Supplementary Information
(Instabilities, defects, and defect ordering in an overdamped active nematic)

Elias Putzig,[1,*] Gabriel S. Redner,[1,†] Arvind Baskaran,[2,‡] and Aparna Baskaran[1,§]

[1] *Martin Fisher School of Physics, Brandeis University, Waltham, MA 02453, USA*
[2] *Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, USA*

[*] efputzig@brandeis.edu
[†] gredner@brandeis.edu
[‡] baskaran@math.uci.edu
[§] aparna@brandeis.edu

I. FREE ENERGY

The dynamics of an equilibrium liquid crystal, which were discussed in the body of the text, can be derived from gradient descent on the well-known Landau-de Gennes free energy [1, 2]:

$$F = \int d^d r \Big[-\frac{\alpha}{2} Tr(\mathbf{Q}^2) + \frac{\beta}{4}\big(Tr(\mathbf{Q}^2)\big)^2 + \chi Q_{ij}\partial_i\partial_j\rho + \frac{1}{2}\kappa(\nabla^2\mathbf{Q})^2 + \frac{1}{2}L_1(\partial_i Q_{kl})^2 + \frac{1}{2}L_2(\partial_i Q_{ik})\partial_j Q_{jk} + \frac{1}{2\rho}L_4 Q_{ij}(\partial_i Q_{kl})\partial_j Q_{kl}\Big] + \Phi[\rho] \tag{1}$$

where the homogeneous terms give a second order phase transition and the terms with coefficients L_i are elastic terms, associated with the energy cost of director distortions. The elastic energy cost is widely described in terms of splay $(K_{11}(\nabla\cdot\hat{n})^2)$ and bend $(K_{33}\big(\hat{n}\times(\nabla\times\hat{n})\big)^2)$ distortion of the director. The parameters in (1) are related to the splay and bend coefficients as: $K_{11} = \rho^2 S^2(2L_1 + L_2 - SL_4)$ and $K_{33} = \rho^2 S^2(2L_1 + L_2 + SL_4)$.

The gradient-descent dynamics from the body of the paper came from taking a derivative of Eq. 1:

$$-\gamma^{-1}\frac{\delta F}{\delta Q_{ij}} = D_r[\alpha - \beta Tr\mathbf{Q}^2]Q_{ij} + 2\bar{D}_E\nabla^2 Q_{ij} + D_\rho(\partial_i\partial_j - \frac{1}{2}\delta_{ij}\nabla^2)\rho - K\nabla^4 Q_{ij} + \frac{D_\delta}{\rho}\Big(2Q_{kl}\partial_k\partial_l Q_{ij} + 2[\partial_k Q_{kl}]\partial_l Q_{ij} - \big([\partial_i Q_{kl}]\partial_j Q_{kl} - \frac{1}{2}\delta_{ij}[\partial_k Q_{lm}]^2\big)\Big) \tag{2}$$

where $D_r = 1/\gamma$, $D_\rho = -\chi/\gamma$, $K = \kappa/\gamma$ and the two mean elastic terms have been consolidated by using the tracelessness and symmetry of Q to group them in the term with coefficient $\bar{D}_E = \frac{1}{2}(L_1 + L_2)/\gamma$. The equilibrium nematic should be stable to director fluctuations $(K_{11}, K_{33} > 0)$, so the differential elastic coefficient, $D_\delta = L_4/\gamma$, should be in a range $|D_\delta| < \frac{3}{S}\bar{D}_E$. The fourth order gradient term, coefficient K, is included in order to ensure smoothness and numerical stability. This role becomes apparent when considering the role of this term in the linear stability.

