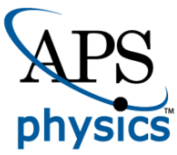

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Excitable Patterns in Active Nematics

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We analyze a model of mutually-propelled filaments suspended in a two-dimensional solvent. The system undergoes a mean-field isotropic-nematic transition for large enough filament concentrations and the nematic order parameter is allowed to vary in space and time. We show that the interplay between non-uniform nematic order, activity and flow results in spatially modulated relaxation oscillations, similar to those seen in excitable media. In this regime the dynamics consists of nearly stationary periods separated by "bursts" of activity in which the system is elastically distorted and solvent is pumped throughout. At even higher activity the dynamics becomes chaotic.

PACS numbers:

Colonies of motile microorganisms, the cytoskeleton and its components, cells and tissues have much in common with soft condensed matter systems (i.e. liquid crystals, amphiphiles, colloids etc.), but in addition they show new phenomena associated with the fact that the constituent particles are active: they consume and dissipate energy to fuel internal changes that generally lead to motion. When active particles have elongated shapes, as seen in cytoskeletal filaments and some cells, they undergo orientational ordering at high concentration to form liquid crystalline phases. The theoretical and experimental study of active materials has disclosed a wealth of emergent behaviors, such as the occurrence of *giant* density fluctuations [1], the emergence of spontaneously flowing states [2], unconventional rheological properties [3] and new spatiotemporal patterns not seen in passive complex fluids [4, 5].

In this Letter, we show that active nematic suspensions behave as excitable media, showing relaxation oscillations that couple activity to spontaneous pulsatile flow with quiescent periods in between, similar to biological pumps. This hydrodynamic phenomenon arises as a consequence of the existence of multiple time scales in the system, when the dynamics of the flow lags with respect to the rate of the active forcing exerted at the microscopic scale and are thus very different from the large scale fluctuations previously observed in simulations with noise and no hydrodynamics [4]. In addition, we see that the orientational dynamics of the system associated with nematic ordering can give rise to large-scale swirling motions resembling those observed in recent motility assay experiments [6] even in the absence of polar order.

Our system consists of a two-dimensional suspension of filaments of length ℓ in a solvent. The filaments are mutually propelled, for example thorough the action of a motor cluster that binds pairs of filaments. The dynamical variables in such a system are the particle concentration c, the solvent flow field $\mathbf{v}$ and the nematic tensor $Q_{ij} = S(n_i n_j - \frac{1}{2}\delta_{ij})$, with S the nematic order parameter and $\mathbf{n}$ the director field, all of which are allowed to vary in space and time. The total density of the system ρ is conserved, so the fluid is assumed to be incompressible. The total number of active particles is also constant, thus the concentration c obeys the continuity equation:

$$\partial_t c = -\nabla \cdot (\mathbf{j}^p + \mathbf{j}^a)\,, \tag{1}$$

where $\mathbf{j}^p$ and $\mathbf{j}^a$ are respectively the passive and active contributions to the current density. The passive current density has the standard form $j_i^p = cv_i - D_{ij}\partial_j c$ where $D_{ij} = D_0\delta_{ij} + D_1 Q_{ij}$ is the anisotropic diffusion tensor, while the active current can be constructed phenomenologically to be of the form $j_i^a = -\alpha_1 c^2 \partial_j Q_{ij}$ or derived from microscopic models [7]. Here the factor c^2 reflects the fact that activity arises from interactions between pairs of rods while the constant α_1 describes the level of activity and is proportional to the concentration of motors and the rate of adenosine-triphosphate (ATP) consumption.

