

Asters, Vortices, and Rotating Spirals in Active Gels of Polar Filaments

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We develop a general theory for active viscoelastic materials made of polar filaments. This theory is motivated by the dynamics of the cytoskeleton. The continuous consumption of a fuel generates a nonequilibrium state characterized by the generation of flows and stresses. Our theory applies to any polar system with internal energy consumption such as active chemical gels and cytoskeletal networks which are set in motion by active processes at work in cells.

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Generalized hydrodynamic theories have been highly successful in describing a large variety of properties of complex fluids such as liquid crystals, polymers, and gels with a small number of measurable parameters [1–3]. Such theories have so far been limited to passive systems. In active systems, energy is continuously supplied by internal or external sources and internally consumed. They represent a new class of materials. Typical examples are polymeric gels driven by chemical reactions, vibrated granular materials, fluidized beds, and biological systems. We propose here a generalized hydrodynamic theory of polar active gels. Such gels can be produced *in vitro* by mixing cytoskeletal filaments and small complexes of motor proteins [4–7] and could provide a paradigm for cell dynamics.

Cells possess a cytoskeleton which is a three-dimensional network of polar elastic filaments [8]. Depending on the length of these filaments and their degree of cross-linking, the cell can control its material properties ranging from a viscous fluid to an elastic gel. In addition, the cell is able to use a large number of associated proteins which interact with the filaments of the cytoskeleton to induce and regulate active dynamic phenomena [9]. A particular example is molecular motors. These highly specialized proteins consume adenosine triphosphate (ATP) which plays the role of a chemical fuel and are able to generate motion along filaments in a direction determined by the filament polarity. In cytoskeletal network, motors induce filament transport, but they also generate forces between the filaments and thus give rise to complex self-organization phenomena [6,7,10–14]. Other processes on the molecular scale contribute to active material properties of the cytoskeleton. Of particular importance is the polymerization and the depolymerization of filaments which generate forces and flow fields [15].

From a general point of view, cytoskeletal networks made of motors interacting with filaments which polymerize and depolymerize are viscoelastic materials

driven away from equilibrium by ATP hydrolysis [16,17]. These networks can have a macroscopic polarity described by a polarization field $\mathbf{p}(\mathbf{x})$ with components p_α defined as the local average of unit vectors characterizing the polarity of individual filaments. The motion of the gel is described by the flow field $\mathbf{v}(\mathbf{x})$ or equivalently by the strain rate tensor $u_{\alpha\beta} = (\partial_\alpha v_\beta + \partial_\beta v_\alpha)/2$. We derive the generalized hydrodynamic equations using Onsager relations which characterize the linear response close to equilibrium. In the spirit of liquid crystal hydrodynamics, we include geometric nonlinearities [18]. We thus systematically expand the fluxes dp_α/dt and $u_{\alpha\beta}$ in terms of their conjugate forces, $h_\alpha = -\delta F/\delta p_\alpha$ and the stress tensor $\sigma_{\alpha\beta}$, respectively, where F is the polarization free energy. In order to drive the system to nonequilibrium steady states, we introduce a further pair of conjugate variables, the rate r of ATP consumption and the chemical potential difference $\Delta\mu$ between ATP and its hydrolysis products. ATP is also involved in the polymerization and the depolymerization of actin.

The generalized flux-force relations for this problem read

$$2\eta u_{\alpha\beta} = \left(1 + \tau \frac{D}{Dt}\right) \times \left\{ \sigma_{\alpha\beta} + \zeta \Delta\mu p_\alpha p_\beta + \bar{\zeta} \Delta\mu \delta_{\alpha\beta} - \frac{\nu_1}{2} (p_\alpha h_\beta + p_\beta h_\alpha) - \bar{\nu}_1 p_\gamma h_\gamma \delta_{\alpha\beta} + \tau A_{\alpha\beta} \right\}, \quad (1)$$

$$\frac{dp_\alpha}{dt} = - (v_\gamma \partial_\gamma) p_\alpha - \omega_{\alpha\beta} p_\beta - \nu_1 u_{\alpha\beta} p_\beta - \bar{\nu}_1 u_{\beta\beta} p_\alpha + \frac{1}{\gamma_1} h_\alpha + \lambda_1 p_\alpha \Delta\mu, \quad (2)$$

$$r = \zeta p_\alpha p_\beta u_{\alpha\beta} + \bar{\zeta} u_{\alpha\alpha} + \lambda \Delta\mu + \lambda_1 p_\alpha h_\alpha. \quad (3)$$

