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Active-filament hydrodynamics: instabilities, boundary conditions and rheology

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Abstract. This paper studies several issues that emerge naturally in the hydrodynamic approach to suspensions of self-driven organisms or filaments (Simha and Ramaswamy 2002 *Phys. Rev. Lett.* **89** 058101; Kruse *et al* 2004 *Phys. Rev. Lett.* **92** 078101; Hatwalne *et al* 2004 *Phys. Rev. Lett.* **92** 118101). These include: a simple pictorial understanding of the instability of orientationally ordered active suspensions; the effect of translational order as well as finite geometries on these instabilities; the role of depolymerization on the possible types of alignment of active polar particles in restricted geometries; and, lastly, speculations on the relation between contractile active matter and jammed granular matter.

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Contents

1. Introduction: background and results

1.1. Background

The equations of active hydrodynamics were initially formulated [1] to describe large-scale ordered states of swimming organisms, such as fish shoals [2] or bacteria [3]. They extended, to these self-driven systems, the broken-symmetry hydrodynamic approach applied so successfully to liquid crystals [4, 5]. The same equations—perhaps unsurprisingly, in hindsight—turn out to provide the theoretical framework for modelling patterns [6, 7] and mechanical response [8] in suspensions of actively contracting filaments such as actomyosin or microtubules, and thus for understanding the mechanics and statistics of the cytoskeleton [9] in particular and living matter in general. The hydrodynamic approach taken in [1, 6] is amply justified by the derivation [10] of the equations from a microscopic description involving motors and filaments. As is now standard, we shall use the term *active* to characterize any object, whether an organism or simply a cell component, that drives itself mechanically by the uptake of chemical energy [11]. A review of the collective dynamics of active particles can be found in [12].

A useful distinction was made in [1, 8] between polar and apolar active particles, as well as between ordered phases with and without macroscopic polarity. Apolar particles or phases, even if orientable, are fore-aft symmetric, whereas polar particles lack this symmetry. In the approach of [1, 8] it was noted that an active particle is an orientable force dipole, so that at a location $\mathbf{r}$ a concentration $c(\mathbf{r})$ of such particles oriented along a locally defined axis $\mathbf{N}(\mathbf{r})$ implies a local stress $\sigma^a(\mathbf{r}) \sim fbc(\mathbf{r})\mathbf{N}(\mathbf{r})\mathbf{N}(\mathbf{r})$ where b and f are respectively the linear dimension of the particle and the force exerted by the active particle on the fluid. Such stresses generate flows in the fluid which in turn reorient $\mathbf{N}$. The consequences of this interplay were shown in [1], [6]–[8], [10] to be most dramatic for systems in or near an oriented state. Of the results obtained in [1, 8], those of potential significance to cytoskeletal dynamics were as follows: (i) A bulk active suspension with uniaxial orientational order—the analogue of a nematic liquid crystal—was inevitably prone to a hydrodynamic instability involving splay or bend of the orientation accompanied by fluid flow. We shall refer to this below as the *generic instability*. In [13] it was shown that a sufficiently strong imposed shear flow suppresses the instability for the contractile case. (ii) A suspension of *contractile* filaments in the isotropic phase, but close to

the threshold for spontaneous orientational order, should show ever stronger viscoelasticity as the system is pushed closer to the ordering transition. Tensile filaments in a similar situation were predicted to show unstable shear-thinning. (iii) Cytoplasmic streaming [11], seen in the crawling of amoebae, emerged naturally in [8] as a particle current arising from activity gradients. Elastotaxis [14] and active mechanosensing [15] are also simply described within our framework.

