

Chemotactic Chiral Active Matter

Yichen Lu

October 23, 2024

Contents

1	Models	2
1.1	Definitions	2
1.1.1	Self-propelled dynamics	2
1.1.2	Polar alignment dynamics	2
1.1.3	Chemotactic dynamics	2
1.1.4	Mixed phase dynamics	3
1.1.5	Coarse graining	3
1.1.6	Angular Fourier expansion of the phase-space distribution	4
1.1.7	Order Parameters	5

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 ($i = 1, 2, \dots, N$):

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

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

where α, β_i^s denote the ‘chemotactic’ coupling strength and $\mathbf{p}_i^s = (\cos \theta_i^s, \sin \theta_i^s)$ 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 Coarse graining

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

$$\rho_i(\mathbf{r}, \theta, \omega, t) = \delta(\mathbf{r}_i(t) - \mathbf{r}) \delta(\theta_i(t) - \theta) g(\omega) , \quad (7)$$

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

$$\rho(\mathbf{r}, \theta, \omega, t) = \sum_{i=1}^N \rho_i(\mathbf{r}, \theta, \omega, t) , \quad (8a)$$

$$\varrho(\mathbf{r}, \theta, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{r}, \theta, \omega, t) d\omega . \quad (8b)$$

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

$$f(\mathbf{r}_i(t), \theta_i(t), \omega_i) = \iiint d\mathbf{r} d\theta d\omega \rho_i(\mathbf{r}, \theta, \omega, t) f(\mathbf{r}, \theta, \omega) . \quad (9)$$

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

$$\begin{aligned} \frac{df(\mathbf{r}_i, \theta_i, \omega_i)}{dt} &= \frac{\partial f(\mathbf{r}_i, \theta_i, \omega_i)}{\partial \mathbf{r}_i} \cdot \frac{d\mathbf{r}_i}{dt} + \frac{\partial f(\mathbf{r}_i, \theta_i, \omega_i)}{\partial \theta_i} \frac{d\theta_i}{dt} + \frac{\partial f(\mathbf{r}_i, \theta_i, \omega_i)}{\partial \omega_i} \frac{d\omega_i}{dt} \\ &= \iiint d\mathbf{r} d\theta d\omega \rho_i(\mathbf{r}, \theta, \omega, t) \left(\frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \mathbf{r}} \cdot \frac{d\mathbf{r}}{dt} + \frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \theta} \frac{d\theta}{dt} + \frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \omega} \frac{d\omega}{dt} \right) \\ &= \iiint d\mathbf{r} d\theta d\omega \left(\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}} \cdot \nabla f(\mathbf{r}, \theta, \omega) + \rho_i(\mathbf{r}, \theta, \omega, t) \dot{\theta} \frac{\partial f(\mathbf{r}, \theta, \omega)}{\partial \theta} \right) . \end{aligned} \quad (10)$$

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

$$\frac{df(\mathbf{r}_i, \theta_i, \omega_i)}{dt} = \iiint d\mathbf{r} d\theta d\omega f(\mathbf{r}, \theta, \omega) \left(-\nabla \cdot (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\theta}) \right) . \quad (11)$$

However, from (9) we may also deduce

$$\frac{df(\mathbf{r}_i, \theta_i, \omega_i)}{dt} = \iiint d\mathbf{r} d\theta d\omega f(\mathbf{r}, \theta, \omega) \frac{\partial \rho_i(\mathbf{r}, \theta, \omega, t)}{\partial t} . \quad (12)$$

Comparing equations (11) and (12) we find (using the fact that f is an arbitrary function) that

$$\frac{\partial \rho_i(\mathbf{r}, \theta, \omega, t)}{\partial t} = -\nabla \cdot (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} (\rho_i(\mathbf{r}, \theta, \omega, t) \dot{\theta}) . \quad (13)$$

