

Chemotactic Chiral Active Matter

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December 25, 2024

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1 Models

1.1 Definitions

1.1.1 Self-propelled dynamics

$$\dot{x}_i = v \cos \theta_i , \quad (1a)$$

$$\dot{y}_i = v \sin \theta_i , \quad (1b)$$

1.1.2 Polar alignment dynamics

- 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:

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

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

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 $\omega_i \sim U(-\omega_{\max}, -\omega_{\min})$.

1.1.3 Chemotactic dynamics

Consider two chemical fields $u(\mathbf{r}, t)$, $v(\mathbf{r}, t)$ that are produced by the ensemble of two symmetrically chiral swarmalators. Swarmalators interact with the chemical field and move towards/against the regions with higher concentration, which can be described by the following equation ($i = 1, 2, \dots, N$):

$$\dot{\mathbf{r}}_i^s = v \mathbf{p}(\theta_i^s) \quad (4a)$$

$$\dot{\theta}_i^s = \omega_i^s + \alpha^s \mathbf{p}_i^s \times \nabla u + \beta^s \mathbf{p}_i^s \times \nabla v \quad (4b)$$

where α, β^s denote the ‘chemotactic’ coupling strength and $\mathbf{p}(\theta) = (\cos \theta, \sin \theta)$ is the unit vector pointing in the direction of the i -th swarmalator, $s \in \{p, n\}$ denotes the two chiral species. Here, we used the notation $\mathbf{a} \times \mathbf{b} = a_1 b_2 - a_2 b_1$.

These two fields evolve as

$$\dot{u} = k_0 \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j^p) - k_d u + D_u \nabla^2 u , \quad (5a)$$

$$\dot{v} = k_0 \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j^n) - k_d v + D_v \nabla^2 v , \quad (5b)$$

where S_+ and S_- are the sets of two chiral swarmalators, k_0 is the production rate, k_d is the decay rate, $D_{u,v}$ are the diffusion coefficients.

1.1.4 Mixed phase dynamics

$$\dot{\mathbf{r}}_i = v \mathbf{p}_i \quad (6a)$$

$$\dot{\theta}_i = \omega_i + \beta_i^u \mathbf{p}_i \times \nabla u + \beta_i^v \mathbf{p}_i \times \nabla v + \frac{K}{N} \sum_{j=1}^N f(|\mathbf{r}_j - \mathbf{r}_i|) \sin(\theta_j - \theta_i) , \quad (6b)$$

1.1.5 Chemotactic Lotka-Volterra dynamics

$$\dot{\mathbf{r}}_i^{1,2} = v \mathbf{p} \left(\theta_i^{1,2} \right) - \sum_{s \in \{1,2\}} \sum_{j=1}^N \frac{H \left(r_c - \left| \mathbf{r}_j^s - \mathbf{r}_i^{1,2} \right| \right)}{\left| \mathbf{r}_j^s - \mathbf{r}_i^{1,2} \right|^\beta} , \quad (7a)$$

$$\dot{\theta}_i^{1,2} = \alpha_{1,2} \mathbf{p} \left(\theta_i^{1,2} \right) \times \nabla c_{1,2} , \quad (7b)$$

$$\dot{c}_1 = D_1 \nabla^2 c_1 + c_1 (k_1 - k_2 c_2) \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j^1) , \quad (7c)$$

$$\dot{c}_2 = D_2 \nabla^2 c_2 + c_2 (k_3 c_1 - k_4) \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j^2) . \quad (7d)$$

2 Short format coarse graining

We begin with Eq. (2), replacing the finite coupling distance alignment interaction with a pseudopotential (the ' δ '-interaction). This substitution is justified when the interaction is sufficiently short-ranged, making the specific shape of the associated interaction potential irrelevant to the dynamics of many swarmalators. The pseudopotential is defined as:

$$\dot{\mathbf{r}}_i^c = v \mathbf{p}(\theta_i^c) , \quad (8a)$$

$$\begin{aligned} \dot{\theta}_i^c &= \omega_i^c + K \sum_{j=1} \delta(\mathbf{r}_j^c - \mathbf{r}_i^c) \sin(\theta_j^c - \theta_i^c) \\ &+ K \sum_{j=1} \delta(\mathbf{r}_j^b - \mathbf{r}_i^b) [\sin(\theta_j^b - \theta_i^b + \alpha_0) - \sin \alpha_0] , \end{aligned} \quad (8b)$$