1.2. Aims of this work; summary of results

In this paper, we address several issues that arise naturally from the findings of [1, 8]. (i) We offer a simple pictorial understanding of the instability of ordered active filaments, whose essence is seen in figures 1 and 2. The instability turns out to be very similar to Euler buckling. (ii) We consider possible translationally ordered states of the filaments, and show that columnar and lamellar translational ordering suppress the instabilities, respectively, of contractile and tensile filaments. (iii) The authors of [1, 8] worked in an unbounded geometry. As expected, we find that confining walls, if close enough, suppress the instability, allowing one to speak meaningfully about the mechanical properties of a uniformly aligned phase of active filaments. (iv) We show also that stationary states with polar filaments oriented with a component normal to the walls are permissible, provided one allows for depolymerization. (v) We argue that the rigidity conferred by the orientation field of an active medium related to that associated with force chains in fragile jammed matter [16].

The remainder of this paper is organized as follows. In section 2, we explain the generic instability and its modification by partial translational ordering. In section 3, we discuss confining walls, boundary conditions, and the role of depolymerization for polar filaments, and comment on the connection to fragile jammed systems.

2. Understanding and suppressing the generic instability

2.1. Physical picture of the instability

The long-wavelength instability [1] of orientationally ordered active suspensions depends only on the existence of contractility (or tensility) and the hydrodynamic interaction, and is unaffected by liquid-crystalline elasticity. Such a robust effect should surely admit a simple physical explanation, as indeed our colleagues have frequently remarked. We provide one in this section. As background, however, a mini-review of the equations [1] of active hydrodynamics and the elementary mathematics leading to the instability is unavoidable. An active suspension is described on large time- and length-scales by three fields: the hydrodynamic velocity field $\mathbf{u}$ of the active suspension, the concentration c of active particles, and the traceless symmetric second-rank orientation tensor $\mathbf{Q}$, as functions of position $\mathbf{x}$ and time t. For *apolar* ordering, the *velocity* of the active filaments relative to the solvent does not enter the hydrodynamic description, since it is neither a conserved nor a broken-symmetry variable in the sense of [4]. For the purpose of understanding the instability in an unbounded system it is enough to consider apolar ordering, which is completely characterized by $\mathbf{Q}$. As shown in [1], the only difference in the polar case as far as the generic instability is concerned is that the unstable mode should travel at a fixed speed as it grows; the growth rate has the same form as in the apolar case. Interesting complications are thus posed by the polar case only when bounding walls are present, as we

shall discuss later. Conservation of the number of active particles is expressed as

$$\partial_t c = -\nabla \cdot \mathbf{J} \tag{1}$$

with a current

$$\mathbf{J} = c\mathbf{u} + D_0 \nabla c + D_1 \mathbf{Q} \cdot \nabla c + W_1 c \nabla \cdot \mathbf{Q} + \boldsymbol{\xi} \tag{2}$$

arising, from left to right on the right-hand side of (2), from advection, isotropic (D_0) and anisotropic (D_1) diffusion, the activity of the particles, characterized by W_1, and noise ($\boldsymbol{\xi}$) of thermal and nonthermal origin.

The orientation tensor $\mathbf{Q}$ evolves by equations familiar from liquid-crystal hydrodynamics [4, 5]:

$$(\partial_t + \mathbf{u} \cdot \nabla)\mathbf{Q} - (\boldsymbol{\Omega} \cdot \mathbf{Q} - \mathbf{Q} \cdot \boldsymbol{\Omega}) = \left[\lambda_0 \mathbf{A} + \lambda_1 \mathbf{A} \cdot \mathbf{Q} - \Gamma \frac{\delta F}{\delta \mathbf{Q}} \right]_{\mathrm{ST}}, \tag{3}$$