The flow velocity obeys an active form of the Navier-Stokes equation

$$\rho\partial_t v_i = \eta\Delta v_i - \partial_i p + \partial_j \tau_{ij}\,, \tag{2}$$

with η the viscosity, p the pressure, and the active stress tensor τ_{ij} given by:

$$\tau_{ij} = -\lambda S H_{ij} + Q_{ik}H_{kj} - H_{ik}Q_{kj} + \alpha_2 c^2 Q_{ij} \tag{3}$$

Here $\nabla\cdot v = 0$, and the first three terms on the right side of Eq. (3) represent the contribution to the elastic stress due to the liquid crystalline nature of the system, with $H_{ij} = -\delta F/\delta Q_{ij}$ the molecular tensor defined from the two-dimensional Landau-De Gennes free energy:

$$F/K = \int dA\,[\tfrac{1}{2}(\nabla\cdot\boldsymbol{Q})^2 + \tfrac{1}{4}(c-c^*)\ \mathrm{tr}\,\boldsymbol{Q}^2 + \tfrac{1}{4}c\,(\mathrm{tr}\,\boldsymbol{Q}^2)^2]$$

where K is both the splay and bending stiffness (in the one-constant approximation). At equilibrium, above the critical concentration c^*, $S = \sqrt{2\,\mathrm{tr}\,\boldsymbol{Q}^2} = \sqrt{1-c^*/c}$ consistent with hard-rod fluid models. The last term in

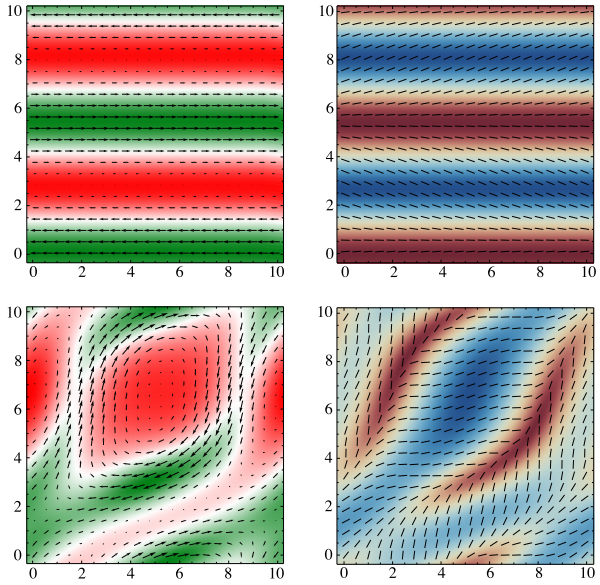

FIG. 1: (Color online) The velocity field (left) and the director field (right) superimposed to a density plot of the concentration and the nematic order parameter for $\alpha_2 = 0.4$ (top) and $\alpha_2 = 3$ (bottom). The colors indicate regions of large (green) and small (red) density and large (blue) and small (brown) nematic order parameter. For moderate values of α_2 the flow consists of two bands traveling in opposite directions with the director field is nearly uniform inside each band. For large α_2 the flow is characterized by large vortices that span lengths of the order of the system size and the director field is organized in grains.

Eq. (3) was first introduced in Ref. [9] and represents the tensile/contractile stress exerted by the active particles in the direction of the director field $\mathbf{n}$, with α_2 a second activity constant.

Finally, the nematic order parameter Q_{ij} satisfies a hydrodynamic equation that can be obtained by constructing all possible traceless-symmetric combinations of the relevant fields, namely the strain-rate tensor $u_{ij} = \frac{1}{2}(\partial_i v_j + \partial_j v_i)$, the vorticity tensor $\omega_{ij} = \frac{1}{2}(\partial_i v_j - \partial_j v_i)$ and the molecular tensor H_{ij} [8], so that

$$[\partial_t + \mathbf{v}\cdot\nabla]Q_{ij} = \gamma^{-1}H_{ij} + \lambda S u_{ij} + Q_{ik}\omega_{kj} - \omega_{ik}Q_{kj} \quad (4)$$

where γ is an orientational viscosity, and the additional terms on the right-hand side describe the coupling between nematic order and flow in two dimensions, with λ the flow-alignment parameter which dictates how the director field rotates in a shear flow and affects the flow and rheology of active systems [2, 3].

