Geometry and topology in active and driven systems

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2 THE GEOMETRY OF THRESHOLDLESS ACTIVE FLOW IN NEMATICS

Active liquids [1] are complex fluids with some components individually capable of converting internal energy into sustained motion. These "active components" can be sub-cellular (such as microtubules powered by molecular motors, and acto-myosin networks [2, 3]), synthetic (e.g., self-propelled colloids [11], or interacting micro-robots), or, alternatively, living organisms [7, 8, 9, 10], such as birds, fish [30], microorganisms [4, 5] or insects [6]. Hybrid systems composed of motile rod-shaped bacteria placed in nontoxic liquid crystals have also been recently realized [31]. All of these systems blur the line between the living and synthetic world, thereby opening up unprecedented opportunities for the design of novel smart materials and technology. At the same time, the far-from-equilibrium nature of active matter leads to exotic phenomena of fundamental interest. Among these are the ability of active fluids to (i) spontaneously break a continuous symmetry in two spatial dimensions [13, 32, 14, 15], (ii) exhibit spontaneous steady state flow [21, 2] in the absence of an external driving force and (iii) support topologically protected excitations (e.g., sound modes) that originate from time-reversal symmetry breaking [33].

A striking example of the phenomenon of spontaneous flow occurs in active nematic liquid crystals [1, 21, 22, 23, 24, 25, 26]. These materials are orientationally ordered but apolar fluids; that is, the active particles share a common axis of motion but, in the homogeneous state, equal numbers of them move in each of the two directions parallel to this axis. As a result, there is no net motion and no net flow. However, if the activity parameter α (defined later) exceeds a *critical threshold* α_c, the undistorted nematic ground state becomes unstable. Once this instability threshold is passed, the active nematics spontaneously deform their state of alignment, triggering macroscopic "turbulent flow" [21, 2, 34, 35, 36, 37]. For nematics, this activity threshold α_c goes to zero as the system size $L \to \infty$: $\alpha_c \sim \frac{K}{L^2}$, where K is a characteristic Frank elastic constant. Equivalently, one can say that the instability-triggered flow does not occur in systems of characteristic size smaller than $L_{\text{inst}} \sim \sqrt{\frac{K}{|\alpha|}}$.

An example of a flow with a threshold for an active nematic in a cylinder [26] is shown in Fig. 10. In their numerical simulations, for small values of activity $\alpha < \alpha_c \approx 0.03$, the director field is aligned

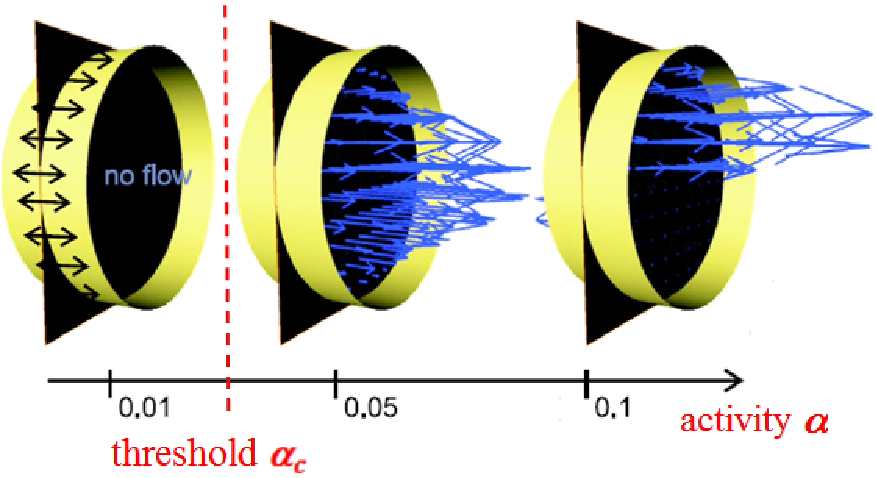

Figure 10: *Numerical simulation of active flow in a nematic cylinder with a threshold taken from [26].* A cross-section of flow in the cylinder is shown for three values of activity α. Flow is observed only for $\alpha < 0.03$.

with the axis of the cylinder and there is no motion; activity in the nematic only starts to induce flow when it exceeds this threshold value.

Other numerical studies of active nematics suggest that some non-uniform director configurations can lead to *laminar* flow for arbitrarily small activity, i.e., well below the instability threshold [34]. However, no systematic study of the mechanisms and criteria behind such "thresholdless active flow" has previously been undertaken. In this thesis, we use a well established hydrodynamic theory of active nematics to identify the class of surface deformations, boundary conditions or external fields that induce a non-uniform director ground-state capable of generating such thresholdless laminar flow. We emphasize that not all spatially non-uniform configurations will induce such flow.

The condition for a given set of boundary conditions and applied fields to induce thresholdless active flow in nematics is most easily expressed in terms of the director field $\hat{\boldsymbol{n}}(\boldsymbol{r})$ [38], which is defined as the local orientation of molecular alignment. It can be stated as follows: if the active force, which is defined in general as

$$\boldsymbol{f}_a \equiv \alpha\left[\hat{\boldsymbol{n}}\left(\nabla\cdot\hat{\boldsymbol{n}}\right)+(\hat{\boldsymbol{n}}\cdot\nabla)\hat{\boldsymbol{n}}\right]=\alpha\left[\hat{\boldsymbol{n}}\left(\nabla\cdot\hat{\boldsymbol{n}}\right)-\hat{\boldsymbol{n}}\times(\nabla\times\hat{\boldsymbol{n}})\right], \tag{1}$$

has non-zero curl, when computed for the director configuration $\hat{\boldsymbol{n}}(\boldsymbol{r})$ that minimizes the Frank elastic free energy (including external fields) of the corresponding equilibrium problem [38], then the active fluid in the same geometry *must* flow (i.e., the velocity field $\boldsymbol{v} \neq \mathbf{0}$). Note that this condition is far more stringent than simply requiring that the nematic ground state orientation be inhomogeneous. For example, *any* pure twist configuration (e.g, a cholesteric, or a twist cell) does not satisfy it, since splay $\nabla \cdot \hat{\boldsymbol{n}}$ and bend $\hat{\boldsymbol{n}} \times \left(\nabla \times \hat{\boldsymbol{n}}\right)$ both vanish in such configurations. The criterion $\nabla \times \boldsymbol{f}_a \neq \mathbf{0}$ is a sufficient but not necessary condition for thresholdless flow.

In the present study, we calculate the resulting flow field $\boldsymbol{v}(\boldsymbol{r})$ explicitly in the "frozen director" approximation, in which the nematic director remains in its equilibrium configuration when activity is turned on. We demonstrate that this approximation is asymptotically exact in the experimentally relevant limit of weak orientational order. Since many nematic to isotropic transitions are weakly first order [38] (at least in equilibrium), this frozen director limit may be realized close to such transitions, and in any case, these approximate solutions provide qualitative insights into the nature of the flow.

Our ideas can also be applied with some modifications to the recently discovered "living liquid crystals" [31]. These systems are a mixture of two components: living bacteria, which provide the activity, and a background medium composed of nematically ordered non-active molecules, but we leave a full discussion of this until chapter 4.

The remainder of this chapter is organized as follows: in section 2.1, we review the "standard model" for the hydrodynamics of active nematics. We also discuss some generalizations of this model, and argue that none of our conclusions will be substantively affected by these generalizations. In sections 2.2 and 2.3, we derive the general criterion for thresholdless active flow and explain the frozen director regime; in section 2.4 we then apply this criterion to the specific case of surfaces of non-zero Gaussian curvature, and show that such surfaces always have non-zero active forces, but need not always have thresholdless flow. We also derive the additional criteria that must be satisfied for thresholdless flow to occur in these systems. In section 2.5, we derive similar results for *bulk* systems with curved boundaries, consider a first example in section 2.6 and then summarise in section 2.7.

