Cooperative Kinetics of Living Liquid Crystals

by

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Overview

(a) Introduction

(b) Modeling of Living Liquid Crystals

(c) Coupled Kinetics and Phase Diagrams

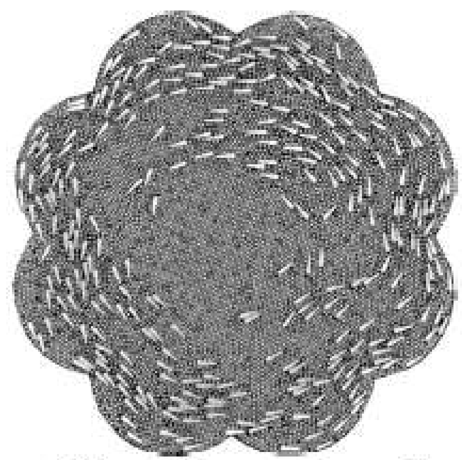
(d) Conclusion

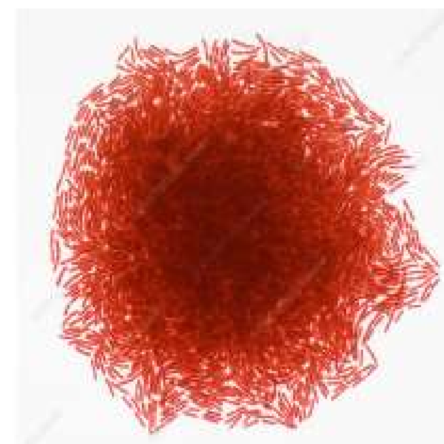
(a) Introduction

- Active matter (AM) is an assembly of self-propelled particles, which consume energy from the surroundings to move. They are intrinsically non-equilibrium systems which violate time-reversal symmetry.


