Chemotactic Chiral Active Matter

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1 The Model

Swarmalators have a spatial position $\mathbf{r}_i = (x_i, y_i)$ and an internal phase θ_i which evolve according to equations:

$$\dot{\mathbf{r}}_i = v\mathbf{p}(\theta_i) \ , \tag{1a}$$

$$\dot{\theta}_i = \omega_i + K \sum_{j \in A_i} [\sin(\theta_j - \theta_i + \alpha_{ij}) - \sin\alpha_{ij}] \ , \tag{1b}$$

for $i = 1, 2, \ldots, N$. Here in Eq. (1a), $\mathbf{p}(\theta) = (\cos\theta, \sin\theta)$, which means each swarmalator rotates with a constant speed v in the direction of its instantaneous phase $\theta_i(t)$. As per Eq. (1b), the sum runs over neighbors within a coupling radius d_0 around swarmalator i:

$$A_i(t) = \{j \mid |\mathbf{r}_i(t) - \mathbf{r}_j(t)| \leqslant d_0\} \ , \tag{2}$$

λ is the coupling strength, and ω_i is the natural frequency of the i-th swarmalator. This means that a swarmalator will rotate with the angular velocity $|\omega_i|$ in the absence of mutual coupling (K), and the sign of ω_i represents the direction of rotation, namely, the tribute of the chirality of the i-th swarmalator. A positive (negative) chirality (ω) describes the counterclockwise (clockwise) rotations of the swarmalator in space. Here, we consider parallels with two types of chiralities with both positive and negative natural frequencies uniformly distributed in two symmetric regimes, namely, half of the swarmalators possess positive natural frequencies $\omega_i \sim U(\omega_{\min}, \omega_{\max})$ and the other half have negative natural frequencies $\omega_i \sim U(-\omega_{\max}, -\omega_{\min})$, where $\omega_{\min,\max} > 0$.

Additionally, α_{ij} is the phase frustration between two neighboring swarmalators, which is defined as:

$$\alpha_{ij} = \begin{cases} \alpha_0, & \omega_i\omega_j < 0 \\ 0, & \omega_i\omega_j \geqslant 0 \end{cases} \tag{3}$$

When $\alpha_0 = 0$, the dynamics reduces to the normal chiral model.

For simplicity, we assume that swarmalators are initially distributed uniformly in a two-dimensional $L \times L$ square with periodic boundary conditions. When two swarmalators are on opposite sides of the square, the absolute value of the difference between at least one of their coordinates is larger than $L/2$. In this case, we take the minimum distance between them, which is the relative distance between the two points in the periodic boundary conditions.

Some order parameters can be introduced to measure the level of spatiotemporal coordination among swarmalators and distinguish the different collective states of the system. Firstly, the usual order parameter to measure the chiral phase separation among swarmalators can be defined as:

$$S(t) = \frac{1}{N} \sum_{i=1}^{N} \frac{\sum_{j \in A_i} H(\omega_i\omega_j)}{|A_i(t)|} \ , \tag{4}$$

where $H(x) = (x > 0)$ is the Heaviside step function. $S(t)$ is the fraction of the pairs of neighboring swarmalators with the same chirality. When $S(t) = 1$, all the neighboring pairs of swarmalators have the same chirality, and the system is in a completely phase-separated state. When $S(t) < 1$, the system is in a mixed state.