The dynamics of such an active nematic suspension is governed by the interplay between the active forcing, whose rate $\tau_{\rm a}^{-1}$ is proportional to the activity parameters α_1 and α_2, and the relaxation of the passive structures, the solvent and the nematic phase, in which energy is dissipated or stored. The response of the passive structures, as described here, occurs at three different time scales: the relaxational time scale of the nematic degrees of freedom $\tau_{\rm p} = \ell^2/(\gamma^{-1}K)$, the diffusive time scale ℓ^2/D_0, and the dissipation time scale of the solvent $\tau_{\rm d} = \rho L^2/\eta$, with L the system size. While the presence of three dimensionless parameters makes for a very rich phenomenology, we temporarily assume that the three passive time scales are of the same magnitude $\tau_{\rm p}$. When $\tau_{\rm a} \gg \tau_{\rm p}$, the active forcing is irrelevant and the system is akin to a passive suspension. On the other hand, when $\tau_{\rm a} \sim \tau_{\rm p}$, a stationary regime can exist wherein the active stresses are balanced by both elastic distortion and flow. Finally, when $\tau_{\rm a} \ll \tau_{\rm p}$ the passive structures will fail to keep up, leading to a dynamical and possibly chaotic interplay between activity, nematic order and flow. To quantify these different regimes, we first make the system dimensionless by scaling all lengths using the rod length ℓ, scaling time with the relaxation time of the director field $\tau_{\rm p}$ and scaling stress using the elastic stress $\sigma = K\ell^{-2}$.

Linear stability analysis about the homogeneous solution reveals that coupling between orientation and flow triggers an instability at a lower critical value of α_2

$$\alpha_2^* = \frac{4\pi^2[2\eta + S_0^2(1-\lambda)^2]}{c_0^2 L^2 S_0(1-\lambda)}\,. \quad (5)$$

and results in a spontaneous flowing banded state shown in Fig. 1 (top). In general, shear flow causes the director field to rotate for $\lambda \neq 1$, which generates elastic stress. For small activity, the elastic stiffness dominates and suppresses flow, while above α_2^* we observe collective motion. This is the spontaneous flow transition already observed in the absence of nematic order parameter fluctuations [2].

To go beyond linear stability analysis, we numerically integrated the equations (1)-(4) on a two-dimensional periodic domain with an initial configuration of a homogeneous system whose director field was aligned along the x axis subject to a small random perturbation in density and orientation, with $\alpha_1 = \alpha_2/2$, $\eta = D_0 = D_1 = 1$, $\lambda = 0.1$ and $L = 10$. We used a vorticity/stream-function finite difference scheme on a collocated grid of lattice spacing $\Delta x = \Delta y = 0.078$. Time integration was performed via a fourth order Runge-Kutta method with time step $\Delta t = 10^3$. As predicted by the linear stability analysis, at low activity the system relaxes to a stationary homogeneous state with $v_x = v_y = 0$ and $S = \sqrt{1 - c^*/c}$. Above the critical value α_2^*, the system forms two bands flowing in opposite directions. The solution is constant along the flow direction (see Fig. 1 top) while the direction of the streamlines (in this case along the x direction) is dictated by the initial conditions. As shown in Fig. 2, the extrema in the flow velocity correspond to the maximal distortion of the director field $\mathbf{n}$. Variations in concentration c and the nematic order parameter S are of order 2% with a minimum in S at the center of a flowing band due to the balance between diffusive and active currents.

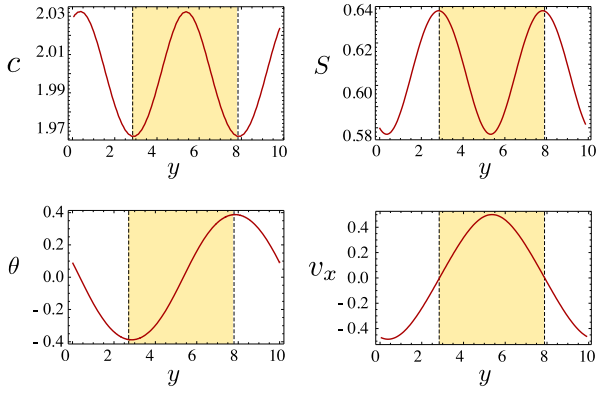

FIG. 2: (Color online) The hydrodynamic fields c, S, θ and v_x along the y axis for $\alpha_2 = 0.4$ The yellow region indicates the band visible in the top panels of Fig. 1

