

Chemotactic Chiral Active Matter

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1 Models

1.1 Definitions

1.1.1 General Model

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

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

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

for $i = 1, 2, \dots, N$. 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 particles, $c(\mathbf{r}, t)$ is the chemical concentration, D is the diffusion coefficient, $F(c)$ is the production rate of the chemical field, $A_i^{1,2} = \{j \mid r_c \geq |\mathbf{r}_j - \mathbf{r}_i|\}$, $\Delta\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$, $\Delta\theta_{ij} = \theta_j - \theta_i$, $\mathbf{I}(\Delta\mathbf{r}_{ij}) = \frac{\Delta\mathbf{r}_{ij}}{|\Delta\mathbf{r}_{ij}|^2}$. The natural frequencies ω_i are distributed with following two cases:

1. **Single-chiral particles:** The natural frequencies ω_i are distributed in $U(\omega_{\min}, \omega_{\max})$ for all particles and $\omega_{\min}\omega_{\max} > 0$.
2. **Double-chiral particles:** The frequencies are distributed in two symmetric uniform distributions, representing two types of chirality. Exactly half of the particles 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:

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

- Mean-field coupling by oscillator number:

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

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:

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

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

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

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

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 $A_i^{1,2} = \{j \mid r_c \geq |\mathbf{r}_j - \mathbf{r}_i^{1,2}|\}$.
Type 2:

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

$$\dot{\theta}_i^{1,2} = \omega + F(\theta, \mathbf{r}), \quad (5b)$$

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

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

Chemotactic Model with Lotka-Volterra Functions

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

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

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

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

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

2 Continuum model

We start with the model as given by Eqs. (6) in the main text but replace the finite range alignment interaction by a pseudopotential (δ -interaction), which is justified if the interaction is short ranged enough, such that the shape of the associated interaction potential is irrelevant to the many particle dynamics:

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

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

where $f^{1,2}(\mathbf{r}, \theta, t)$ is the probability density of particles of species 1 or 2 at position \mathbf{r} and orientation θ at time t , and $\mathbf{v}_r^{1,2}$ and $v_\theta^{1,2}$ are the velocity fields in the position and orientation space, respectively.

The velocity fields are given by

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

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

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

$$\begin{aligned} \frac{\partial}{\partial t} f^{1,2}(\mathbf{r}, \theta, t) = & -v\mathbf{p}(\theta) \cdot \nabla f^{1,2} - \nabla \cdot \mathbf{F}_{\text{coll}}^{1,2}(\mathbf{r}, \theta, t) \\ & - \omega \partial_\theta f^{1,2} - |\nabla c_{1,2}| \partial_\theta [f^{1,2} \sin(\varphi_{c_{1,2}} - \theta)] , \end{aligned} \quad (9)$$

where

$$\mathbf{F}_{\text{coll}}^{1,2}(\mathbf{r}, \theta, t) = \int d\theta' d\mathbf{r}' f^{1,2}(\mathbf{r}', \theta', t) f^{1,2}(\mathbf{r}, \theta, t) \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2} , \quad (10)$$

and

$$\begin{aligned} \nabla \cdot \mathbf{F}_{\text{coll}}^{1,2}(\mathbf{r}, \theta, t) &= \nabla \cdot \int d\theta' d\mathbf{r}' f^{1,2}(\mathbf{r}', \theta', t) f^{1,2}(\mathbf{r}, \theta, t) \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2} \\ &= \int d\theta' d\mathbf{r}' f^{1,2}(\mathbf{r}', \theta', t) \nabla \cdot \left[f^{1,2}(\mathbf{r}, \theta, t) \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2} \right] \\ &= \int d\theta' d\mathbf{r}' f^{1,2}(\mathbf{r}', \theta', t) \left[-2\pi \delta(\mathbf{r}' - \mathbf{r}) f^{1,2}(\mathbf{r}, \theta, t) + \nabla f^{1,2}(\mathbf{r}, \theta, t) \cdot \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2} \right] \\ &= -2\pi f^{1,2}(\mathbf{r}, \theta, t) \int_0^{2\pi} d\theta' f^{1,2}(\mathbf{r}, \theta', t) + \nabla f^{1,2}(\mathbf{r}, \theta, t) \cdot \int d\theta' d\mathbf{r}' f^{1,2}(\mathbf{r}', \theta', t) \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2} \end{aligned} \quad (11)$$