Bird flocks

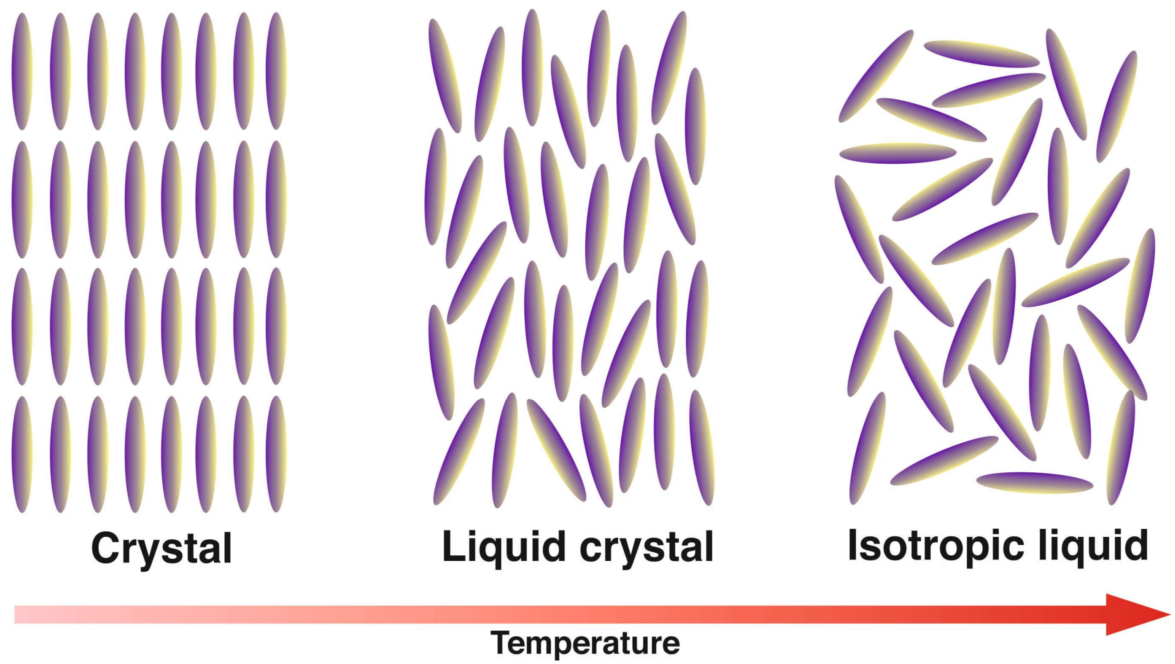

Fish shoals


Vibrated granular rods


Bacterial colony

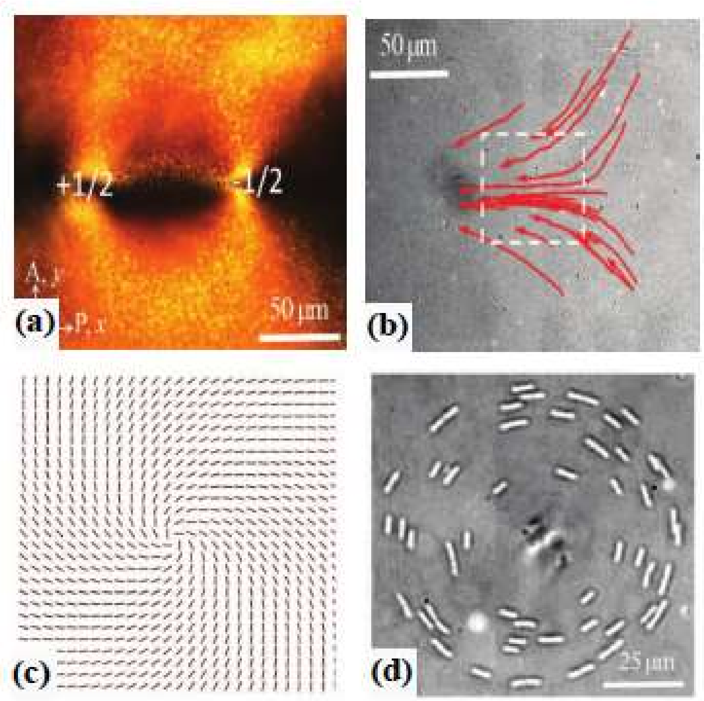
M.C. Marchetti, J.F. Joanny, S. Ramaswamy et al., Rev. Mod. Phys. **85**, 1143 (2013).

- Nematic liquid crystals are an assembly of rod-shaped particles which have properties intermediate to those of liquids (no positional order) and crystals (orientational order).



P.G. de Gennes and J. Prost, The Physics of Liquid Crystals, International Series of Monographs on Physics **83**, OUP (1993).

- Living liquid crystals (LLCs) are nematic LCs with active particles. They have potential applications in micro-fluidic devices and synthetic systems which model mobile cells in a medium.
- Experiments on bacillus subtilis in NLCs show novel phenomenology.



(a) Picture of defect pair in NLCs.

(b) Bacteria migrate to defects.

(d) Director channels bacteria.

S. Zhou, A. Sokolov, O.D. Lavrentovich and I.S. Aranson, PNAS **11**, 1265 (2014);
C. Peng, T. Turiv, Y. Guo, Q.-H. Wei and O.D. Lavrentovich, Science 354, 882 (2016).

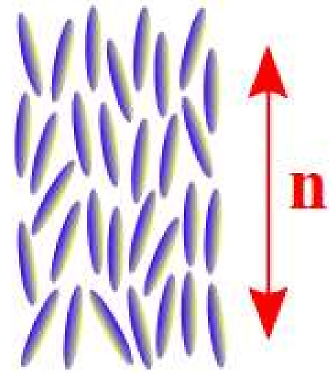
(b) Modeling of Living Liquid Crystals

A. Vats, P.K. Yadav, V. Banerjee and S. Puri, Phys. Rev. E **108**, 024701 (2023).

- Landau-de Gennes free energy for NLCs

$$Q_{ij} = \mathcal{S}\left(n_i n_j - \frac{\delta_{ij}}{2}\right)$$

$$\mathrm{Tr}(\mathbf{Q}) = 0; \quad \mathrm{Tr}(\mathbf{Q}^2) = 2(Q_{11}^2 + Q_{12}^2) = \mathcal{S}^2/2; \quad \mathrm{Tr}(\mathbf{Q}^3) = 0$$



