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Cite as: J. Chem. Phys. 150, 064909 (2019); https://doi.org/10.1063/1.5085282
Submitted: 11 December 2018 . Accepted: 26 January 2019 . Published Online: 13 February 2019

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ABSTRACT
We numerically study the dynamics of two-dimensional blue phases in active chiral liquid crystals. We show that introducing contractile activity results in stabilised blue phases, while small extensile activity generates ordered but dynamic blue phases characterised by coherently moving half-skyrmions and disclinations. Increasing extensile activity above a threshold leads to the dissociation of the half-skyrmions and active turbulence. We further analyse isolated active half-skyrmions in an isotropic background and compare the activity-induced velocity fields in simulations to an analytical prediction of the flow. Finally, we show that confining an active blue phase can give rise to a system-wide circulation, in which half-skyrmions and disclinations rotate together.

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I. INTRODUCTION

Active matter is continuously driven out of equilibrium by the injection of energy at the level of its individual constituent particles, leading to phenomena such as spontaneous flow generation\(^1,2\) and active turbulence.\(^3,4\) Furthermore, liquid crystal features including long-range orientational order and topological defects emerge in systems composed of anisotropic active particles, such as rod-shaped bacteria\(^5,6\) or cytoskeletal filaments.\(^7\) Owing to their widespread relevance to biological systems—from subcellular actomyosin mixtures\(^8\) to bacterial biofilms\(^9\) and tissues\(^10-13\)—active liquid crystals have become one of the key model systems for understanding active materials.\(^14,15\)

Previous studies of active liquid crystals have however mostly focused on achiral particles. In nature, chirality is ubiquitous, ranging from the helical structure of DNA\(^16\) and bacterial flagella\(^17\) to numerous biopolymers such as actin, chitin, and microtubules.\(^18\) On a more macroscopic level, the mitotic spindle is chiral due to torques within microtubule bundles,\(^19\) cells can develop chiral actomyosin patterns,\(^20\) and there is even tissue-scale chirality in spontaneous cellular shear flow.\(^21\) Motivated by this common occurrence of chirality in biological systems, in this paper, we explore the combined effects of activity and chirality on pattern formation within active chiral liquid crystals.

In the absence of any activity, a particular case of chiral patterning in liquid crystals occurs when there is helical ordering in more than one direction. Topological constraints mean that it is not possible to construct such a state without introducing defects or disclination lines. If the free energy advantage of twisting offsets the cost of introducing topological defects, it is however possible to obtain local regions of double-twist surrounded by negative disclinations positioned, in two dimensions, in a hexagonal lattice. This structure, occurring in the temperature range between the isotropic and the cholesteric phases, is generally known as a blue phase in the context of passive liquid crystals.\(^22\)

The double-twisted regions can be regarded as vortex-like excitations without singularities at their centre, referred to as "half-skyrmions" (Fig. 1). Although the original work by Skyrme\(^23\) dealt with three-dimensional topological excitations, two-dimensional full- and half-skyrmions have recently
attracted considerable attention in condensed matter systems. A lattice of two-dimensional half-skyrmions has been observed experimentally in the precursor state of a bulk cubic helimagnet using neutron scattering and recently also in thin films of passive chiral liquid crystals by direct optical means.

In this paper, we simulate quasi-two-dimensional active chiral liquid crystals. We show that stable vortex lattices form due to the presence of an internal chiral structure in an active two-dimensional blue phase and demonstrate a threshold for dissociation into unbound vortices for the case of extensile activity. For contractile activity, however, the vortex lattice remains stable for any activity strength considered. Furthermore, we compare analytical and computational flow-fields around isolated active half-skyrmions in an isotropic background and show that these structures are stable under contractile activity, but unstable for the case of extensile activity. This is consistent with the suppression of the splay instability reported for active cholesterics, but can more intuitively be understood in terms of the stability of the half-skyrmions. Finally, we simulate an active two-dimensional blue phase in square confinement and find a dynamically ordered state around isolated active half-skyrmions in an isotropic background.

