Screened Hydrodynamics In An Active Nematic

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Active turbulence in dense active systems is characterised by high vorticity on a length scale large compared to that of individual entities. We describe the properties of active turbulence as momentum propagation is screened by frictional damping. As friction is increased, the spacing between the walls in the nematic director field decreases as a consequence of the more rapid velocity decays. This leads to, firstly, a regime with more walls and an increased number of topological defects, and then to a jammed state in which the walls delimitate bands of opposing flow, analogous to the shear bands observed in passive complex fluids.

Active materials intrinsically exist out of equilibrium driven by a continuous input of energy. Many such systems are of biological origin, including suspensions of cytoskeletal elements, cells and bacteria. Vibrated granular rods and active colloids provide examples of inanimate active materials [1, 2]. Dense active systems often exhibit collective behaviour producing long range spatial and temporal correlations that are much larger than the typical length and time scales associated with individual particles [3–6]. Active turbulence, observed in active nematics, is a canonical example of this behaviour, which is characterised by rapidly varying flow fields with a high degree of vorticity. Recently it has been proposed that there are links between active turbulence and the appearance of lines of kinks, or walls, in the director field and the formation of topological defects also appears to be relevant in defining the active turbulent state [4, 7–11].

Active turbulence has been observed in experiments on systems as diverse as dense suspensions of bacteria [3], microtubules and molecular motors [4], cells [5], mixtures of bacteria and liquid crystals [10], and vertically vibrated rods [6]. Diverse simulations from those considering discrete particles [11, 12], eg driven, self-avoiding rods of high aspect ratio, to those based on differing continuum theories, eg active nematohydrodynamics, [7, 8, 13] all see the hallmarks of active turbulence. However we still lack a predictive theory of this dynamical state, or an understanding of which of the properties of active turbulence are universal and which are system specific.

A classification often applied to active nematics is the relevance of momentum conservation in determining their dynamics [2]. Systems that conserve momentum (eg a free-standing fluid layer) are termed ‘wet’, those with no momentum conservation (eg vibrated granular rods) ‘dry’. In reality completely wet or dry systems are two ends of a continuum, parametrised by the ratio of viscous to frictional dissipation. The aim of this paper is to study the crossover between active turbulence in wet and in dry nematics to understand any connections between these limits.

Understanding the crossover between wet and dry systems is also of relevance because many of the experiments studying active matter are performed in two dimensions with the system in contact with a solid or fluid substrate which will lead to some degree of frictional damping. Experiments using microtubules and molecular motors are conducted on an oil-water interface [4] and so frictional damping will be small, pattern formation studies of amoeboid cells [14], collective migration [5] and structured flows [15] of epithelial cells are performed on a solid substrate and therefore both viscous and frictional damping will be relevant, whereas for vertically vibrated granular rods [6] friction will dominate.

We show that substrate friction promotes shear banding, thus changing the structure and characteristic length scales of active turbulence. We first illustrate this concept in one dimension, and then present the results of simulations demonstrating its consequences in two dimensions.

We consider the hydrodynamic equations of motion for an active nematic modified by an additional frictional term [16, 17],

\[ \rho (\partial_t + u_k \partial_k) u_i = \partial_j \Pi_{ij} - \gamma u_i, \]
\[ (\partial_t + u_k \partial_k) Q_{ij} - S_{ij} = \Gamma H_{ij} \]

where \( \gamma \) is the friction coefficient. The evolution of orientational order is described by a tensor order parameter \( Q \), familiar in standard liquid crystal hydrodynamics [18]. The generalised advection term, \( S_{ij} = (\lambda E_{ik} + \Omega_{ik})(Q_{kj} + \delta_{kj}/3) + (Q_{ik} + \delta_{ik}/3)(\lambda E_{kj} - \Omega_{kj}) - 2\lambda(Q_{ij} + \delta_{ij}/3)(Q_{kl}\delta_{kl}u_i) \), describes the response of \( Q \) to velocity gradients. Here \( E_{ij} = (\partial_i u_j + \partial_j u_i)/2 \) is the strain rate tensor, \( \Omega_{ij} = (\partial_i u_k - \partial_k u_i)/2 \) is the vorticity tensor and \( \lambda \) is the alignment parameter. We use \( \lambda = 0.7 \), which corresponds to aligning rods [18, 19].

