Chemotactic Chiral Active Matter

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1 Models

1.1 Definitions

1.1.1 General Model

$$\dot{\mathbf{r}}_i(t) = v\mathbf{p}(\theta_i) + \sum_{j\in A_i^{1,2}} \mathbf{I}(\Delta\mathbf{r}_{ij}) , \tag{1a}$$

$$\dot{\theta}_i(t) = \omega_i + G(\mathbf{r},\theta,c) + \sum_{j\neq i} H(\Delta\theta_{ij},\Delta\mathbf{r}_{ij}) , \tag{1b}$$

$$\dot{c}(\mathbf{r},t) = D\nabla^2 c + F(c)\sum_{j=1} \delta(\mathbf{r}-\mathbf{r}_i) , \tag{1c}$$

for $i = 1, 2, \cdots, N$. Here, $\mathbf{r}_i$ is the position of the i-th particle, θ_i is the orientation of the i-th particle, v is the self-propulsion velocity, $\mathbf{p}(\theta_i) = (\cos\theta_i, \sin\theta_i)$ is the unit vector pointing in the direction of the i-th particle, ω_i is the natural frequency of the i-th particle, $G(\mathbf{r},\theta,c)$ is the coupling function between particles and chemical fields, $H(\Delta\theta_{ij},\Delta\mathbf{r}_{ij})$ is the coupling function between partials, $c(\mathbf{r},t)$ is the chemical concentration, D is the diffusion coefficient, $F(c)$ is the production rate of the chemical field, $A_i^{1,2} = \{j \mid r_c \geqslant |\mathbf{r}_j - \mathbf{r}_i|\}$, $\Delta\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$, $\Delta\theta_{ij} = \theta_j - \theta_i$, $\mathbf{I}(\Delta\mathbf{r}_{ij}) = \frac{\Delta\mathbf{r}_{ij}}{|\Delta\mathbf{r}_{ij}|^2}$. The natural frequencies ω_i are distributed with following two cases:

1. **Single-chiral swarmalators:** The natural frequencies ω_i are distributed in $U(\omega_{\min},\omega_{\max})$ for all swarmalators and $\omega_{\min}\omega_{\max} > 0$.

2. **Double-chiral swarmalators:** The frequencies are distributed in two symmetric uniform distributions, representing two types of chirality. Exactly half of the swarmalators have natural frequencies $\omega_i \sim U(\omega_{\min},\omega_{\max})$ and the other half have natural frequencies $\omega_i \sim U(-\omega_{\max},-\omega_{\min})$.

1.1.2 Polar alignment Interaction

- Additive coupling:

$$\dot{\theta}_i = \omega_i + K\sum_{j=1}^{N} f(r_{ij})\sin(\theta_j - \theta_i + \alpha) , \tag{2}$$

- Mean-field coupling by oscillator number:

$$\dot{\theta}_i = \omega_i + \frac{K}{N}\sum_{j=1}^{N} f(r_{ij})\sin(\theta_j - \theta_i + \alpha) , \tag{3}$$

  which is similar to the swarmalator model.

Here, $f(r_{ij})$ is a function of $r = |\mathbf{r}_i - \mathbf{r}_j|$, and K is the coupling strength. The function $f(r)$ can be defined as

1. $f_H(r) = H(d_0 - r),\ r_0 > 0$;

2. $f_E(r) = e^{-\frac{r}{d_0}},\ r_0 > 0$.

1.1.3 Chemotactic Interaction

General Chemotactic Model For Two Species

Type 1:

$$\dot{\mathbf{r}}_i^{1,2} = v\mathbf{p}\left(\theta_i^{1,2}\right) - \sum_{j\in A_i^{1,2}} \mathbf{I}_{ij}^{1,2} \,, \tag{4a}$$

$$\dot{\theta}_i^{1,2} = \omega_i + \left|\nabla c_{1,2}\right| \sin\left(\varphi_{c_{1,2}} - \theta_i^{1,2}\right) + F\left(\theta, \mathbf{r}\right) \,, \tag{4b}$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + F_1\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^1\right) \,, \tag{4c}$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + F_2\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^2\right) \,, \tag{4d}$$

where $\mathbf{I}_{ij}^{1,2} = \frac{\mathbf{r}_j - \mathbf{r}_i^{1,2}}{|\mathbf{r}_j - \mathbf{r}_i^{1,2}|^2}$, $\varphi_{c_{1,2}} = \arctan\left(\frac{\partial_y c_{1,2}}{\partial_x c_{1,2}}\right)$ and $A_i^{1,2} = \left\{ j \mid r_c \geqslant |\mathbf{r}_j - \mathbf{r}_i^{1,2}| \right\}$.
Type 2:

$$\dot{\mathbf{r}}_i^{1,2} = v\mathbf{p}\left(\theta_i^{1,2}\right) + \alpha_{1,2}\nabla c_{1,2} - \sum_{j\in A_i^{1,2}} \mathbf{I}_{ij}^{1,2} \,, \tag{5a}$$

$$\dot{\theta}_i^{1,2} = \omega_i + F\left(\theta, \mathbf{r}\right) \,, \tag{5b}$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + F_1\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^1\right) \,, \tag{5c}$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + F_2\left(c_1, c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^2\right) \,, \tag{5d}$$

Chemotactic Model with Lotka-Volterra Functions

Let $F_1\left(c_1, c_2\right) = c_1\left(k_1 - k_2 c_2\right)$ and $F_2\left(c_1, c_2\right) = c_2\left(k_3 c_1 - k_4\right)$, where k_1, k_2, k_3, k_4 are constants.

$$\dot{\mathbf{r}}_i^{1,2} = v\mathbf{p}\left(\theta_i^{1,2}\right) - \sum_{j\in A_i^{1,2}} \mathbf{I}_{ij}^{1,2} \,, \tag{6a}$$

$$\dot{\theta}_i^{1,2} = \omega_i + \left|\nabla c_{1,2}\right| \sin\left(\varphi_{c_{1,2}} - \theta_i^{1,2}\right) + F\left(\theta, \mathbf{r}\right) \,, \tag{6b}$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + c_1\left(k_1 - k_2 c_2\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^1\right) \,, \tag{6c}$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + c_2\left(k_3 c_1 - k_4\right) \sum_{j=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_j^2\right) \,, \tag{6d}$$

2 Continuum model

In the thermodynamic limit $N \to \infty$, the Eqs. (6a) and (6b) give rise to the following continuum model:

$$\frac{\partial}{\partial t}\rho^{1,2}\left(\mathbf{r}, \theta, t\right) = -\frac{\partial}{\partial \theta}\left(\rho^{1,2} v_\theta^{1,2}\right) - \nabla \cdot \left(\rho^{1,2}\mathbf{v}_{\mathbf{r}}^{1,2}\right) \,, \tag{7}$$

where $\rho^{1,2}\left(\mathbf{r}, \theta, t\right)$ is the probability density of swarmalators of species 1 or 2 at position $\mathbf{r}$ and orientation θ at time t, and $\mathbf{v}_{\mathbf{r}}^{1,2}$ and $v_\theta^{1,2}$ are the velocity fields in the position and orientation space, respectively. The velocity fields are given by

$$v_\theta^{1,2}\left(\mathbf{r}, \theta, t\right) = \omega + \left|\nabla c_{1,2}\right| \sin\left(\varphi_{c_{1,2}} - \theta\right) + F\left(\theta, \mathbf{r}\right) \,, \tag{8a}$$

$$\mathbf{v}_{\mathbf{r}}^{1,2}\left(\mathbf{r}, \theta, t\right) = v\mathbf{p}\left(\theta\right) - \int d\theta' d\mathbf{r}' \rho^{1,2}\left(\mathbf{r}', \theta', t\right) \mathbf{I}\left(\mathbf{r} - \mathbf{r}'\right) \,, \tag{8b}$$

where $\mathbf{I}(\mathbf{r}) = |\mathbf{r}|^{-2}\mathbf{r}$. By substituting Eqs. (8) into Eq. (7), we obtain

$$\begin{aligned}\frac{\partial}{\partial t}\rho^{1,2}(\mathbf{r},\theta,t) =& -\omega\partial_\theta\rho^{1,2} - |\nabla c_{1,2}|\,\partial_\theta\left[\rho^{1,2}\sin\left(\varphi_{c_{1,2}}-\theta\right)\right] \\ & - v\mathbf{p}(\theta)\cdot\nabla\rho^{1,2} - \nabla\cdot\int d\theta\prime d\mathbf{r}\prime\rho^{1,2}(\mathbf{r}\prime,\theta\prime,t)\,\mathbf{I}(\mathbf{r}-\mathbf{r}\prime)\,.\end{aligned} \tag{9}$$

3 Behaviors