

Active Matter



Flocking, Self-propelled, Chiral & Chemotactic

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

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

for $i = 1, 2, \dots, N$. Here, \mathbf{r}_i and θ_i is the position and orientation of the i -th particle, respectively, v is the self-propulsion velocity, $\mathbf{p}(\theta_i) = (\cos \theta_i, \sin \theta_i)$ is the instantaneous unit orientation, ω_i is the natural frequency, $H(\Delta \theta_{ij}, \Delta \mathbf{r}_{ij})$ is the coupling function between partials, $\Delta \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\Delta \theta_{ij} = \theta_i - \theta_j$.

$$\mathbf{I}(\Delta \mathbf{r}) = \frac{\Delta \mathbf{r}}{|\Delta \mathbf{r}|} k(R_r - |\Delta \mathbf{r}|) \Theta(R_r - |\Delta \mathbf{r}|) \quad (2)$$

$$H(\Delta \theta, \Delta \mathbf{r}) = K \sin(\Delta \theta) \Theta(R_\theta - |\Delta \mathbf{r}|) \quad (3)$$

In the thermodynamic limit $N \rightarrow \infty$, the agent-based model gives rise to the following continuum form:

$$\frac{\partial}{\partial t} f(\mathbf{r}, \theta, t) = -\frac{\partial}{\partial \theta} (f v_\theta) - \nabla \cdot (f \mathbf{v}_\mathbf{r}) , \quad (4)$$

where $f(\mathbf{r}, \theta, t)$ is the probability density of particles at position \mathbf{r} and orientation θ at time t , and $\mathbf{v}_\mathbf{r}$ and v_θ are the velocity fields in the position and orientation space, respectively. The velocity fields are given by

$$v_\theta(\mathbf{r}, \theta, t) = \omega + K \int d\theta' f(\mathbf{r}, \theta', t) \sin(\theta' - \theta) , \quad (5a)$$

$$\mathbf{v}_\mathbf{r}(\mathbf{r}, \theta, t) = v\mathbf{p}(\theta) + \int d\theta' d\mathbf{r}' f(\mathbf{r}', \theta', t) \mathbf{I}(\mathbf{r} - \mathbf{r}') . \quad (5b)$$

By substituting Eqs. (5) into Eq. (4), we obtain

$$\begin{aligned} \frac{\partial}{\partial t} f(\mathbf{r}, \theta, t) = & -v\mathbf{p}(\theta) \cdot \nabla f - \nabla \cdot \left[f(\mathbf{r}, \theta, t) \int d\theta' d\mathbf{r}' f(\mathbf{r}', \theta', t) \mathbf{I}(\mathbf{r} - \mathbf{r}') \right] \\ & - \omega \partial_\theta f - K \partial_\theta \left[f(\mathbf{r}, \theta, t) \int d\theta' f(\mathbf{r}, \theta', t) \sin(\theta' - \theta) \right] , \end{aligned} \quad (6)$$

$$\begin{aligned} \frac{\partial}{\partial t} f(\mathbf{r}, \theta, t) = & -v\mathbf{p}(\theta) \cdot \nabla f - \nabla \cdot \left[f(\mathbf{r}, \theta, t) \int d\theta' d\mathbf{r}' f(\mathbf{r}', \theta', t) \mathbf{I}(\mathbf{r} - \mathbf{r}') \right] \\ & - \omega \partial_{\theta} f - K \partial_{\theta} \int d\theta' d\mathbf{r}' f(\mathbf{r}, \theta', t) \sin(\theta' - \theta), \end{aligned} \quad (7)$$

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

$$f(\mathbf{r}, \theta, t) = \sum_{k=-\infty}^{\infty} f_k(\mathbf{r}, t) e^{ik\theta}, \quad (8)$$

with the projection

$$f_k(\mathbf{r}, t) = \frac{1}{2\pi} \int d\theta f(\mathbf{r}, \theta, t) e^{-ik\theta}, \quad (9)$$

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

$$\rho(\mathbf{r}, t) \equiv \int_0^{2\pi} d\theta f(\mathbf{r}, \theta, t) = 2\pi f_0(\mathbf{r}, t) \quad (10a)$$

$$\begin{aligned} p(\mathbf{r}, t) &\equiv \int_0^{2\pi} d\theta \mathbf{p}(\theta) f(\mathbf{r}, \theta, t) \\ &= \int_0^{2\pi} d\theta \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} f(\mathbf{r}, \theta, t) = \int_0^{2\pi} d\theta \frac{1}{2} \begin{bmatrix} e^{i\theta} + e^{-i\theta} \\ i(e^{-i\theta} - e^{i\theta}) \end{bmatrix} f(\mathbf{r}, \theta, t) \\ &= \pi \begin{bmatrix} f_1(\mathbf{r}, t) + f_{-1}(\mathbf{r}, t) \\ i(f_1(\mathbf{r}, t) - f_{-1}(\mathbf{r}, t)) \end{bmatrix} \end{aligned} \quad (10b)$$

In the following, the different contributions to the continuum model, are analyzed separately.