Upon increasing the value of the activity parameter above $\alpha_2 = 0.41$, the spontaneously flowing state evolves into a pulsatile flow. Fig. 3 (top left panel) shows a plot of the x and y components of the flow velocity in the center of the box for $\alpha_2 = 1.5$. In this regime the dynamics consists of a sequence of almost stationary passive periods separated by active "bursts" in which the director switches abruptly between two orthogonal orientations. During passive periods, c and S are nearly uniform, there is virtually no flow and the director field is either parallel or perpendicular to the x direction. Eventually this configuration breaks down and the director field rotates by 90° (see Fig. 3). The rotation of the director field is initially localized along lines, generating a band of flow similar to those in Fig. 1 (top). The flow terminates after the director field rotates and a uniform orientation is restored. The process then repeats.

The rotation of the director field occurs through a temporary "melting" of the nematic phase. As shown in Fig. 3, during each passive period the nematic order parameter is equal to its equilibrium value $S_0 = \sqrt{1 - c^*/c}$, but drops to $\sim (2/5)\, S_0$ during rotation. The reduction of order is system-wide, but, as shown in the middle in the bottom-left panel of Fig. 3, is most pronounced along the boundaries between bands. Without transient melting, the distortions of the director field required for a burst are unfavorable for any level of activity.

Oscillatory phenomena have been shown to arise from nonlinear stress-strain relationships in models of passive complex fluids under shear [10]. Here we show that excitability can arise in a model for active nematic fluids without external forcing, driven by the competing timescales of internal activity, flow, and microstructure relaxation. To understand this quantitatively, we construct a minimal set of equations that captures this competition between timescales and retains the minimal features responsible for excitability: the coupling between active forcing and the fluid microstructure and the variable nematic order embedded in the Landau-De Gennes free energy. We approximate Q_{xx}^2 as a constant and $u_{xx} \approx 0$, let $u = -u_{xy}$ and $Q = Q_{xy}$, and drop the coupling between Q_{ij} and ω_{ij}. Eqs. (2) and (4) can then be expressed in Fourier space as:

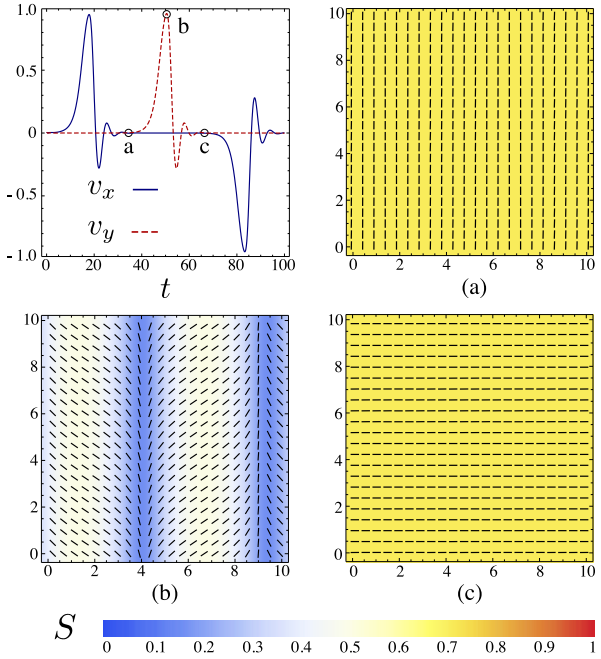

FIG. 3: (Color online) Dynamics of active "burst" for $\alpha_2 = 1.5$. The flow velocity at the point $x = y = L/3$ is shown as a function of time over the course of a director field rotation (top left) and the director field is shown for the three labeled time points. Between two consecutive bursts the system is homogeneous and uniformly aligned. During a burst, nematic order is drastically reduced in the whole system and the director undergoes a distortion with a consequent formation of two bands flowing in opposite directions. Concentration fluctuates by only about 10%. After a burst, a stationary state is restored with the director field rotated of 90° with respect to its previous orientation.

