Shear flow induced isotropic to nematic transition in a suspension of active filaments

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Abstract. – We study the effects of externally applied shear flow on a model of suspensions of motors and filaments, via the equations of active hydrodynamics [PRL **89** (2002) 058101; **92** (2004) 118101]. In the absence of shear, the orientationally ordered phase of *both* polar and apolar active particles is always unstable at zero-wavenumber. An imposed steady shear large enough to overcome the active stresses stabilises both apolar and moving polar phases. Our work is relevant to *in vitro* studies of active filaments, the reorientation of endothelial cells subject to shear flow and shear-induced motility of attached cells.

The collective behaviour of suspensions of active particles[1] is fundamentally different from that of their passive counterparts, as highlighted by recent studies on hydrodynamic instabilities [1,2], rheology [3] and steady state patterns [4–6] of active particle systems. Recent experimental studies on model systems such as motor-filament extracts [7,8] and suspensions of swimming bacteria [9–11] or spermatocytes [12] have also reported strong departures from *equilibrium* behaviour.

One surprising prediction [1] is that, unlike in passive suspensions, long-range uniaxial orientational order in active Stokesian[2] suspensions of polar particles is *always* destroyed by a hydrodynamic instability. This is because the flow generated by a small, long-wavelength splay or bend deformation imposed on an oriented configuration always acts instantaneously (in the Stokesian regime) to further increase the deformation [1, 13].

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[1]By active particle we mean an object which absorbs energy from its surroundings and dissipates it in the process of carrying out internal movements; examples include self-propelled organisms, motor-filament complexes, and agitated monolayers of granular particles.
[2]where viscosity dominates and inertia is ignored

If only this instability could be controlled, we would have an orientationally ordered phase of active particles with rather unusual rheological properties [13]. We already noted two dramatic rheological consequences [2,3]: (i) the orientationally ordered phase is characterised by a nonzero steady-state average of the deviatoric stress – a kind of yield stress – and (ii) on approaching the orientationally ordered state from the isotropic fluid, a suspension of active *contractile* elements exhibits solid-like behaviour *without translational arrest*. However to obtain this novel material we would first need to stabilise this orientationally ordered phase.

In this paper we ask whether an imposed shear flow can suppress this instability of active Stokesian suspensions. We address this question by constructing a set of coarse-grained equations for the hydrodynamics of the active particle suspensions. We consider apolar (nematic) as well as polar order, keeping in mind that the latter correspond to phases with a nonzero drift velocity of the active particles. Here is a summary of our results, valid in both 2 and 3 dimensions. (i) The instability obtained in [1] occurs for *apolar* ordered suspensions as well; (ii) Imposed shear larger than a critical strain rate $\dot{\gamma}_c$ stabilises the orientationally ordered phase yielding a stability diagram (Fig. 4) controlled by two variables, a flow alignment parameter λ and the the ratio of the shear to active stress. The drift velocity of the vector-ordered phase depends on $\dot{\gamma}$ and λ. Possible experimental tests and some complications regarding boundary conditions and back-flow are discussed at the end of the paper. We now turn to the details of our calculations.

(A) Hydrodynamic equations : The hydrodynamic variables for a suspension of active particles [1,3] are the total momentum density $\mathbf{g} = \rho\mathbf{u}$ of the particles + fluid, where $\mathbf{u}$ is the hydrodynamic velocity field and ρ the density, the concentration $c(\mathbf{r}, t)$ of active particles, and the orientational order parameter field. For *polar* systems, the order parameter is the polarisation vector $\mathbf{p}(\mathbf{r}, t)$ of the force dipoles associated with the active particles. Active systems being out of thermal equilibrium, a local polarisation always implies a local average drift velocity of the active particle relative to the fluid. We thus take $\mathbf{p}$ to be the velocity field of the active particles relative to the fluid. *Apolar* nematic orientational order is characterised by a traceless symmetric tensor $\boldsymbol{Q} \equiv S(\mathbf{pp} - p^2 (1/d)\boldsymbol{I})$, where $\mathbf{p}$ is now the director and S is the scalar nematic order parameter [14]. We focus on the polar case, and indicate differences where appropriate for the apolar case. Momentum conservation in the Stokesian limit means $\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = 0$, where the total stress tensor $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}^a + \boldsymbol{\sigma}^r + \boldsymbol{\sigma}^d$ is the sum of contributions from activity, order-parameter gradients and viscous dissipation, and overall incompressibility of the suspension means $\boldsymbol{\nabla} \cdot \mathbf{u} = 0$, $\rho = \rho_0$, the mean density.