2.1 THE HYDRODYNAMICS OF ACTIVE NEMATICS

We take as our model for an incompressible one-component active nematic fluid the following three coupled equations [21]:

$$\rho_0 \frac{Dv_k}{Dt} = -\partial_k P + \eta \nabla^2 v_k + \alpha \partial_j \left(n_j n_k\right) + \partial_j (\lambda_{ijk} \frac{\delta F}{\delta n_i}) \tag{2a}$$

$$\frac{Dn_i}{Dt} = \lambda_{ijk} \partial_j v_k - \frac{1}{\gamma_1} \left[\frac{\delta F}{\delta n_i} - \left(\frac{\delta F}{\delta \hat{n}} \cdot \hat{n} \right) n_i \right] \tag{2b}$$

$$\nabla \cdot \boldsymbol{v} = 0, \tag{2c}$$

where $D/Dt \equiv \partial_t + \boldsymbol{v} \cdot \nabla$ is the convective derivative and the tensor λ_{ijk} is given by

$$\lambda_{ijk} \equiv \left(\frac{\lambda+1}{2} \right) n_j \delta_{ik} + \left(\frac{\lambda-1}{2} \right) n_k \delta_{ij} - \lambda n_i n_j n_k. \tag{3}$$

The first Eq. (2a) is a modified Navier-Stokes equation describing the evolution of the velocity field $\boldsymbol{v}(\boldsymbol{r}, t)$; Eq. (2b) is the nematodynamic equation describing the evolution of the director field $\hat{\boldsymbol{n}}(\boldsymbol{r}, t)$, which responds both to the flow $\boldsymbol{v}$, and to its own molecular field $\frac{\delta F}{\delta \boldsymbol{n}}$ (described in more detail below), and (2c) is the incompressibility condition, which is required since we take the density ρ_0 to be constant. We denote by P the dynamic pressure, η the shear viscosity, which we take to be isotropic for simplicity, and γ_1 the director field rotational viscosity. The dimensionless flow-alignment parameter λ captures the anisotropic response of the nematogens to shear. Note that the only difference between Eq. (2a-2c) and the equations of motion for an equilibrium nematic [38] is the active force term $\alpha \partial_j \left(n_j n_k\right)$ in the Navier-Stokes Eq. (2a), which may be contractile ($\alpha > 0$) or extensile ($\alpha < 0$), depending on the system [21]. The molecular field $\frac{\delta F}{\delta \boldsymbol{n}}$, derived from the Frank free energy

$$F = \frac{1}{2} \int d^3\boldsymbol{r} [K_1 \left(\nabla \cdot \hat{\boldsymbol{n}}\right)^2 + K_2 \left(\hat{\boldsymbol{n}} \cdot \left(\nabla \times \hat{\boldsymbol{n}}\right)\right)^2 + K_3 \left|\hat{\boldsymbol{n}} \times \left(\nabla \times \hat{\boldsymbol{n}}\right)\right|^2], \tag{4}$$

is parametrized respectively by three independent elastic constants $K_{1,2,3}$ for splay, twist, and bend deformations of the director.

Note that, strictly speaking, Eq. (2a-2c) are not the most general set of equations for a one-component active nematic. Specifically, there are two ways in which they could be generalized:

1) The free energy F that appears in the velocity equation of motion (2a) need not, in a non-equilibrium system, be the same as that in the

director equation of motion (2b). Both free energies have to have the same *form* as (4), since that form is required by rotation invariance, but the Frank constants $K_{1,2,3}$ that appear in them need not be equal.
2) The viscosity need not be isotropic: there are in general six Leslie coefficients [42] characterizing this anisotropic response.

However, both of these concerns can safely be ignored in the small activity regime which we are considering. We deal with 2) later in this chapter in section 2.3 while 1) we discuss now.

To see why non-equilibrium molecular fields may be ignored in the hydrodynamic theory, first we rewrite the equations of motion (2a-2c) taking into account this difference in Frank free energies:

$$\rho_0 \frac{Dv_k}{Dt} = -\partial_k P + \eta \nabla^2 v_k + \alpha \partial_j \left(n_j n_k\right) + \partial_j (\lambda_{ijk} h_{vi}) \tag{5a}$$

$$\frac{Dn_i}{Dt} = \lambda_{ijk}\partial_j v_k - \frac{1}{\gamma_1}\left[h_{ni} - \left(\boldsymbol{h}_n \cdot \hat{\boldsymbol{n}}\right) n_i\right] \tag{5b}$$

$$\nabla \cdot \boldsymbol{v} = 0, \tag{5c}$$

where the molecular fields $\boldsymbol{h}_\nu$, $\nu = [v, n]$ appearing in these equations are given by $\boldsymbol{h}_\nu = \frac{\delta F_\nu}{\delta \hat{\boldsymbol{n}}}$, which implies

$$\begin{aligned} \boldsymbol{h}_\nu &\equiv \frac{\delta F_\nu}{\delta \hat{\boldsymbol{n}}} = 2(K_{2\nu} - K_{3\nu})\left(\hat{\boldsymbol{n}} \cdot \left(\nabla \times \hat{\boldsymbol{n}}\right)\right) \nabla \times \hat{\boldsymbol{n}} \\ &- K_{3\nu} \nabla^2 \hat{\boldsymbol{n}} + (K_{3\nu} - K_{2\nu}) \hat{\boldsymbol{n}} \times \nabla \left(\hat{\boldsymbol{n}} \cdot \nabla \times \hat{\boldsymbol{n}}\right) \\ &+ (K_{3\nu} - K_{1\nu}) \nabla \left(\nabla \cdot \hat{\boldsymbol{n}}\right). \end{aligned} \tag{6}$$

Here the the F_ν's, $\nu = [v, n]$ are the non-equilibrium generalizations of the equilibrium Frank free energy F. They are constrained by rotation invariance in exactly the same way as in equilibrium, and must, therefore, both take the usual Frank free energy [38] form:

$$\begin{aligned} F_\nu = \frac{1}{2} \int d^3 r [K_{1\nu} \left(\nabla \cdot \hat{\boldsymbol{n}}\right)^2 + K_{2\nu} \left(\hat{\boldsymbol{n}} \cdot \left(\nabla \times \hat{\boldsymbol{n}}\right)\right)^2 \\ + K_{3\nu} \left|\hat{\boldsymbol{n}} \times \left(\nabla \times \hat{\boldsymbol{n}}\right)\right|^2], \end{aligned} \tag{7}$$

Although the form of the two free energies must be the same, away from equilibrium, the values of the Frank constants $K_{1,2,3}$ need not be the same in the two free energies. Only in equilibrium, in which the activity parameter $\alpha = 0$, do the two Frank free energies become equal ($F_v = F_n$). In an active system, however, the fundamentally non-equilibrium nature of the problem means that there are no such requirements of equality; that is, $F_v \neq F_n$ away from equilibrium, in contrast to the equations of motion (2a-2c) of the main text, in which we took $F_v = F_n = F$. This is not necessarily true but we do expect [21] that both α and the difference between F_v and F_n will be proportional to the density of active particles, and so will be very small when that density is small. Since we are interested in the small activity (i.e., low active particle density) limit, we can ignore the difference between F_v and F_n.

To see this, note that, even when α is very small, the terms involving $\boldsymbol{h}_v$ in (5a) are always negligible, relative to the α terms. This is because, in the small activity limit, $\boldsymbol{h}_v \to \boldsymbol{h}_n$, with the difference $\boldsymbol{h}_v - \boldsymbol{h}_n \propto \alpha$, since, as noted earlier, the difference between $\boldsymbol{h}_v$ and $\boldsymbol{h}_n$ is a purely active effect. However, we have already shown that $\boldsymbol{h}_n \parallel \hat{\boldsymbol{n}}$; it is straightforward to show that when $\boldsymbol{h}_v \parallel \hat{\boldsymbol{n}}$, the terms involving $\boldsymbol{h}_v$ in eq. (5a) vanish. Hence, the only piece of those terms that can survive must arise from the difference $\boldsymbol{h}_v - \boldsymbol{h}_n$, which, as we have just shown, is proportional to α. However, these terms also involve more spatial derivatives of $\hat{\boldsymbol{n}}$ than the α term and so on dimensional grounds, we expect the ratio of the $\boldsymbol{h}_v$ terms to the α terms to be $\mathcal{O}\left(\frac{a}{L}\right)^2$, where a is a microscopic length (e.g., the size of the active particles), while L is the macroscopic length scale over which $\hat{\boldsymbol{n}}$ varies. Hence, the $\boldsymbol{h}_v$ terms in eq. (5a) are negligible, regardless of the value of α, in a macroscopic geometry.

Note that the length a that appears in this estimate cannot be the instability length $L_{\text{inst}} \sim \sqrt{\frac{K}{\alpha}}$ discussed at the start of this chapter, since the ratio of the $\boldsymbol{h}_v$ to the α term must be independent of α.