The rotational diffusivity is denoted as \( \Gamma \) and the Landau-de Gennes free energy, \( F = K(\partial_k Q_{ij})^2/2 + A Q_{ij} Q_{ji}/2 + B Q_{ij} Q_{jk} Q_{ki}/3 + C(Q_{ij} Q_{ji})^2/4 \), governs the relaxation of the orientational order by determining the molecular field \( H_{ij} = -\delta F/\delta Q_{ij} + (\delta_{ij}/3)\Pi(\delta F/\delta Q_{kl}) \) in Eq. (2). \( A, B \) and \( C \) are material constants and \( K \) is the elastic constant.

The standard, passive liquid crystal contributions to the stress are the viscous stress, \( \Pi_{ij}^{\text{viscous}} = 2\mu E_{ij} \), and the elastic stress, \( \Pi_{ij}^{\text{passive}} = -P\delta_{ij} + 2\lambda(Q_{ij} + \delta_{ij}/3)(Q_{kl}\delta_{kl}u_i) \).
$$\delta_{ij}/3(Q_{kl}H_{lk} - \lambda H_{ik}(Q_{kj} + \delta_{ij}/3) - \lambda(Q_{ik} + \delta_{ij}/3)H_{kj} - \partial_i Q_{kl} \frac{\partial P}{\partial Q_{kl}} + Q_{ik}H_{kj} - H_{ik}Q_{kj}$$

where $P$ is the pressure. The active contribution to the stress is a consequence of the dipolar nature of the active system, $\Pi_{ij}^{active} = -\zeta Q_{ij}$ [20]. Thus any gradient in $Q$ generates a flow field and $\zeta$, the activity coefficient, determines the strength of this flow field. We consider $\zeta > 0$, corresponding to extensile systems. Details of the model can be found in [18, 21–23].

The numerical solution of Eqs. (1) and (2) uses a hybrid lattice Boltzmann method on a $D3Q15$ lattice [22]. The parameters used are $\Gamma = 0.34$, $A = 0.0$, $B = -0.3$, $C = 0.3$, $K = 0.01$, $\zeta = 0.01$, $\mu = 2/3$, in lattice units, unless mentioned otherwise. As usual discrete space and time steps are chosen as unity and therefore all quantities can be converted to physical units appropriately depending on the material of interest [8, 24]. The frictional force $\gamma u$ was incorporated into the lattice Boltzmann scheme as a force density in a way analogous to the gravity [22, 25].

Before presenting results for the full 2D model it is instructive to consider 1D solutions, confining the active nematic between $y = 0$ and $y = L = 100$, with periodic boundary conditions along $y$, and assuming translational symmetry in the $x$ direction. The nematic field can now be represented by a single variable, $\theta(y)$ describing the angle between the direction of orientation and the $x$ axis. A consequence of the active stress is that gradients in $\theta(y)$ generate a velocity in the $x$ direction $u_x(y)$. This system shows strong hysteresis, with the final state depending on the initial conditions [26]. Therefore we chose the protocol of always initialising the simulation with four pairs of oppositely oriented bend deformations along $y$ (see legend in Fig. 1(a)). It relaxed to a variety of different steady states depending on the values of the friction $\gamma$ and the activity $\zeta$, as summarised in Fig. 1(a). Other initial conditions give qualitatively similar results.

