

Supplemental Material: Active Transport of Cargo-Carrying and Interconnected Chiral Particles

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1 Outline

We present the detailed derivation of the steady state density distribution of the active-passive composite, for the cases where they are connected by an infinitely stiff spring and a spring with zero rest length. These notes are organised as follows: In Sections 2 and 3, we perform the coarse graining of the Fokker-Planck equation by integrating out the rotational and bond degrees of freedom. Section 4 describes the approximations employed to arrive at the close form solution of the steady state density distribution. In Section 5, we show the calculation for the tactic parameter for both the infinitely stiff spring and the spring with zero rest length. This is followed by simulation results on the tactic behavior of chains of chiral active particles in Section 6. We end with the details of the Langevin dynamics simulations in Section 7.

2 Eliminating the orientational degrees of freedom

We begin with the stochastic equations of motion that govern the dynamics of the active-passive composite (Eq. (1) in the main text). These are given by:

$$\frac{d\mathbf{r}_1}{dt} = \frac{1}{\gamma}\mathbf{F} + \frac{1}{\gamma}f_s(\mathbf{r}_1)\mathbf{p} + \sqrt{\frac{2T}{\gamma}}\boldsymbol{\xi}_1(t), \quad (\text{SI 1a})$$

$$\frac{d\theta}{dt} = \omega + \sqrt{2D_R}\eta(t), \quad (\text{SI 1b})$$

$$\frac{d\mathbf{r}_2}{dt} = -\frac{1}{q\gamma}\mathbf{F} + \sqrt{\frac{2T}{q\gamma}}\boldsymbol{\xi}_2(t). \quad (\text{SI 1c})$$

It is convenient to make a coordinate transformation to the collective coordinate of the composite, which are identified as the center of friction and the bond coordinates, given by:

$$\begin{aligned} \mathbf{R} &= \frac{1}{1+q}\mathbf{r}_1 + \frac{q}{1+q}\mathbf{r}_2, \\ \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2. \end{aligned} \quad (\text{SI 2})$$

We now switch to an equivalent description in terms of the Fokker-Planck equation (FPE) for the probability density $P(\mathbf{R}, \mathbf{r}, \theta, t) \equiv P$, given by:

$$\begin{aligned} \frac{\partial}{\partial t}P &= -\nabla_{\mathbf{R}} \cdot \left[\frac{1}{1+q}\frac{1}{\gamma}f_s\mathbf{p}P - \frac{1}{1+q}\frac{T}{\gamma}\nabla_{\mathbf{R}}P \right] \\ &\quad - \nabla_{\mathbf{r}} \cdot \left[\frac{1+q}{q}\frac{1}{\gamma}\mathbf{F}P + \frac{1}{\gamma}f_s\mathbf{p}P - \frac{1+q}{q}\frac{T}{\gamma}\nabla_{\mathbf{r}}P \right] \\ &\quad - \omega\partial_{\theta}P + D_R\partial_{\theta}^2P, \end{aligned} \quad (\text{SI 3})$$

where the symbol \cdot represents a single contraction, and $\nabla_{\mathbf{R}}$ and $\nabla_{\mathbf{r}}$ represent derivatives with respect to \mathbf{R} and \mathbf{r} , respectively. ∂_{θ} is the rotation operator in two dimensions and ∂_{θ}^2 is the Laplacian on a unit circle.

Following the analysis introduced in [1], we start by expanding the probability density in the eigenfunctions of ∂_θ^2 operator:

$$P(\mathbf{R}, \mathbf{r}, \theta, t) = \phi + \boldsymbol{\sigma} \cdot \mathbf{p} + \boldsymbol{\mu} : \mathbf{Q} + \Theta(P). \quad (\text{SI } 4)$$

Here, the 1, \mathbf{p} and $\mathbf{Q} = \mathbf{p}\mathbf{p} - \mathbf{1}/2$ are the first three eigenfunctions of ∂_θ^2 operator with eigenvalues 0, -1 and -4 respectively, and $:$ denotes double contraction. Note that these eigenfunctions are equivalent to the 0th, 1st and 2nd order moments in the angular multipole expansion in two dimensions, and correspond to physically relevant observables. Specifically, $\phi(\mathbf{R}, \mathbf{r}, t)$ is the positional probability density, $\boldsymbol{\sigma}(\mathbf{R}, \mathbf{r}, t)$ is proportional to the average orientation and $\boldsymbol{\mu}(\mathbf{R}, \mathbf{r}, t)$ is related to the nematic order parameter. $\Theta(P)$ contains the dependencies on all the higher order moments.