2.2 THRESHOLDLESS FLOW IN ACTIVE NEMATICS

In certain geometries, the consitutive equations (2a-2c) lead to steady state macroscopic fluid flow for arbitrarily small activity.

We will estalish the nature of the geometrical conditions by contradiction. If there is no fluid flow (i.e., if the velocity field $\boldsymbol{v} = \mathbf{0}$), then the equation of motion (2b) for the director field implies that, in a steady state, for which $\frac{Dn_i}{Dt} = 0$, $\frac{\delta F}{\delta \hat{\boldsymbol{n}}} - (\hat{\boldsymbol{n}} \cdot \frac{\delta F}{\delta \hat{\boldsymbol{n}}}\hat{\boldsymbol{n}}) = \mathbf{0}$ (which also holds in the case of anisotropic viscosity). This is simply the Euler-Lagrange equation for minimizing the Frank free energy F subject to the constraint $|\hat{\boldsymbol{n}}| = 1$. The contradiction arises when we insert such an equilibrium solution for the nematic director into the equation of motion for the velocity field (2a).

The last term on the right hand side of Eq. (2a), involving $\frac{\delta F}{\delta \hat{\boldsymbol{n}}}$, vanishes when $\frac{\delta F}{\delta \hat{\boldsymbol{n}}} \parallel \hat{\boldsymbol{n}}$, which is the case when the director field is in its ground state. Since the velocity field $\boldsymbol{v}$ vanishes, Eq. (2a) reduces to $\nabla P = \alpha\left(\hat{\boldsymbol{n}} \cdot \nabla\hat{\boldsymbol{n}} + \hat{\boldsymbol{n}}\nabla \cdot \hat{\boldsymbol{n}}\right) \equiv \boldsymbol{f}_a$. Hence the pressure gradient must cancel the active force to prevent flow, but if the active force has a non-vanishing curl, this is not possible. In such cases, $\boldsymbol{v} = \mathbf{0}$ can never be a solution in the presence of activity; the fluid must flow, no matter how small the activity. Thus, a sufficient (but not necessary) condition for thresholdless active flow is

$$\nabla \times \boldsymbol{f}_a \neq \mathbf{0}, \tag{8}$$

which has also been implicit in other work such as [41].

One class of director configurations for which the condition in Eq. (8) is not satisfied is that of "pure twist" configurations; that is, configurations in which the twist does not vanish (i.e., $\hat{\boldsymbol{n}} \cdot \left(\nabla \times \hat{\boldsymbol{n}}\right) \neq 0$), but the splay and bend do (i.e., $\nabla \cdot \hat{\boldsymbol{n}} = 0$ and $\hat{\boldsymbol{n}} \times \left(\nabla \times \hat{\boldsymbol{n}}\right) = \mathbf{0}$, respectively). This can be seen by using the vector calculus identity $\left[\hat{\boldsymbol{n}} \times \left(\nabla \times \hat{\boldsymbol{n}}\right)\right]_i = n_j \nabla_i n_j - \hat{\boldsymbol{n}} \cdot \nabla n_i = \frac{1}{2}\nabla_i |\hat{\boldsymbol{n}}|^2 - \hat{\boldsymbol{n}} \cdot \nabla n_i = -\hat{\boldsymbol{n}} \cdot \nabla n_i$, where in the last equality we have used the fact that $\hat{\boldsymbol{n}}$ is a unit vector to set $\nabla_i |\hat{\boldsymbol{n}}|^2 = \nabla_i 1 = 0$. Using this, the active force $\boldsymbol{f}_a$ may be rewritten as

$$\boldsymbol{f}_a = \alpha \left[\hat{\boldsymbol{n}}\, \nabla \cdot \hat{\boldsymbol{n}} - \hat{\boldsymbol{n}} \times \left(\nabla \times \hat{\boldsymbol{n}}\right)\right], \tag{9}$$

which implies that a director field with pure twist has zero active force, and, hence, no flow for sufficiently small activity.

One might wonder whether active flow in this case can be induced by the activity-induced difference between $\boldsymbol{h}_v$ and $\boldsymbol{h}_n$; we'll now prove that this is not the case.

To see this, note that in a pure twist state, since $\hat{\boldsymbol{n}} \times (\nabla \times \hat{\boldsymbol{n}}) = \mathbf{0}$, $\nabla \times \hat{\boldsymbol{n}}$ must be parallel to $\hat{\boldsymbol{n}}$ itself. This implies

$$\nabla \times \hat{\boldsymbol{n}} = g(\boldsymbol{r}) \hat{\boldsymbol{n}}(\boldsymbol{r}) \tag{10}$$

where $g(\boldsymbol{r})$ is some scalar function of $\boldsymbol{r}$. Furthermore, since $\hat{\boldsymbol{n}}$ is divergenceless in a pure twist state ($\nabla \cdot \hat{\boldsymbol{n}} = 0$), a well-known identity of vector calculus implies $\nabla^2 \hat{\boldsymbol{n}} = -\nabla \times (\nabla \times \hat{\boldsymbol{n}})$; using (10) in this identity gives

$$\nabla^2 \hat{\boldsymbol{n}} = -g \nabla \times \hat{\boldsymbol{n}} - \nabla g \times \hat{\boldsymbol{n}} = -g^2 \hat{\boldsymbol{n}} + \hat{\boldsymbol{n}} \times \nabla g\,, \tag{11}$$

where in the second equality we have used (10) a second time. Using (10), (11) and $\nabla \cdot \hat{\boldsymbol{n}} = 0$ in our expression (34) for the molecular field $\boldsymbol{h}_n$ gives

$$\boldsymbol{h}_n = (2K_{2n} - K_{3n}) g^2 \hat{\boldsymbol{n}} - K_{2n} \hat{\boldsymbol{n}} \times \nabla g\,. \tag{12}$$

However, for this to be parallel to $\hat{\boldsymbol{n}}$, which is required to satisfy the director equation of motion (5b) with $\boldsymbol{v} = \mathbf{0}$, we must have $\nabla g \parallel \hat{\boldsymbol{n}}$. For such a g, (12) implies

$$\boldsymbol{h}_n = (2K_{2n} - K_{3n}) g^2 \hat{\boldsymbol{n}}\,, \tag{13}$$

and, by the same reasoning,

$$\boldsymbol{h}_v = (2K_{2v} - K_{3v})g^2\hat{\boldsymbol{n}}\,. \tag{14}$$

Thus, for any pure twist configuration that gives $\boldsymbol{h}_n \propto \hat{\boldsymbol{n}}$ (which is just the condition for minimizing the Frank energy F_n subject to the constraint $|\hat{\boldsymbol{n}}| = 1$), the active force $\boldsymbol{f}_a$ vanishes, and both $\boldsymbol{h}_v$ and $\boldsymbol{h}_n$ are everywhere parallel to $\hat{\boldsymbol{n}}$. But the latter conditions imply, as noted earlier, that all of the terms involving $\boldsymbol{h}_v$ and $\boldsymbol{h}_n$ in (5a) and (5b) vanish. Since $\boldsymbol{f}_a$ does as well, and all of the other terms in those equations vanish when $\boldsymbol{v} = \mathbf{0}$, we can conclude that, if $\hat{\boldsymbol{n}}$ is in a pure twist configuration that minimizes F_n, there will be no thresholdless active flow.

2.3 FROZEN DIRECTOR REGIME

When we consider specific examples of thresholdless active flow in chapter 3, we will determine analytically the velocity field $\boldsymbol{v}(\boldsymbol{r}, t)$. In general, this is a difficult, non-linear calculation, since the flow field reorients the nematic director. However, in the "frozen director" limit $\gamma_1 \ll \eta$, turning on activity (and thereby inducing thresholdless flow) does not lead to an appreciable change in the nematic director configuration from that in equilibrium, which is obtained by minimizing the Frank free energy. We now show that there is a very natural, generic, and well-defined limit in which γ_1 will always be much less than η: namely, the limit of weak nematic order.