The complete derivation of these constitutive equations of the material, valid for small $\Delta\mu$, will be described

elsewhere [19]. Equation (1) is a generalization of the Maxwell model for a physical gel with viscosity η and elastic modulus $E = \eta/\tau$ to a situation, where stresses and material currents are generated by active processes. The tensor, $A_{\alpha\beta}$, summarizes nonlinear reactive terms which are familiar in the classical nonlinear viscoelastic models [20] and are not relevant in the following. We have used the convective derivative of a tensor field [20]

$$\frac{D\sigma_{\alpha\beta}}{Dt} \equiv \frac{\partial\sigma_{\alpha\beta}}{\partial t} + (v_\gamma\partial_\gamma)\sigma_{\alpha\beta} + [\omega_{\alpha\gamma}\sigma_{\gamma\beta} + \omega_{\beta\gamma}\sigma_{\gamma\alpha}], \quad (4)$$

where $\omega_{\alpha\beta} \equiv \frac{1}{2}(\partial_\alpha v_\beta - \partial_\beta v_\alpha)$ is the local vorticity. Equation (2) describes the dynamics of the polarization which is coupled to the flow and driven by active processes characterized by $\Delta\mu$. The rotational viscosity, γ_1 , and the reactive coefficients, ν_1 and $\bar{\nu}_1$, determine the orientation of the polarization in a simple shear flow and a compressional flow, respectively, as in conventional nematohydrodynamics [18]. The coefficients ζ , $\bar{\zeta}$, and λ_1 have been introduced phenomenologically to characterize all active terms allowed by symmetry and satisfy the Onsager symmetry relations. Equation (3) describes the rate of ATP hydrolysis assuming that the ATP concentration remains uniform in the system. The diagonal coefficient λ characterizes the ATP consumption in the absence of mechanochemical couplings. The signs of the off-diagonal terms in the flux-force relations (1)–(3) are imposed by the Onsager symmetry relations and time inversion symmetry. We ignore here chiral terms which we expect to have a small effect.

We now solve these equations for a particular case. We consider a defect of the polarization field with topological charge one and rotational symmetry in a cylindrical geometry. Such a point defect could represent an aster, where all filaments are oriented radially, a vortex, where they are oriented orthoradially, or a spiral defect. We use polar coordinates (r, θ) and represent the polarization vector by an angle ψ , with $p_r = \cos\psi$ and $p_\theta = \sin\psi$, such that the polarization modulus is fixed to $\mathbf{p}^2 = 1$. This implies that the material is polar and far from an isotropic to polar phase transition. We introduce the components of the conjugate field to the polarization, parallel and perpendicular to the polarization

$$h_{\parallel} = h_r \cos\psi + h_\theta \sin\psi, \quad h_{\perp} = -h_r \sin\psi + h_\theta \cos\psi. \quad (5)$$

If we assume rotational symmetry, $u_{rr} = dv_r/dr$, $u_{\theta\theta} = v_r/r$. We assume for simplicity that the gel is incompressible, $u_{rr} + u_{\theta\theta} = 0$. This imposes the radial velocity profile $v_r = \alpha/r$. In the absence of polymerization at the boundaries, v_r vanishes at the boundaries which implies $\alpha = 0$, $v_r = 0$, and $u_{rr} = u_{\theta\theta} = 0$. The angular component of the velocity v_θ determines $u_{r\theta} = (r/2)\frac{d}{dr}(v_\theta/r)$ and $\omega_{r\theta} = (1/2r)\frac{d}{dr}(rv_\theta)$. In a steady state Eq. (2) reads

$$\nu_1 u_{r\theta} \sin 2\psi = h_{\parallel}/\gamma_1 + \lambda_1 \Delta\mu, \quad (6)$$

$$u_{r\theta}[1 - \nu_1 \cos 2\psi] = -h_{\perp}/\gamma_1. \quad (7)$$

Similarly, in the absence of externally imposed flows Eq. (1) leads to linear order in $\Delta\mu$ to

$$2\eta u_{r\theta} = \sigma_{r\theta} + \frac{\zeta}{2}\Delta\mu \sin 2\psi - \frac{\nu_1}{2}(h_{\parallel} \sin 2\psi + h_{\perp} \cos 2\psi). \quad (8)$$