We conducted numerical simulations to investigate the performance and characteristics of our system under various conditions. All the numerical simulations of the model Eq. (1) were run on Python using Euler integration with box size of $L = 10$, population sizes of $N = 500, 1000$ for single/double-chiral swarmalators, respectively, maximum and minimum absolute values of natural frequencies $\omega_{\max} = 3$, $\omega_{\min} = 1$, coupling strength λ in $[0.01, 0.1] \cup [0.1, 1]$ with step length 0.1, 0.05, respectively, action radius of d_0 in $[0.1, 1] \cup [1, 2]$ with step length 0.05, 0.5, respectively, a time step $\Delta t = 0.01$, and total number of iterations of $T = 60000$. Unless otherwise stated, each data point of order parameters R, R_c and N_r was collected by averaging last 1000 time steps of the simulation to discard the transients.
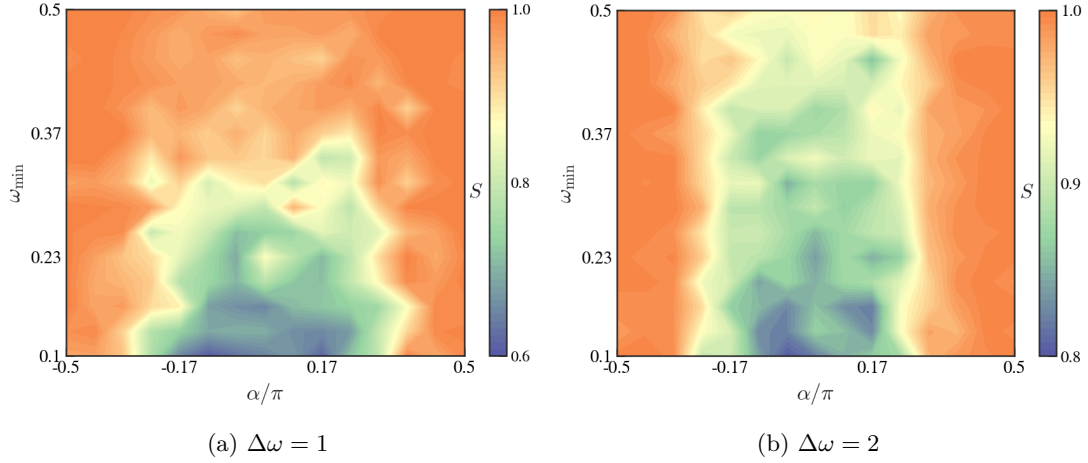
Figure 1: Phase diagrams of the system with different natural frequency differences $\Delta\omega$. The color represents the order parameter S of the system.

2   Frustration-enhanced phase separation

3   Coarse grained equations and phase diagrams

We begin with Eq. (1), 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:

$$\dot{\mathbf{r}}_i^c = v\mathbf{p}\left(\theta_i^c\right) \ , \tag{5a}$$

$$\dot{\theta}_i^c = \omega_i^c + K\sum_{j=1}\delta\left(\mathbf{r}_j^c - \mathbf{r}_i^c\right)\sin\left(\theta_j^c - \theta_i^c\right)$$

$$+ K\sum_{j=1}\delta\left(\mathbf{r}_j^b - \mathbf{r}_i^b\right)\left[\sin\left(\theta_j^b - \theta_i^b + \alpha_0\right) - \sin\alpha_0\right] \ , \tag{5b}$$

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

$$\rho^c\left(\mathbf{r},\theta,t\right) = \sum_{i=1}\rho_i^c\left(\mathbf{r},\theta,t\right) \ , \tag{6}$$

where $\rho_i^c\left(\mathbf{r},\theta,t\right) = \delta\left(\mathbf{r}_i^c\left(t\right) - \mathbf{r}\right)\delta\left(\theta_i^c\left(t\right) - \theta\right)$ 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. (1) 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:

$$\frac{\partial\rho_i^c}{\partial t} = -\nabla\cdot\left(\rho_i^c v_{\mathbf{r}}\right) - \frac{\partial}{\partial\theta}\left(\rho_i^c v_\theta^{c,i}\right) \ . \tag{7}$$

Here, the velocity fields read

$$v_{\mathbf{r}}\left(\mathbf{r},\theta,t\right) = v\mathbf{p}\left(\theta\right) \ , \tag{8a}$$

$$v_\theta^{c,i}\left(\mathbf{r},\theta,t\right) = \omega_i^c + K\int\mathrm{d}\phi\rho^c\left(\mathbf{r},\phi,t\right)\sin\left(\phi - \theta\right)$$

$$+ K\int\mathrm{d}\phi\rho^b\left(\mathbf{r},\phi,t\right)\left[\sin\left(\phi - \theta + \alpha_0\right) - \sin\alpha_0\right] \ . \tag{8b}$$

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Summing Eq. (7) over the i and c indices, and using the definition of the density ρ^c in Eq. (6), we obtain

$$
\begin{aligned}
\frac{\partial \rho^c (\mathbf{r}, \theta, t)}{\partial t} = & -v\mathbf{p}(\theta) \cdot \nabla \rho^c (\mathbf{r}, \theta, t) - \frac{\partial}{\partial \theta} \Omega (\mathbf{r}, \theta, t) \\
& + K \frac{\partial}{\partial \theta} \rho^c \int \mathrm{d}\phi \rho^c (\mathbf{r}, \phi, t) \sin (\phi - \theta) \\
& + K \frac{\partial}{\partial \theta} \rho^c \int \mathrm{d}\phi \rho^b (\mathbf{r}, \phi, t) [\sin (\phi - \theta + \alpha_0) - \sin \alpha_0] ,
\end{aligned}
\tag{9}
$$