We begin by noting that if the active and viscous terms are balanced in Eq. (2a), this implies schematically that if the system has a characteristic length scale L, then $\eta v/L^2 \sim \alpha/L$ and so $v \sim \alpha L/\eta$. This last result implies that the Reynolds number $Re \equiv \frac{\rho_0 v L}{\eta} = \frac{\rho_0 L^2 \alpha}{\eta^2}$. Using this estimate of v in Eq. (2b), we see that

$$\frac{1}{\gamma_1}\frac{\delta F}{\delta \hat{\boldsymbol{n}}} \sim \alpha/\eta. \tag{15}$$

Assuming that α is small enough that $Re \ll 1$, we can make the familiar Stokes approximation of neglecting the inertial terms on the left hand side of Eq. (2a). We may neglect the λ term in Eq. (2a), which is of order $\frac{\gamma_1}{\eta}\frac{\alpha}{L}$, and is therefore smaller than the unperturbed active force by a factor of $\frac{\gamma_1}{\eta}$.

We also need to take into account the change in the active force resulting from the change in the director field $\delta\hat{\boldsymbol{n}} \equiv \hat{\boldsymbol{n}} - \hat{\boldsymbol{n}}_0$ induced by the flow; here $\hat{\boldsymbol{n}}_0$ is the equilibrium configuration of the nematic director (that is, the one that minimizes the Frank free energy, or, equivalently, the field that is present before the activity is switched on). Since schematically the molecular field $\frac{\delta F}{\delta \hat{\boldsymbol{n}}} \sim \frac{K\delta n}{L^2}$ (note that δn appears in this expression rather than n because $\left(\frac{\delta F}{\delta \hat{\boldsymbol{n}}}\right)_{\hat{\boldsymbol{n}}=\hat{\boldsymbol{n}}_0} = \mathbf{0}$), our estimate (15) of that field implies that the magnitude δn of the perturbation in the director field must be of order $\frac{\alpha\gamma_1 L^2}{\eta K} \sim \frac{\gamma_1}{\eta}\left(\frac{L}{L_{\text{inst}}}\right)^2$, where L_{inst} is the length-scale beyond which the uniform state becomes unstable. Since we are considering systems which are smaller than this length, and since we are also assuming $\gamma_1 \ll \eta$, the change δn in $\hat{\mathbf{n}}$ is $\ll \hat{\mathbf{n}}_0$, the undistorted director configuration, and, hence, negligible.

To summarize: in the "frozen director" regime, defined as $\gamma_1 \ll \eta$, and small activity $\alpha \ll K/L^2$, we can determine the flow field simply by balancing the viscous force $\eta\nabla^2\mathbf{v}$ plus the pressure gradient ∇P against the active force $\boldsymbol{f}_a$ computed for the unperturbed, equilibrium configuration $\hat{\mathbf{n}}_0$ which minimizes the Frank free energy; that is, we can take the active force

$$\boldsymbol{f}_a = \alpha\left(\hat{\boldsymbol{n}}\cdot\nabla\hat{\boldsymbol{n}} + \hat{\boldsymbol{n}}\nabla\cdot\hat{\boldsymbol{n}}\right) \approx \alpha\left(\hat{\boldsymbol{n}}_0\cdot\nabla\hat{\boldsymbol{n}}_0 + \hat{\boldsymbol{n}}_0\nabla\cdot\hat{\boldsymbol{n}}_0\right) . \qquad (16)$$

Making this substitution, and neglecting the λ-term in (2a), simplifies (2a)-(2c) to:

$$0 \;=\; -\nabla P + \eta\nabla^2\boldsymbol{v} + \alpha\left(\hat{\boldsymbol{n}}_{\mathbf{0}}\cdot\nabla\hat{\boldsymbol{n}}_{\mathbf{0}} + \hat{\boldsymbol{n}}_{\mathbf{0}}\nabla\cdot\hat{\boldsymbol{n}}_{\mathbf{0}}\right) \qquad (17)$$

with $\nabla\cdot\boldsymbol{v} = 0$.

We now justify the isotropic viscosity approximation which we raised in section 2.1. In the limit of weak order, which in the notation of Kuzuu and Doi [43] is the limit $S_2, S_4 \ll 1$, our isotropic viscosity approximation becomes valid because the isotropic piece of the viscosity α_4 is much greater than the anisotropic pieces $\alpha_{1,5,6}$ of the viscosity, since the latter all vanish when $S_{2,4} \to 0$) with , $\eta = \alpha_4/2 \approx \eta^* C^3 r^2$. Furthermore, the coefficient $\gamma_1 = \alpha_3 - \alpha_2 = 10\eta^* C^3 r^2 S_2/\lambda$. Taking the ratio γ_1/η then gives $\gamma_1/\eta \approx 10 S_2/\lambda$, which, is always much less than 1 when the order is weak, since the flow alignment parameter λ is typically $O(1)$, and $S_2 \ll 1$ when the order is weak.

We therefore expect our analytic solutions for the velocity fields, which assumed both isotropic viscosity and $\gamma_1 \ll \eta$ (to justify the "frozen director" approximation) to be quantitatively accurate in all active systems in which the nematic order is weak.

Note that no matter how strong the order is, at sufficiently long wavelengths, fluctuations in the nematic order parameter are much smaller than fluctuations in the nematic director. Hence, the director field representation is always a good approximation at sufficiently long wavelengths. In the case of weak nematic order, the nematic correlation length is of order a/S where a is a molecular length (~ 1nm) and S is the nematic order parameter. Taking $S \sim 0.01$, the nematic correlation length is of order 100nm, much smaller than the size of a millimeter-sized sample.

We also note that this in particular implies that the "frozen director" approximation will always be valid for systems close to a weakly first order nematic to isotropic (NI) transition; since many NI transitions are, indeed, weakly first order [38], this means it should be quite easy to experimentally test our quantitative predictions for the flow field.

Next, in the remainder of this section we extend the results of section 2.2 in the case of a *simply connected* sample in the "frozen director" approximation, in which case the condition for thresholdless flow $\nabla \times \boldsymbol{f_a} \neq \mathbf{0}$ is necessary as well as sufficient. We consider the case in which the director field that minimizes F_n is pure splay, by which we mean $\nabla \times \hat{\boldsymbol{n}} = \mathbf{0}$. The curl of the active force is now given by

$$\begin{aligned}\nabla \times \boldsymbol{f}_a &= \alpha \nabla \times \left[\hat{\boldsymbol{n}}\, \nabla \cdot \hat{\boldsymbol{n}}\right] \\ &= \alpha \nabla \left(\nabla \cdot \hat{\boldsymbol{n}}\right) \times \hat{\boldsymbol{n}},\end{aligned} \tag{18}$$

which is also zero when the pure splay director field is a ground state of F_n, because the Euler-Lagrange equations that arise from minimizing F_n then require that $\boldsymbol{h}_n \parallel \hat{\boldsymbol{n}}$, which in turn, from (34), requires that $\nabla \left(\nabla \cdot \hat{\boldsymbol{n}}\right)$ is parallel to $\hat{\boldsymbol{n}}$. Furthermore, when $\nabla \times \hat{\boldsymbol{n}} = \mathbf{0}$, we can write $\hat{\boldsymbol{n}} = \nabla \Phi(\boldsymbol{r})$, which then implies $\boldsymbol{h}_v = -K_{1v} \nabla^2 \nabla \Phi$, and $\boldsymbol{h}_n = -K_{1n} \nabla^2 \nabla \Phi$. Thus, $\boldsymbol{h}_v \parallel \boldsymbol{h}_n$, so, if $\boldsymbol{h}_n \parallel \hat{\boldsymbol{n}}$ everywhere, $\boldsymbol{h}_v \parallel \hat{\boldsymbol{n}}$ everywhere as well. Hence, once again, the $\boldsymbol{h}_v$ and $\boldsymbol{h}_n$ terms in (5a) and (5b), respectively, vanish, as does the curl of the active force. Under the conditions of this section we can conclude that there is no flow.