The equation accounts for self-propulsion, and short-range repulsion between particles, rotational diffusion and chemotactic alignment. From here, we expand $f^{1,2}(\mathbf{r}, \theta, t)$ in a Fourier series

$$f^{1,2}(\mathbf{r}, \theta, t) = \sum_{k=-\infty}^{\infty} f_k^{1,2}(\mathbf{r}, t) e^{ik\theta} , \quad (12)$$

with the projection

$$f_k^{1,2}(\mathbf{r}, t) = \frac{1}{2\pi} \int d\theta f^{1,2}(\mathbf{r}, \theta, t) e^{-ik\theta} , \quad (13)$$

and define the coefficients as the particle density $\rho(\mathbf{r}, t)$ and the density-weighted polar order $\mathbf{p}(\mathbf{r}, t)$ by relating them to the harmonics via the Fourier expansion:

$$\rho^{1,2}(\mathbf{r}, t) \equiv \int_0^{2\pi} d\theta f^{1,2}(\mathbf{r}, \theta, t) = 2\pi f_0^{1,2}(\mathbf{r}, t) \quad (14a)$$

$$\begin{aligned} \mathbf{p}^{1,2}(\mathbf{r}, t) &\equiv \int_0^{2\pi} d\theta \mathbf{p}(\theta) f^{1,2}(\mathbf{r}, \theta, t) \\ &= \int_0^{2\pi} d\theta \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} f^{1,2}(\mathbf{r}, \theta, t) = \int_0^{2\pi} d\theta \frac{1}{2} \begin{bmatrix} e^{i\theta} + e^{-i\theta} \\ i(e^{-i\theta} - e^{i\theta}) \end{bmatrix} f^{1,2}(\mathbf{r}, \theta, t) \\ &= \pi \begin{bmatrix} \frac{1}{2\pi} \int_0^{2\pi} d\theta (e^{i\theta} + e^{-i\theta}) f^{1,2}(\mathbf{r}, \theta, t) \\ \frac{1}{2\pi} \int_0^{2\pi} d\theta i(e^{-i\theta} - e^{i\theta}) f^{1,2}(\mathbf{r}, \theta, t) \end{bmatrix} = \pi \begin{bmatrix} f_1^{1,2}(\mathbf{r}, t) + f_{-1}^{1,2}(\mathbf{r}, t) \\ i(f_1^{1,2}(\mathbf{r}, t) - f_{-1}^{1,2}(\mathbf{r}, t)) \end{bmatrix} \end{aligned} \quad (14b)$$

In the following, the different contributions to the continuum model, Eq. (7), are analyzed separately. First, in order to derive expressions for the self-propulsion, $-v\mathbf{p}(\theta) \cdot \nabla f^{1,2}$, we apply the projection

operator, Eq. (13), onto the corresponding term in Eq. (7) and obtain

$$\begin{aligned}
\frac{\partial}{\partial t} f_{k,\text{prop}}^{1,2} &= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} [-v\mathbf{p}(\theta) \cdot \nabla f^{1,2}] \\
&= -\frac{v}{4\pi} \int_0^{2\pi} d\theta e^{-ik\theta} \left[\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2} (e^{i(m+1)\theta} + e^{i(m-1)\theta}) + i\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2} (e^{i(m-1)\theta} - e^{i(m+1)\theta}) \right] \\
&= -\frac{v}{4\pi} \int_0^{2\pi} d\theta \left[\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2} (e^{i(m-k+1)\theta} + e^{i(m-k-1)\theta}) + i\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2} (e^{i(m-k-1)\theta} - e^{i(m-k+1)\theta}) \right] \\
&= -\frac{v}{2} \left\{ \partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2} [\delta(m-k+1) + \delta(m-k-1)] + i\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2} [\delta(m-k-1) - \delta(m-k+1)] \right\}. \tag{15}
\end{aligned}$$