At low activities, the system regains a nematic configuration, with the director field aligned along $y$, and no flow. Using a mathematical analogy to the Fredericks transition in passive nematic liquid crystals Voituriez et al. [27] showed that, for $\gamma = 0$, the nematic ordering is unstable to a state with spontaneous flow at a critical activity $\zeta_{C_w} = \pi^2 K(4\Gamma_1 + (\lambda_1 - 1)^2)/[2L^2(\lambda_1 + 1)]$. Here $\pi$ denotes an instability driven by small deviations from initial angles $\theta = 0$ and $\theta = \pi/2$ respectively. Also $\Gamma_1 = 2\Gamma/9g^2$ and $\lambda_1 = (3q + 4)\lambda/9g$ where $q$ is the magnitude of the nematic order, the largest eigenvalue of $Q$ [22]. The approach in [27] generalises to non-zero $\gamma$ by replacing $\zeta$ by an effective activity $\zeta_{\gamma} - \frac{2\Gamma_1 K}{\lambda_1 + 1}$. For flow aligning nematics ($\lambda_1 > 1$), the threshold of activity required for the spontaneous flow transition is therefore increased due to the presence of frictional dissipation to $\zeta_{C_w} = \zeta_{C_w} + \frac{2\Gamma_1 K}{\lambda_1 + 1}$. These curves, plotted as continuous lines in Fig. 1, match the numerical calculations.

For small $\gamma$ the analytical and numerical results show that the spontaneous flow transition is to a state where the director field exhibits a pair of oppositely oriented bend deformations, symmetrically placed in the domain, as illustrated in Fig. 1(a). This bidirectional flow, referred to as shear banding, is a consequence of unstable regions in the stress-strain curve for active nematics [22, 24]. As activity is increased, the number of such bend deformations increases, until at $\zeta \sim 0.01$ they are no longer stable, and are replaced by splay deformations (see Fig. 1(a)) as observed in [9]. As $\gamma$ increases the critical activity required to drive the transition to a flowing state also increases. Moreover the number of pairs of oppositely oriented bend deformations increases for a given activity.

To motivate why higher frictional dissipation leads to a reduction in width of the shear bands Fig. 1(b) shows the director angle, $\theta$, (top) and the associated velocity field, $u_x$, (bottom) corresponding to a single bend deformation. Variation in the director field, localised around $y/L =$
generates active forces and acts to drive the flow [19, 28]. When \( \gamma = 0 \) the source flow decays slowly with a constant shear rate due to viscous damping, giving a characteristic triangular flow profile. As \( \gamma \) increases the additional friction accelerates the decay of the velocity field.

Considering a balance between the dissipative terms and modelling the source of flow generation as a point force of strength \( F \) located at \( y = y_0 \), we see that

\[
\mu \frac{\partial^2 y}{\partial t^2} - \gamma y = F\delta(y - y_0).
\]

This indicates an exponential relaxation of velocity over a characteristic length

\[ l_{diss} = \sqrt{\frac{\mu}{\gamma}}. \]

For small friction this length scale is not relevant, but at large \( \gamma \), it can be small so that momentum is lost over much shorter lengths than expected from viscosity alone. This is explicitly demonstrated in Fig. 1(b) where the continuous vertical lines show \( l_{wall} + 2l_{diss} \) indicating the faster decay of velocity field with increasing \( \gamma \). Here \( l_{wall} \) is a measure of the width of the bend deformation itself which, as shown in the figure, is very weakly dependent on the friction.

This shortfall of viscous momentum transfer in the transverse direction supports the formation of more closely spaced shear bands. Similar effects are important in fully developed active turbulence. To demonstrate this we now present the results of simulations on a two dimensional domain of size \( 400 \times 400 \) with periodic boundary conditions, a system that exhibits active turbulence. For no friction any nematic is unstable to the active stress. The instability leads to the formations of walls, lines of kinks in the director field. Generally the walls are generated in pairs (as indicated in Fig. 2(a)). They are analogous to the bend deformations observed in 1D but, unlike in 1D, they are unstable to both transverse fluctuations and, for sufficiently large activities, to the generation of pairs of topological defects, which move apart and hence locally restore nematic order. Typical configurations of director field and defects, and of velocity and vorticity fields, are illustrated in Fig. 2(a) and (b) respectively.