We now turn to the case of a pure bend field (i.e., one for which $\nabla \cdot \hat{\boldsymbol{n}} = \hat{\boldsymbol{n}} \cdot \nabla \times \hat{\boldsymbol{n}} = 0$). Using the identity $\nabla(\boldsymbol{A} \cdot \boldsymbol{B}) = (\boldsymbol{A} \cdot \nabla)\boldsymbol{B} + (\boldsymbol{B} \cdot \nabla)\boldsymbol{A} + \boldsymbol{A} \times (\nabla \times \boldsymbol{B}) + \boldsymbol{B} \times (\nabla \times \boldsymbol{A})$, with $\boldsymbol{A} = \hat{\boldsymbol{n}}$ and $\boldsymbol{B} = \nabla \times \hat{\boldsymbol{n}}$, and recalling that $\hat{\boldsymbol{n}} \cdot \nabla \times \hat{\boldsymbol{n}}$ must vanish in a pure bend field, gives:

$$(\hat{\boldsymbol{n}} \cdot \nabla)\nabla \times \hat{\boldsymbol{n}} + (\nabla \times \hat{\boldsymbol{n}} \cdot \nabla)\hat{\boldsymbol{n}} + \hat{\boldsymbol{n}} \times (\nabla \times \nabla \times \hat{\boldsymbol{n}}) = 0. \tag{19}$$

If this pure bend state is also a ground state of F_n, the Euler-Lagrange Eq. (34) for F_n is satisfied. For pure bend, that equation reduces to $\nabla^2 \hat{\boldsymbol{n}} \parallel \hat{\boldsymbol{n}}$, so that $\hat{\boldsymbol{n}} \times (\nabla \times \nabla \times \hat{\boldsymbol{n}}) = -\hat{\boldsymbol{n}} \times \nabla^2 \hat{\boldsymbol{n}} = \mathbf{0}$, thereby eliminating the last term of (19). To compute $\nabla \times \boldsymbol{f}_a$, we now use the identity $\nabla \times (\boldsymbol{A} \times \boldsymbol{B}) = \boldsymbol{A}(\nabla \cdot \boldsymbol{B}) - \boldsymbol{B}(\nabla \cdot \boldsymbol{A}) + (\boldsymbol{B} \cdot \nabla)\boldsymbol{A} - (\boldsymbol{A} \cdot \nabla)\boldsymbol{B}$, again with $\boldsymbol{A} = \hat{\boldsymbol{n}}$ and $\boldsymbol{B} = \nabla \times \hat{\boldsymbol{n}}$, for $-\hat{\boldsymbol{n}} \times (\nabla \times \hat{\boldsymbol{n}})$, to get

$$\nabla \times \boldsymbol{f}_a = (\hat{\boldsymbol{n}} \cdot \nabla)\nabla \times \hat{\boldsymbol{n}} - (\nabla \times \hat{\boldsymbol{n}} \cdot \nabla)\hat{\boldsymbol{n}}. \tag{20}$$

Using our previous result (19) together with $\hat{\boldsymbol{n}} \times (\nabla \times \nabla \times \hat{\boldsymbol{n}}) = \mathbf{0}$, we can rewrite this equation as

$$\nabla \times \boldsymbol{f}_a = 2(\hat{\boldsymbol{n}} \cdot \nabla)\nabla \times \hat{\boldsymbol{n}} = -2(\nabla \times \hat{\boldsymbol{n}} \cdot \nabla)\hat{\boldsymbol{n}}. \tag{21}$$

This is as far as we can go considering completely general pure bend configurations. To proceed further, we will now, in addition to imposing pure bend, add the additional restriction to "2D" configurations, by which we mean that $\hat{\boldsymbol{n}}$ only depends on x and y, and has no z component, in some Cartesian coordinate system. Then $\nabla \times \hat{\boldsymbol{n}}$ is in the z-direction, and so $(\nabla \times \hat{\boldsymbol{n}} \cdot \nabla)\hat{\boldsymbol{n}} = 0$, which implies from (21) that $\nabla \times \boldsymbol{f}_a = \boldsymbol{0}$ as well. Similarly we have that $\boldsymbol{h}_n = -K_{3n}\nabla^2\hat{\boldsymbol{n}} \parallel \hat{\boldsymbol{n}}$ by virtue of the Euler-Lagrange equations. Since $\boldsymbol{h}_v = -K_{3v}\nabla^2\hat{\boldsymbol{n}}$, this is also parallel to $\hat{\boldsymbol{n}}$ and so the $\boldsymbol{h}_v$ terms vanish, contributing nothing to Eq. (5a).

We can thus conclude that under the conditions of this section, a two-dimensional active nematic with a director field in its ground state must have *both splay and bend* for there to be thresholdless flow in the absence of external fields.

For fully three-dimensional configurations of an active nematic, on the other hand, for which there is also twist to take into account, it is unclear whether or not both splay and bend are necessary for thresholdless flow to occur in the absence of external fields.

What we can conclude though is that, under the conditions of this section and in the absence of external fields, the ground state director field must at the very least either have both splay and twist, or have bend, in order to induce thresholdless active flow.

In summary, we have identified three large classes of spatially non-uniform director configurations, namely, all pure twist and in the case of simply connected geometries in the "frozen director" approximation, all pure splay, and pure 2D bend, which do not induce thresholdless active flow. Thus, the requirements for thresholdless active flow are far more stringent than the mere existence of a spatially non-uniform director field.

2.4 TWO-DIMENSIONAL CURVED SYSTEMS

Having introduced and discussed the concept of thresholdless active flow, we now look at geometric conditions which can apply on 2D curved surfaces which will firstly lead to a non-zero active force, and secondly to non-zero flow.

Consider an active nematic material confined to a curved monolayer shell, such as that shown in Fig. 11. Such systems are of special interest since many active nematics synthesized to date are monolayers or thin shells with planar anchoring [22, 25]. In this section, we will show that, in general, a shell with non-vanishing Gaussian curvature G generates a non-vanishing active force $\boldsymbol{f}_a$. To prove this result, we first assume that, if the shell is very thin, the component of $\hat{\boldsymbol{n}}$ perpendicular to

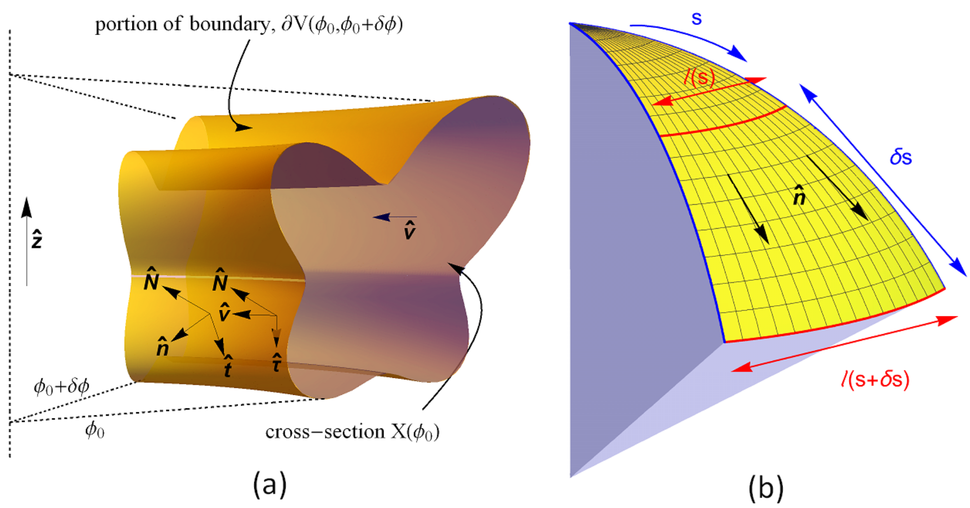

Figure 11: *Orthonormal set of unit vectors and geodesics on a curved surface.* (a) A volume V' of arbitrary cross-section with torsional symmetry. The normal to the bounding surface is $\hat{\boldsymbol{N}}$ and 2 orthonormal sets of unit vectors are shown: (i) director field $\hat{\boldsymbol{n}}$ tangential to the bounding surface with $\hat{\boldsymbol{t}} = \hat{\boldsymbol{N}} \times \hat{\boldsymbol{n}}$; and (ii) direction of symmetry $\hat{\boldsymbol{\nu}}$ also tangential to bounding surface with $\hat{\boldsymbol{\tau}} = \hat{\boldsymbol{N}} \times \hat{\boldsymbol{\nu}}$; and (b) In the case of planar anchoring of the director $\hat{\boldsymbol{n}}$ on a surface with Gaussian curvature, the distance between geodesics $\ell(s)$ as a function of the arc-length s.