where the subscript 'ST' means we must take the symmetric traceless part of the entire right-hand side of (3), $\mathbf{A}$ and $\boldsymbol{\Omega}$ are the symmetric and skew parts of the velocity gradient tensor $\nabla \mathbf{u}$, λ_0 and λ_1 are positive reversible kinetic coefficients related to flow-alignment, $F[\mathbf{Q}, c]$ is a free-energy functional favouring a steady state with a nonzero $\mathbf{Q}$, imposing costs for spatial gradients in $\mathbf{Q}$, and containing permitted coupling between c and $\mathbf{Q}$. The hydrodynamic velocity field, ignoring inertia, obeys the Stokes equation of force balance $\nabla \cdot \boldsymbol{\sigma} = 0$. The total stress $\boldsymbol{\sigma}$ comprises contributions from viscosity η, pressure p, and the orientation tensor $\mathbf{Q}$. The first two are familiar from ordinary fluid mechanics. The contribution from $\mathbf{Q}$ is the sum of terms standard to nematic hydrodynamics [4, 5], and a crucial *active* term $W_2 c\mathbf{Q}$ where W_2 is a phenomenological parameter characterizing the strength of the force dipole carried by each active particle. What this means is that in an active system a state with $\mathbf{Q} \neq 0$ has a nonzero deviatoric stress. If we associate the principal axis of $\mathbf{Q}$ with the orientation of the underlying filaments, then positive and negative W_2 correspond respectively to tensile and contractile filaments. In what follows we shall treat both cases for generality; while the contractile case is of relevance to cytoskeletal filaments, many swimming organisms are macroscopically tensile. The Stokes equation thus reads

$$-\eta \nabla^2 \mathbf{u} = \nabla \cdot \left[\left(\lambda_0 \frac{\delta F}{\delta \mathbf{Q}} - \lambda_1 \mathbf{Q} \cdot \frac{\delta F}{\delta \mathbf{Q}} \right)_{\mathrm{ST}} - W_2 c \mathbf{Q} \right] - \nabla p. \tag{4}$$

To see the instability, assume the system is in a quiescent ($\mathbf{u} = 0$) state of uniform orientational order with filaments pointing along $\hat{\mathbf{z}}$, $\mathbf{Q} = \mathrm{diag}(-Q/3, -Q/3, 2Q/3)$. The concentration c plays no role here so we set it to its mean value c_0. Consider a long-wavelength perturbation with filaments tilting slightly along $\pm x$, i.e., a small Q_{xz}. Two cases are easiest to analyse: (i) splay: variation only along x and $\mathbf{u} = u(x)\hat{\mathbf{z}}$; (ii) bend: variation only along z (bend) and $\mathbf{u} = u(z)\hat{\mathbf{x}}$. Project out the pressure and work to lowest order in wavenumber q: (4) then becomes a balance between active and viscous stresses only. Solving for $\mathbf{u}$ and inserting it in (3) yields, to lowest order in q,

$$\partial_t Q_{xz} = -\frac{\alpha c_0 W_2}{\eta} Q_{xz} \tag{5}$$

for splay and

$$\partial_t Q_{xz} = +\frac{\alpha c_0 W_2}{\eta} Q_{xz} \tag{6}$$

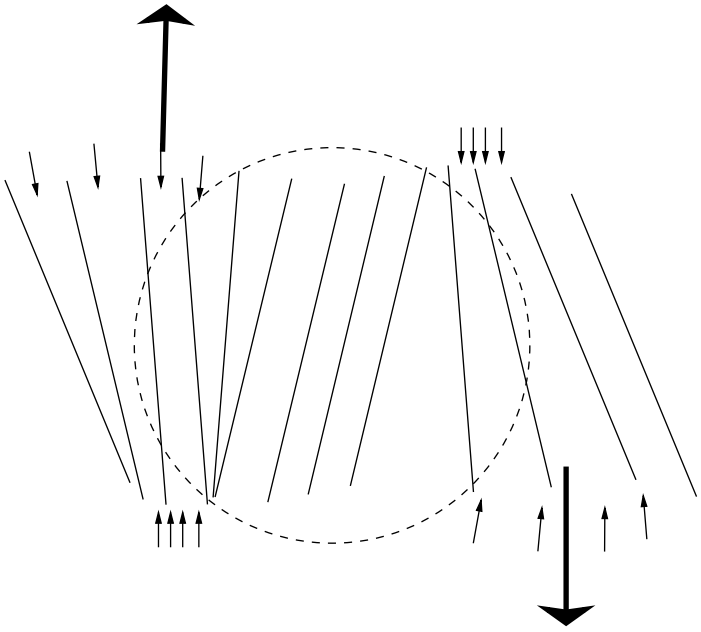

Figure 1. Understanding the splay instability of contractile filaments: splayed sets of filaments pumps fluid out their open ends, shearing the filaments in between so they tilt further.