$$\boxed{F_Q[\mathbf{Q}] = \int \mathrm{d}\mathbf{r} \left\{ \frac{A}{2}\mathrm{Tr}(\boldsymbol{Q}^2) + \frac{B}{3}\mathrm{Tr}(\boldsymbol{Q}^3) + \frac{C}{4}[\mathrm{Tr}(\boldsymbol{Q}^2)]^2 + \frac{L}{2}\left|\nabla \mathbf{Q}\right|^2 \right\}}$$

$$\boxed{\frac{\partial \mathbf{Q}}{\partial t} = -\Gamma_{\mathbf{Q}} \frac{\delta F_Q[\mathbf{Q}]}{\delta \mathbf{Q}},}$$

- Free energy for AM

Polarization vector (**P**) and density

$$F_a[\rho,\mathbf{P}] = \int \mathrm{d}\mathbf{r} \left[\frac{\alpha(\rho)}{2}|\mathbf{P}|^2 + \frac{\beta}{4}|\mathbf{P}|^4 + \frac{\kappa}{2}|\nabla\mathbf{P}|^2 + \frac{w}{2}|\mathbf{P}|^2\nabla\cdot\mathbf{P} - \frac{v_1}{2}(\nabla\cdot\mathbf{P})\frac{\delta\rho}{\rho_0} + \frac{D_\rho}{2}(\delta\rho)^2\right]$$

Toner-Tu kinetic equations

$$\frac{\partial\rho}{\partial t} = -v_0\nabla\cdot(\mathbf{P}\rho) - \nabla\cdot\left(-\Gamma_\rho\nabla\frac{\delta F_a}{\delta\rho}\right),$$

$$\frac{\partial\mathbf{P}}{\partial t} = \lambda_1(\mathbf{P}\cdot\nabla)\mathbf{P} - \Gamma_P\frac{\delta F_a}{\delta\mathbf{P}}.$$

- Proposed free energy for LLCs

$$F[\mathbf{Q},\rho,\mathbf{P}] = F_a + F_Q - c_0\sum_{i,j} Q_{ij}P_iP_j$$

$$-(\mathbf{n}\cdot\mathbf{P})^2$$

- Kinetic equations for LLCs in dimensionless variables

$$\frac{\partial Q_{11}}{\partial t} = \xi_1 \left[\pm Q_{11} - (Q_{11}^2 + Q_{12}^2) Q_{11} + \nabla^2 Q_{11} \right] + c_0 (P_1^2 - P_2^2),$$

$$\frac{\partial Q_{12}}{\partial t} = \xi_1 \left[\pm Q_{12} - (Q_{11}^2 + Q_{12}^2) Q_{12} + \nabla^2 Q_{12} \right] + 2 c_0 P_1 P_2,$$

$$\frac{1}{\Gamma}\frac{\partial P_1}{\partial t} = \xi_2 \Bigg[\left(\frac{\rho}{\rho_c} - 1 - \mathbf{P}\cdot\mathbf{P} \right) P_1 - \frac{v_1'}{2\rho_0} \nabla_x \rho + \lambda_1' (\mathbf{P}\cdot\nabla) P_1 + \lambda_2' \nabla_x (|\mathbf{P}|^2)$$

$$+ \lambda_3' P_1 (\nabla \cdot \mathbf{P}) + K' \nabla^2 P_1 \Bigg] + c_0 (Q_{11} P_1 + Q_{12} P_2),$$

$$\frac{1}{\Gamma}\frac{\partial P_2}{\partial t} = \xi_2 \Bigg[\left(\frac{\rho}{\rho_c} - 1 - \mathbf{P}\cdot\mathbf{P} \right) P_2 - \frac{v_1'}{2\rho_0} \nabla_y \rho + \lambda_1' (\mathbf{P}\cdot\nabla) P_2 + \lambda_2' \nabla_y (|\mathbf{P}|^2)$$

$$+ \lambda_3' P_2 (\nabla \cdot \mathbf{P}) + K' \nabla^2 P_2 \Bigg] + c_0 (Q_{12} P_1 - Q_{11} P_2),$$

$$\frac{1}{\Gamma'}\frac{\partial \rho}{\partial t} = -v_0' \nabla \cdot (\mathbf{P}\rho) + D_\rho' \nabla^2 \rho.$$