II. LINEAR STABILITY

The equations of an overdamped active nematic,

$$\partial_t\rho = D\nabla^2\rho + D_Q\partial_i\partial_j Q_{ij} \tag{3}$$

and Eq **??**, admit a homogeneous uni-axial nematic state with average density $\rho_0 > 1$, and the order parameter $\mathbf{Q} = \rho_0 S_0(\hat{\boldsymbol{x}}\hat{\boldsymbol{x}} - \frac{1}{2}\mathbf{I})$ with $S_0 = \sqrt{\frac{2(\rho_0-1)}{\rho_0+1}}$. Without loss of generality, we have picked coordinates so that the direction of nematic ordering is along the x-axis of our coordinate system. We parameterize the fluctuations about this state in the form $\rho(\mathbf{r},t) = \rho_0 + \delta\rho(\mathbf{r},t)$, $Q_{xx}(\mathbf{r},t) = \frac{1}{2}\rho_0 S_0 + \delta Q_{xx}(\mathbf{r},t)$ and $Q_{xy}(\mathbf{r},t) = \delta Q_{xy}(\mathbf{r},t)$. Further, we introduce a Fourier transform $\tilde{X} = \int d\mathbf{r}e^{i\mathbf{k}\cdot\mathbf{r}}X(\mathbf{r},t)$. The resulting linearized equations in Fourier space are

$$\partial_t\delta\tilde{\rho} = -Dk^2\delta\tilde{\rho} - D_Q k^2\cos(2\phi)\delta\tilde{Q}_{xx} - D_Q k^2\sin(2\phi)\delta\tilde{Q}_{xy} \tag{4a}$$

$$\begin{aligned}\partial_t\delta\tilde{Q}_{xx} &= \Big(C_0 - \tfrac{1}{2}D_\rho k^2\cos(2\phi)\Big)\delta\tilde{\rho} \\ &- \Big(2\alpha_0 + 2D_E k^2 + (D_\delta - \tfrac{1}{2}\lambda_S)S_0 k^2\cos(2\phi) + Kk^4\Big)\delta\tilde{Q}_{xx} \\ &+ \tfrac{1}{2}\lambda_S S_0 k^2\sin(2\phi)\delta\tilde{Q}_{xy}\end{aligned} \tag{4b}$$

$$\begin{aligned}\partial_t\delta\tilde{Q}_{xy} = &- \tfrac{1}{2}D_\rho k^2\sin(2\phi)\delta\tilde{\rho} \\ &- \tfrac{\lambda_R}{2}S_0 k^2\sin(2\phi)\delta\tilde{Q}_{xx} \\ &- \Big(2D_E k^2 - \tfrac{\lambda_R}{2}S_0 k^2\cos(2\phi) + D_\delta S_0 k^2\cos(2\phi) + Kk^4\Big)\delta\tilde{Q}_{yx}\end{aligned} \tag{4c}$$

where ϕ is the angle between the director (along the x axis in our coordinates) and the spatial gradient vector $\mathbf{k}$. The effective mean elastic term, $D_E = \bar{D}_E - \lambda_E$ comes from the Laplacian term in Eqs. 2 and **??** and, we have defined parameters $C_0 = \sqrt{\frac{2(\rho_0-1)}{\rho_0+1}}\left(\frac{\rho_0^2+\rho_0-1}{\rho_0+1}\right)$, and $\alpha_0 = \rho_0 - 1$ for notational compactness.

The stability of these equations is best explicated by considering spatial fluctuations along ($\phi = 0$) or perpendicular to ($\phi = \frac{\pi}{2}$) the direction of ordering. In these two sectors, the fluctuations in the direction of ordering $\delta\tilde{Q}_{xy}$ decouple form those in the magnitude of ordering $\delta\tilde{Q}_{xx}$ and the density $\delta\tilde{\rho}$, thereby enabling a clear identification of mechanisms at play.

The decoupled fluctuations in the direction of ordering, $\delta\tilde{Q}_{xy}$, are of the following form:

$$\partial_t \delta\tilde{Q}_{xy} = -\Big(\big(2D_E \mp \frac{S_0}{2}(\lambda_R - 2D_\delta)\big)k^2 + Kk^4\Big)\delta\tilde{Q}_{xy} \tag{5}$$

where upper sign in the coefficient of the quadratic term (k^2) is for bend fluctuations (along the director: $\phi = 0$) and the lower is for splay fluctuations (perpendicular to the director: $\phi = \pi/2$). When the coefficient of the quadratic term becomes negative there will be an instability in the direction of order at large wavelengths (small wave-vector, k). The fourth-order gradient term, with coefficient K guarantees that, when there is an instability in this mode, the ordered solution will restabilize at finite wavelength. This is required in order to retain a smooth solution at the smallest length scales, which is a physical condition which should be satisfied by fields such as the ones we describe here. It is also necessary, in order to achieve numerical stability, that fluctuations on wavelengths comparable to the step size used in the discretization of space are suppressed.