The equations for the active polar order parameter $\mathbf{p}$ read

$$\partial_t\mathbf{p} + (\mathbf{u} \cdot \boldsymbol{\nabla})\,\mathbf{p} - \frac{1}{2}\,(\boldsymbol{\nabla} \times \mathbf{u}) \times \mathbf{p} + \left[\lambda_1\,(\mathbf{p} \cdot \boldsymbol{\nabla})\,\mathbf{p} + \lambda_2\,(\boldsymbol{\nabla} \cdot \mathbf{p})\,\mathbf{p} + \lambda_3\boldsymbol{\nabla}|\mathbf{p}|^2\right]$$
$$= \frac{\lambda}{2}\,\left(\boldsymbol{\nabla}\,\mathbf{u} + (\boldsymbol{\nabla}\,\mathbf{u})^T\right) \cdot \mathbf{p} - \zeta\,\boldsymbol{\nabla}c(\mathbf{r}, t) + \Gamma\,\mathbf{h} + \dots \tag{1}$$

In (1), the first three terms on the left are the material derivative of $\mathbf{p}$ (co-moving and co-rotating with the suspension) and the square brackets (as well as the ζ term on the right) contain symmetry-allowed *polar* contributions [15] (of which the λ_1 term alone [2] is active), ruled out in apolar nematohydrodynamics, whether passive [14, 16] or active [1]. The first term on the right, together with the $\boldsymbol{\nabla} \times \mathbf{u}$ term on the left, lead to flow-alignment [14]. The relaxation dynamics is contained in the order-parameter molecular field $\mathbf{h} = c(r, t)\left[\alpha\mathbf{p} - \beta|\mathbf{p}|^2\mathbf{p} + K\nabla^2\mathbf{p}\right]$ which favours a fixed length for $\mathbf{p}$ and assigns an elastic cost to inhomogeneities in the one-Frank-constant approximation.

Conservation of active particles states

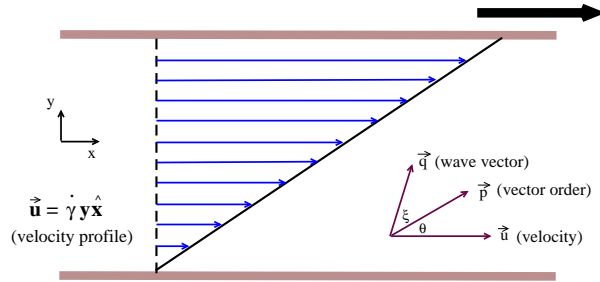$$\partial_t c = -\boldsymbol{\nabla} \cdot \left[\,c\,(\mathbf{u} + \mathbf{p})\right]. \tag{2}$$

Fig. 1 – Suspension of active vector ordered particles subject to an imposed velocity along the $\hat{\boldsymbol{x}}$-axis, $u_0 = \dot{\gamma} y \hat{\boldsymbol{x}}$ with a gradient along the $\hat{\boldsymbol{y}}$-axis. The shear alignment angle θ and the angle ξ between the wavevector $\mathbf{q}$ and the ordering direction are also shown.

The reactive stress from order-parameter gradients is

$$\boldsymbol{\sigma}^r = -\frac{\lambda}{2} \left(\mathbf{p}\,\mathbf{h} + (\mathbf{h}\,\mathbf{p})^T \right) + \Pi\,\mathbf{I} \tag{3}$$

where Π is a generalised pressure; and the viscous stress is $\boldsymbol{\sigma}^d = \frac{\eta}{2} \left(\boldsymbol{\nabla}\,\mathbf{u} + (\boldsymbol{\nabla}\,\mathbf{u})^T \right) \equiv \eta\,\mathbf{A}$, where η the bare shear viscosity of the suspension.

To determine the active stress, we make use of the fact that the simplest active particle, on long timescales, is a permanent force dipole [1,3]. To leading order the deviatoric part of the stress coming from activity is given by

$$\boldsymbol{\sigma}^a\left(\mathbf{r}, t\right) = W c\left(\mathbf{r}, t\right) \left(\mathbf{p}\,\mathbf{p} - p^2 \frac{1}{d}\mathbf{I} \right) , \tag{4}$$

where d is the spatial dimension, and the magnitude and *sign* of W characterise the nature of the elementary force dipoles [1,3].

