepsilon e_{33} n_3 n_3) n_3); \end{aligned} \quad (\text{A.5})$$

$$\varepsilon (q_t + v_k q_{,k}) - \frac{2}{3} (q+2) \xi (\varepsilon e_{11} n_1 n_1 + e_{13} n_1 n_3 + e_{31} n_3 n_1 + \varepsilon e_{33} n_3 n_3)$$

$$\begin{aligned}
&= -4qL_1\Gamma \left(\varepsilon^2 |n_{1,1}|^2 + |n_{1,3}|^2 + \varepsilon^2 |n_{3,1}|^2 + |n_{3,3}|^2 \right) + \\
&\quad L_1\Gamma \left(\varepsilon^2 q_{,11} + q_{,33} \right) + L_1\Gamma \left(a^2 q - \frac{c^2 q^3}{2} \right) + \varepsilon \lambda_1 \Delta \chi q,
\end{aligned} \tag{A.6}$$

where

$$T_{11}^E = L_1 \left(\frac{3}{4} |q_{,1}|^2 + 2q^2 |n_{k,1}|^2 \right), \tag{A.7a}$$

$$T_{13}^E = T_{31}^E = L_1 \left(\frac{3}{4} q_{,1} q_{,3} + 2q^2 n_{k,1} n_{k,3} \right), \tag{A.7b}$$

$$T_{33}^E = L_1 \left(\frac{3}{4} |q_{,3}|^2 + 2q^2 |n_{k,3}|^2 \right), \tag{A.7c}$$

$$\begin{aligned}
\tilde{T}_{11} = & \alpha_1 (\varepsilon n_1 n_1 e_{11} n_1 n_1 + n_1 n_3 e_{13} n_1 n_1 + n_3 n_1 e_{31} n_1 n_1 + \varepsilon n_3 n_3 e_{33} n_1 n_1) \\
& + \alpha_2 N_1 n_1 + \alpha_3 N_1 n_1 + \alpha_4 \varepsilon e_{11} \\
& + \alpha_5 (\varepsilon e_{11} n_1 n_1 + e_{13} n_3 n_1) + \alpha_6 (\varepsilon e_{11} n_1 n_1 + e_{13} n_3 n_1) \\
& + \frac{\varepsilon}{\Gamma} \frac{\xi q}{2} n_1 n_1 (q_t + v_k q_{,k}) + \frac{\varepsilon}{\Gamma} [\xi \lambda_1 (1 - q^2) - \zeta] \Delta \chi q (n_1 n_1 - 1/2),
\end{aligned} \tag{A.7d}$$

$$\begin{aligned}
\tilde{T}_{13} = & \alpha_1 (\varepsilon n_1 n_1 e_{11} n_1 n_3 + n_1 n_3 e_{13} n_1 n_3 + n_3 n_1 e_{31} n_1 n_3 + \varepsilon n_3 n_3 e_{33} n_1 n_3) \\
& + \alpha_2 N_1 n_3 + \alpha_3 N_3 n_1 + \alpha_4 e_{13} \\
& + \alpha_5 (\varepsilon e_{11} n_1 n_3 + e_{13} n_3 n_3) + \alpha_6 (e_{31} n_1 n_1 + \varepsilon e_{33} n_3 n_1) \\
& + \frac{\varepsilon}{\Gamma} \frac{\xi q}{2} n_1 n_3 (q_t + v_k q_{,k}) + \frac{\varepsilon}{\Gamma} [\xi \lambda_1 (1 - q^2) - \zeta] \Delta \chi q n_1 n_3,
\end{aligned} \tag{A.7e}$$

$$\begin{aligned}
\tilde{T}_{31} = & \alpha_1 (\varepsilon n_1 n_1 e_{11} n_3 n_1 + n_1 n_3 e_{13} n_3 n_1 + n_3 n_1 e_{31} n_3 n_1 + \varepsilon n_3 n_3 e_{33} n_3 n_1) \\
& + \alpha_2 N_3 n_1 + \alpha_3 N_1 n_3 + \alpha_4 e_{31} \\
& + \alpha_5 (e_{31} n_1 n_1 + \varepsilon e_{33} n_3 n_1) + \alpha_6 (\varepsilon e_{11} n_1 n_3 + e_{13} n_3 n_3) \\
& + \frac{\varepsilon}{\Gamma} \frac{\xi q}{2} n_3 n_1 (q_t + v_k q_{,k}) + \frac{\varepsilon}{\Gamma} [\xi \lambda_1 (1 - q^2) - \zeta] \Delta \chi q n_3 n_1,
\end{aligned} \tag{A.7f}$$