where $c \in \{+, -\}$ is the chirality of the swarmalator i and $b = +$ if $c = -$ and vice versa. Then following [1] we derive a continuum equation of motion for the combined N -swarmalator probability density

$$\rho^c(\mathbf{r}, \theta, t) = \sum_{i=1} \rho_i^c(\mathbf{r}, \theta, t) , \quad (9)$$

where $\rho_i^c(\mathbf{r}, \theta, t) = \delta(\mathbf{r}_i^c(t) - \mathbf{r}) \delta(\theta_i^c(t) - \theta)$ is the probability density of finding i -th swarmalator at position \mathbf{r} with phase θ and chirality c at time t . Since the deterministic dynamical equation Eq. (??) conserves the number of oscillators with a given natural frequency over time, the distribution function evolves according to a continuity equation of the following form:

$$\frac{\partial \rho_i^c}{\partial t} = -\nabla \cdot (\rho_i^c v_{\mathbf{r}}) - \frac{\partial}{\partial \theta} \left(\rho_i^c v_{\theta}^{c,i} \right) . \quad (10)$$

Here, the velocity fields read

$$v_{\mathbf{r}}(\mathbf{r}, \theta, t) = v \mathbf{p}(\theta) , \quad (11a)$$

$$\begin{aligned} v_{\theta}^{c,i}(\mathbf{r}, \theta, t) &= \omega_i^c + K \int d\phi \rho^c(\mathbf{r}, \phi, t) \sin(\phi - \theta) \\ &+ K \int d\phi \rho^b(\mathbf{r}, \phi, t) [\sin(\phi - \theta + \alpha_0) - \sin \alpha_0] . \end{aligned} \quad (11b)$$

Summing Eq. (10) over the i and c indices, and using the definition of the density ρ^c in Eq. (9), we obtain

$$\begin{aligned} \frac{\partial \rho^c(\mathbf{r}, \theta, t)}{\partial t} &= -v \mathbf{p}(\theta) \cdot \nabla \rho^c(\mathbf{r}, \theta, t) - \frac{\partial}{\partial \theta} \Omega(\mathbf{r}, \theta, t) \\ &+ K \frac{\partial}{\partial \theta} \rho^c \int d\phi \rho^c(\mathbf{r}, \phi, t) \sin(\phi - \theta) \\ &+ K \frac{\partial}{\partial \theta} \rho^c \int d\phi \rho^b(\mathbf{r}, \phi, t) [\sin(\phi - \theta + \alpha_0) - \sin \alpha_0], \end{aligned} \quad (12)$$

where $\Omega(\mathbf{r}, \theta, t) = \sum_{i=1} \rho_i^c(\mathbf{r}, \theta, t) \omega_i^c$. Spatiotemporal dynamics of the ISS indicates $\forall i, c, \rho_i^c(\mathbf{r}, \theta, t) \equiv \rho_{\text{ISS}}(\mathbf{r}, \theta, t)$, which yields

$$\Omega(\mathbf{r}, \theta, t) = \rho^c(\mathbf{r}, \theta, t) \frac{(\omega_{\max} + \omega_{\min})}{2}. \quad (13)$$

Transforming Eq. (12) to Fourier space, yields an equation of motion for the Fourier modes $\varrho_k^c(\mathbf{r}, t) = \int \rho^c(\mathbf{r}, \theta, t) e^{ik\theta} d\theta$ of ρ^c :

$$\begin{aligned} \frac{\partial \varrho_k^c}{\partial t} &= -\frac{v}{2} \left[\frac{\partial}{\partial x} (\varrho_{k+1}^c + \varrho_{k-1}^c) - i \frac{\partial}{\partial y} (\varrho_{k+1}^c - \varrho_{k-1}^c) \right] \\ &- \left[\frac{ik(\omega_{\max} + \omega_{\min})}{2} \varrho_k^c - k^2 \right] \varrho_k^c \\ &+ \frac{iKk}{2\pi} \sum_{m=-\infty}^{\infty} \varrho_{k-m}^c F_{-m} \varrho_m^c \end{aligned} \quad (14)$$