**II. GOVERNING EQUATIONS**

In a recent paper, we simulated quasi-2D membranes of a passive cholesteric liquid crystal using a nematohydrodynamic approach. Here, we use the nematohydrodynamic equations of liquid crystals, modified to account for the stresses generated by active constituent elements. The total density $\rho$ and the velocity field $\mathbf{u}$ obey the incompressible Navier–Stokes equations

$$\nabla \cdot \mathbf{u} = 0, \quad (\text{I})$$

where $\Pi$ is the stress tensor. To account for the macroscopic orientational order of the microscopic active and anisotropic particles, the nematic tensor $Q = \frac{S_0}{2} (m - 1/3)$ is introduced. This tensor is symmetric and traceless, and $S_0$ is the coarse-grained magnitude of the nematic order. $n$ is the local nematic director, and $I$ is the identity matrix. The nematic tensor evolves as

$$\frac{\partial Q}{\partial t} + \mathbf{u} \cdot \nabla Q = \frac{1}{\tau} (Q - I), \quad (\text{II})$$

with $\tau$ being the rotational diffusivity. The co-rotation term $S_3$ is given by

$$S = \left[ \frac{1}{3} \left( \frac{Q + 1/3}{Q} \right) - \frac{2}{3} \nabla \left( \frac{Q + 1/3}{Q} \right) \right] Q,$$  

$$\nabla \cdot \mathbf{u} = 0, \quad (\text{III})$$

where $\mathbf{u}$ is the local nematic director. Finally, we simulate an active two-dimensional blue phase in square confinement and find a dynamically ordered state around isolated active half-skyrmions in an isotropic background.

**FIG. 1.** Top view of a single half-skyrmion. The director twists through an angle of $\pi/2$, from a vertical orientation in the centre of the half-skyrmion to a horizontal orientation at the edge. The angle $\phi_0$ is $\pi/2$ in equilibrium, but changes under the influence of activity, leading to a “swirl”-like profile.
which includes the pressure, $P$. The active stress is proportional to the nematic tensor $\Pi = -\zeta Q$ such that any gradient in the nematic tensor generates a flow field, with strength determined by the activity parameter, $\zeta$. Positive $\zeta$ corresponds to extensile activity, where constituent active particles drag fluid in towards their sides and expel it along their elongation axis. For contractile activity $\zeta < 0$, and fluid is pulled in along the length of the particles and pushed out from their sides. Explicit chiral active terms such as those introduced in Ref. 35 are not necessary in our case since we are dealing with the full three-dimensional nematic tensor, while the two-dimensional tensor in Ref. 35 does not include any twist. Moreover, in the active stress, we do not include any contribution from active torques that could arise, for example, in E. coli bacteria due to the counter-rotation of the head and tail. Instead, here we are interested in the combined effects of active force-dipoles and passive chirality of the particles.

III. RESULTS

A. Dynamic blue phases

The active nematohydrodynamics equations (1)–(3) are solved using a hybrid lattice Boltzmann–finite difference method. The time step and lattice spacing are set to unity. The parameters used are $\Lambda_0 = 1.5$, $\gamma = 2.85$, $L_4 = 0.04$, $L_C = 0.085$, $\Omega_0 = 2\pi/10.3$, $\Gamma = 0.7$, $\xi = 0.5 - 0.9$, $\eta = 2/3$, and $\rho = 1$, in lattice Boltzmann units. We model a two-dimensional velocity field, but in order to allow for twist, the director is free to point in three dimensions. For sufficiently high chirality, the ground state of the system is a hexagonal lattice of double-twist cylinders surrounded by negative disclinations. These double-twist cylinders are structures with a topological skyrmion number $N = \frac{1}{2\pi} \int dx dy \cdot \left( \frac{\partial^2 (\omega y^2)}{\partial x^2} - \frac{\partial^2 (\omega x^2)}{\partial y^2} \right) = \frac{1}{2}$, and they are therefore termed half-skyrmions (see Fig. 1).