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 (13) over the i and using the definition of the density ρ we obtain

$$\frac{\partial \rho(\mathbf{r}, \theta, \omega, t)}{\partial t} = -\nabla \cdot (\rho(\mathbf{r}, \theta, \omega, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} (\rho(\mathbf{r}, \theta, \omega, t) \dot{\theta}) . \quad (14)$$

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

$$\begin{aligned} \frac{\partial \rho(\mathbf{r}, \theta, \omega, t)}{\partial t} &= -\nabla \cdot (\rho(\mathbf{r}, \theta, \omega, t) v \mathbf{p}(\theta)) - \frac{\partial}{\partial \theta} \left(\rho(\mathbf{r}, \theta, \omega, t) \left(\omega + G \sum_{j=1}^N \sin(\theta_j - \theta) \delta(\mathbf{r}_j - \mathbf{r}) \right) \right) \\ &= -v \mathbf{p}(\theta) \cdot \nabla \rho(\mathbf{r}, \theta, \omega, t) - \omega \frac{\partial}{\partial \theta} \rho(\mathbf{r}, \theta, \omega, t) \\ &\quad - G \frac{\partial}{\partial \theta} \rho(\mathbf{r}, \theta, \omega, t) \iiint d\mathbf{r}' d\theta' d\omega' \rho(\mathbf{r}', \theta', \omega', t) \sin(\theta' - \theta) \delta(\mathbf{r}' - \mathbf{r}), \end{aligned} \quad (15)$$

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

$$\begin{aligned} \frac{\partial \varrho(\mathbf{r}, \theta, t)}{\partial t} &= -v \mathbf{p}(\theta) \cdot \nabla \varrho(\mathbf{r}, \theta, t) - \frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho(\mathbf{r}, \theta, \omega, t) d\omega \\ &\quad - G \frac{\partial}{\partial \theta} \varrho(\mathbf{r}, \theta, t) \iint d\mathbf{r}' d\theta' \varrho(\mathbf{r}', \theta', t) \sin(\theta' - \theta) \delta(\mathbf{r}' - \mathbf{r}) \end{aligned} \quad (16)$$

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

$$\begin{aligned} \frac{\partial \rho^s(\mathbf{r}, \theta, \omega, t)}{\partial t} &= -\nabla \cdot (\rho^s(\mathbf{r}, \theta, \omega, t) v \mathbf{p}(\theta)) - \frac{\partial}{\partial \theta} (\rho^s(\mathbf{r}, \theta, \omega, t) (\omega + \alpha^s \mathbf{p}(\theta) \times \nabla u + \beta^s \mathbf{p}(\theta) \times \nabla v)) \\ &= -v \mathbf{p}(\theta) \cdot \nabla \rho^s(\mathbf{r}, \theta, \omega, t) - \omega \frac{\partial}{\partial \theta} \rho^s(\mathbf{r}, \theta, \omega, t) \\ &\quad - \frac{\partial}{\partial \theta} \rho^s(\mathbf{r}, \theta, \omega, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)] \end{aligned} \quad (17)$$

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

$$\begin{aligned} \frac{\partial \varrho^s(\mathbf{r}, \theta, t)}{\partial t} &= -v \mathbf{p}(\theta) \cdot \nabla \varrho^s(\mathbf{r}, \theta, t) - \frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega \\ &\quad - \frac{\partial}{\partial \theta} \varrho^s(\mathbf{r}, \theta, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)] \end{aligned} \quad (18)$$

Next, let's determine the value of item

$$\int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega. \quad (19)$$

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

$$\int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega = \begin{cases} \frac{1}{2} \rho^s(\mathbf{r}, \theta, \omega, t) (\omega_{\max}^2 - \omega_{\min}^2), & \text{SingleChirality} \\ 0, & \text{DoubleChirality} \end{cases}. \quad (20)$$