With the definitions, Eqs. (14a) and (14b), we obtain for the field variables

$$\begin{aligned}
\frac{\partial}{\partial t} \rho_{\text{prop}}^{1,2} &= 2\pi \frac{\partial}{\partial t} f_{0,\text{prop}}^{1,2} \\
&= -v\pi \left[\partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2} [\delta(m+1) + \delta(m-1)] + i\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2} [\delta(m-1) - \delta(m+1)] \right] \tag{16} \\
&= -v\pi \left[\partial_x (f_{-1}^{1,2} + f_1^{1,2}) + i\partial_y (f_1^{1,2} - f_{-1}^{1,2}) \right] \\
&= -v\nabla \cdot \mathbf{p}_{\text{prop}}^{1,2},
\end{aligned}$$

and because of

$$\begin{aligned}
\partial_t f_1^{1,2} &= -\frac{v}{2} \left\{ \partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2} [\delta(m) + \delta(m-2)] + i\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2} [\delta(m-2) - \delta(m)] \right\} \\
&= -\frac{v}{2} \left[\partial_x (f_0^{1,2} + f_2^{1,2}) + i\partial_y (f_2^{1,2} - f_0^{1,2}) \right] \tag{17a}
\end{aligned}$$

$$\begin{aligned}
\partial_t f_{-1}^{1,2} &= -\frac{v}{2} \left\{ \partial_x \sum_{m=-\infty}^{\infty} f_m^{1,2} [\delta(m-2) + \delta(m)] + i\partial_y \sum_{k=-\infty}^{\infty} f_m^{1,2} [\delta(m) - \delta(m-2)] \right\} \\
&= -\frac{v}{2} \left[\partial_x (f_0^{1,2} + f_2^{1,2}) + i\partial_y (f_0^{1,2} - f_2^{1,2}) \right], \tag{17b}
\end{aligned}$$

we have

$$\frac{\partial}{\partial t} \mathbf{p}_{\text{prop}}^{1,2} = \pi \begin{bmatrix} \partial_t (f_1^{1,2} + f_{-1}^{1,2}) \\ i\partial_t (f_1^{1,2} - f_{-1}^{1,2}) \end{bmatrix} = \pi \begin{bmatrix} -v\partial_x (f_0^{1,2} + f_2^{1,2}) \\ v\partial_y (f_2^{1,2} - f_0^{1,2}) \end{bmatrix} \approx -\frac{v}{2} \begin{bmatrix} \partial_x f_0^{1,2} \\ \partial_y f_0^{1,2} \end{bmatrix} = -\frac{v}{2} \nabla \rho_{\text{prop}}^{1,2}. \tag{18}$$

Next, we turn to the short-range repulsion, $-\nabla \cdot \mathbf{F}_{\text{coll}}^{1,2}(\mathbf{r}, \theta, t)$. We apply the projection operator, Eq. (13), onto the corresponding term in Eq. (7) and obtain

$$\begin{aligned}
\frac{\partial}{\partial t} f_{k,\text{coll}}^{1,2} &= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} [\nabla \cdot \mathbf{F}_{\text{coll}}^{1,2}(\mathbf{r}, \theta, t)] \\
&= -4\pi^2 f_{0,\text{coll}}^{1,2}(\mathbf{r}, t) f_{k,\text{coll}}^{1,2}(\mathbf{r}, t) + 2\pi \nabla f_{k,\text{coll}}^{1,2}(\mathbf{r}, t) \cdot \int d\mathbf{r}' f_{0,\text{coll}}^{1,2}(\mathbf{r}, t) \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2}, \tag{19}
\end{aligned}$$