An example of the response to activity for a rod-like system with $\zeta = 0.9$ can be viewed in Fig. 2 (Multimedia view). Upon application of contractile activity, the director field deforms from a double-twist cylinder configuration to a vortex-like “swirl” [Fig. 2(a) (Multimedia view)]. The swirls all generate rotational flow with the same handedness, with regions of opposite vorticity in between [Fig. 2(b) (Multimedia view)]. This type of vortex lattice is remarkably similar to that reported in active nematics with substrate friction, where hydrodynamic screening stabilised the vortices, while here the additional length introduced by the intrinsic pitch of the cholesteric sets the vortex scale.

The hexagonal structure of the two-dimensional blue phase is stable for all contractile activity strengths considered. Figure 3(a) shows the velocity–velocity correlation function $C_{uu}(r) = \langle u(r,t) \cdot u(0,0) \rangle / \langle u(0,0) \rangle^2$ for a range of contractile activities, where $r = \sqrt{x^2 + y^2}$. There is order over several pitch lengths. The vorticity–vorticity correlation function $C_{\omega\omega}(r) = \langle \omega(r,t) \cdot \omega(0,0) \rangle / \langle \omega(0,0) \rangle^2$, where $\omega$ is the vorticity, shows the same behaviour [Fig. 3(b)].

These two-dimensional blue phases are however unstable to extensile active stresses. An example of the director field [Fig. 2(c) (Multimedia view)] and the velocity field
[Fig. 2(d) (Multimedia view)] show that under sufficiently large extensile activity, the two-dimensional blue phase breaks up and active-turbulence-like behaviour emerges. This is further exemplified by the velocity-velocity correlation functions in Fig. 3(c), which show a reduction in order with increasing extensile activity. Figure 3(d) shows something unexpected, however: even though for intermediate extensile activities the correlation functions show that order over multiple pitch lengths is lost, the vorticity-vorticity correlation function still indicates the existence of a well-defined coherence length. This is because the active turbulence state is first developed for relatively coherent patches with the half-skyrmions moving as coherent units, in a turbulent-like fashion. Only for larger activity numbers is this coherence lost.

In addition, measurements of the number of half-skyrmions in the system highlight the difference between contractile and extensile driving (Fig. 4). For contractile systems, the number of half-skyrmions does not change substantially with increasing activity. The small increase in the number density is due to the stabilising effect of the contractile activity which helps the lattice become more regular so that it can fit slightly more half-skyrmions. For extensile systems, however, the behaviour is different. The initial increase in the number of half-skyrmions for extensile activity is due to the breakup of short cholesteric stripes, which are present at low activity. More importantly, the number density of half-skyrmions drops significantly when the coherence is lost. This dissociation of half-skyrmions and the onset of active turbulence occur at approximately \( \zeta_{cr} \approx 4Kq_0^2 (A_{cr} \approx 2) \), and it is accompanied by a faster increase in the root mean squared velocity \( \nu_{rms} \) (Fig. 4, inset). This threshold can be explained by considering the competition between the pitch length set by the intrinsic chirality of the particles, \( p = 2\pi/q_0 \), and the active length scale set by the activity \( \zeta \) and orientational elasticity \( K \) of the system, \( l_a \sim \sqrt{K/\zeta} \). As the activity is increased to the level where the active length scale becomes smaller than the pitch length, the half-skyrmions break up and the active turbulence is established. The number of half-skyrmions does not go to zero in the active turbulence regime, since there is no topological difference between a double-twist cylinder and a cholesteric stripe of finite length. In order to explain the
different behaviour for contractile and extensile systems, we next consider an isolated active half-skyrmion in an isotropic background.