(c) Coupled Kinetics and Phase Diagrams

- Three cases of interest

Case 1: LC intrinsically disordered (-), AM intrinsically ordered
Case 2: LC intrinsically ordered (+), AM intrinsically disordered
Case 3: LC intrinsically ordered (+), AM intrinsically ordered

- Stationary or fixed point (FP) solutions

$$\begin{aligned}
&\pm Q_{11}^* - ({Q_{11}^*}^2 + {Q_{12}^*}^2)Q_{11}^* + c_0(P_1^{*2} - P_2^{*2}) = 0,\\
&\pm Q_{12}^* - ({Q_{11}^*}^2 + {Q_{12}^*}^2)Q_{12}^* + 2c_0 P_1^* P_2^* = 0,\\
&(g_0 - |\mathbf{P}^*|^2)P_1^* + c_0(Q_{11}^* P_1^* + Q_{12}^* P_2^*) = 0,\\
&(g_0 - |\mathbf{P}^*|^2)P_2^* + c_0(Q_{12}^* P_1^* - Q_{11}^* P_2^*) = 0,
\end{aligned}$$

$$g_0 = \rho_0/\rho_c - 1$$

Rotational invariance

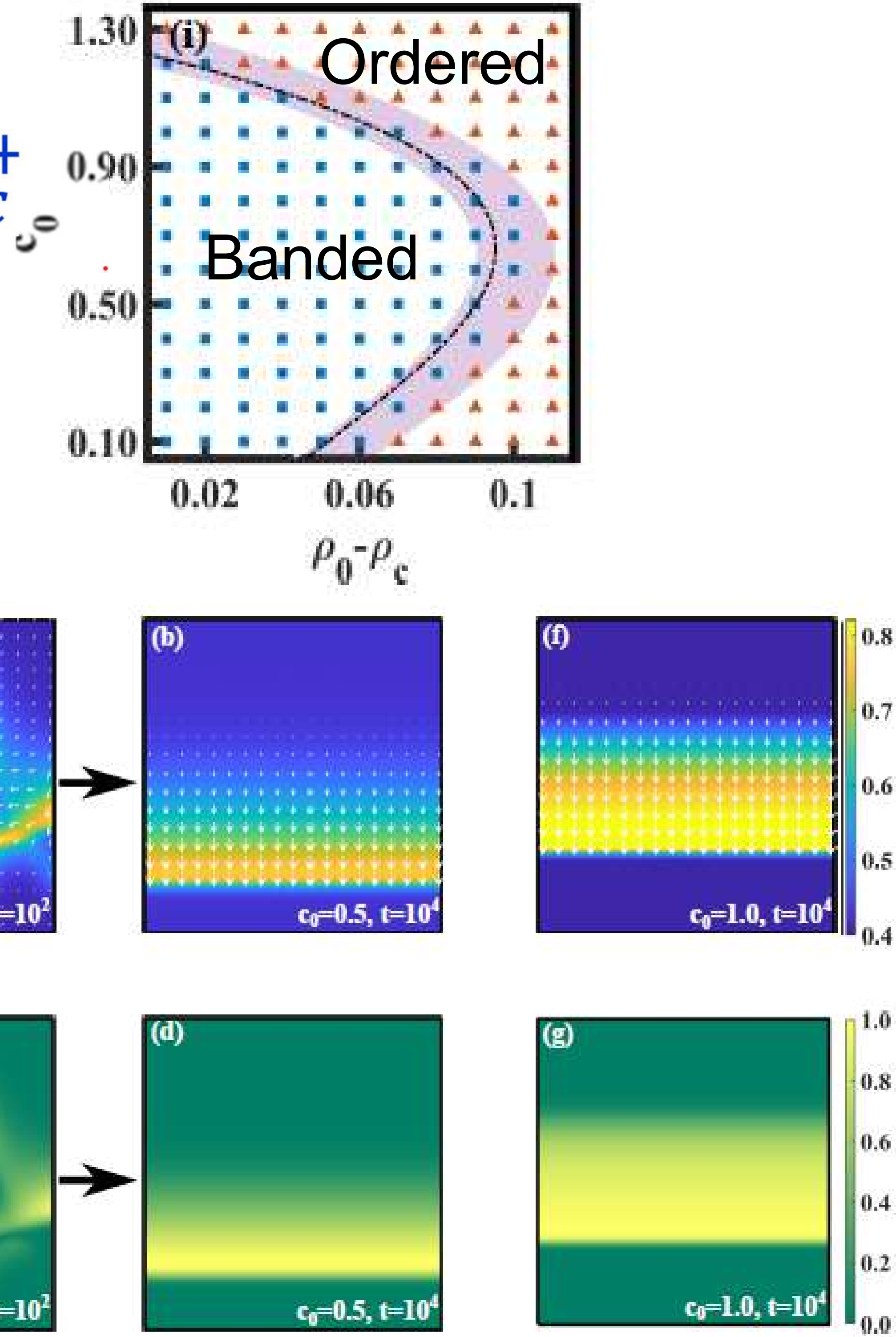
$$Q_{11}^* = r_Q \cos 2\theta, \quad Q_{12}^* = r_Q \sin 2\theta; \quad P_1^* = r_P \cos\theta, \quad P_2^* = r_P \sin\theta.$$