for bend, where $\alpha > 0$ depends on Q, λ_0 and λ_1, and the finite timescales in the $q \to 0$ limit are a consequence of the long-ranged nature of the Stokesian hydrodynamic interaction. As promised, there is a linear instability of the splay mode for contractile filaments $W_2 < 0$ and the bend mode for tensile filaments $W_2 > 0$. Let us use the remarkably simple forms (5), (6) to see what is going on physically.

A single contractile filament pulls fluid in from both ends of its long axis, and ejects fluid in the plane normal to it, and a single tensile filament does precisely the opposite. Now consider long-wavelength splay imposed on an initially parallel collection of contractile filaments. In figure 1 the filaments in the left half of the figure are more spread apart at the top end than at the bottom, and those in the right half are the other way around. Fluid is thus pulled in more strongly at the bottom in the left half and at the top in the right half. This results in a shear flow over the central portion, with extensional axis oriented in such a way as to tilt the filaments further in the direction in which they were already perturbed. Similarly, a single tensile filament pushes fluid out at both ends along its long axis, and thus sucks fluid radially inward in the perpendicular plane. Figure 2 shows a configuration of tensile elements with long-wavelength bend. The curvature now means that the fluid is sucked in more from the right in the top half and from the left in the bottom half of the picture. Thus the mid-section is sheared in such a way as to increase its tilt. This completes our admittedly *ex post facto* rationalization of the generic instability of ordered active filaments in suspension. It should be noted that by assuming that the fluid flow due to a given configuration of filaments sets in everywhere at once, the arguments were implicitly using the Stokesian approximation. It should be added that the instability of tensile filaments to bend is very similar to the buckling instability of a column [17].

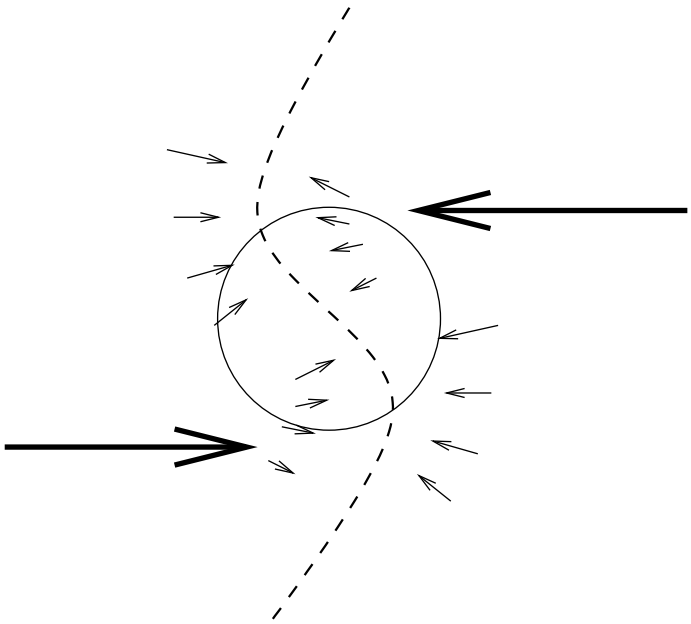

Figure 2. Understanding the bend instability of tensile filaments: bent sets of filaments shear the filaments in between so they tilt further.