B. Isolated half-skyrmions

1. Theory

We begin by presenting an analytical model of a single half-skyrmion in an isotropic fluid. Moving radially outwards, the director twists through an angle of π/2, from a vertical orientation at the centre of the skyrmion to a horizontal orientation in the azimuthal direction at the edge. The director field can be written as

\[ \mathbf{n}(r) = (\cos \Phi(r) \sin \Theta(r), \sin \Phi(r) \sin \Theta(r), \cos \Theta(r)) \]

where the polar coordinates \( r = (r \cos \phi, r \sin \phi) \) are introduced, and

\[ \Phi(\phi) = \phi + \phi_0 \] (with \( \phi_0 = \pm \pi/2 \) depending on handedness), and

\[ \Theta(r) = r/R \] for \( 0 \leq r \leq R\pi/2 \).

We consider the three elastic modes, splay, twist, and bend, usually written as the Frank free energy in terms of the director field \( \mathbf{n} \)

\[ \mathcal{F}_{\text{Frank}} = \frac{K_1}{2} (\nabla \cdot \mathbf{n})^2 + \frac{K_2}{2} (\nabla \times \mathbf{n})^2 + \frac{K_3}{2} (\mathbf{n} \times (\nabla \times \mathbf{n}))^2. \] (9)

We have omitted the saddle-splay contribution \( K_{24} \), since earlier work showed it is not necessary to stabilise a two-dimensional blue phase. Inserting the director field in Eq. (9), it can be readily seen that a half-skyrmion is free of splay, but not of bend. It is well established that contractile stresses drive an instability of the nematic state to splay deformations, while extensile stresses yield bend deformations. In active chiral nematics, however, the cholesteric order contributes a passive bend term that acts to screen the nematic splay mode. Instability only sets in when the activity exceeds a threshold and only for extensile activity. Due to the cholesteric order in half-skyrmions, it can therefore be expected that a half-skyrmion is unstable to extensile stresses above a finite threshold in activity, but stable to contractile stresses.

An intuitive way to understand the stabilising effect of contractile stresses observed in the simulations is by considering the half-skyrmion as a +1-topological defect that has escaped into the third dimension (Fig. 5). If the +1 defect is split into two +1/2 topological defects, the direction of spontaneous motion of active +1/2-defects can be used to interpret the observed behaviour: extensile active stresses drive the two defects apart [Fig. 5(a)], whereas contractile active stresses push the two defects together [Fig. 5(b)]. Since the undeformed half-skyrmion is a topological excitation without a singularity at its centre, introducing +1/2-defects will come with an energy cost. This explains the existence of a threshold for vortex dissociation in extensile systems.

It is obvious from a simple calculation that the undeformed half-skyrmion director field cannot generate rotational flow. If the Stokesian regime of Eq. (2) is considered, and the elastic terms in the stress tensor that generate backflow...
are neglected, the velocity obeys

\[ \eta \Delta u - \nabla p = - \mathbf{f} = \zeta \nabla \cdot \mathbf{Q} = \frac{3S \zeta}{2} \nabla \cdot \mathbf{m}. \tag{10} \]

using the definition of \( Q \). The radial component of the force will be balanced by the pressure because of incompressibility, and the azimuthal gradient of the pressure is zero due to symmetry. The equation that has to be solved is therefore simply

\[ \eta \Delta u_\phi = -f_\phi = \frac{3S \zeta}{2R} \sin \left( \frac{r}{R} \right) \left( \frac{r}{R} + R \sin \left( \frac{r}{R} \right) \right) \sin 2\phi. \tag{11} \]

The symmetry of the undeformed director field, with \( \phi_0 = \pm \pi/2 \), cannot give rise to a flow \( (u_\phi = 0) \). However, if the constant phase in \( \Phi(\phi) \) is now perturbed, this will lead to a rotational flow.

The change in the constant phase is due to the director field deforming from pure bend deformations (in order to adapt the preferred twist) to a configuration that also accommodates splay to counterbalance the active stress. The case with constant phase \( \phi_0 = \pi/4 \) deserves particular attention since it corresponds to the bend-splay \(+1\) defect that has recently been studied in the context of active stress. The constancy of the order parameter \( Q \) in the isotropic phase, but nevertheless obtain good agreement with the simulation results (Fig. 6). It should be noted that the model only holds for contractile activity or small extensile activity. In the case of large extensile activity, the approximation that the director field is constant in time is no longer valid.