Cases	FP solutions $(Q^*_{11}, Q^*_{12}, P^*_1, P^*_2) = (r_Q, 0, r_P, 0)$
Case 1 $(T > T_c,\ \rho_0 = \rho_c^+)$	$r_Q = -2^{1/3}(1+c_0^2)a_1^{-1/3} + a_1^{1/3}(2^{1/3}3)^{-1}$ $r_P^2 = c_0 r_Q + \lvert g_0\rvert$ $a_1 = 27\lvert g_0\rvert c_0 + \sqrt{(27\lvert g_0\rvert c_0)^2 + 4(3-3c_0^2)^3}$
Case 2 $(T < T_c,\ \rho_0 = \rho_c^-)$	$r_Q = 2^{1/3}(1+c_0^2)a_1^{-1/3} + a_1^{1/3}(2^{1/3}3)^{-1}$ $r_P^2 = c_0 r_Q - \lvert g_0\rvert$ $a_1 = -27\lvert g_0\rvert c_0 + \sqrt{(27\lvert g_0\rvert c_0)^2 + 4(3-3c_0^2)^3}$
Case 3 $(T < T_c,\ \rho_0 = \rho_c^+)$	$r_Q = 2^{1/3}(1+c_0^2)a_1^{-1/3} + a_1^{1/3}(2^{1/3}3)^{-1}$ $r_P^2 = c_0 r_Q + \lvert g_0\rvert$ $a_1 = 27\lvert g_0\rvert c_0 + \sqrt{(27\lvert g_0\rvert c_0)^2 + 4(3-3c_0^2)^3}$

TABLE 1. FP solutions for *Cases 1-3*.

Examine linear stability of FPs to get the phase diagrams.