$$\begin{aligned}
\tilde{T}_{33} = & \alpha_1 (\varepsilon n_1 n_1 e_{11} n_3 n_3 + n_1 n_3 e_{13} n_3 n_3 + n_3 n_1 e_{31} n_3 n_3 + \varepsilon n_3 n_3 e_{33} n_3 n_3) \\
& + \alpha_2 N_3 n_3 + \alpha_3 N_3 n_3 + \alpha_4 \varepsilon e_{33} \\
& + \alpha_5 (e_{31} n_1 n_3 + \varepsilon e_{33} n_3 n_3) + \alpha_6 (e_{31} n_1 n_3 + \varepsilon e_{33} n_3 n_3) \\
& + \frac{\varepsilon}{\Gamma} \frac{\xi q}{2} n_3 n_3 (q_t + v_k q_{,k}) + \frac{\varepsilon}{\Gamma} [\xi \lambda_1 (1 - q^2) - \zeta] \Delta \chi q (n_3 n_3 - 1/2),
\end{aligned} \tag{A.7g}$$

$$e_{11} = \partial_1 v_1, \quad \omega_{11} = 0, \tag{A.8a}$$

$$e_{13} = \frac{1}{2} (\partial_3 v_1 + \varepsilon^2 \partial_1 v_3), \quad \omega_{13} = \frac{1}{2} (\partial_3 v_1 - \varepsilon^2 \partial_1 v_3), \tag{A.8b}$$

$$e_{31} = \frac{1}{2} (\varepsilon^2 \partial_1 v_3 + \partial_3 v_1), \quad \omega_{31} = \frac{1}{2} (\varepsilon^2 \partial_1 v_3 - \partial_3 v_1), \tag{A.8c}$$

$$e_{33} = \partial_3 v_3, \quad \omega_{33} = 0, \tag{A.8d}$$

$$N_1 = \varepsilon \partial_t n_1 + \varepsilon v_j \partial_j n_1 - \frac{1}{2} \partial_3 v_1 n_3 + \varepsilon^2 \frac{1}{2} \partial_1 v_3 n_3, \quad (\text{A.9a})$$

$$N_3 = \varepsilon \partial_t n_3 + \varepsilon v_j \partial_j n_3 - \varepsilon^2 \frac{1}{2} \partial_1 v_3 n_1 + \frac{1}{2} \partial_3 v_1 n_1. \quad (\text{A.9b})$$

In turn, at the substrate $x_3 = 0$, the non-dimensional boundary conditions are

$$v_1 = 0, \quad v_3 = 0, \quad (\text{A.10a})$$

$$n_3 = \cos \theta_1, \quad (\text{A.10b})$$

$$q = q_1, \quad (\text{A.10c})$$

and at the free surface, $x_3 = \eta(x_1, t)$, they are

$$\eta_t = v_3 - v_1 \partial_1 \eta, \quad (\text{A.11a})$$

$$\begin{aligned} -p + \frac{\varepsilon}{(1 + \varepsilon^2 \eta_{1,1}^2)} \left[(\varepsilon^2 T_{11}^E + \tilde{T}_{11}) \eta_{1,1}^2 \right. \\ \left. - (\varepsilon T_{13}^E + \tilde{T}_{13}) \eta_{1,1} - (\varepsilon T_{31}^E + \tilde{T}_{31}) \eta_{1,1} \right. \\ \left. + (T_{33}^E + \tilde{T}_{33}) \right] = \frac{\eta_{,11}}{(1 + \varepsilon^2 \eta_{1,1}^2)^{3/2}}, \end{aligned} \quad (\text{A.11b})$$

$$\begin{aligned} -\varepsilon \eta_{1,1} (\varepsilon^2 T_{11}^E + \tilde{T}_{11}) - \varepsilon^2 \eta_{1,1}^2 (\varepsilon T_{13}^E + \tilde{T}_{13}) \\ + (\varepsilon T_{31}^E + \tilde{T}_{31}) + \varepsilon \eta_{1,1} (T_{33}^E + \tilde{T}_{33}) = 0, \end{aligned} \quad (\text{A.11c})$$

$$\frac{-\varepsilon \eta_{1,1} n_1 + n_3}{(1 + \varepsilon^2 \eta_{1,1}^2)^{1/2}} = \cos \theta_2, \quad (\text{A.11d})$$

$$q = q_2, \quad (\text{A.11e})$$

where in the normal stress equation we have used again our earlier choice for ε in (3.5).