Similarly, equation (8b) can be rewritten as

$$\varrho^s(\mathbf{r}, \theta, t) = \rho^s(\mathbf{r}, \theta, \omega, t) \int_{-\infty}^{+\infty} d\omega = \begin{cases} 2(\omega_{\max} - \omega_{\min}) \rho^s(\mathbf{r}, \theta, \omega, t), & \text{SingleChirality} \\ 0, & \text{DoubleChirality} \end{cases}. \quad (21)$$

Substituting equations (21) into (20), we obtain

1.1.6 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

$$\hat{\varrho}_k(\mathbf{r}, t) = \int_{-\pi}^{\pi} \varrho(\mathbf{r}, \theta, t) e^{ik\theta} d\theta. \quad (22)$$

The inverse Fourier transform is

$$\varrho(\mathbf{r}, \theta, t) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \hat{\varrho}_k(\mathbf{r}, t) e^{ik\theta}. \quad (23)$$

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 (16) and (18) by $e^{i\theta}$ and integrate over θ from $-\pi$ to π . For equation (18), we obtain ($j = 1, 2$)

$$\frac{\partial}{\partial t} \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) \varrho(\mathbf{r}, \theta, t) d\theta + v \sum_{l=1}^2 \frac{\partial}{\partial \mathbf{r}_l} \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) \mathbf{e}_l(\theta) \varrho(\mathbf{r}, \theta, t) d\theta = \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) (I_{\text{freq}} + I_{\text{chem}}) d\theta, \quad (24)$$

where

$$I_{\text{freq}} = -\frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega, \quad (25a)$$

$$I_{\text{chem}} = -\frac{\partial}{\partial \theta} \varrho^s(\mathbf{r}, \theta, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)]. \quad (25b)$$

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 (24) in such complex notations. For later use, we shall write it in a slightly more general form, replacing $e^{i\theta}$ by $e^{ik\theta}$:

$$\frac{\partial}{\partial t} \int_{-\pi}^{\pi} e^{ik\theta} \varrho(\mathbf{r}, \theta, t) d\theta + v \sum_{l=1}^2 \frac{\partial}{\partial \mathbf{r}_l} \int_{-\pi}^{\pi} e^{ik\theta} \mathbf{e}_l(\theta) \varrho(\mathbf{r}, \theta, t) d\theta = \int_{-\pi}^{\pi} e^{ik\theta} (I_{\text{freq}} + I_{\text{chem}}) d\theta. \quad (26)$$

Equation (24) 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

$$Q_l^{(k)}(\mathbf{r}, t) = \int_{-\pi}^{\pi} d\theta e^{ik\theta} \mathbf{e}_l(\theta) f(\mathbf{r}, \theta, t). \quad (27)$$

The following relations are then easily obtained:

$$\begin{aligned} Q_1^{(k)}(\mathbf{r}, t) &= \frac{1}{2} [\hat{f}_{k+1}(\mathbf{r}, t) + \hat{f}_{k-1}(\mathbf{r}, t)], \\ Q_2^{(k)}(\mathbf{r}, t) &= \frac{1}{2i} [\hat{f}_{k+1}(\mathbf{r}, t) - \hat{f}_{k-1}(\mathbf{r}, t)]. \end{aligned} \quad (28)$$

The right-hand side of equation (26) is computed by inserting the Fourier series expansion (23) into equations (25). After a rather straightforward calculation, one finds

1.1.7 Order Parameters

Some order parameters can be introduced to measure the level of spatiotemporal coordinations among swarms and distinguish the different collective states of the system. Firstly, the usual order parameter to measure the global phase synchronization among swarms can be defined as the following complex function:

$$Z(t) = R(t) e^{i\psi(t)} = \frac{1}{N} \sum_{j=1}^N e^{i\theta_j(t)}, \quad (29)$$

where $i = \sqrt{-1}$. The degree modulus $R(t) = |Z(t)|$ is the absolute value of the mean of the complex numbers $e^{i\theta_i}$, which can be interpreted as the absolute value of the mean normalized velocity of all

swarmalators. When $R \approx 1$, swarmalators are fully phase synchronized, and when $R \approx 0$, swarmalators are phase incoherent.