Case 1:
AM ordered $\rho_0 = \rho_c^+$
LC disordered T>T$_C$



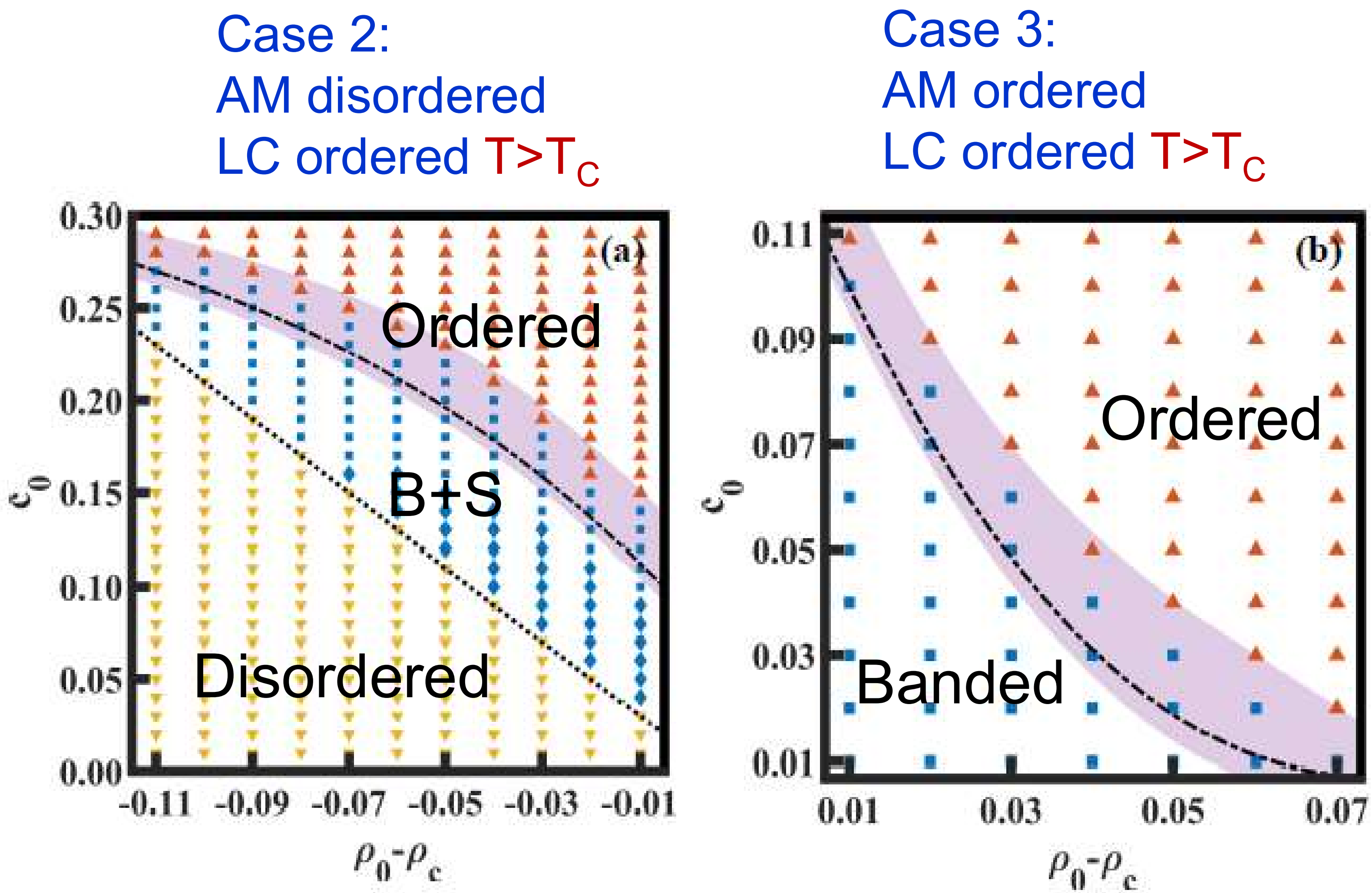


FIG. 3. Phase diagram for (a) *Case 2*: $T < T_c, \rho_0 = \rho_c^-$; and (b) *Case 3*: $T < T_c, \rho_0 = \rho_c^+$ showing different phases: disordered (▼), chimera (■), soliton plus chimera (♦), and ordered (▲). The phase boundaries shown by the dotted and dashed lines are obtained analytically in SII. The smear indicates the corresponding numerical phase boundary for the chimera → ordered transition.