2.2. Effect of translational ordering

Elongated particles can form translationally ordered phases as well at large concentration. Start with an ordered phase with active filaments with orientation given by the director field $\hat{\mathbf{N}} = \hat{\mathbf{z}} + \delta\mathbf{N}_\perp$ where the mean orientation is taken along $\hat{\mathbf{z}}$ and the transverse directions x and y are collectively labelled $\perp$. This phase is subject to the instability we just discussed in section 2.1. Now change conditions so that the system undergoes a transition to (a) a columnar hexagonal (hereafter H) phase, for example, with 2-dimensional translational (2D) order in the plane perpendicular to the filaments, or (b) a lamellar (hereafter L) phase with 1D translational order along the filaments. Case (a) is of particular relevance for biofilaments because of their tendency to bundle. Translational order introduces new broken-symmetry variables and corresponding elastic restoring forces [5]. The H phase is endowed with a two-component displacement field $\mathbf{u} = (u_x, u_y)$ and the L phase with a one-component displacement field u. The preferred intercolumn or interlayer spacing slaves the director deviation [5]: $\delta\mathbf{N}_\perp \simeq -\partial_z\mathbf{u}$ in the H phase and $\delta\mathbf{N}_\perp \simeq -\nabla_\perp u$ in the L phase. Thus, a splay deformation in the H phase will thus dilate or compress the intercolumn spacing, and a bend in the L phase will do likewise to the interlayer spacing. In the absence of active stresses, for a system with viscosity η and typical elastic moduli B, the displacement fields, in the viscosity-dominated regime, have an exponential relaxation rate B/η. Hence, by the slaving principle just mentioned, so do splay in the H and bend in the L phase. Recall from (5) and (6) that the instability growth rates in the absence of translational order are proportional to $W_2 c_0/\eta$ where W_2 is a measure of the activity. Elastic and active stresses thus compete here. If the elastic moduli B, which encode interfilament interactions (whether energetic or entropic), are large enough, the presence of translation ordering will suppress the splay instability of contractile filaments, in the H phase, and the bend instability of tensile filaments, in the L phase. Note that contractile filaments

with L order, or tensile filaments with 2D translational order, are not saved from their generic instability.

Generalizing the preceding arguments, it is clear that a *single*, active, fluid membrane [18]–[21] with contractile or tensile proteins of force W and 2D concentration ϕ disposed normal to it is like a membrane under in-plane tension of magnitude $W\phi$, negative for the contractile and positive for the tensile case. Undulations of such a membrane should thus have a characteristic relaxation or growth rate $W\phi q/\eta$ at 2D wavenumber q, as one can see by imitating the calculation of the dynamics of a tense membrane with hydrodynamic interaction [22]. Relaxational or unstable modes of this form do not arise in earlier analyses of active membranes [18, 19, 21] because the dependence of the active stress on the membrane orientation was not included.

3. The mechanics of confined active filaments

3.1. Confinement suppresses the generic instability

It was shown in [8] that active suspensions with homogeneous long-range orientational order have a nonzero deviatoric stress, and that a contractile suspension approaching such an ordered state behaves like a passive systems near *translational* freezing. However, reference [8], unlike [10], was conservative about identifying active ordered suspensions as a kind of yield stress material, because of the generic instability [1] discussed in section 2. To be able to measure the novel viscoelastic properties of a homogeneously ordered active suspension, one must suppress the instability. One way is to impose shear [13], which does stabilize the filaments at an angle to the flow, but only past a threshold shear-rate. Instead, confine the suspension to a film of thickness b in the z-direction, and assume the system size in the $xy = \perp$ plane is much larger than b. This is different from [7] where the important boundary condition is imposed on walls in the xy plane. The two standard boundary conditions on the filaments at the walls are homeotropic (normal to the walls) and homogeneous (parallel to the walls but otherwise unconstrained). Neither of these picks out a direction in the $\perp$ plane. The velocity field obeys no slip at the walls, so the slowest velocity mode has z component of its wavevector equal to π/d. The effective viscous damping for a mode with in-plane wavevector $\mathbf{q}_\perp$ is now $\eta(q_\perp^2 + (\pi/d)^2$. If we repeat the hydrodynamic analysis of section 2 for splay modes, and now include the usual contribution to the relaxation from director elasticity, with Frank constant K, equation (5) is replaced by

$$\partial_t Q_{xz} = -\left[\frac{\alpha c_0 W_2}{q_x^2 + (\pi/b)^2} + K\right]\frac{q_x^2}{\eta} Q_{xz}. \tag{7}$$