The field $h_{\perp} = -\delta F/\delta\psi$ can be calculated from a polarization free energy similar to that used for nematic liquid crystals

$$F = \int d^2x \left[\frac{K}{2}(\nabla \cdot \mathbf{p})^2 + \frac{K + \delta K}{2}(\mathbf{p} \cdot \nabla \mathbf{p})^2 + k\nabla \cdot \mathbf{p} - h_{\parallel} \mathbf{p}^2 \right], \quad (9)$$

where $K_1 = K$ and $K_3 = K + \delta K$ are the splay and bend elastic moduli, respectively, and k describes the spontaneous splay allowed by symmetry. Note that there is no twist term for cylindrical symmetry and that we assume that \mathbf{p}^2 is constant. The spontaneous splay leads to boundary terms which are unimportant in the following [21]. We obtain

$$h_{\perp} = (K + \delta K \cos^2\psi) \left[\psi'' + \frac{\psi'}{r} \right] - \frac{\delta K}{2} \sin 2\psi \left[\frac{1}{r^2} + \psi'^2 \right], \quad (10)$$

where the primes denote derivatives with respect to r . The field h_{\parallel} is a Lagrange multiplier added to impose the constraint $\mathbf{p}^2 = 1$. The condition of mechanical equilibrium reads

$$\partial_\alpha(\sigma_{\alpha\beta} - P\delta_{\alpha\beta}) = 0. \quad (11)$$

The radial component of Eq. (11) determines the pressure P . The tangential component is solved by $\sigma_{r\theta} = B/r^2$, where $B = 0$ corresponds to the condition that no stress is applied at the boundaries which we assume in the following.

At equilibrium, $\Delta\mu = 0$, our equations correspond to a ferroelectric nematic liquid crystal and no motion occurs. Four types of topological defects of charge one are possible. They correspond to asters with constant angle $\psi = 0$ and $\psi = \pi$ and to vortices with $\psi = \pm\pi/2$. With appropriate boundary conditions, asters are stable for positive δK , while vortices are stable for negative δK . If $\delta K = 0$, defects with constant angle $\psi = \psi_0$ are solutions for all ψ_0 . We call these solutions spiral defects since all trajectories following polarization are spirals given by $r(\theta) = r_0 \exp[\cot(\psi_0)\theta]$.

For an active system, $\Delta\mu \neq 0$, spiral defects are required by symmetry to rotate. They can most easily be discussed for $\delta K = 0$, where the dynamic equations have only four solutions selected by Eq. (7) with a polarization orientation

$$\cos 2\psi_0 = 1/\nu_1. \quad (12)$$

We assume here that $|\nu_1| > 1$ [22]. These are the same as the orientation angles of a nematic liquid crystal in a shear flow. The rotation speed is obtained by inserting

Eq. (6) in Eq. (8) which leads to

$$v_\theta(r) = \omega_0 r \log\left(\frac{r}{r_0}\right), \quad (13)$$

$$\omega_0 = \frac{2 \sin 2\psi_0}{4\eta + \gamma_1 \nu_1^2 \sin^2 2\psi_0} \tilde{\zeta} \Delta \mu,$$

where $\tilde{\zeta} = \zeta + \nu_1 \gamma_1 \lambda_1$. The velocity gradient is $u_{r\theta} = \omega_0/2$. For a system of finite size with maximal radius R , we have $r_0 = R$ if we impose that no motion occurs at the boundaries. A sketch of the polarization and velocity fields for a rotating spiral defects is given on Fig. 1.

