How the Active Liquid Crystal Got Its Cusps

Lyotropic Active Nematics
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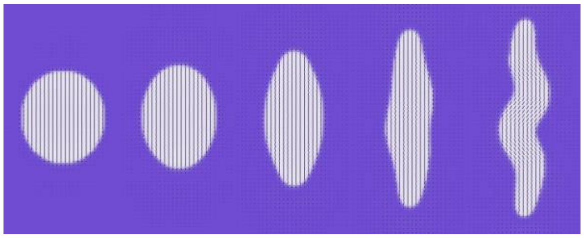
Recommended with a commentary by Jonathan V. Selinger, Kent State University

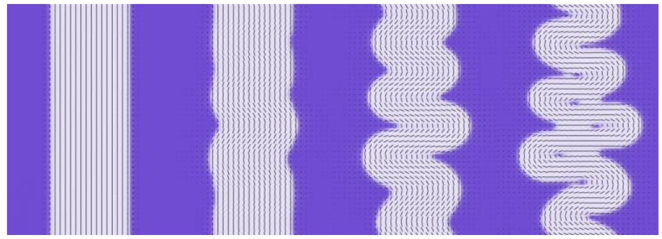
Liquid crystals are soft materials that exhibit partial order: they have orientational order, with molecules aligned along some axis, but not full crystalline positional order. In typical liquid crystals, such as those used in display devices, this partial order occurs in thermal equilibrium, and results from a competition between energy and entropy. By contrast, in recent years there has been growing interest in a new class of materials, called *active liquid crystals*, which are not in thermal equilibrium.[1] These materials are composed of particles that constantly consume energy and propel themselves, and hence form a dynamic order. In this dynamic order, the material is constantly in motion, swirling and undulating, with topological defects forming and annihilating. Indeed, in an ingenious illustration, the group of Zvonimir Dogic at Brandeis University has used an experimental video of active liquid crystals as the background for Vincent van Gogh's famous painting *Starry Night*.[2]

Active liquid crystals have been studied through a range of theoretical techniques, including agent-based simulations (with agents representing swarming bacteria, flocking animals, or other self-propelled particles), hydrodynamic theories (using long-wavelength equations of motion with all symmetry-allowed terms), and computational fluid dynamics (with coupled fluids representing the self-propelled particles and the solvent). Based on these theoretical studies, many of the properties of active liquid crystals are now well established. Even so, for theorists with backgrounds in equilibrium statistical mechanics, it is often challenging to develop an intuitive understanding of the behavior. We are so accustomed to thinking about order, disorder, and phase transitions of condensed matter systems in terms of the free energy that we have to ask: If a system does not minimize its free energy, what does it do? We may have hydrodynamic equations to predict the behavior, but we need intuitive stories to rationalize the predictions—my light-hearted analogy would be the classic *Just So Stories* of Rudyard Kipling, which include tales like "How the Camel Got His Hump."

The current preprint by Blow, Thampi, and Yeomans[3] sets out to describe a new class of active liquid crystals that are *lyotropic*, meaning that the phase behavior is controlled mainly by concentration rather than temperature. In these materials, the active material coexists with an isotropic fluid. Under the influence of the activity, the mixture can phase-separate into active nematic liquid crystal droplets surrounded by the passive isotropic phase (or isotropic droplets surrounded by active liquid crystal, depending on the composition). The investigators can then calculate the shape of the droplets and the texture of the nematic director field. Most of the work reported here uses a hybrid lattice Boltzmann method of computational fluid dynamics. However, I think the most striking features of the paper are the stories that provide a useful way to think about the behavior, by comparison with equilibrium liquid crystals.

One important story concerns the behavior that the authors call *active anchoring* at interfaces. In equilibrium liquid crystals, surface anchoring is an important part of the physics. For example, the nematic director field may be anchored in one direction along the rubbed glass surface of a liquid-crystal cell, and in another direction at a free surface exposed to air. Indeed,





liquid-crystal display devices usually operate through the competition between one alignment induced by surface anchoring and another alignment induced by an electric field. In the current preprint, the material makes its own interfaces between active nematic regions and passive isotropic regions. One must then ask how the interface affects the alignment of the director, and how the director affects the shape of the interface. The preprint shows that there are two mechanisms for active anchoring. The first mechanism tends to align the director parallel to the interface, and to make the interface extend parallel to the director. The second mechanism tends to induce shear flow whenever the director is oblique with respect to the interface. This induced shear flow then rotates the director further, leading to an instability. Hence, we see that a droplet of liquid crystal will tend to extend and then buckle, as shown in Fig. 1 from the preprint. This buckled shape will then sharpen to form cusps, shown in Fig. 2. That is a very satisfying story, because active liquid crystals commonly form such highly distorted shapes. In homage to Kipling, I would call it "How the Active Liquid Crystal Got Its Cusps."

Another interesting story in this preprint concerns how to account for topological defect charges. In bulk active nematic liquid crystals, topological defects of charge +1/2 and −1/2 form in pairs, and the +1/2 defects then move rapidly, leading to a dynamic state of defect creation and annihilation.[4] What is the analogous process in active lyotropic liquid crystals? The preprint shows that +1/2 defects form at the isotropic/nematic interface when the interface shape buckles. As the interface sharpens to form cusps, the +1/2 defects move into the interior of the nematic regions. What happens to the remaining negative topological charge? Naively, one might just say that it is left behind in the isotropic regions. However, the preprint considers this question more quantitatively by generalizing the usual definition of topological charge to nonuniform nematic order. By this definition, the negative change becomes diffuse and spread over long regions of the curved interface, while the positive charge is concentrated at points inside the nematic regions. This concept of topological charge is novel and intriguing; we will need to see whether it can be applied consistently to other liquid-crystal interfacial problems.

Apart from these intuitive stories, the preprint presents a thorough study using computational fluid dynamics to simulate the evolution of structures, and correlation functions to analyze the results. These calculations provide detailed examples of the behavior that can be expected in active liquid crystals that are free to phase separate. Even so, I find the simple stories to be particularly helpful for my intuition, and perhaps also for other readers.

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[1] For a detailed review of research on active liquid crystals, see M. C. Marchetti, J. F. Joanny, S. Ramaswamy, T. B. Liverpool, J. Prost, M. Rao, and R. A. Simha, Rev. Mod. Phys. **85**, 1143 (2013).
[2] See https://www.youtube.com/watch?v=gB_LO-ODgkw.
[3] M. L. Blow, S. P. Thampi, and J. M. Yeomans, arXiv:1407.7493.
[4] L. Giomi, M. J. Bowick, X. Ma, and M. C. Marchetti, Phys. Rev. Lett. **110**, 228101 (2013).