Firstly, in order to derive expressions for the self-propulsion, $-v\mathbf{p}(\theta) \cdot \nabla f$, we apply the projection operator, $f_k(\mathbf{r}, t) = \frac{1}{2\pi} \int d\theta f(\mathbf{r}, \theta, t) e^{-ik\theta}$, onto the corresponding term and obtain

$$\begin{aligned}
 \frac{\partial}{\partial t} f_{k,\text{prop}} &= \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} [-v\mathbf{p}(\theta) \cdot \nabla f] \\
 &= -\frac{v}{4\pi} \int_0^{2\pi} d\theta \left\{ e^{-ik\theta} \left[\partial_x \sum_{m=-\infty}^{\infty} f_m (e^{i(m+1)\theta} + e^{i(m-1)\theta}) \right. \right. \\
 &\quad \left. \left. + i\partial_y \sum_{k=-\infty}^{\infty} f_m (e^{i(m-1)\theta} - e^{i(m+1)\theta}) \right] \right\} \quad (11) \\
 &= -\frac{v}{2} \left\{ \partial_x \sum_{m=-\infty}^{\infty} f_m [\delta(m-k+1) + \delta(m-k-1)] \right. \\
 &\quad \left. + i\partial_y \sum_{k=-\infty}^{\infty} f_m [\delta(m-k-1) - \delta(m-k+1)] \right\}.
 \end{aligned}$$

With the definitions of $\rho(\mathbf{r}, t)$ and $p(\mathbf{r}, t)$, we obtain for the field variables

$$\begin{aligned}
 \frac{\partial}{\partial t} \rho_{\text{prop}} &= 2\pi \frac{\partial}{\partial t} f_{0,\text{prop}} \\
 &= -v\pi \left[\partial_x \sum_{m=-\infty}^{\infty} f_m (\delta_{m+1} + \delta_{m-1}) + i\partial_y \sum_{k=-\infty}^{\infty} f_m (\delta_{m-1} - \delta_{m+1}) \right] \\
 &= -v\pi [\partial_x (f_{-1} + f_1) + i\partial_y (f_1 - f_{-1})] \\
 &= -v\nabla \cdot p_{\text{prop}} ,
 \end{aligned} \tag{12}$$

and because of

$$\partial_t f_1 = -\frac{v}{2} [\partial_x (f_0 + f_2) + i\partial_y (f_2 - f_0)] , \tag{13a}$$

$$\partial_t f_{-1} = -\frac{v}{2} [\partial_x (f_0 + f_2) + i\partial_y (f_0 - f_2)] , \tag{13b}$$

we have

$$\frac{\partial}{\partial t} p_{\text{prop}} = \pi \begin{bmatrix} -v\partial_x (f_0 + f_2) \\ v\partial_y (f_2 - f_0) \end{bmatrix} \approx -\frac{v}{2} \begin{bmatrix} \partial_x f_0 \\ \partial_y f_0 \end{bmatrix} = -\frac{v}{2} \nabla \rho_{\text{prop}} \tag{14}$$

Next, we turn to the rotational diffusion, $-\omega\partial_\theta f$.

$$\begin{aligned}
 \frac{\partial}{\partial t} f_{k,\text{rota}}(\mathbf{r}, t) &= -\frac{\omega}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} \partial_\theta f(\mathbf{r}, \theta, t) \\
 &= -\frac{\omega}{2\pi} \sum_{m=-\infty}^{\infty} i m f_{m,\text{rota}}(\mathbf{r}, t) \int_0^{2\pi} d\theta e^{i(m-k)\theta} \\
 &= -\omega \sum_{m=-\infty}^{\infty} i m f_{m,\text{rota}}(\mathbf{r}, t) \delta(m-k) \\
 &= -ik\omega f_{k,\text{rota}}(\mathbf{r}, t)
 \end{aligned} \tag{15}$$

With the definitions of $\rho(\mathbf{r}, t)$ and $p(\mathbf{r}, t)$, we obtain for the field variables

$$\begin{aligned}
 \frac{\partial}{\partial t} \rho_{\text{rota}} &= 0, \\
 \frac{\partial}{\partial t} p_{\text{rota}} &= \omega\pi \begin{bmatrix} i(f_{-1,\text{rota}} - f_{1,\text{rota}}) \\ f_{-1,\text{rota}} + f_{1,\text{rota}} \end{bmatrix} = \omega p_{\text{rota},\perp},
 \end{aligned} \tag{16}$$

where $p_{\text{rota},\perp} = (-p_{\text{rota},y}, p_{\text{rota},x})$.