B Derivation of the thin-film model for the active Eriksen-Leslie-Parodi theory

B.1 Governing equations

In this appendix, we give a brief account of the derivation of the thin-film model for the Eriksen-Leslie-Parodi theory augmented by activity terms. Conventions and notations carry over from the main text. The conservation of mass, linear and angular momentum balance equations are given by

$$0 = \partial_i v_i, \quad (\text{B.1})$$

$$0 = -\partial_i p - \partial_j (\partial_{\partial_j n_k} W \partial_i n_k) + \partial_j \tilde{T}_{ij} \quad (\text{B.2})$$

$$0 = h_i - \gamma_1 N_i - \gamma_2 e_{ij} n_j + \lambda_1^{ELP} \Delta \chi^{ELP} n_i, \quad (\text{B.3})$$

The bulk free energy density W is

$$\begin{aligned} 2W = & K_1 (\nabla \cdot \mathbf{n})^2 + K_2 (\mathbf{n} \cdot \text{curl } \mathbf{n})^2 \\ & + K_3 (\mathbf{n} \times \text{curl } \mathbf{n})^2 + (K_2 + K_4) [\text{tr}(\nabla n)^2 - (\nabla \cdot \mathbf{n})^2] \end{aligned} \quad (\text{B.4})$$

The parameters K_1 , K_2 and K_3 are the splay, twist and bend elastic moduli (see de Gennes & Prost [64]), and $K_2 + K_4$ is the saddle-splay constant. Notice that in the case of strong anchoring, the final term does not contribute to the governing equations [17], and that in 2D, there is also no twist term. Again, we will assume that all the $K_1 = K_2 = K_3 \equiv K$ and $K_4 = 0$. This assumption is discussed for liquid crystals in section 3.1.3.2 of [64], and we use it here for simplification; see also [12]. Notice that under this assumption the elastic energy is reduced to the Dirichlet energy (see also equation (4) in [17])

$$2W = K \partial_k n_i \partial_k n_i. \quad (\text{B.5})$$

In turn, the rate of change of the director with respect to the background fluid N_i is defined as in (2.22). The molecular field is given by

$$h_i = \gamma n_i - \frac{\delta W}{\delta n_i} \quad (\text{B.6})$$

where γ appears as a Lagrange multiplier in the variational formulation to satisfy the condition $n_i n_i = 1$ and may in general depend on x_i and t .

Here and in the following sections, we consider several stress tensors. The total stress tensor is given by

$$T_{ij} = -p \delta_{ij} + T_{ij}^E + \tilde{T}_{ij}, \quad (\text{B.7})$$

where the Eriksen-Leslie tensor is

$$T_{ij}^E = -\partial_{\partial_i n_k} W \partial_j n_k \quad (\text{B.8})$$

and the extra stress tensor is

$$\begin{aligned} \tilde{T}_{ij} = & \alpha_1 n_k n_p e_{kp} n_i n_j + \alpha_2 N_i n_j + \alpha_3 N_j n_i + \alpha_4 e_{ij} \\ & + \alpha_5 e_{ik} n_k n_j + \alpha_6 e_{jk} n_k n_i + \zeta^{ELP} \Delta \chi^{ELP} n_i n_j. \end{aligned} \quad (\text{B.9})$$

We remark that in some of the literature, e.g. [34], T_{ij} includes an additional term $-W \delta_{ij}$, which, however, amounts to a redefinition of the pressure [17]. As in the nematic system (2.4)-(2.6) we introduced in system (B.1)-(B.3) two active parameters λ_1^{ELP} and ζ^{ELP} .