The stability diagram of asters and vortices for $\delta K \neq 0$ can be obtained by studying their linear stability as a function of $\tilde{\zeta} \Delta \mu$. In general ψ is a solution to

$$h_\perp [4\eta + \gamma_1 \nu_1 (\nu_1 - \cos 2\psi)] = \gamma_1 \tilde{\zeta} \Delta \mu \times \sin 2\psi (\nu_1 \cos 2\psi - 1), \quad (14)$$

where h_\perp is given by Eq. (10). The stability limit of asters ($\delta K > 0$) is assessed by linearizing Eq. (14) around $\psi = 0$ and looking for nontrivial solutions. For simplicity, we impose $\psi = 0$ at the boundary $r = R$ and assume $\nu_1 > 1$. Asters are unstable if $\tilde{\zeta} \Delta \mu$ is smaller than a critical value given by

$$\tilde{\zeta} \Delta \mu_c^A = -\left(\frac{z_n}{R}\right)^2 \frac{[4\eta + \gamma_1 \nu_1 (\nu_1 - 1)]}{2\gamma_1 (\nu_1 - 1)} (K + \delta K). \quad (15)$$

Here, $n = [\delta K / (K + \delta K)]^{1/2}$ and z_n is the first positive zero of the Bessel function $J_n(z)$ of degree n . In this case, we expect as for $\delta K = 0$ stable rotating spiral defects to exist. Note, however, that these states are solutions to Eq. (14) which do not correspond to a constant angle ψ . A similar analysis reveals an instability of vortices ($\delta K < 0$) for negative $\tilde{\zeta} \Delta \mu$ smaller than a critical value

$$\tilde{\zeta} \Delta \mu_c^V = -\left(\frac{z_m}{R}\right)^2 \frac{[4\eta + \gamma_1 \nu_1 (\nu_1 + 1)]}{2\gamma_1 (\nu_1 + 1)} K, \quad (16)$$

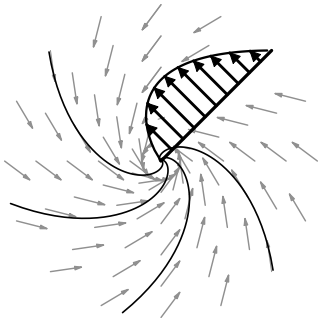


FIG. 1. Schematic representation of a rotating spiral defect for vanishing elastic anisotropy $\delta K = 0$ and in the presence of actively generated stresses $\tilde{\zeta} \Delta \mu \neq 0$ in the gel. Gray arrows represent the polarization vector. The solid lines follow the polarization which spirals to the center. The velocity field of the gel motion is orthoradial and represented by a schematic plot of the velocity profile as a function of the radius.

where $m = (-\delta K / K)^{1/2}$. The resulting stability diagram in the $(\tilde{\zeta} \Delta \mu, \delta K)$ plane is displayed in Fig. 2.

For a thin quasi-two-dimensional system, additional dissipation is due to friction with the substrate that we assume proportional to the local velocity. The force balance Eq. (11) reads $\partial_\alpha (\sigma_{\alpha\beta} - P \delta_{\alpha\beta}) = \xi v_\beta$, where ξ is a friction per unit area. For a rotating spiral defect, friction forces are balanced by the tangential stress

$$\sigma_{r\theta} = \frac{\xi}{r^2} \int_0^r dr' r'^2 v_\theta(r'). \quad (17)$$

Using this relation in Eq. (8) leads again, for $\delta K = 0$, to spiral defects with constant angle ψ_0 given by Eq. (12). The velocity profile in an infinite system is

$$v_\theta(r) = 2\omega_0 \lambda_f \{K_1(r/\lambda_f) - (\lambda_f/r)\}, \quad (18)$$

where K_1 is the modified Bessel function of the second kind defined in Ref. [23], the friction length is given by $\lambda_f = (4\eta + \gamma_1 \nu_1 \sin^2 2\psi_0)^{1/2} / 2\xi^{1/2}$, and ω_0 is given by Eq. (13). At short distances ($r \ll \lambda_f$), the dissipation is dominated by the viscosity η and the velocity field is the same as in the absence of friction. For large distances, the dissipation is dominated by the substrate friction ξ and the velocity v_θ decays to zero. Therefore, the qualitative features of the stability diagram in the presence of the substrate friction can be inferred from the diagram shown in Fig. 2 by replacing R by λ_f .