Next, we turn to the alignment interactions,

$$\begin{aligned}
\frac{\partial}{\partial t} f_{\text{align}}(\mathbf{r}, \theta, t) &= -K \partial_{\theta} \left[f(\mathbf{r}, \theta, t) \int d\theta' f(\mathbf{r}, \theta', t) \sin(\theta' - \theta) \right] \\
&= K i \pi \left(e^{-i\theta} f_{-1, \text{align}} - e^{i\theta} f_{1, \text{align}} \right) \sum_{-\infty}^{+\infty} m f_{k, \text{align}} e^{im\theta} + \\
&\quad K \pi \left(e^{-i\theta} f_{-1, \text{align}} + e^{i\theta} f_{1, \text{align}} \right) f_{\text{align}}
\end{aligned} \tag{17}$$

and

$$\begin{aligned}
\frac{\partial}{\partial t} f_{k, \text{align}}(\mathbf{r}, t) &= \frac{1}{2\pi} \int d\theta f_{\text{align}}(\mathbf{r}, \theta, t) e^{-ik\theta} \\
&= -K \pi \left(f_{-1, \text{align}} \sum_{-\infty}^{+\infty} m f_{k, \text{align}} \delta_{k-m+1} - f_{1, \text{align}} \sum_{-\infty}^{+\infty} m f_{k, \text{align}} \delta_{k-m-1} \right) \\
&\quad + K \pi (f_{k+1, \text{align}} f_{-1, \text{align}} + f_{k-1, \text{align}} f_{1, \text{align}}) \\
&= -K \pi [(k+1) f_{-1, \text{align}} f_{k, \text{align}} - (k-1) f_{1, \text{align}} f_{k, \text{align}}] \\
&\quad + K \pi (f_{k+1, \text{align}} f_{-1, \text{align}} + f_{k-1, \text{align}} f_{1, \text{align}})
\end{aligned} \tag{18}$$

With the definitions of $\rho(\mathbf{r}, t)$ and $p(\mathbf{r}, t)$, we obtain for the field variables

$$\begin{aligned}\frac{\partial}{\partial t}\rho_{\text{align}} &= 0, \\ \frac{\partial}{\partial t}p_{\text{align}} &= \pi \left[\begin{array}{c} \partial_t [f_1(\mathbf{r}, t) + f_{-1}(\mathbf{r}, t)] \\ i\partial_t [f_1(\mathbf{r}, t) - f_{-1}(\mathbf{r}, t)] \end{array} \right] = K\rho_{\text{align}}p_{\text{align}}\end{aligned}\tag{19}$$

because of

$$\begin{aligned}\frac{\partial}{\partial t}f_1 &= K\pi(f_2f_{-1} + f_0f_1 - 2f_{-1}f_1) = K\pi f_1(f_0 - 2f_{-1}) \\ \frac{\partial}{\partial t}f_{-1} &= K\pi(f_0f_{-1} + f_{-2}f_1 - 2f_{-1}f_1) = K\pi f_{-1}(f_0 - 2f_1)\end{aligned}\tag{20}$$

Next, we turn to the short-range repulsion

$$\begin{aligned}
 \int F_{\text{sr}} f(\mathbf{r}', \theta', t) d\mathbf{r}' d\theta' &= 2\pi \int \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} k(R_r - |\mathbf{r} - \mathbf{r}'|) \Theta(R_r - |\mathbf{r} - \mathbf{r}'|) f(\mathbf{r}', t) d\mathbf{r}' \\
 &= 2\pi \int_0^{R_r} \int_0^{2\pi} \mathbf{p}(\phi) k(R_r - d) [f(0, t) + d \nabla f(\mathbf{r}', t)] dd d\phi \\
 &= \frac{4\pi^2}{3} R_r^4 \nabla f(\mathbf{r}', t)
 \end{aligned}
 \tag{21}$$

To summarize, the continuum model can be written as

$$\dot{\rho}^{1,2}(\mathbf{r}, t) = -v \nabla \cdot p^{1,2} + D \nabla^2 \rho^{1,2} , \quad (22a)$$

$$\dot{p}^{1,2}(\mathbf{r}, t) = -\frac{v}{2} \nabla \rho^{1,2} + D \nabla^2 p^{1,2} + \omega p_{\perp}^{1,2} - K \rho p , \quad (22b)$$