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 $\forall i, c, \rho_i^c (\mathbf{r}, \theta, t) \equiv \rho_{\mathrm{ISS}} (\mathbf{r}, \theta, t)$, which yields

$$
\Omega (\mathbf{r}, \theta, t) = \rho^c (\mathbf{r}, \theta, t) \frac{(\omega_{\max} + \omega_{\min})}{2} .
\tag{10}
$$

Transforming Eq. (9) to Fourier space, yields an equation of motion for the Fourier modes $\varrho_k^c (\mathbf{r}, t) = \int \rho^c (\mathbf{r}, \theta, t) \, \mathrm{e}^{\mathrm{i}k\theta} \mathrm{d}\theta$ of ρ^c:

$$
\begin{aligned}
\frac{\partial \varrho_k^c}{\partial t} = & -\frac{v}{2} \left[\frac{\partial}{\partial x} \left(\varrho_{k+1}^c + \varrho_{k-1}^c \right) - \mathrm{i} \frac{\partial}{\partial y} \left(\varrho_{k+1}^c - \varrho_{k-1}^c \right) \right] \\
& - \left[\frac{\mathrm{i}k (\omega_{\max} + \omega_{\min})}{2} \varrho_k^c - k^2 \right] \varrho_k^c \\
& + \frac{\mathrm{i}Kk}{2\pi} \sum_{m=-\infty}^{\infty} \varrho_{k-m}^c F_{-m} \varrho_m^c
\end{aligned}
\tag{11}
$$

3.1 Coarse graining

We now follow the strategy in [1] to consider the evolution of the density function for i-th particle

$$
\rho_i (\mathbf{r}, \theta, t) = \delta (\mathbf{r}_i (t) - \mathbf{r}) \delta (\theta_i (t) - \theta) ,
\tag{12}
$$

which denotes the probability of finding i-th particle at position $\mathbf{r}$, with orientation θ. 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

$$
\rho (\mathbf{r}, \theta, t) = \sum_{i=1}^{N} \rho_i (\mathbf{r}, \theta, t) ,
\tag{13}
$$

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

$$
f (\mathbf{r}_i (t), \theta_i (t)) = \int \mathrm{d}\mathbf{r} \mathrm{d}\theta \rho_i (\mathbf{r}, \theta, t) f (\mathbf{r}, \theta) .
\tag{14}
$$

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

$$
\begin{aligned}
\frac{\mathrm{d} f (\mathbf{r}_i, \theta_i)}{\mathrm{d}t} = & \frac{\partial f (\mathbf{r}_i, \theta_i)}{\partial \mathbf{r}_i} \cdot \frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} + \frac{\partial f (\mathbf{r}_i, \theta_i)}{\partial \theta_i} \frac{\mathrm{d}\theta_i}{\mathrm{d}t} \\
= & \int \mathrm{d}\mathbf{r} \mathrm{d}\theta \rho_i (\mathbf{r}, \theta, t) \left(\frac{\partial f (\mathbf{r}, \theta)}{\partial \mathbf{r}} \cdot \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} + \frac{\partial f (\mathbf{r}, \theta)}{\partial \theta} \frac{\mathrm{d}\theta}{\mathrm{d}t} \right) \\
= & \iiint \mathrm{d}\mathbf{r} \mathrm{d}\theta \left(\rho_i (\mathbf{r}, \theta, t) \dot{\mathbf{r}} \cdot \nabla f (\mathbf{r}, \theta) + \rho_i (\mathbf{r}, \theta, t) \dot{\theta} \frac{\partial}{\partial \theta} f (\mathbf{r}, \theta) \right) .
\end{aligned}
\tag{15}
$$

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

$$
\frac{\mathrm{d} f (\mathbf{r}_i, \theta_i)}{\mathrm{d}t} = \int \mathrm{d}\mathbf{r} \mathrm{d}\theta f (\mathbf{r}, \theta) \left(-\nabla \cdot (\rho_i (\mathbf{r}, \theta, t) \dot{\mathbf{r}}) - \frac{\partial}{\partial \theta} \left(\rho_i (\mathbf{r}, \theta, t) \dot{\theta} \right) \right) ,
\tag{16}
$$

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However, from (14) we may also deduce

$$\frac{\mathrm{d}f\left(\mathbf{r}_i, \theta_i\right)}{\mathrm{d}t} = \iiint \mathrm{d}\mathbf{r}\mathrm{d}\theta f\left(\mathbf{r}, \theta\right) \frac{\partial \rho_i\left(\mathbf{r}, \theta, t\right)}{\partial t} . \tag{17}$$