the surface is negligible everywhere inside the shell [44, 45, 46], i.e., planar anchoring conditions. In this case, we can decompose the active force $\boldsymbol{f}_a(\boldsymbol{x})$ at position $\boldsymbol{x}$ along three orthogonal directions: (i) the local surface normal $\hat{\boldsymbol{N}}$, (ii) the nematic director $\hat{\boldsymbol{n}}$ and (iii) the tangent vector $\hat{\boldsymbol{t}}$ perpendicular to both $\hat{\boldsymbol{N}}$ and $\hat{\boldsymbol{n}}$, shown in Fig. 11(a) (which in addition shows a second orthonormal set of unit vectors $(\hat{\boldsymbol{N}}, \hat{\boldsymbol{\nu}}, \hat{\boldsymbol{\tau}})$ used below in Section 2.4). The active force reads

$$\boldsymbol{f}_a(\boldsymbol{x}) = \alpha \left[\hat{\boldsymbol{n}}(\boldsymbol{x}) \; \nabla \cdot \hat{\boldsymbol{n}}(\boldsymbol{x}) + \hat{\boldsymbol{t}}(\boldsymbol{x}) \; \kappa_g(\boldsymbol{x}) + \hat{\boldsymbol{N}}(\boldsymbol{x}) \; \kappa_n(\boldsymbol{x}) \right] \tag{22}$$

where $\kappa_n = \hat{\boldsymbol{N}} \cdot \left(\hat{\boldsymbol{n}} \cdot \nabla \right) \hat{\boldsymbol{n}}$ denotes the local normal curvature of the nematic director field $\hat{\boldsymbol{n}}(\boldsymbol{x})$ and $\kappa_g = \hat{\boldsymbol{t}} \cdot \left(\hat{\boldsymbol{n}} \cdot \nabla \right) \hat{\boldsymbol{n}}$ denotes its geodesic curvature [47, 48], which quantifies deviations from the local geodesic tangent to $\hat{\boldsymbol{n}}$.

Since the set of vectors $(\hat{\boldsymbol{N}}, \hat{\boldsymbol{n}}, \hat{\boldsymbol{t}})$ is orthonormal, the active force can only vanish if all three of its components vanish. In particular, this implies that $\kappa_g = 0$. However, we now show that the condition $\kappa_g = 0$ forces the $\hat{\boldsymbol{n}}$ component of $\boldsymbol{f}_a$ (which is proportional to $\nabla \cdot \hat{\boldsymbol{n}}$) to be non-zero, on any surface with non-zero Gaussian curvature. To prove this statement, note that if $\kappa_g = 0$, the nematic director must lie on geodesics everywhere on the surface, as illustrated in Fig. 11(b). Consider an infinitesimal patch bounded by two geodesics (along which the nematic director is aligned) and their normals, drawn in red in Fig. 11(b). These perpendicular arcs have length equal to the distance $\ell(s)$ between the two geodesics parametrized by the arc-length s along one of them. We now apply the divergence theorem to the director field $\hat{\boldsymbol{n}}$ on this small patch, whose area is approximately given by ds times $\ell(s)$. The $\hat{\boldsymbol{n}}$ flux vanishes along the two geodesics, and it is equal to $\ell(s + ds)$ and $-\ell(s)$ along the two red arcs, which yields

$$\nabla \cdot \hat{\boldsymbol{n}} = \frac{1}{\ell} \frac{d\ell}{ds}. \tag{23}$$

The right hand side of Eq. (23) cannot be identically zero because $\frac{d^2\ell}{ds^2} = -G(s)\,\ell$ on an arbitrary surface with non-vanishing $G(x)$ [51]. Intuitively, Gaussian curvature forces geodesics to either converge or diverge, which in turn implies that $\nabla \cdot \hat{\boldsymbol{n}} \neq 0$. The converse statement also holds, namely that $\nabla \cdot \hat{\boldsymbol{n}} = 0$ requires $\kappa_g \neq 0$. Thus we have proved that non-vanishing Gaussian curvature G implies a non-vanishing active force $\boldsymbol{f}_a$. The incompatibility relation derived above has a purely geometric origin and is independent of the values of elastic constants and other material parameters, such as the viscosity tensor. It is also responsible for the geometric frustration of nematic (and more generally orientational and crystalline) order in curved space.

A non-vanishing Gaussian curvature always enforces a non-zero in-plane active force, but thresholdless flow will occur only if this active force $\boldsymbol{f}_a$ cannot be balanced by the pressure gradient. Since ∇P is by definition a conservative force, a sufficient condition for thresholdless flow is therefore

$$G(\boldsymbol{x}) \neq 0 \tag{24}$$

at some point $\boldsymbol{x}$ on the shell, and

$$\oint_C d\boldsymbol{l} \cdot \boldsymbol{f}_a \neq 0 \tag{25}$$

for some closed loop C on the shell.

Our derivation of this condition never assumed that the director configuration was free of topological defects (i.e., disclinations); hence the active force must be non-zero for any surface with non-vanishing Gaussian curvature, even if, as often happens [49, 50], that Gaussian curvature induces disclinations on the surface. Topological defects actually make flow highly likely (a result first noted in references [23, 24] for flat surfaces), since they induce large director gradients near their core.

Note, however, the condition (25) will not be satisfied for all surfaces with non-zero Gaussian curvature, even though the active force must be non-zero for all such surfaces. In the next chapter, we consider a specific example that illustrates this point.

2.5 THREE-DIMENSIONAL SYSTEMS WITH CURVED BOUNDARIES

We now look at how the geometry of the boundaries and anchoring conditions of the director can also force thresholdless flow in bulk active nematics under confinement. This may be of practical importance, since controlling boundaries and boundary conditions for liquid crystals is a highly developed technology, that has long been used for the construction of liquid crystal displays. Efforts are under way to extend such control to the active regime [31, 55, 56].

Consider non-planar alignment of the director to the walls of a three-dimensional channel with torsional symmetry (by which we mean equivalently that the sample is bounded by a surface of revolution about the $z-$axis as shown in Fig. 11(a)). The nematic liquid crystal fills the bulk bound by the surface. If we make the additional assumption that the pressure gradient vanishes along the direction of torsional symmetry, which we denote by $\hat{\boldsymbol{\nu}}$, a non-zero component of the active force along $\hat{\boldsymbol{\nu}}$ will result in thresholdless flow.

A small section of a channel V' bounded by an arbitrarily shaped surface with torsional symmetry along $\hat{\boldsymbol{\nu}}$ is shown in Fig. 11(a), where the local surface normal is represented by the unit vector $\hat{\mathbf{N}}(\boldsymbol{x})$. Denoting the torsional coordinate by ϕ, the volume V' is the section of the three-dimensional channel bounded by the surfaces $\phi = \phi_o$ and $\phi = \phi_o + \delta\phi$. The *integrated* force $\boldsymbol{F}(\phi_o)$ acting on the volume V' can then be obtained by integrating the force density, $(f_a)_i = \alpha\, \partial_j(n_i n_j)$, over the infinitesimal volume V'. Applying the divergence theorem, we obtain the projection of $\boldsymbol{F}(\phi_o)$ along $\hat{\boldsymbol{\nu}}(\phi_o)$ in terms of the anchoring conditions of the nematic director at the boundary, leading to the sufficient condition for thresholdless flow:

$$\begin{aligned} 0 \neq \boldsymbol{F}(\phi_o) \cdot \hat{\boldsymbol{\nu}}(\phi_o) &= \alpha \int_{\partial V(\phi_o, \phi_o+\delta\phi)} dS (\hat{\mathbf{N}} \cdot \hat{\boldsymbol{n}})\, (\hat{\boldsymbol{\nu}} \cdot \hat{\boldsymbol{n}}) \\ &+ \alpha\, \delta\phi \int_{X(\phi_o)} dS (\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{z}} \cdot \hat{\boldsymbol{n}})\, (\hat{\boldsymbol{\nu}} \cdot \hat{\boldsymbol{n}}) \end{aligned} \tag{26}$$

where $\hat{\boldsymbol{z}}$ is the axis of torsional symmetry (see Fig. 11(a)), so that in cylindrical coordinates centered on the axis of symmetry, $\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{z}}$ is a unit vector in the radial direction. A detailed derivation of Eq. (26) in the case of general curvilinear coordinates under suitable assumptions follows in section 2.5.1. Here, we note that in the case of a sample with *high slenderness* (for which the radius of curvature along $\hat{\boldsymbol{\nu}}$ is much greater than in the directions perpendicular to it), the second term may be dropped relative to the first term. Once this simplification is made, condition (26) becomes

$$0 \neq \boldsymbol{F}(\phi_0) \cdot \hat{\boldsymbol{\nu}}(\phi_0) = \alpha \int_{\partial V(\phi_0, \phi_0 + \delta\phi)} dS(\hat{\boldsymbol{N}} \cdot \hat{\boldsymbol{n}})\,(\hat{\boldsymbol{\nu}} \cdot \hat{\boldsymbol{n}}) \tag{27}$$

which we see is met as long as the nematic director $\hat{\mathbf{n}}$ is not perpendicular to $\hat{\mathrm{N}}$ or $\hat{\boldsymbol{\nu}}$ on all the surfaces bounding the volume element.