With the definitions, Eqs. (14a) and (14b), we obtain for the field variables

$$\begin{aligned}
\frac{\partial}{\partial t} \rho_{\text{coll}}^{1,2} &= 2\pi \frac{\partial}{\partial t} f_{0,\text{coll}}^{1,2} \\
&= -2\pi \left[f_{0,\text{coll}}^{1,2}(\mathbf{r}, t) \right]^2 + \nabla f_{0,\text{coll}}^{1,2}(\mathbf{r}, t) \cdot \int d\mathbf{r}' f_{0,\text{coll}}^{1,2}(\mathbf{r}, t) \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2}, \tag{20}
\end{aligned}$$

and

$$\frac{\partial}{\partial t} \mathbf{p}_{\text{coll}}^{1,2} = -2\pi \rho_{\text{coll}}^{1,2} \mathbf{p}_{\text{coll}}^{1,2} + \dots \tag{21}$$

Next, we turn to the rotational diffusion, $-\omega\partial_\theta f^{1,2}$. We apply the projection operator, Eq. (13), onto the corresponding term in Eq. (7) and obtain

$$\begin{aligned}
\frac{\partial}{\partial t} f_{k,\text{rota}}^{1,2}(\mathbf{r}, t) &= -\frac{\omega}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} \partial_\theta f^{1,2}(\mathbf{r}, \theta, t) \\
&= -\frac{\omega}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} \sum_{m=-\infty}^{\infty} f_{m,\text{rota}}^{1,2}(\mathbf{r}, t) \partial_\theta e^{im\theta} \\
&= -\frac{\omega}{2\pi} \int_0^{2\pi} d\theta \sum_{m=-\infty}^{\infty} im f_{m,\text{rota}}^{1,2}(\mathbf{r}, t) e^{i(m-k)\theta} \\
&= -\frac{\omega}{2\pi} \sum_{m=-\infty}^{\infty} im f_{m,\text{rota}}^{1,2}(\mathbf{r}, t) \int_0^{2\pi} d\theta e^{i(m-k)\theta} \\
&= -\omega \sum_{m=-\infty}^{\infty} im f_{m,\text{rota}}^{1,2}(\mathbf{r}, t) \delta(m-k) \\
&= -ik\omega f_{k,\text{rota}}^{1,2}(\mathbf{r}, t)
\end{aligned} \tag{22}$$

With the definitions, Eqs. (14a) and (14b), we obtain for the field variables

$$\frac{\partial}{\partial t} \rho_{\text{rota}}^{1,2} = 0, \tag{23}$$

and

$$\frac{\partial}{\partial t} \mathbf{p}_{\text{rota}}^{1,2} = \pi \begin{bmatrix} \partial_t f_{1,\text{rota}}^{1,2} + \partial_t f_{-1,\text{rota}}^{1,2} \\ i \left(\partial_t f_{1,\text{rota}}^{1,2} - \partial_t f_{-1,\text{rota}}^{1,2} \right) \end{bmatrix} = \omega \pi \begin{bmatrix} i \left(f_{-1,\text{rota}}^{1,2} - f_{1,\text{rota}}^{1,2} \right) \\ f_{-1,\text{rota}}^{1,2} + f_{1,\text{rota}}^{1,2} \end{bmatrix} = \omega \mathbf{p}_{\text{rota},\perp}^{1,2}, \tag{24}$$

where $\mathbf{p}_{\text{rota},\perp}^{1,2} = (-p_{\text{rota},y}^{1,2}, p_{\text{rota},x}^{1,2})$.

Next, we turn to the chemotactic alignment, $-\omega\partial_\theta f^{1,2}$. We apply the projection operator, Eq. (13), onto the corresponding term in Eq. (7) and obtain

$$\frac{\partial}{\partial t} \rho_{\text{chem}}^{1,2} = 0, \tag{25}$$

and

$$\frac{\partial}{\partial t} \mathbf{p}_{\text{chem}}^{1,2} = \rho_{\text{chem}}^{1,2} \nabla c_{1,2}. \tag{26}$$

3 Behaviors