Here we use this hydrodynamic description to study the effect of shear flow on the ordering and stability of active particle suspensions.

(B) Shear flow : We impose a planar shear flow (Fig. 1) along the $\hat{\boldsymbol{x}}$-axis, with a velocity gradient along $\hat{\boldsymbol{y}}$, giving rise to an imposed velocity field $\mathbf{u}_0 = \dot{\gamma} y \hat{\boldsymbol{x}}$.

The instability of the orientationally ordered phase [1] and its stabilisation due to shear is most simply seen in two dimensions ($d = 2$); we therefore present detailed calculations in $d = 2$, and merely state results in $d = 3$.

We look for homogeneous steady states of (1), (2); the steady state concentration is a uniform $c(r, t) = c_0$. The amplitude and phase of the steady state active vector order parameter

are, respectively,

$$p_0^2 = \frac{\alpha}{\beta} + \frac{\dot\gamma}{2\beta}\sqrt{\lambda^2 - 1} \tag{5}$$

$$\tan\theta = \sqrt{\frac{\lambda - 1}{\lambda + 1}}. \tag{6}$$

The flow alignment parameter λ can take values between 1 and ∞, corresponding to $0 \le \theta \le \pi/4$. Note that while p_0 *increases* with shear rate, the phase θ is *independent* of it.

(C) Stability of orientational order: To determine the stability of this homogeneous steady state, we set $\mathbf{p}(\mathbf{r}, t) = p_0(\cos\theta, \sin\theta) + \delta\mathbf{p}(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t) = \mathbf{u}_0 + \delta\mathbf{u}(\mathbf{r}, t)$ and $c(\mathbf{r}, t) = c_0 + \delta c(\mathbf{r}, t)$, where the perturbations are assumed small. It is convenient to decompose $\delta\mathbf{p}$ and $\delta\mathbf{u}$ parallel and perpendicular to the ordering direction $\mathbf{p}_0$, e.g., $\delta\mathbf{p} = (\delta p_\parallel, \delta p_\perp)$, and to eliminate the "massive" field $\delta p_\parallel$ in favour of the remaining variables yielding, after a spatial fourier transform,

$$\left[\partial_t + iq_\parallel\lambda_1 p_0 + 2iq_\perp F\lambda_3 p_0 + \dot\gamma\sqrt{\lambda^2 - 1}\right]\delta p_\perp(q) + \frac{\dot\gamma}{2}\left(F\cos\theta - \sin\theta\right)\frac{\partial}{\partial q_y}\left(q_\perp\delta p_\perp(q)\right)$$
$$= \left[\frac{ip_0 q^2}{2\rho_0 q_\parallel}\left(1 + \lambda\cos 2\xi\right)\right]\delta g_\perp(q) + \left[\frac{i\dot\gamma q_\parallel}{2}D_0 + \frac{i\lambda\dot\gamma q_\parallel}{2}D_0\cos 2\theta\right]\delta c_q, \tag{7}$$

where $P = 2\Gamma\alpha + \dot\gamma\left(\lambda^2 - 1\right)$, $F = \dot\gamma/P$ and $D_0 = \zeta/P$. Since the instability we are interested in has maximum growth rate [1] at zero wavenumber, we ignore the term $q_i\frac{\partial}{\partial q_j}$ operating on the fields, whose effect can be shown to vanish for $q \to 0$.

Fluctuations in the hydrodynamic velocity field, $\delta\mathbf{u} \equiv \delta\mathbf{g}/\rho_0$, to linear order are governed by the Stokes equation. Imposing incompressibility and eliminating the pressure, eliminating $\delta p_\parallel$ in favour of the remaining fields as above, and fourier-transforming in space, we find $q_\parallel = q_x\cos\theta + q_y\sin\theta$ to obtain,

$$0 = - \eta q^2\delta g_\perp(q) + \left(\frac{iW q_\parallel^2 q_\perp}{q^2}\right)\delta c_q + \left[\frac{2iW c_0 q_\parallel q_\perp}{p_0 q^2}\right]q_\perp\delta p_\perp(q) - \frac{iW c_0 q_\parallel}{p_0}\delta p_\perp(q). \tag{8}$$

Concentration fluctuations to linear order are given by

$$\partial_t\delta c_q = -i\, q_\parallel\, p_0\delta c_q - ic_0\left(q_\perp - Fq_\parallel\right)\delta p_\perp(q). \tag{9}$$

We are now in a position to compute the full fluctuation spectrum. While we have analysed the linear stability of the orientationally ordered phase in the basis spanned by $\delta\mathbf{u}$, $\delta\mathbf{p}$ and δc, we find that the origin of instability and its recovery by the shear flow can be understood even in the absence of the concentration equation. Thus, to make the subsequent analysis more transparent, we drop the concentration fluctuation terms at the outset.