2.5.1 *Geometric integral conditions for thresholdless active flow*

To derive the geometric integral formula (26) above, for a sample with symmetry and arbitrary smooth cross-section X, parametrised by general orthogonal curvilinear coordinates $\xi_{1,2,3}$ shown in Fig. 12. Above we make the replacements in notation $\hat{\boldsymbol{\xi}}_{\mathbf{1}} \rightarrow \hat{\boldsymbol{N}}$, the normal to the bounding surface ∂V, $\hat{\boldsymbol{\xi}}_{\mathbf{2}} \rightarrow \hat{\boldsymbol{\nu}}$, the direction of symmetry and $\hat{\boldsymbol{\xi}}_{\mathbf{3}} \rightarrow \hat{\boldsymbol{\tau}} = \hat{\boldsymbol{N}} \times \hat{\boldsymbol{\nu}}$. The net active force $\boldsymbol{F}(\phi_0)$ acting on this volume is given by

$$\boldsymbol{F}(\phi_0) = \int_{V'} h_1 h_2 h_3 d\xi_1 d\xi_2 d\xi_3 \boldsymbol{f}_a\,, \tag{28}$$

where the geometrical scale factors $h_{1,2,3}$ are the ratios of the infinitesimal distances to infinitesimal changes $d\xi_{1,2,3}$ in the curvilinear coordinates (and should not, of course, be confused with the components of the "molecular fields" $\boldsymbol{h}$). Applying the divergence theorem to the component of $\boldsymbol{F}(\phi_0)$ along the direction $\hat{\boldsymbol{\xi}}_{\mathbf{2}}$ enables us to convert the volume integral in (28) into an integral over the surface $\partial V'$ of V':

$$\boldsymbol{F}(\phi_0) \cdot \hat{\boldsymbol{\xi}}_{\mathbf{2}}(\phi_0) = \alpha \int_{\partial V'} dS(\hat{\boldsymbol{\xi}}_{\mathbf{1}} \cdot \hat{\boldsymbol{n}})(\hat{\boldsymbol{\xi}}_{\mathbf{2}} \cdot \hat{\boldsymbol{n}}). \tag{29}$$

To evaluate this surface integral, we note that the surface $\partial V'$ of V' can be divided into three parts: the portion of the sample surface $\partial V(\phi_0, \phi_0 + \delta\phi)$ that borders V', and the two cross-sectional "caps" $X(\phi_0)$ and $X(\phi_0 + \delta\phi)$ (see Fig. 12). Doing so gives three surface integrals to evaluate, the first of which is:

$$I^{\alpha}_{\partial V(\phi_0, \phi_0 + \delta\phi)} \quad = \quad \alpha \hat{\boldsymbol{\xi}}_{\mathbf{2}}(\phi_0) \cdot \int_{\phi_0}^{\phi_0 + \delta\phi} d\xi_2 \int d\xi_3 h_2 h_3 n_1 n_i \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}\,.$$

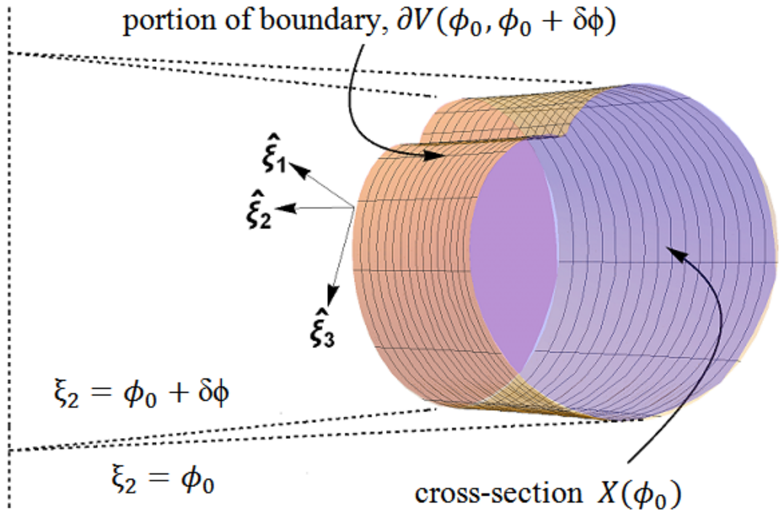

Figure 12: *General co-ordinates* $\xi_{1,2,3}$ *for a shape with torsional symmetry.* Volume V' with cross-section X bounded by the surfaces $\xi_2 = \phi_o$ and $\phi_o + \delta\phi$. The faces of V' are $\partial V(\phi_o, \phi_o + \delta\phi), X(\phi_o)$ and $X(\phi_o + \delta\phi)$.

Using the facts that the element of surface area $dS = d\xi_2 d\xi_3 h_2 h_3$, $n_1 = \hat{\boldsymbol{N}} \cdot \hat{\boldsymbol{n}}$, $\hat{\boldsymbol{n}} = n_i \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}$ and, in the notation of the main text, $\hat{\boldsymbol{\xi}}_{\boldsymbol{2}}(\phi_o) = \hat{\boldsymbol{\nu}}$, we obtain the first term on the right hand side of Eq. (26):

$$I^{\alpha}_{\partial V(\phi_o,\phi_o+\delta\phi)} \approx \alpha \int_{\partial V(\phi_o,\phi_o+\delta\phi)} dS(\hat{\boldsymbol{N}} \cdot \hat{\boldsymbol{n}})(\hat{\boldsymbol{\nu}} \cdot \hat{\boldsymbol{n}}). \tag{30}$$

Now evaluating the integrals across the cross-sections, it is convenient to combine them as follows:

$$\begin{aligned} I^{\alpha}_{X(\phi_o)} &= \alpha \hat{\boldsymbol{\xi}}_{\boldsymbol{2}}(\phi_o) \cdot \int d\xi_1 d\xi_3 h_1 h_3 n_2 \left(-n_i \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}(\phi_o)\right) \\ I^{\alpha}_{X(\phi_o+\delta\phi)} &= \alpha \hat{\boldsymbol{\xi}}_{\boldsymbol{2}}(\phi_o) \cdot \int d\xi_1 d\xi_3 h_1 h_3 n_2 \left(n_i \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}(\phi_o + \delta\phi)\right) \end{aligned}$$

so that

$$\begin{aligned} I^{\alpha}_{X(\phi_o)} + I^{\alpha}_{X(\phi_o+\delta\phi)} &\approx \alpha \delta\phi \hat{\boldsymbol{\xi}}_{\boldsymbol{2}} \cdot \int d\xi_1 d\xi_3 h_1 h_3 n_2 n_i \partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}(\phi_o) \\ &\approx \alpha \delta\phi \int d\xi_1 d\xi_3 h_1 h_3 n_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{2}} \cdot \left(n_i \partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}\right) \end{aligned} \tag{31}$$

again taking $\hat{\boldsymbol{\xi}}_{\boldsymbol{2}}$ inside the integral sign. The second term $I^{\alpha}_{X(\phi_o)} + I^{\alpha}_{X(\phi_o+\delta\phi)}$ can be simplified by noting that $\hat{\boldsymbol{\xi}}_{\boldsymbol{2}} \cdot \partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{i}} = \partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{2}} \cdot \hat{\boldsymbol{\xi}}_{\boldsymbol{i}} - \hat{\boldsymbol{\xi}}_{\boldsymbol{i}} \cdot \partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{2}}$.