Panels (c) and (d) of Fig. 2 compare similar snapshots, but for \( \gamma = 0.01 \). Just as for shear-banding in the 1D systems, the addition of friction reduces the spacing between walls resulting in a larger number of walls, and thus defects, in the steady state. Distortions in the director field act as sources of flow and therefore walls and defects are the main sources of vorticity. Since the number of such distortions is increased, the flow field also changes substantially. This is apparent when comparing Fig. 2(b) and (d): the decrease in the characteristic length of circulating regions is noticeable.

The very different behaviour of the active nematic for large friction, \( \gamma = 0.5 \), is shown in the snapshots in panels (e) and (f) of Fig. 2. The induced flow velocities are smaller and no defects are generated. Instead one observes closely spaced walls jammed approximately parallel to each other (but with some quenched disorder) supporting anti-parallel shearing flows very reminiscent of the multiple bend configurations observed in 1D. Reducing \( l_{diss} \) further decreased the width of the shear bands to an unphysical limit set by lattice spacing. We comment that walls which do not decay into defects are also observed in active turbulence at \( \gamma = 0 \) for sufficiently small activities. However these are highly unstable to lateral perturbations; they continually collide and show chaotic and transient behaviour [8].

FIG. 2. Left panel: director field and topological defects (with +1/2 and −1/2 defects denoted by red and blue dots) and right panel: vorticity, denoted by the colour scale from +ve (red) to -ve (blue) normalised to its maximum value, and velocity field (arrows). (a),(b): no solid friction (\( \gamma = 0 \)). (c),(d): \( \gamma = 0.01 \) and (e),(f): \( \gamma = 0.5 \). (a),(c),(e) correspond to the left bottom quarter of (b),(d),(f) respectively. The formation of a pair of walls is identified in (a).
coefficient it is substantially reduced.

Fig. 3(b) plots the number of defects as a function of the friction coefficient for each value of $K$. This first increases with friction, as the number of walls which finally decay into defects increases, and then decreases as there is not enough energy available to create defects for high frictional damping. The maximum occurs for smaller $\gamma$ at larger $K$ because the defect energy increases with increasing elastic constant.

In 1D we argued that the distance between walls (or equivalently the width of the shear bands) is determined by the dissipation length $l_{diss} = \sqrt{\mu/\gamma}$ which controls the decay of the velocity field. We now present evidence that the same is true in the 2D case. We measured the normalised order parameter correlation function $C_{QQ}(R) = (\langle Q(R) : Q(0) \rangle - \langle Q(\infty) : Q(0) \rangle) / (\langle Q(0)^2 \rangle - \langle Q(\infty) : Q(0) \rangle)$ and estimated the distance between walls $l_n$ as the point at which $C_{QQ}$ reaches its minimum value. This is justified because $C_{QQ}$ measures the size of nematically oriented regions. We plot this distance as a function of the dissipation length in Fig. 3(c). As can be seen, $l_n$ is essentially independent of the friction $\gamma$ as long as $l_n < l_{diss}$. Once these two quantities become comparable, the distance between the walls is set by $l_{diss}$ and therefore decreases with $\gamma$. The region between $l_n^{wet}$ (i.e. $l_n$ for $\gamma = 0$) and $2l_n^{wet}$ which is highlighted in each case corresponds to the transition to the over damped limit.

To summarise, we describe here the implications of frictional damping due, for example, to flow over a substrate, in a wet active nematic. The dissipation length, $l_{diss}$, the characteristic length scale describing the decay of momentum from a source, is irrelevant for small friction. However for larger friction this length scale sets the spacing between walls. $l_{diss}$ decreases with increasing friction and therefore the number of walls and the number of defects formed by their decay, increases. At higher friction, as the walls become even more closely spaced, they form a jammed state where wall fluctuations and break up, and hence defect formation, are suppressed. In this limit the walls are reminiscent of the boundaries between velocity bands seen in sheared passive fluids. It will be interesting to test the consequences of momentum screening in experiments by using substrates with varying friction coefficients, and to consider whether similar effects are seen in compressible active nematics where density fluctuations are relevant.

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