Following [1], we express the fluctuation spectrum in terms of the splay fluctuation $\Phi = \nabla_\perp\delta p_\perp$, the in-plane expansion rate $\Theta = \nabla_\perp\delta g_\perp$, and the angle ξ made by $\mathbf{q}$ with the ordering direction:

$$\left[\partial_t + iq_\parallel\lambda_1 p_0 + \dot\gamma\sqrt{\lambda^2 - 1}\left(1 - \frac{1}{4\lambda}\right) + O(\dot\gamma^2)\right]\Phi_q - \left[\frac{ip_0 q^2}{2\rho_0 q_\parallel}\left(1 + \lambda\cos 2\xi\right)\right]\Theta_q = 0 \tag{10}$$

and

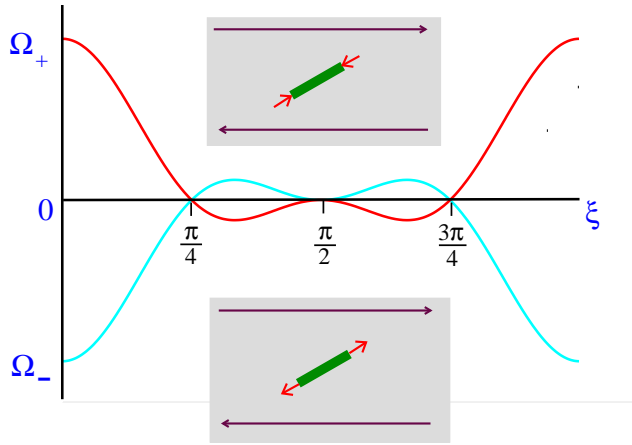$$0 = -\eta q^2\Theta_q - \left[\frac{iW c_0 q_\parallel\cos 2\xi}{p_0}\right]\Phi_q \tag{11}$$

Fig. 2 – The growth rates $\Omega_{\pm}(q = 0)$ versus 2ξ (angle between perturbing and the ordering direction), for either sign of activity W. Inset shows the induced flow lines arising from active rods subject to a flow.

This implies that the splay fluctuations Φ_q have a growth rate

$$\Omega = \frac{Wc_0}{2\eta}\cos 2\xi\,(1 + \lambda\cos 2\xi) - \dot{\gamma}\sqrt{\lambda^2 - 1}\left(1 - \frac{1}{4\lambda}\right) + O(\dot{\gamma}^2). \qquad (12)$$

First recall the generic instability when $\dot{\gamma} = 0$: the oriented phase is *always* unstable, either to splay or to bend fluctuations, depending on the sign of W [1]. This can be seen *even at* $q = 0$, where the growth rate $\Omega_+(0) > 0$ for $-\pi/4 > \xi > \pi/4$ when $W > 0$, and $\Omega_-(0) > 0$ for $\pi/4 > \xi > 3\pi/4$, when $W < 0$ (Fig. 2). The dispersion curve $\Omega_{\pm}$ is shown in Fig. 3 : fluctuations with wavenumber $q < q_0 \propto |W|$ grow in time; this sets the scale over which orientational order can be stabilised. Note that *both* the polar phase, as noted by [1], and the apolar nematic as well, are generically unstable in the absence of shear. This is clear, since the polar terms containing $\{\lambda_i\}$ and ζ in (1), do not appear in the growth rate equation (3).

The imposed shear flow represented by a horizontal line $\dot{\gamma} = $ const. in Fig. 3, cuts this dispersion curve at $q^*(\dot{\gamma})$, suggesting that fluctuations whose scale is *smaller* than $1/q^*$ are the first to be stabilised by the shear flow. Our estimate of q^* is qualitative : the crossover from Ω-dominated to $\dot{\gamma}$-dominated at nonzero q cannot strictly be evaluated in our treatment, since we dropped the $q_x\partial q_y$ terms on the grounds that they wouldn't matter at $q = 0$ where the instability is fastest. As $\dot{\gamma}$ is increased, $q^*(\dot{\gamma})$ decreases, till at $\dot{\gamma} = \dot{\gamma}_c$, this cutoff scale moves to zero, as $q^* = (\dot{\gamma} - \dot{\gamma}_c)^{1/2}$. At this shear rate $\dot{\gamma}_c$, the oriented phase is completely stabilised by the shear flow. This defines a stability boundary as a function of λ and W.