One condition which always leads to an instability in the direction of order is when the effective mean elastic term, $D_E < 0$. This is analogous to the generic instability which has been discussed in theories of active nematic suspensions [3–6], as they both arise due to shearing, though in this case it is self-induced shearing, rather than shear flow of a fluid. In this case, the existence of this instability requires that $\lambda_E = \frac{f}{\xi}\lambda_1 > \bar{D}_E$, which can occur when the system consists of extensile ($f > 0$) rod-like particles which align with a shear ($\lambda_1 > 0$). It may also occur for contractile ($f < 0$) disc-like particles which align perpendicular to a shear ($\lambda_1 < 0$). The fastest growing mode for this instability will always be bend when $(\lambda_R - 2D_\delta) > 0$, and will be splay otherwise. We find, therefore, that the bend instability will dominate in extensile ($\lambda_R > 0$) rod-like particles, and the splay instability will dominate in contractile ($\lambda_R < 0$) disc-like particles, unless there is a significantly greater energetic cost to either bend or splay deformations ($|D_\delta| > \frac{1}{2}\lambda_R$). This differs from what was seen in active suspensions in that here, in the overdamped case, there is no concept of flow-alignment VS flow-tumbling. This also differs in that the active suspension theories make the one-constant ($D_\delta = 0$) approximation, so they do not discuss the dependence of the mode of the instability on the energetic penalties for splay VS bend distortions.

The other instability in the direction of order arises due to the rotation of the director by the active torque when $D_E > 0$. The active torque must exceed a threshold $\lambda_R > (4D_E/S_0 + 2D_\delta)$ to overcome the elastic terms. This threshold is larger when the energetic penalty to bend distortions of the director is higher than that of splay distortions, and $D_\delta > 0$. In order to define a 'distance' from the bend instability, is useful to define a bend instability parameter $\psi \equiv \frac{\lambda_R - 2D_\delta}{D_E \cdot \Lambda(\rho_0)}$, where $\Lambda(\rho_0) = 4/S_0 = 4\sqrt{\frac{\rho_0+1}{2(\rho_0-1)}}$. The ordered state is unstable to bend fluctuations when $\psi > 1$. Note that if the nematic was contractile, λ_R is negative and hence there exists a splay instability, which occurs when $\psi < -1$. We have, however, focused on extensile systems for this study of the overdamped dynamics, and left the study of the contractile, overdamped dynamics to future work.

III. ADDITIONAL NUMERICAL PHENOMENOLOGY

[1] P.-G. De Gennes and J. Prost, *The physics of liquid crystals*, Vol. 23 (Clarendon press Oxford, 1993).
[2] A. N. Beris and B. J. Edwards, *Thermodynamics of flowing systems: with internal microstructure* (Oxford University Press, 1994).
[3] S. Ramaswamy and M. Rao, New J. Phys. **9**, 423 (2007).