Director field boundary conditions. At the substrate $x_3 = 0$, the strong anchoring condition reads

$$n = \sin \theta_1 e_1 + \cos \theta_1 e_3, \quad (\text{B.10})$$

where e_1 and e_3 are the canonical unit vectors, and at the free surface $x_3 = \eta(x, t)$, we have analogously

$$n = \cos \theta_2 \nu + \sin \theta_2 t. \quad (\text{B.11})$$

Flow field and stress boundary conditions. For the boundary conditions of the flow field we assume at the substrate $x_3 = 0$ no-slip and impermeability, respectively

$$v_1 = 0, \quad v_3 = 0, \quad (\text{B.12})$$

and at the interface $x_3 = \eta(x_1, t)$, we have the kinematic condition

$$\partial_t \eta = v_3 - v_1 \partial_1 \eta. \quad (\text{B.13})$$

The interfacial stress boundary condition is

$$\nu_i T_{ij} = -g_0 \partial_i \nu_i \nu_j, \quad (\text{B.14})$$

or in components

$$\nu_i T_{ij} \nu_j = -g_0 \partial_i \nu_i, \quad (\text{B.15})$$

$$\nu_i T_{ij} t_j = 0. \quad (\text{B.16})$$

From (B.7), we obtain for the normal bulk stress

$$\nu_i T_{ij} \nu_j = -p + \nu_i T_{ij}^E \nu_j + \nu_i \tilde{T}_{ij} \nu_j, \quad (\text{B.17})$$

$$\nu_i T_{ij}^E \nu_j = -\nu_i \partial_{\partial_i n_k} W \partial_j n_k \nu_j, \quad (\text{B.18})$$

$$\begin{aligned} \nu_i \tilde{T}_{ij} \nu_j &= \alpha_1 n_k n_p e_{kp} \nu_i n_i n_j \nu_j + \alpha_2 \nu_i N_i n_j \nu_j + \alpha_3 \nu_i N_j n_i \nu_j \\ &\quad + \alpha_4 \nu_i e_{ij} \nu_j + \alpha_5 \nu_i e_{ik} n_k n_j \nu_j + \alpha_6 \nu_i e_{jk} n_k n_i \nu_j \\ &\quad + \zeta^{ELP} \Delta \chi^{ELP} \nu_i n_i n_j \nu_j. \end{aligned} \quad (\text{B.19})$$

Similarly, we obtain for the tangential boundary condition

$$\nu_i T_{ij} t_j = \nu_i T_{ij}^E t_j + \nu_i \tilde{T}_{ij} t_j, \quad (\text{B.20})$$

$$\nu_i T_{ij}^E t_j = -\nu_i \partial_{\partial_i n_k} W \partial_j n_k t_j, \quad (\text{B.21})$$

$$\begin{aligned} \nu_i \tilde{T}_{ij} t_j &= \alpha_1 n_k n_p e_{kp} \nu_i n_i n_j t_j + \alpha_2 \nu_i N_i n_j t_j + \alpha_3 \nu_i N_j n_i t_j \\ &\quad + \alpha_4 \nu_i e_{ij} t_j + \alpha_5 \nu_i e_{ik} n_k n_j t_j + \alpha_6 \nu_i e_{jk} n_k n_i t_j \\ &\quad + \zeta^{ELP} \Delta \chi^{ELP} \nu_i n_i n_j t_j. \end{aligned} \quad (\text{B.22})$$

B.2 Thin-film approximation

Using the same nondimensionalisation (3.1)–(3.5) as before together with $W = \mathcal{E} \bar{W}$ and

$$\mathcal{E} = \frac{K}{\varepsilon^2 L^2}, \quad (\text{B.23})$$

we obtain that the non-dimensional bulk free energy becomes

$$2\bar{W} = (\partial_3 n_3)^2 + (\partial_3 n_1)^2 + O(\varepsilon^2). \quad (\text{B.24})$$

The scaled molecular field is then to leading order

$$\bar{h}_1 = n_1 + \partial_3^2 n_1 + O(\varepsilon^2) \quad (\text{B.25})$$

$$\bar{h}_3 = n_3 + \partial_3^2 n_3 + O(\varepsilon^2) \quad (\text{B.26})$$

Further on, we introduce the dimensionless parameters

$$\bar{\alpha}_i = \alpha_i / \mu, \quad \bar{\gamma}_i = \gamma_i / \mu, \quad \Delta \bar{\chi}^{ELP} = \frac{\varepsilon L}{\mu U} \Delta \chi^{ELP}, \quad \bar{\zeta}^{EPL} = \zeta^{EPL} / \mu, \quad (\text{B.27})$$