3 Coarse graining

We now follow the strategy in [1] to consider the evolution of the density function for a single particle

$$\rho_i(\mathbf{r}, \theta, \omega, t) = \delta(\mathbf{r}_i(t) - \mathbf{r}) \delta(\theta_i(t) - \theta) g(\omega), \quad (15)$$

which denotes the probability of finding a particle at position \mathbf{r} , with orientation θ and natural frequency ω , where $g(\omega)$ is the time independent swarmalator frequency distribution. The density function ρ_i satisfies the continuity equation, and we shall then demonstrate how one may write a closed equation for the global density

$$\rho(\mathbf{r}, \theta, \omega, t) = \sum_{i=1}^N \rho_i(\mathbf{r}, \theta, \omega, t), \quad (16a)$$

$$\varrho(\mathbf{r}, \theta, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{r}, \theta, \omega, t) d\omega. \quad (16b)$$

The derivation follows a well known argument. Consider an arbitrary function f defined on the coordinate space of the system. Using the definition of the density it is a tautology that

$$f(\mathbf{r}_i(t), \theta_i(t), \omega_i) = \iiint d\mathbf{r} d\theta d\omega \rho_i(\mathbf{r}, \theta, \omega, t) f(\mathbf{r}, \theta, \omega). \quad (17)$$

Expanding the differential equation over the next time step δt one obtains

$$\begin{aligned} \frac{df(\mathbf{r}_i, \theta_i, \omega_i)}{dt} &= \frac{\partial f(\mathbf{r}_i, \theta_i, \omega_i)}{\partial \mathbf{r}_i} \cdot \frac{d\mathbf{r}_i}{dt} + \frac{\partial f(\mathbf{r}_i, \theta_i, \omega_i)}{\partial \theta_i} \frac{d\theta_i}{dt} + \frac{\partial f(\mathbf{r}_i, \theta_i, \omega_i)}{\partial \omega_i} \frac{d\omega_i}{dt} \\ &= \iiint d\mathbf{r} d\theta d\omega \rho_i(\mathbf{r}, \theta, \omega, t) \left(\frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \mathbf{r}} \cdot \frac{d\mathbf{r}}{dt} + \frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \theta} \frac{d\theta}{dt} + \frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \omega} \frac{d\omega}{dt} \right) \\ &= \iiint d\mathbf{r} d\theta d\omega \left(\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}} \cdot \nabla f(\mathbf{r}, \theta, \omega) + \rho_i(\mathbf{r}, \theta, \omega, t) \dot{\theta} \frac{\partial}{\partial \theta} f(\mathbf{r}, \theta, \omega) \right). \end{aligned} \quad (18)$$

Re-arranging the above integral by integration by parts we obtain

$$\frac{df(\mathbf{r}_i, \theta_i, \omega_i)}{dt} = \iiint d\mathbf{r} d\theta d\omega f(\mathbf{r}, \theta, \omega) \left(-\nabla \cdot (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\theta}) \right). \quad (19)$$

However, from (17) we may also deduce

$$\frac{df(\mathbf{r}_i, \theta_i, \omega_i)}{dt} = \iiint d\mathbf{r} d\theta d\omega f(\mathbf{r}, \theta, \omega) \frac{\partial \rho_i(\mathbf{r}, \theta, \omega, t)}{\partial t}. \quad (20)$$

Comparing equations (19) and (20) we find (using the fact that f is an arbitrary function) that

$$\frac{\partial \rho_i(\mathbf{r}, \theta, \omega, t)}{\partial t} = -\nabla \cdot (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\theta}). \quad (21)$$

We emphasize that this argument is standard and the only subtlety is that we have not carried out any thermal averaging at this point. Summing equation (21) over the i and using the definition of the density ρ we obtain

$$\frac{\partial \rho(\mathbf{r}, \theta, \omega, t)}{\partial t} = -\nabla \cdot (\rho(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} (\rho(\mathbf{r}, \theta, \omega, t) \dot{\theta}). \quad (22)$$