For $q_x \to 0$, as b is changed from large to small values, the director diffusivity $(K + \alpha c_0 W_2 b^2)/\eta$ goes from negative (unstable) to positive (stable) for the contractile case $W_2 < 0$. Thus, a sufficiently closely confined sample of an active nematic suspension is stable and one can talk meaningfully about its mechanically response to small perturbations.

A similar analysis can of course be repeated for tensile filaments and the bend instability. In either case, liquid-crystal physicists will note the close analogy to the undulational instability [5] of a smectic under tension. The difference here is that the tension is internally generated by the activity.

3.2. Filament orientation, forces at a wall, and an analogy to granular matter

Filaments at a wall, whether polar or apolar, in general are expected to lie normal to or parallel to the wall, corresponding to the two standard boundary conditions of liquid crystal physics discussed above. It is interesting to note that these have an important consequence in the present context: they correspond to two types of active force centres at a boundary. Such forces can thus push or pull on boundaries, or transport material actively along the boundary. The normal forces are those which enter, for instance, in motility based on actin polymerization [23], while the parallel forces have received less attention.

Let us turn to the special issues arising in the case of polar filaments in a finite geometry. On general grounds of symmetry [24], a polar object under nonequilibrium conditions should have a nonzero drift velocity. Passive filaments in a shear flow, if parameters are in the right range, will align in the bulk at an angle to the flow. Switching on activity and polarity, we see that the filaments will now try to move. Since they cannot penetrate the wall they must lie parallel to it. Two possibilities present themselves: the filament configuration in the plane of the walls can be isotropic, like the actin meshwork in the cortex of a cell, or more ordered, like microtubules. However, the filaments could move in the bulk of the sample, and lose their motility at the walls simply by depolymerizing. Let c and m be the volume fractions of polymeric filaments and monomers, with a simple reaction between n monomers and one filament, with forward and backward reaction rate constants k_+ and k_-. Let the filaments have a velocity $\mathbf{v}$ in the bulk of the sample cell and zero at the walls, and let us say the monomers have only diffusive, not directed, motion, with diffusivity D. Ignore filament diffusion. Then the balance between monomer and filament reads

$$\partial_t c = -k_- c + k_+ m^n c - \nabla \cdot (c\mathbf{v}); \tag{8}$$

$$\partial_t m = nk_- c - nk_+ m^n c + D\nabla^2 m. \tag{9}$$

It is straightforward to see from these equations that a steady state can be found with a return flux of monomer balancing the forward flux of filaments decreasing to zero as it reaches a wall. The rheological consequences of depolymerization remain to be investigated.

3.2.1. Analogy to fragile jammed granular matter. Lastly, the form $\sigma^a \sim \mathbf{NN}$ for the active stress of filaments with macroscopic orientation $\mathbf{N}$, as discussed in [1, 8] and at the start of this paper is strongly reminiscent of the constitutive equation proposed for fragile jammed matter [16] with force chains, if we identify the filament axis $\mathbf{N}$ with the force-chain director in [16]. Consider an ordered suspension of contractile filaments, with sample size small enough to evade the generic instability. Impose a small shear; it will orient at the flow-alignment angle for that shear geometry. If the shear is switched off, it will then display solid-like elasticity provide static shear is applied with the same principal axes as before. If now the sample is sheared in a different direction, it will *flow* and rearrange and jam once again with angle consistent with the new shear, and will then support static stresses with respect to this new direction. This appears to us to be completely analogous to the behaviour outlined in [16]. Of course, the stress in granular jams is externally imposed whereas here it is generated by the particles. Moreover, contractile filaments align with their axes in the extensional direction of an imposed stress, while in granular matter the chains are along the compressional axis.

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