Comparing equations (16) and (17) we find (using the fact that f is an arbitrary function) that

$$\frac{\partial \rho_i\left(\mathbf{r}, \theta, t\right)}{\partial t} = -\nabla \cdot \left(\rho_i\left(\mathbf{r}, \theta, t\right) \dot{\mathbf{r}}\right) - \frac{\partial}{\partial \theta}\left(\rho_i\left(\mathbf{r}, \theta, t\right) \dot{\theta}\right) . \tag{18}$$

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

$$\frac{\partial \rho\left(\mathbf{r}, \theta, \omega, t\right)}{\partial t} = -\nabla \cdot \left(\rho\left(\mathbf{r}, \theta, \omega, t\right) \dot{\mathbf{r}}\right) - \frac{\partial}{\partial \theta}\left(\rho\left(\mathbf{r}, \theta, \omega, t\right) \dot{\theta}\right) . \tag{19}$$

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

$$\begin{aligned}
\frac{\partial \rho\left(\mathbf{r}, \theta, \omega, t\right)}{\partial t} &= -\nabla \cdot \left(\rho\left(\mathbf{r}, \theta, \omega, t\right) v\mathbf{p}\left(\theta\right)\right) - \frac{\partial}{\partial \theta}\left(\rho\left(\mathbf{r}, \theta, \omega, t\right)\left(\omega + G\sum_{j=1}^{N} \sin\left(\theta_j - \theta\right) \delta\left(\mathbf{r}_j - \mathbf{r}\right)\right)\right) \\
&= -v\mathbf{p}\left(\theta\right) \cdot \nabla \rho\left(\mathbf{r}, \theta, \omega, t\right) - \omega\frac{\partial}{\partial \theta}\rho\left(\mathbf{r}, \theta, \omega, t\right) \\
&\quad - G\frac{\partial}{\partial \theta}\rho\left(\mathbf{r}, \theta, \omega, t\right) \iiint \mathrm{d}\mathbf{r}'\mathrm{d}\theta'\mathrm{d}\omega' \rho\left(\mathbf{r}', \theta', \omega', t\right) \sin\left(\theta' - \theta\right) \delta\left(\mathbf{r}' - \mathbf{r}\right) ,
\end{aligned} \tag{20}$$

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

$$\begin{aligned}
\frac{\partial \varrho\left(\mathbf{r}, \theta, t\right)}{\partial t} &= -v\mathbf{p}\left(\theta\right) \cdot \nabla \varrho\left(\mathbf{r}, \theta, t\right) - \frac{\partial}{\partial \theta}\int_{-\infty}^{+\infty} \omega\rho\left(\mathbf{r}, \theta, \omega, t\right) \mathrm{d}\omega \\
&\quad - G\frac{\partial}{\partial \theta}\varrho\left(\mathbf{r}, \theta, t\right) \iint \mathrm{d}\mathbf{r}'\mathrm{d}\theta' \varrho\left(\mathbf{r}', \theta', t\right) \sin\left(\theta' - \theta\right) \delta\left(\mathbf{r}' - \mathbf{r}\right)
\end{aligned} \tag{21}$$

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

$$\begin{aligned}
\frac{\partial \rho^s\left(\mathbf{r}, \theta, \omega, t\right)}{\partial t} &= -\nabla \cdot \left(\rho^s\left(\mathbf{r}, \theta, \omega, t\right) v\mathbf{p}\left(\theta\right)\right) - \frac{\partial}{\partial \theta}\left(\rho^s\left(\mathbf{r}, \theta, \omega, t\right)\left(\omega + \alpha^s\mathbf{p}\left(\theta\right) \times \nabla u + \beta^s\mathbf{p}\left(\theta\right) \times \nabla v\right)\right) \\
&= -v\mathbf{p}\left(\theta\right) \cdot \nabla \rho^s\left(\mathbf{r}, \theta, \omega, t\right) - \omega\frac{\partial}{\partial \theta}\rho^s\left(\mathbf{r}, \theta, \omega, t\right) \\
&\quad - \frac{\partial}{\partial \theta}\rho^s\left(\mathbf{r}, \theta, \omega, t\right) \alpha^s\left[|\nabla u|\sin\left(\theta + \varphi_u\right) + |\nabla v|\sin\left(\theta + \varphi_v\right)\right]
\end{aligned} \tag{22}$$

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

$$\begin{aligned}
\frac{\partial \varrho^s\left(\mathbf{r}, \theta, t\right)}{\partial t} &= -v\mathbf{p}\left(\theta\right) \cdot \nabla \varrho^s\left(\mathbf{r}, \theta, t\right) - \frac{\partial}{\partial \theta}\int_{-\infty}^{+\infty} \omega\rho^s\left(\mathbf{r}, \theta, \omega, t\right) \mathrm{d}\omega \\
&\quad - \frac{\partial}{\partial \theta}\varrho^s\left(\mathbf{r}, \theta, t\right) \alpha^s\left[|\nabla u|\sin\left(\theta + \varphi_u\right) + |\nabla v|\sin\left(\theta + \varphi_v\right)\right]
\end{aligned} \tag{23}$$