(1) For the case of the phase coupling dynamics, the equation for the density ρ is

$$\begin{aligned} \frac{\partial \rho(\mathbf{r}, \theta, \omega, t)}{\partial t} &= -\nabla \cdot (\rho(\mathbf{r}, \theta, \omega, t) v \mathbf{p}(\theta)) - \frac{\partial}{\partial \theta} \left(\rho(\mathbf{r}, \theta, \omega, t) \left(\omega + G \sum_{j=1}^N \sin(\theta_j - \theta) \delta(\mathbf{r}_j - \mathbf{r}) \right) \right) \\ &= -v \mathbf{p}(\theta) \cdot \nabla \rho(\mathbf{r}, \theta, \omega, t) - \omega \frac{\partial}{\partial \theta} \rho(\mathbf{r}, \theta, \omega, t) \\ &\quad - G \frac{\partial}{\partial \theta} \rho(\mathbf{r}, \theta, \omega, t) \iiint d\mathbf{r}' d\theta' d\omega' \rho(\mathbf{r}', \theta', \omega', t) \sin(\theta' - \theta) \delta(\mathbf{r}' - \mathbf{r}), \end{aligned} \quad (23)$$

where $\mathbf{p}(\theta) = (\cos \theta, \sin \theta)$. Then for the density ϱ we have

$$\begin{aligned} \frac{\partial \varrho(\mathbf{r}, \theta, t)}{\partial t} &= -v \mathbf{p}(\theta) \cdot \nabla \varrho(\mathbf{r}, \theta, t) - \frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho(\mathbf{r}, \theta, \omega, t) d\omega \\ &\quad - G \frac{\partial}{\partial \theta} \varrho(\mathbf{r}, \theta, t) \iint d\mathbf{r}' d\theta' \varrho(\mathbf{r}', \theta', t) \sin(\theta' - \theta) \delta(\mathbf{r}' - \mathbf{r}) \end{aligned} \quad (24)$$

(2) For the case of the chemotactic dynamics, the equation for the density ρ^s is

$$\begin{aligned} \frac{\partial \rho^s(\mathbf{r}, \theta, \omega, t)}{\partial t} &= -\nabla \cdot (\rho^s(\mathbf{r}, \theta, \omega, t) v \mathbf{p}(\theta)) - \frac{\partial}{\partial \theta} (\rho^s(\mathbf{r}, \theta, \omega, t) (\omega + \alpha^s \mathbf{p}(\theta) \times \nabla u + \beta^s \mathbf{p}(\theta) \times \nabla v)) \\ &= -v \mathbf{p}(\theta) \cdot \nabla \rho^s(\mathbf{r}, \theta, \omega, t) - \omega \frac{\partial}{\partial \theta} \rho^s(\mathbf{r}, \theta, \omega, t) \\ &\quad - \frac{\partial}{\partial \theta} \rho^s(\mathbf{r}, \theta, \omega, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)] \end{aligned} \quad (25)$$

where $\varphi_c = \arg(-\partial_y c + i \partial_x c)$, $c = u, v$. Then for the density ϱ^s we have

$$\begin{aligned} \frac{\partial \varrho^s(\mathbf{r}, \theta, t)}{\partial t} &= -v \mathbf{p}(\theta) \cdot \nabla \varrho^s(\mathbf{r}, \theta, t) - \frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega \\ &\quad - \frac{\partial}{\partial \theta} \varrho^s(\mathbf{r}, \theta, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)] \end{aligned} \quad (26)$$

Next, let's determine the value of item

$$\int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega. \quad (27)$$

The uniform distribution of disorder state indicates $g(\omega) = [2(\omega_{\max} - \omega_{\min})]^{-1}$, which is an ω -independent constant. Then we have

$$\int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega = \begin{cases} \frac{1}{2} \rho^s(\mathbf{r}, \theta, \omega, t) (\omega_{\max}^2 - \omega_{\min}^2), & \text{SingleChirality} \\ 0, & \text{DoubleChirality} \end{cases}. \quad (28)$$

Similarly, equation (16b) can be rewritten as

$$\varrho^s(\mathbf{r}, \theta, t) = \rho^s(\mathbf{r}, \theta, \omega, t) \int_{-\infty}^{+\infty} d\omega = \begin{cases} 2(\omega_{\max} - \omega_{\min}) \rho^s(\mathbf{r}, \theta, \omega, t), & \text{SingleChirality} \\ 0, & \text{DoubleChirality} \end{cases}. \quad (29)$$