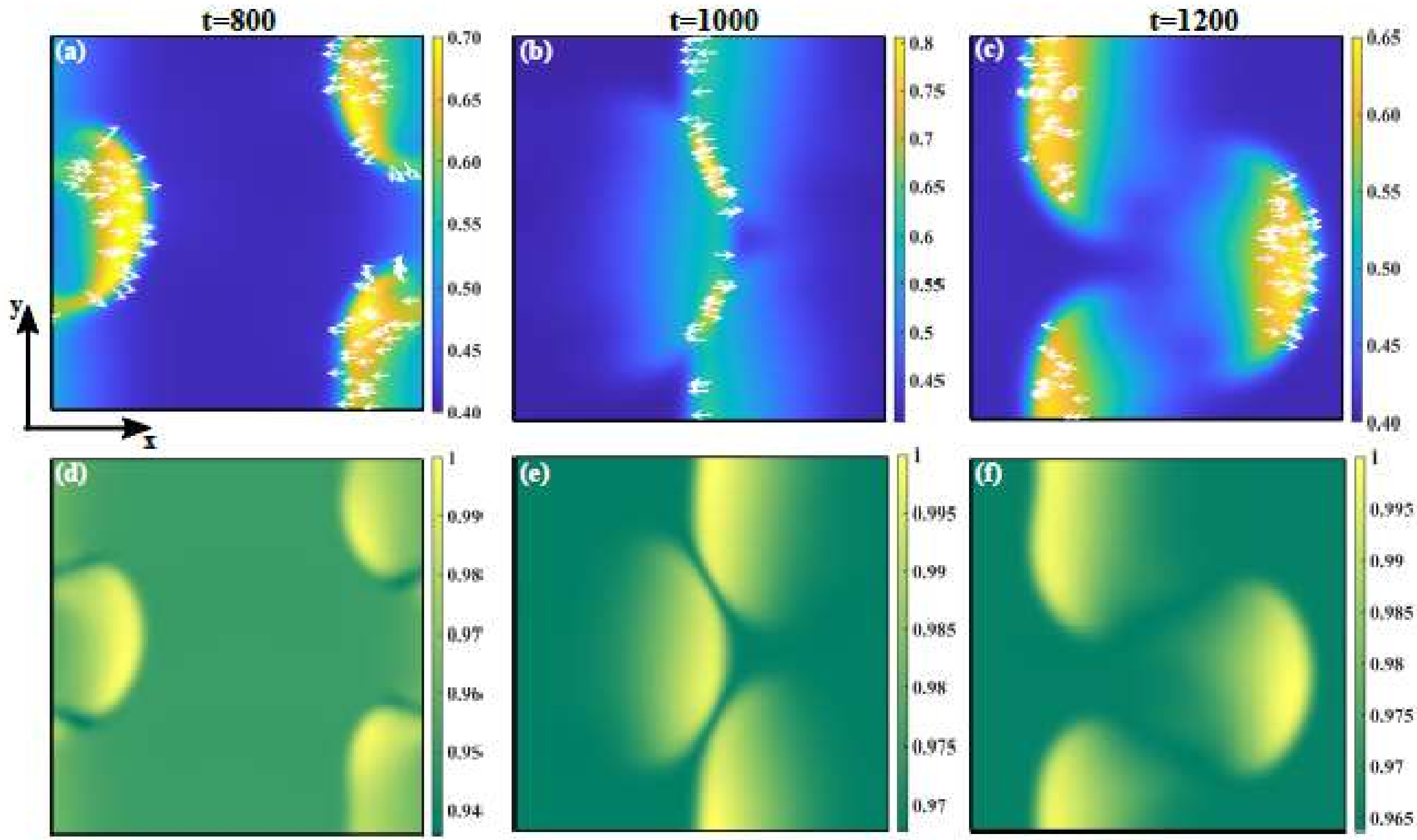


FIG. 2. Morphology snapshots of the active field (top row) and nematic field (bottom row) for *Case 2* with $T < T_c, \rho_0 = \rho_c^- = 0.48$ and $c_0 = 0.1$. The arrows in the active morphologies correspond to the polarization field in the high density regions ($\rho > 0.6$), and denote the direction of motion of the active field. The $\mathcal{S}$-field is normalized by (d) $\mathcal{S}_m = 2.104$, (e) $\mathcal{S}_m = 2.066$, (f) $\mathcal{S}_m = 2.0737$ respectively.

(d) Conclusion

- We have formulated a Ginzburg-Landau model of living liquid crystals (LLCs), where the two components are treated on equal footing.
- The active particles align parallel to the nematic liquid crystals in our model, but one can also model AM at an arbitrary angle to LCs.
- We have studied the phase diagram and kinetics of this model. The ordered component can drag the disordered component into chimera and 2-dimensional soliton states.