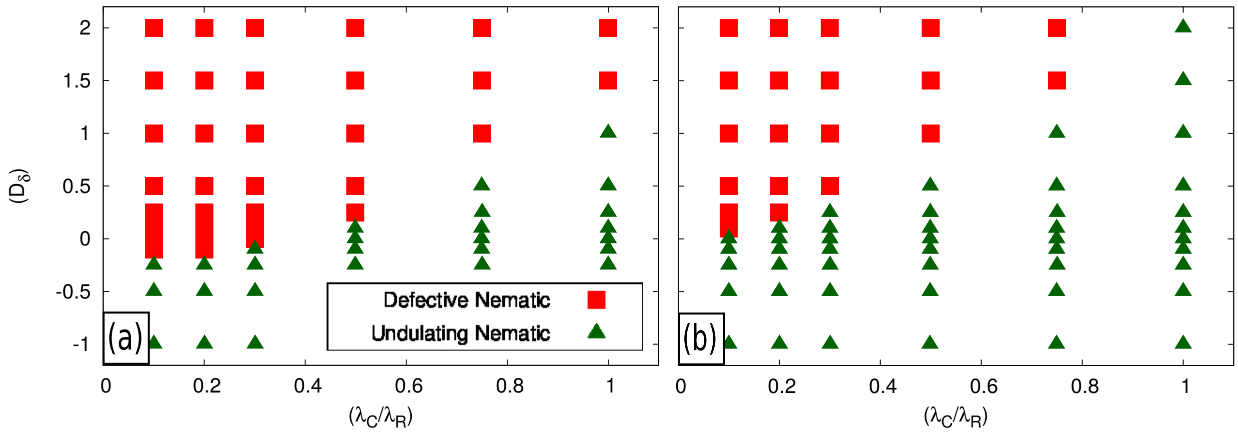

FIG. 1. These plots indicate whether an undulating nematic, or a turbulent, defective nematic state formed out of nematic initial conditions, from a point near the bend instability ($\psi = 1.05$, $\rho_0 = 2.0$) with (a) $\lambda_S = -1.0$ and (b) $\lambda_S = 1.0$. The formation of defects near the critical density is facilitated by having a strength of active convection which is small compared to the strength of the active torque ($\lambda_C/\lambda_R < 1$), and by a large energetic penalty to bend deformations, compared to the penalty to splay deformations ($D_\delta > 0$). The value of λ_S, however, seems to make little difference.

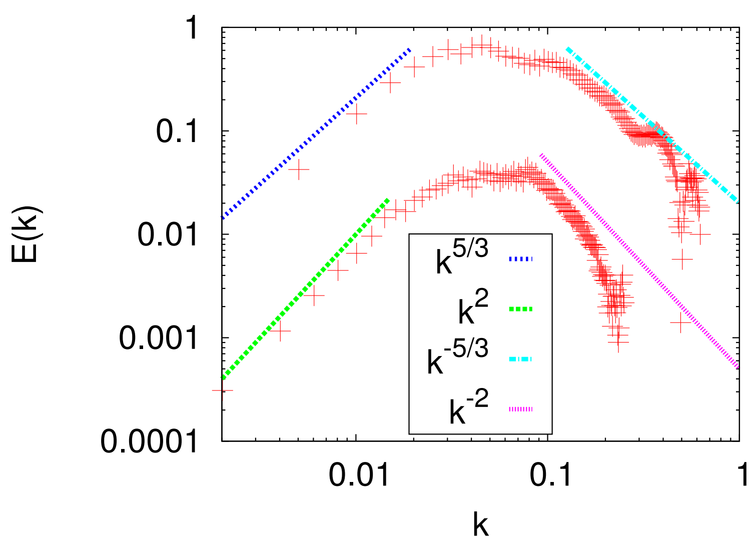

FIG. 2. Log-scale plots of the following approximation of the energy spectral density $E(k) = \frac{k}{2\pi}\int d^2Re^{ik\cdot R}\langle\vec{v}(0)\cdot\vec{v}(R)\rangle$. Data shows two sets of parameters. Top: $(\rho_0, \lambda_R, D_\delta)$=$(2, 8, 1)$ and Bottom: $(3, 10, 0.5)$; scaled by multiplicative constants for comparison. The energy density seems to scale with a power laws of $k^{5/3}$ (k^2) for small wave-vector, and $k^{-5/3}$ (k^{-2}) and for large wave-vector for the upper (lower) curve. These u-shaped energy spectra are similar to what is seen in mixing flow in three dimensions, and is reminiscent of that seen in bacterial turbulence and a reversing-rod model [7].

[4] L. Giomi, L. Mahadevan, B. Chakraborty, and M. F. Hagan, Nonlinearity **25**, 2245 (2012).

[5] L. Giomi, M. J. Bowick, P. Mishra, R. Sknepnek, and M. C. Marchetti, Phil. Trans. R. Soc. A **372**, 20130365 (2014).

[6] S. P. Thampi, R. Golestanian, and J. M. Yeomans, Phil. Trans. R. Soc. A **372**, 20130366 (2014).

[7] H. H. Wensink, J. Dunkel, S. Heidenreich, K. Drescher, R. E. Goldstein, H. Lowen, and J. M. Yeomans, Proc. Nat. Acad. Sci. U.S.A. **109**, 14308 (2012), 1208.4239v1.