Substituting equations (29) into (28), we obtain

3.0.1 Angular Fourier expansion of the phase-space distribution

As $\varrho(\mathbf{r}, \theta, t)$ is a periodic function of θ , it can be expanded in a Fourier series, defined as

$$\hat{\varrho}_k(\mathbf{r}, t) = \int_{-\pi}^{\pi} \varrho(\mathbf{r}, \theta, t) e^{ik\theta} d\theta. \quad (30)$$

The inverse Fourier transform is

$$\varrho(\mathbf{r}, \theta, t) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \hat{\varrho}_k(\mathbf{r}, t) e^{ik\theta}. \quad (31)$$

In this framework, the uniform distribution $\varrho_0(\mathbf{r}, \theta, t) = (2\pi)^{-1} \varrho_0^*$ corresponds to $\hat{\varrho}_k(\mathbf{r}, \omega, t) = (2\pi)^{-1} \varrho_0^*$ for $k = 0$.

Let us use as a basis of the plane the two orthogonal vectors $\mathbf{p}_1 = (1, 0)$ and $\mathbf{p}_2 = (0, 1)$. In order to obtain an evolution equation for the velocity field, we multiply equations (24) and (26) by $e(\theta)$ and integrate over θ from $-\pi$ to π . For equation (26), we obtain ($j = 1, 2$)

$$\frac{\partial}{\partial t} \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) \varrho(\mathbf{r}, \theta, t) d\theta + v \sum_{l=1}^2 \frac{\partial}{\partial \mathbf{r}_l} \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) \mathbf{e}_l(\theta) \varrho(\mathbf{r}, \theta, t) d\theta = \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) (I_{\text{freq}} + I_{\text{chem}}) d\theta, \quad (32)$$

where

$$I_{\text{freq}} = -\frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega, \quad (33a)$$

$$I_{\text{chem}} = -\frac{\partial}{\partial \theta} \varrho^s(\mathbf{r}, \theta, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)]. \quad (33b)$$

To proceed further, it is convenient to identify complex numbers with two-dimensional vectors, in such a way that $\mathbf{e}(\theta)$ is mapped onto $e^{i\theta}$. Then, in the same way, $v \hat{\varrho}_1(\mathbf{r}, t)$ is associated with the momentum field $\mathbf{w}(\mathbf{r}, t) = \rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t)$. Hence, we wish to rewrite equation (32) in such complex notations. For later use, we shall write it in a slightly more general form, replacing $e^{i\theta}$ by $e^{ik\theta}$:

$$\frac{\partial}{\partial t} \int_{-\pi}^{\pi} e^{ik\theta} \varrho(\mathbf{r}, \theta, t) d\theta + v \sum_{l=1}^2 \frac{\partial}{\partial \mathbf{r}_l} \int_{-\pi}^{\pi} e^{ik\theta} \mathbf{e}_l(\theta) \varrho(\mathbf{r}, \theta, t) d\theta = \int_{-\pi}^{\pi} e^{ik\theta} (I_{\text{freq}} + I_{\text{chem}}) d\theta. \quad (34)$$

Equation (32) is recovered for $k = 1$, up to the mapping between complex numbers and two-dimensional vectors. The first term on the left-hand side is simply $\partial \hat{\varrho}_k / \partial t$. The second term on the left-hand side can be evaluated as follows: For $l = 1, 2$ and k integer, let us define the complex quantity $Q_l^{(k)}(\mathbf{r}, t)$ as

$$Q_l^{(k)}(\mathbf{r}, t) = \int_{-\pi}^{\pi} d\theta e^{ik\theta} \mathbf{e}_l(\theta) f(\mathbf{r}, \theta, t). \quad (35)$$

The following relations are then easily obtained:

$$\begin{aligned} Q_1^{(k)}(\mathbf{r}, t) &= \frac{1}{2}[\hat{f}_{k+1}(\mathbf{r}, t) + \hat{f}_{k-1}(\mathbf{r}, t)], \\ Q_2^{(k)}(\mathbf{r}, t) &= \frac{1}{2i}[\hat{f}_{k+1}(\mathbf{r}, t) - \hat{f}_{k-1}(\mathbf{r}, t)]. \end{aligned} \tag{36}$$

The right-hand side of equation (34) is computed by inserting the Fourier series expansion (31) into equations (33). After a rather straightforward calculation, one finds

References

- [1] David S Dean. Langevin equation for the density of a system of interacting langevin processes. *Journal of Physics A: Mathematical and General*, 29(24):L613, dec 1996.