The essential result of this Letter is to show that topological defects start to rotate for sufficiently strong driving by active processes according to the state diagram shown in Fig. 2. In recent experiments, spiral defects were observed in an *in vitro* assay which for increasing motor concentration became asters [6,7]. This sequence of

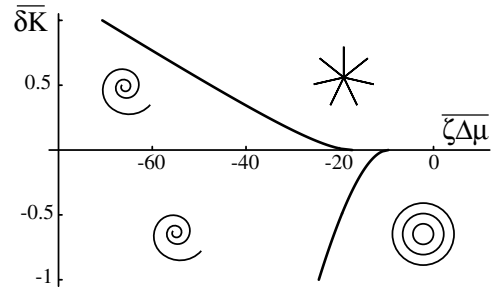


FIG. 2. Stability diagram of asters, vortices, and spirals which are topological defects in an active gel of polar filaments. Asters are stable for $\delta K > 0$ in the region with actively generated stresses $\tilde{\zeta} \Delta \mu$ larger than a critical value $\tilde{\zeta} \Delta \mu_c^A$. This critical value is negative, corresponding to contractile stresses in the gel. Vortices are stable for $\delta K < 0$ and $\tilde{\zeta} \Delta \mu > \tilde{\zeta} \Delta \mu_c^V$. For other parameter values, rotating spirals occur via a symmetry breaking dynamic instability. Here, $\overline{\delta K} = \delta K / K$ is a dimensionless ratio of two elastic moduli and $\overline{\zeta} \Delta \mu = R^2 \tilde{\zeta} \Delta \mu / K$ is a dimensionless measure of active stresses. Note that both rotation senses occur with equal probability on symmetry grounds. The diagram was evaluated for the choice $\eta / \gamma_1 = 1$ and $\nu_1 = 2$ of Onsager coefficients of the system.

structures is found in our stability diagram upon increasing δK and/or decreasing the active stress. It is not obvious how the generated stress is modified as the motor concentration is varied, albeit one might expect that increasing motor concentrations lead to increased contractile stresses which would favor spirals. However, motors which cross-link filaments near their ends penalize vortices as compared to asters which leads to an effective increase of both K and δK . This could be the dominant effect in these experiments. It is interesting to note that similar spiral motion as discussed here can also be observed in artificial systems and described using an active nematic hydrodynamics [24,25].

The dynamic and mechanical properties of spiral defects could also be important for fragments of fish keratocytes which spontaneously move on a substrate when their symmetry is broken, for example, by a mechanical action [26]. The flat, almost two-dimensional fragments contain actin filaments and myosin motors. In the front part, the actin filaments are polarized in a direction with the plus ends pointing toward the advancing front of the fragment. In the rear part, filaments are oriented parallel to the fragment edge. This pattern of filament orientation can be generated by two spiral defects which rotate in opposite directions. While a single spiral defect rotates at a fixed position, two counterrotating spirals move in a direction perpendicular to the axis connecting their centers. This filament pattern thus provides a mechanism for the motion of keratocyte fragments. The velocity of motion is of order $\omega_0 D$, where D is the distance between spiral centers and of the order of the cell size. However, a more specific description of cell locomotion requires a careful description of the adhesion on the substrate [27].

We can estimate the rotation rate ω_0 (13) induced by the motor activity. Stresses generated by motor activity in a filament system have been discussed in weakly interacting filament bundles using microscopic arguments [11]. Applying these arguments to our situation, we find $\sigma_{\text{act}} \approx \eta v_m^2 \tau_i \ell / (da^2)$, where v_m is a typical velocity of the motors, τ_i is the typical time a motor stays attached to a filament end after it arrives there, d is the spacing between motors along the filaments, a is the distance between filaments, and ℓ is the length of the filaments. The rotation speed is thus of order $\omega_0 \approx v_m^2 \tau_i \ell / (da^2)$. We estimate it as $\omega_0 \approx 0.1 \text{ min}^{-1}$ for myosins on actin leading to fragment velocities of the order of $1 \mu\text{m}/\text{min}$.

We have presented here a general hydrodynamic description of active gels which contains all relevant terms allowed by symmetry. In particular, it includes the viscoelasticity of the gel, and it can be coupled to the chemical kinetics of filament polymerization and the dynamics of the motor distribution. These effects will be the subject of a separate publication [19].

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