C. Coherent rotation of a confined active blue phase

When active matter is confined, the otherwise turbulent-like motion can become coherent. For example, cell monolayers, dense bacterial suspensions, and microtubule/kinesin motor mixtures can all self-organise into a single circulating unit inside a circular or square box. Therefore, we next ask if the active blue phase can behave in a similar way. Simulating the dissociation threshold in an extensile system, the half-skyrmions stay largely intact [see Fig. 7(a) (Multimedia view)] and indeed move collectively to set up a coherent rotational flow [see Figs. 7(a) and 7(b) (Multimedia view)]. The emergence of coherent rotation is best illustrated by calculating the ratio of the average orthoradial to radial velocity [Fig. 7(c)]. For extensile activity above the dissociation

\[ \frac{\langle r \rangle}{\langle r^2 \rangle} \text{ normalized by the characteristic pitch}. \]

2. Simulations

The analytical result is only valid for single half-skyrmions and does not take into account the interactions between the half-skyrmions, or the presence of the six \(-1/2\)-defects surrounding each cylinder in a blue phase. Therefore, in order to provide a closer comparison between our analytical prediction and the numerical results, we next simulate half-skyrmions in an isotropic background by quenching from infinite temperature to \( \gamma = 2.74 \), with \( q_0 = 2\pi/13 \), and applying an external field in the out of plane direction to stabilise the half-skyrmion. To this end, an external field free energy \( \mathcal{F}_{\text{ext}} = -D \cdot \mathbf{Q} \cdot \mathbf{D} \) is added to the total free energy, where \( D = 0.15\zeta \) is the applied external field. The resulting velocity field for a contractile activity \( A = -3.27 \) is shown in Fig. 6(a). In our analytical model we neglect the change in the magnitude of the nematic order parameter \( Q \) going from a half-skyrmion cylinder into the isotropic phase, but nevertheless obtain good agreement with the simulation results (Fig. 6). It should be noted that the model only holds for contractile activity or small extensile activity. In the case of large extensile activity, the approximation that the director field is constant in time is no longer valid.
threshold, circulation persists [Fig. 7(c)], but without the hexagonal symmetry found in the two-dimensional blue phase. This is evident from the vorticity–vorticity correlation functions in Fig. 7(d) (dashed-dotted line), which show that for large extensile activity the coherence is lost. For contractile activity, no coherent rotational flow is observed as the blue phase remains unperturbed.

IV. DISCUSSION

Combining active stresses of self-propelled particles with two-dimensional helical ordering in the blue phase provides a framework for studying non-equilibrium topological states in active matter. Compared to the few existing theoretical studies that treat chiral active materials, we explicitly introduce topological states in chiral liquid crystals and connect the director structure to the resulting dynamics. We show that half-skyrmions are stable to contractile stresses, but that there is an active instability threshold for extensile active particles analogous to the pitch–splay mode in active cholesterics. This can be understood by regarding the topological excitation as a +1-defect that has escaped into the third dimension. A small perturbation will lead to two +1/2-defects, which are driven apart for extensile active stresses but driven together for contractile active stresses. For small extensile activity, the half-skyrmions do not dissociate, and they set up a coherent rotational flow when enclosed, reminiscent of collective cell behaviour in confinement.

A number of directions for future work can be envisaged. For instance, the linear stability analysis performed for active nematics, smectics, and cholesterics could be extended to the two-dimensional blue phase, introducing new symmetries to the framework. Second, the third dimension could be made finite, both in a linear stability analysis and in simulations, to study the onset of active instabilities along the axis of half-skyrmions. Third, a three-dimensional active blue phase could be simulated to investigate whether these are also stable to contractile active stresses.

ACKNOWLEDGMENTS

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the DIStruc Marie Skłodowska-Curie Grant Agreement No. 641839. A.D. was supported by a Royal Commission for the Exhibition of 1851 Research Fellowship.