The order parameter R is not enough to measure the emergence of partial clustered phase synchronization of swarmalators. Therefore a local order parameter can be introduced to measure the clustered synchronization:

$$Z_c^k(t) = R_c^k(t) e^{i\psi_c^k(t)} = \frac{1}{|C_k(t)|} \sum_{j \in C_k(t)} e^{i\theta_j(t)}, \quad (30)$$

N_c is the number of clusters, C_k is the k -th cluster, and $|C_k|$ is the number of swarmalators in the k -th cluster (see the details of the determination of clusters in Appendix). An averaged global order parameter can be further introduced as

$$R_c(t) = \frac{1}{N_c(t)} \sum_{k=1}^{N_c(t)} R_c^k(t). \quad (31)$$

As the swarmalators within the k -th cluster are fully synchronized, $R_c^k \approx 1$, and therefore also globally $R_c \approx 1$.

Except the study for phase coherence, other order parameters can be defined to further describe the locking of the frequencies of swarmalators under the chiral condition. One first introduce a cluster frequency difference to measure the chiral synchronizability of swarmalators within a cluster as

$$\Delta\Omega_c^k = \frac{1}{|C_k|^2} \sum_{i,j \in C_k} \left(\langle \dot{\theta}_i \rangle - \langle \dot{\theta}_j \rangle \right)^2, \quad (32)$$

where $\langle \dot{\theta}_i \rangle$ is the average phase velocity of the i -th cluster, which can be defined by

$$\langle \dot{\theta}_i \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{t_0}^{t_0+T} \dot{\theta}_i(t) dt. \quad (33)$$

Then a global frequency difference of clusters is

$$\Delta\Omega_c = \frac{1}{N_c} \sum_{k=1}^{N_c} \Delta\Omega_c^k. \quad (34)$$

For any cluster k , one can assume that $\langle \dot{\theta}_i \rangle \in [a, b]$. Then the expectation of $\Delta\Omega_c^k$ can be calculated as

$$E(\Delta\Omega_c^k) = 2E\left(\langle \dot{\theta}_i \rangle^2\right) - 2E\left(\langle \dot{\theta}_i \rangle \langle \dot{\theta}_j \rangle\right). \quad (35)$$

For different cases of bounds, the value is

$$E(\Delta\Omega_c^k) \begin{cases} = 0, & ab \geq 0 \\ > 0, & ab < 0 \end{cases} \quad (36)$$

Therefore, if $n \rightarrow \infty$ and the average phase velocities of swarmalators within the cluster are all positive, all negative, $\Delta\Omega_c^k \approx 0$, and we name this case as the *chirality-locked cluster*. Otherwise, $\Delta\Omega_c^k > 0$. When $\Delta\Omega_c \approx 0$, the swarmalators will organize to form several clusters, within each cluster swarmalators are chirality-locked. Note that chirality locking is different from phase locking, as the chirality-locked swarmalators can have different phase velocities, which also means that they can have different rotational radii. Obviously, chirality locking is a more loose condition than phase locking.

All the above order parameters measure different aspects of coordination in the phases of swarmalators. Because the phase variable describes the alignment of a swarmalator, various synchrony states imply the motion alignment of swarmalators in the swarming dynamics. In the following discussions, we further define an order parameter to depict the spatial swarming ordering:

$$N_r(t) = \frac{1}{N} \frac{1}{N_c(t)} \sum_{k=1}^{N_c(t)} |C_k(t)|. \quad (37)$$

N_r is the relative number of swarmalators in the clusters, which measures the spatial condensation of swarmalators. When $N_r \approx 1$, swarmalators are fully spatially condensed, and when $N_r \approx 0$, swarmalators are spatially dispersed.

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.