where μ is the kinematic viscosity. Then we nondimensionalize (B.3) to obtain (upon neglecting lower order terms) that

$$0 = \left(\frac{K}{\varepsilon^2 L^2} \right) \bar{h}_1 - \left(\frac{\alpha_2}{\mu} \right) \left(\frac{\mu U}{\varepsilon L} \right) n_3 \partial_3 \bar{v}_1 + \frac{\mu U}{\varepsilon L} \bar{\lambda}_1^{ELP} \Delta \bar{\chi}^{ELP} n_1 \quad (\text{B.28})$$

$$0 = \left(\frac{K}{\varepsilon^2 L^2} \right) \bar{h}_3 - \left(\frac{\alpha_3}{\mu} \right) \left(\frac{\mu U}{\varepsilon L} \right) n_1 \partial_3 \bar{v}_1 + \frac{\mu U}{\varepsilon L} \bar{\lambda}_1^{ELP} \Delta \bar{\chi}^{ELP} n_3 \quad (\text{B.29})$$

If $K/\varepsilon^2 L^2 \gg \mu U/\varepsilon L$ the flow field decouples from the director field in these equations. Therefore, we require the case of weak elasticity $K/\varepsilon \mu U L = O(1)$, so that all three terms in each of the equations (B.28) and (B.29) remain.

The scale P for the pressure is obtained, as before, by balancing it with the dominant viscous contributions in the horizontal momentum equation (B.2) (i.e. for $i = 1$). We drop the overbars from this point onwards and introduce θ as in (3.12). The leading order bulk equations then are

$$0 = v_{1,1} + v_{3,3}, \quad (\text{B.30a})$$

$$0 = -p_{,1} + \frac{1}{2}(v_{1,3} f_A(\theta))_{,3} + \zeta^{ELP} \Delta \chi^{ELP} (\sin(2\theta))_{,3}, \quad (\text{B.30b})$$

$$0 = -p_{,3}, \quad (\text{B.30c})$$

$$0 = \gamma \sin \theta + K(\sin \theta)_{,33} + \frac{1}{2}(\gamma_1 - \gamma_2) v_{1,3} \cos \theta + \lambda_1^{ELP} \Delta \chi^{ELP} \sin \theta, \quad (\text{B.30d})$$

$$0 = \gamma \cos \theta + K(\cos \theta)_{,33} - \frac{1}{2}(\gamma_1 + \gamma_2) v_{1,3} \sin \theta + \lambda_1^{ELP} \Delta \chi^{ELP} \cos \theta, \quad (\text{B.30e})$$

with the Lagrange parameter γ and

$$f_A(\theta) = (\alpha_1/2) \sin^2(2\theta) + (\alpha_5 - \alpha_2) \cos^2 \theta + (\alpha_3 + \alpha_6) \sin^2 \theta + \alpha_4. \quad (\text{B.30f})$$

Notice that in the above all terms in $\partial_j (\partial_{\partial_j n_k} W \partial_1 n_k)$ are of order ε or smaller and hence do not contribute. The leading order boundary conditions are as follows: At $x_3 = 0$, we have

$$v_1 = 0, \quad v_3 = 0, \quad (\text{B.31a})$$

$$\theta = \theta_1, \quad (\text{B.31b})$$

and at the free surface, $x_3 = \eta(x_1, t)$,

$$\eta_t = v_3 - v_1 \partial_1 \eta, \quad (\text{B.32a})$$

$$-p = \eta_{,11}, \quad (\text{B.32b})$$

$$\frac{1}{2} v_{1,3} f_B(\theta_2) = -\frac{\zeta^{ELP} \Delta \chi^{ELP}}{2} \sin(2\theta_2), \quad (\text{B.32c})$$

$$\theta = \theta_2, \quad (\text{B.32d})$$

where we have defined

$$f_B(\theta) = (\alpha_1/2) \sin^2(2\theta) + (\alpha_6 - \alpha_3) \cos^2 \theta + (\alpha_2 + \alpha_5) \sin^2 \theta + \alpha_4. \quad (\text{B.33})$$

Similarly as it was done in [17] for its passive counterpart, the system (B.30)–(B.33) can be partly integrated to yield the active thin-film model (3.27) based on the Leslie-Erickson-Parodi theory. In particular, the mass conservation relation (3.27a) can be derived from (B.30a), (B.32a) and (B.31a).

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