Next, let's determine the value of item

$$\int_{-\infty}^{+\infty} \omega\rho^s\left(\mathbf{r}, \theta, \omega, t\right) \mathrm{d}\omega . \tag{24}$$

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

$$\int_{-\infty}^{+\infty} \omega\rho^s\left(\mathbf{r}, \theta, \omega, t\right) \mathrm{d}\omega = \begin{cases} \frac{1}{2}\rho^s\left(\mathbf{r}, \theta, \omega, t\right)\left(\omega_{\max}^2 - \omega_{\min}^2\right), & \mathrm{SingleChirality} \\ 0, & \mathrm{DoubleChirality} \end{cases} . \tag{25}$$

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Similarly, equation (13) can be rewritten as

$$\varrho^s(\mathbf{r}, \theta, t) = \rho^s(\mathbf{r}, \theta, \omega, t) \int_{-\infty}^{+\infty} d\omega = \begin{cases} 2(\omega_{\max} - \omega_{\min}) \rho^s(\mathbf{r}, \theta, \omega, t), & \text{SingleChirality} \\ 0, & \text{DoubleChirality} \end{cases}. \tag{26}$$

Substituting equations (26) into (25), we obtain

3.1.1 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

$$\hat{\varrho}_k(\mathbf{r}, t) = \int_{-\pi}^{\pi} \varrho(\mathbf{r}, \theta, t) e^{ik\theta} d\theta. \tag{27}$$

The inverse Fourier transform is

$$\varrho(\mathbf{r}, \theta, t) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \hat{\varrho}_k(\mathbf{r}, t) e^{ik\theta}. \tag{28}$$

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 (21) and (23) by $e(\theta)$ and integrate over θ from $-\pi$ to π. For equation (23), we obtain ($j = 1, 2$)

$$\frac{\partial}{\partial t} \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) \varrho(\mathbf{r}, \theta, t) d\theta + v \sum_{l=1}^{2} \frac{\partial}{\partial \mathbf{r}_l} \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) \mathbf{e}_l(\theta) \varrho(\mathbf{r}, \theta, t) d\theta = \int_{-\pi}^{\pi} \mathbf{e}_j(\theta) (I_{\text{freq}} + I_{\text{chem}}) d\theta, \tag{29}$$

where

$$I_{\text{freq}} = -\frac{\partial}{\partial \theta} \int_{-\infty}^{+\infty} \omega \rho^s(\mathbf{r}, \theta, \omega, t) d\omega, \tag{30a}$$

$$I_{\text{chem}} = -\frac{\partial}{\partial \theta} \varrho^s(\mathbf{r}, \theta, t) \alpha^s [|\nabla u| \sin(\theta + \varphi_u) + |\nabla v| \sin(\theta + \varphi_v)]. \tag{30b}$$

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

$$\frac{\partial}{\partial t} \int_{-\pi}^{\pi} e^{ik\theta} \varrho(\mathbf{r}, \theta, t) d\theta + v \sum_{l=1}^{2} \frac{\partial}{\partial \mathbf{r}_l} \int_{-\pi}^{\pi} e^{ik\theta} \mathbf{e}_l(\theta) \varrho(\mathbf{r}, \theta, t) d\theta = \int_{-\pi}^{\pi} e^{ik\theta} (I_{\text{freq}} + I_{\text{chem}}) d\theta. \tag{31}$$

Equation (29) 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

$$Q_l^{(k)}(\mathbf{r}, t) = \int_{-\pi}^{\pi} d\theta e^{ik\theta} e_l(\theta) \varrho(\mathbf{r}, \theta, t). \tag{32}$$

The following relations are then easily obtained:

$$Q_1^{(k)}(\mathbf{r}, t) = \frac{1}{2} [\hat{\varrho}_{k+1}(\mathbf{r}, t) + \hat{\varrho}_{k-1}(\mathbf{r}, t)],$$
$$Q_2^{(k)}(\mathbf{r}, t) = \frac{1}{2i} [\hat{\varrho}_{k+1}(\mathbf{r}, t) - \hat{\varrho}_{k-1}(\mathbf{r}, t)]. \tag{33}$$

The right-hand side of equation (31) is computed by inserting the Fourier series expansion (28) into equations (30). After a rather straightforward calculation, one finds

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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.