Since $\hat{\boldsymbol{\xi}}_{\boldsymbol{2}} \cdot \hat{\boldsymbol{\xi}}_{\boldsymbol{i}} = \delta_{i2}$, which is independent of ϕ, the first term vanishes. The argument of the integral in (31) can then be rewritten $\hat{\boldsymbol{\xi}}_{\boldsymbol{2}} \cdot \left(n_i \partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{i}}\right) = -n_i \hat{\boldsymbol{\xi}}_{\boldsymbol{i}} \cdot \left(\partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{2}}\right) = -\hat{\boldsymbol{n}} \cdot \left(\boldsymbol{\partial_2} \hat{\boldsymbol{\xi}}_{\boldsymbol{2}}\right)$, where we've used the fact that $n_i \hat{\boldsymbol{\xi}}_{\boldsymbol{i}} = \hat{\boldsymbol{n}}$ (this simply being the decomposition of $\hat{\boldsymbol{n}}$ along the local coordinate axes $\hat{\boldsymbol{\xi}}_{\boldsymbol{i}}$). Now, using the fact that $\partial_2 \hat{\boldsymbol{\xi}}_{\boldsymbol{2}} = \partial_\phi \hat{\boldsymbol{\phi}} = -\hat{\boldsymbol{r}}$, where $\hat{\boldsymbol{r}}$ is the unit vector in the radial direction from the axis of toroidal symmetry, we obtain

$$I^{\alpha}_{X(\phi_0)} + I^{\alpha}_{X(\phi_0+\delta\phi)} \approx \alpha\, \delta\phi \int\limits_{X(\phi_0)} dS \left((\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{z}}) \cdot \hat{\boldsymbol{n}} \right) \, (\hat{\boldsymbol{\nu}} \cdot \hat{\boldsymbol{n}}) \tag{32}$$

where $\hat{\boldsymbol{r}} = \hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{z}}$. Adding this expression for the contribution of the cross sections $X(\phi_0)$ and $X(\phi_0 + \delta\phi)$ to the net toroidal force to that of the boundary ∂V as given by (30) immediately gives Eq. (26) above.

High slenderness limit In the case of torsional symmetry with an arbitrary (smooth) cross-section X where the volume has a high slenderness, σ, the second term in eq. (26) may be dropped if the first term is non-zero. To see this, suppose that the length-scale in the $\hat{\boldsymbol{\xi}}_{\boldsymbol{1}}$- and $\hat{\boldsymbol{\xi}}_{\boldsymbol{3}}$-directions is L, while in the $\hat{\boldsymbol{\xi}}_{\boldsymbol{2}}$-direction it has a length scale of σL. A very slender sample will therefore have $\sigma \gg 1$, whereas a "fat" sample will have $\sigma \approx 1$. The first term in eq. (26) is proportional to $L^2\sigma$, whereas the second term is proportional to L^2 and so can be neglected compared with the first term.

2.6 A FIRST EXAMPLE

We now look at a first example - an active nematic confined between two infinite parallel plates, one with perpendicular and the other with planar anchoring, shown in Fig. 13. The director field and flow profile for this system were determined numerically in Ref. [34] but we work it analytically in chapter 3. Here, we deduce the main features of the flow using simple geometric arguments without carrying out explicit calculations. Firstly, notice that because of the symmetry in the $y-$direction, this system is the high slenderness limit of a similar torsionally symmetric system. This can be seen by giving the system torsional symmetry by revolving the figure about, say, the point $(-R, 0)$ in the $(x, y)-$plane to create an annulus. The high slenderness limit is obtained by sending $R \to \infty$ and recovering Fig. 13, in which case Eq. (27) is exact. However, $\boldsymbol{F} \cdot \hat{\boldsymbol{\nu}} = 0$ in this cell because $(\hat{\boldsymbol{N}} \cdot \hat{\boldsymbol{n}}) = 0$ on one plate and $(\hat{\boldsymbol{\nu}} \cdot \hat{\boldsymbol{n}}) = 0$ on the other. Nonetheless, active nematics flow at arbitrary small α in such a mixed alignment cell. This can be

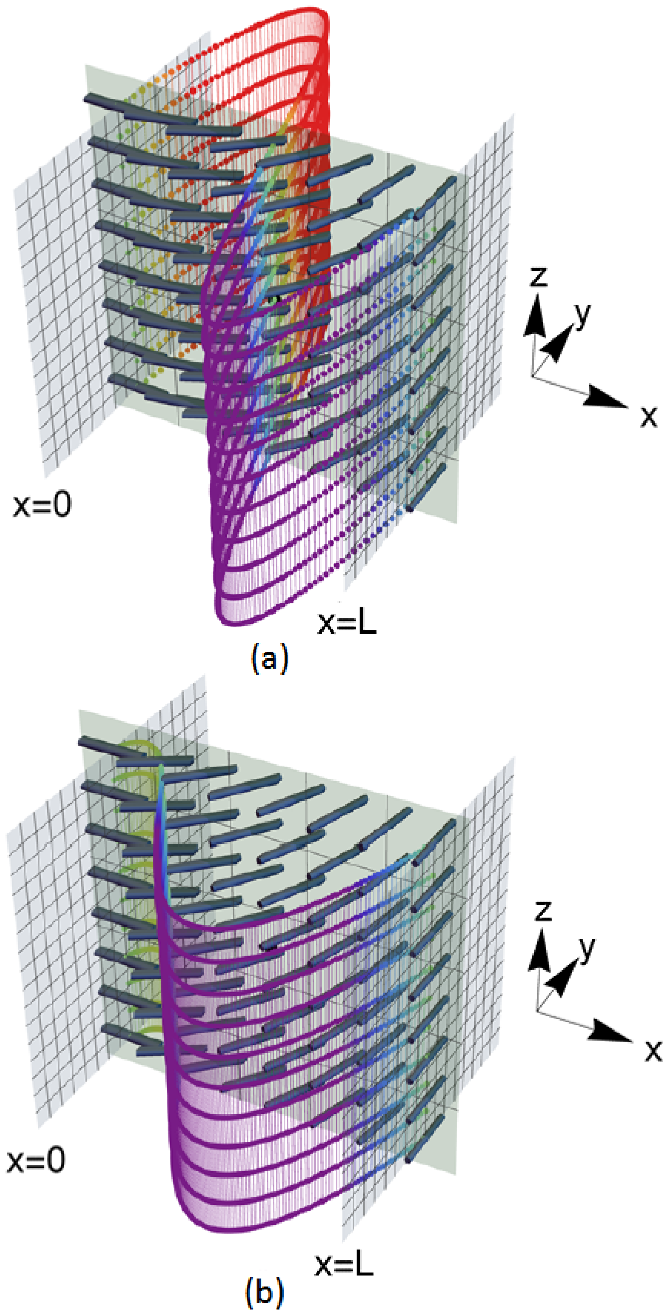

Figure 13: *Flow profile and director field ground state generated with mixed boundary conditions in 2 dimensions* (a) in the isotropic case $K_1 = K_3$ and (b) in the anisotropic case $K_1 \gg K_3$. Red denotes maximum flow in the $\hat{\boldsymbol{y}}$-direction, violet maximum flow in the $-\hat{\boldsymbol{y}}$-direction and green no flow.

explained by applying Eq. (27) to either of the two portions of the cell, on opposite sides of the plane (parallel to both walls), whose surface normal $\hat{\mathbf{N}}$ makes an angle of $\pi/4$ with $\hat{\boldsymbol{n}}$. The boundary conditions on θ, and continuity ensure that such a plane exists, though it will not, for arbitrary and unequal values of the Frank constants $K_{1,2,3}$, be the midplane. According to Eq. (27), the resulting active forces in each of the two portions will be non-zero but of opposite sign; hence, the two sides must flow in opposite directions. In the special case of equal Frank constants $K_1 = K_2 = K_3$, the midplane is the plane on which the surface normal $\hat{\boldsymbol{N}}$ makes an angle of $\pi/4$ with $\hat{\boldsymbol{n}}$, and the flow in the two halves cancels out, leading to zero net flow in the whole cell. In the generic case of unequal Frank constants, this cancellation does not occur, leading to non-zero net flow, as we discuss more fully in chapter 3.

2.7 SUMMARY

We have introduced the topic of active nematic systems and reviewed the "standard model" for the hydrodynamics of active nematics. We then considered some generalizations of this model, and explained why none of our conclusions are significantly affected by these generalizations. After that, we derived the general criterion for thresholdless active flow and explained the frozen director regime and then went on to apply this criterion to the specific case of surfaces of non-zero Gaussian curvature. We showed that these surfaces always have non-zero active forces and then also derived the additional criteria that must be satisfied for thresholdless flow to occur in these systems.

We then considered the case of 3D bulk systems and concluded with an introductory simple 3D example of parallel plates with mixed boundary conditions. In the next chapter we will develop this further and work several more examples in both 2D as well as 3D.