$$\dot{Q} = aQ - bQ^3 - u \tag{6a}$$

$$\dot{u} = k^2(\alpha Q - \eta u) \tag{6b}$$

where k is a wave number of an arbitrary spatial mode and a and b are proportional to the inverse rotational viscosity γ^{-1}. Eqs. (6) has the form of the FitzHugh-Nagumo model for excitable dynamical systems [11]. For $\alpha < \alpha_c = \eta(2a + \eta k^2)/3$ the system rapidly relaxes to a state characterized by a finite strain-rate that balances the active stress with $\eta u = \alpha Q = \alpha\sqrt{(a - \alpha/\eta)/b}$. For $\alpha > \alpha_c$, this state becomes unstable and the trajectory converges to a limit cycle with a frequency $\nu \sim k^2\alpha$. In comparison, the frequency of oscillations as a function of α_2 for the full equations is shown in Fig. 4. As anticipated, when the active and passive time-scales are comparable the active forcing is accommodated by the mi-

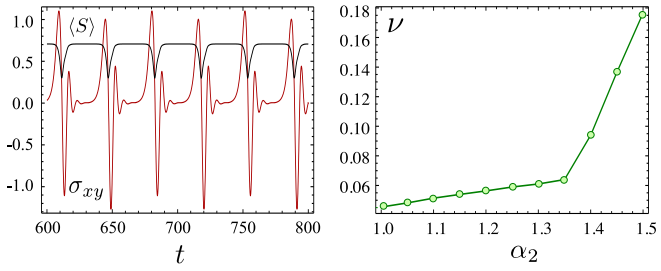

FIG. 4: (Color online) (Left) The average nematic order parameter $\langle S \rangle$ and the total shear stress σ_{xy} are shown over several bursts for $\alpha_2 = 1.5$. (right) The frequency of bursts is shown as a function of α_2.

crostructure leading to a distortion of the director filed and a steady flow. However, when the active forcing rate is increased, the microstructure dynamics lag, resulting in relaxation oscillations. The critical active rate can be obtained by rewriting α_c in terms of timescales defined above to give $3\tau_a^{-1} = (2a\tau_p^{-1} + \ell^2 k^2 \tau_d^{-1})$, with $\tau_a = \eta/\alpha$. The origins of the kink at $\alpha_2 = 1.35$ are unclear at present, but it does not correspond to excitation of a spatial mode of larger wave-number.

Returning to the full equations, when the activity is further increased, the sequence of bursts and the flow patterns becomes more complex and eventually chaotic. Fig. 1 (bottom) shows a typical snapshot of the flow velocity and the director field superimposed to a density plot of the concentration and the nematic order parameter respectively. The flow is characterized by large vortices with patches, or "grains", where the director field is uniformly oriented. The relatively narrow grain boundaries span the entire system and are the fastest flowing regions in the system. In this regime, the dynamics is characterized by sets of grains of approximatively uniform orientation that swirl around each other and continuously merge and reform. Other examples of chaotic flows in active fluids have been reported in models of dilute bacterial suspensions with no liquid crystalline elasticity [12] (see also Ref. [2]e).

Our analysis of the hydrodynamics of active nematic suspensions in two dimensions shows that allowing spatiotemporal fluctuations in the magnitude of the nematic order parameter S qualitatively changes the flow behavior as compared to systems in which S is constrained to be uniform, most notably leading to excitable behavior. We note that both the flip-flop dynamics (Fig. 3) and the swirling motion (Fig. 1 bottom) resemble behavior observed in the motility assay experiments of Schaller *et al* [6]. While those experiments consider polar filaments, our analysis of mutually-propelled rods with nematic order suggests that these classes of patterns can emerge even in the absence of polar order. Finally, we note that excitability is crucial to many biological functions, such as cardiac rhythms and the nervous system. While relaxation oscillations in those systems arise from heavily regulated networks of chemical and electrical signals, the predictions of our model suggest that they can also emerge directly from the physical interactions among constituent components of a cell.

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