The stability phase diagram is best represented by defining a dimensionless *active* Peclet number, $Pe_a = 2\eta\dot{\gamma}/|W|c_0$, as the ratio of the imposed shear rate to the typical shear-rate produced around the active particles. As one crosses from the unstable to the stable region in the plane of Pe_a and flow-alignment parameter λ (Fig. 4) the orientational order parameter sets in at the value given by Eq. (6), which in effect gives a discontinuous transition since the
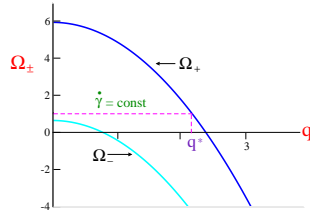
Fig. 3 – Dispersion curves $\Omega_{\pm}$ versus q, for ξ corresponding to maximum growth rate. The horizontal line corresponding to a frequency $\dot{\gamma}\sqrt{\lambda^2 - 1}\left(1 - \frac{1}{4\lambda}\right)$ defines the scale q^* beyond which fluctuations are stabilised. As $\dot{\gamma}$ increases towards $\dot{\gamma}_c$, the stabilisation scale goes to zero as $(\dot{\gamma} - \dot{\gamma}_c)^{1/2}$.

order parameter in the hydrodynamically unstable region is zero. For polar active particles, the shear-stabilised oriented phase has a nonzero drift of the particles with respect to the solvent.

Note that the critical shear rate required to stabilise the oriented phase $\dot{\gamma}_c$ is larger for positive W than negative. This is consistent with our earlier observation [3], that the flow induced by the active stresslets, oppose the imposed flow when $W > 0$ and enhance it when $W < 0$.

(D) Shear flow induced stabilisation in $d = 3$: The calculation of the stability diagram is more tedious in $d = 3$; however since the spirit is the same, we merely quote results and point out differences. To start with, we note that $\mathbf{p}_0$, the steady state orientational conformation in the presence of the shear flow $\mathbf{u}_0 = \dot{\gamma}y\hat{\boldsymbol{x}}$ is the same as (6), i.e.. it still lies in the plane of the imposed velocity and its gradient (the xy plane). We then decompose the fluctuations
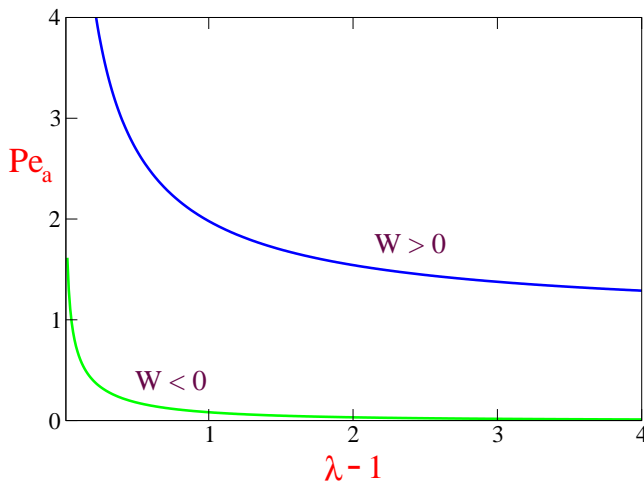

Fig. 4 – Stability diagram in the plane of Active Peclet number Pe_a and flow-alignment parameter λ.

in an appropriate orthonormal basis, viz., $\delta\mathbf{p} = (\delta p_\parallel, \delta p_\perp, \delta p_z)$, where $\delta p_\parallel = \delta\mathbf{p} \cdot \mathbf{p}_0$, $\delta p_\perp = \delta\mathbf{p} \cdot (\hat{\mathbf{z}} \times \mathbf{p}_0)$ and $\delta p_z = \delta\mathbf{p} \cdot \hat{\mathbf{z}}$ (similarly for $\delta\mathbf{g}$). As before we ignore concentration fluctuations.

Once again, $\delta p_\parallel$ is massive, and we rewrite the order parameter fluctuations in terms of the in-plane splay $\Phi_\perp = \nabla_\perp \delta p_\perp$ and $\Phi_z = \nabla_z \delta p_z$. Similarly invoking incompressibility, we rewrite the momentum fluctuations as the in-plane expansion rate $\Theta_\perp = \nabla_\perp \delta g_\perp$ and $\Theta_z = \nabla_z \delta g_z$. Eliminating the momentum fluctuations via force-balance, we find that the resulting linearised dynamical equations for $\Phi_\perp$ and Φ_z give rise to an eigenvalue spectrum qualitatively resembling (3). Thus even in $d = 3$, one may define a stability phase diagram in the $Pe_a - \lambda$ plane; a large enough shear rate stabilises an orientationally ordered phase.

Note that the vector-ordered phase has a non-zero drift velocity v_d, with a magnitude proportional to $c_0 \, p_0$ (6). This macroscopic *particle current* will result in a counter *solvent flow* of the same magnitude.

Experimental realisations in a planar shear flow geometry will necessarily have to contend with finite boundaries; it is therefore important to specify boundary conditions for the active order parameter $\mathbf{p}$. This is especially important in the polar case, since the local polarisation implies a local average drift velocity of the active particle relative to the fluid. Assuming the active particles cannot penetrate the walls, $\mathbf{p}$ must be tangent to the confining walls (the homogeneous boundary conditions of liquid crystal physics). In plane Couette flow, however, this is at odds with the flow-alignment requirement of $\mathbf{p}$ pointing at an angle to the suspension velocity as in Eq. (6). This conflict must be resolved by a boundary layer in $\mathbf{p}$ at the walls. The case of wall-normal (homeotropic [14]) alignment will be discussed elsewhere.

In conclusion we have shown how to stabilise the orientationally ordered phase of an active particle suspension by imposing a uniform shear flow. We have determined the nonequilibrium phase diagram in the plane of "active Peclet number" and flow-alignment parameter. This sets the stage for a study of the unusual rheological features of this shear-stabilised oriented phase of active matter [13]. In a forthcoming submission we will use this framework to study the dynamics of reorientation of endothelial cells subject to shear flow [17].

REFERENCES

[1]   R.A. Simha and S. Ramaswamy, Phys. Rev. Lett. **89**, 058101 (2002).
[2]   T. B. Liverpool and M. C. Marchetti, Phys. Rev. Lett. **90**, 138102 (2003), Europhys. Lett. **69** (2005) 846 and cond-mat/0607285; A. Ahmadi *et al.*, cond-mat/0607287 and 0507590.
[3]   Y. Hatwalne, S. Ramaswamy, M. Rao and R. Aditi Simha, Phys. Rev. Lett. **92**, 118101 (2004).
[4]   H. Y. Lee and M. Kardar, Phys. Rev. E **64**, 056113 (2001).
[5]   K. Kruse, J. F. Joanny, F. Julicher, J. Prost, and K. Sekimoto, Phys. Rev. Lett. **92** 078101 (2004); Eur. Phys. J. E **16**, 5 (2005).
[6]   S. Sankararaman, G.I. Menon and P.B.S. Kumar, Phys. Rev. E. **70**, 031905 (2004).
[7]   D. Humphrey et al., Nature **416**, 413 (2002).
[8]   F. Nédélec, T. Surrey, A. C. Maggs and S. Leibler, Nature **389**, 305 (1997); F. Nédélec, T. Surrey and E. Karsenti, Curr. Opin. Cell Biol. **15**, 118 (2003).
[9]   X.L. Wu and A. Libchaber, Phys. Rev. Lett. **84**, 3017 (2000).
[10] G. Soni et al., Biophys. J. **84**, 26342637 (2003).
[11] C. Dombrowski, L. Cisneros, S. Chatkaew, R.E. Goldstein, and J.O. Kessler, Phys. Rev. Lett. **93** (2004) 098103.
[12] I. H. Riedel, K. Kruse and J. Howard, Science **309**, 300 (2005).
[13] S. Muhuri, S. Ramaswamy and M. Rao, in preparation.
[14] P.G. de Gennes and J. Prost, *The Physics of Liquid Crystals*, Clarendon, Oxford (1995).

[15] J. Toner and Y. Tu, Phys. Rev. E **58**, 4828 (1998).

[16] L.D. Landau and E.M. Lifshitz, *Theory of Elasticity*, Pergamon Press, NY (1998).

[17] S. Noria et al., Am. J. Pathol. **164**, 1211 (2004).