Since we eventually want to know the collective position of the active-passive composite in the steady state, we will integrate out the orientational degrees of freedom. This forms our first coarse-graining step. To this end, we introduce the inner product:

$$\langle f(\mathbf{p}(\theta)), g(\mathbf{p}(\theta)) \rangle = \int_0^{2\pi} d\theta f(\mathbf{p}(\theta)) g(\mathbf{p}(\theta)). \quad (\text{SI } 5)$$

We can now project the FPE onto the eigenfunctions of ∂_θ^2 operator to get the time evolution of the moments. To do this, we will need to use the following relations involving the orthogonality of the eigenfunctions of our expansion:

$$\begin{aligned} \langle 1, 1 \rangle &= 2\pi, \\ \langle \mathbf{p}, 1 \rangle &= 0, \\ \langle \mathbf{Q}, 1 \rangle &= 0, \\ \langle 1, P \rangle &= 2\pi\phi, \\ \langle \mathbf{p}, P \rangle &= \pi\boldsymbol{\sigma}, \\ \langle \mathbf{Q}, P \rangle &= \frac{\pi}{2}\boldsymbol{\mu}, \\ \langle \mathbf{p}, \partial_\theta P \rangle &= -\pi\boldsymbol{\varepsilon} \cdot \boldsymbol{\sigma}, \\ \langle 1, \Theta(P) \rangle &= 0, \\ \langle \mathbf{p}, \Theta(P) \rangle &= 0, \\ \langle \mathbf{Q}, \Theta(P) \rangle &= 0. \end{aligned} \quad (\text{SI } 6)$$

Note that, we have evaluated the inner product $\langle \mathbf{p}, \partial_\theta P \rangle$ as follows:

$$\langle \mathbf{p}, \partial_\theta P \rangle = - \int_0^{2\pi} d\theta (\partial_\theta \mathbf{p}) P = - \int_0^{2\pi} d\theta \boldsymbol{\varepsilon} \cdot \mathbf{p} P = -\boldsymbol{\varepsilon} \cdot \langle \mathbf{p}, P \rangle = -\pi \boldsymbol{\varepsilon} \cdot \boldsymbol{\sigma},$$

where we have used integration by parts and introduced the two dimensional *Levi-Civita* tensor $\boldsymbol{\varepsilon}$:

$$\boldsymbol{\varepsilon} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

To get the equation of motion for the positional probability density $2\pi\phi(\mathbf{r}_1, \mathbf{r}_2, t) = \int_0^{2\pi} d\theta P(\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}, t)$, we project eq. (SI 4) onto the identity eigenfunction and get:

$$\frac{\partial}{\partial t} \phi = -\nabla_{\mathbf{R}} \cdot \left[-\frac{T}{\gamma} \frac{1}{1+q} \nabla_{\mathbf{R}} \phi + \frac{1}{1+q} \frac{1}{2\gamma} f_s \boldsymbol{\sigma} \right] - \nabla_{\mathbf{r}} \cdot \left[\frac{1}{2\gamma} f_s \boldsymbol{\sigma} + \frac{1+q}{q} \frac{1}{\gamma} \mathbf{F} \phi - \frac{T}{\gamma} \frac{1+q}{q} \nabla_{\mathbf{r}} \phi \right]. \quad (\text{SI } 7)$$

Similarly, taking the inner product of eq. (SI 4) with \mathbf{p} gives:

$$\left\{ \frac{\partial}{\partial t} + (D_R \mathbb{1} - \omega \boldsymbol{\varepsilon}) \cdot \right\} \boldsymbol{\sigma} = -\frac{1}{\gamma} \left(\frac{1}{1+q} \nabla_R + \nabla_r \right) (f_s \phi) - \frac{1}{\gamma} \frac{1+q}{q} \nabla_r \cdot (\mathbf{F} \boldsymbol{\sigma}) \\ + \frac{T}{\gamma} \left(\frac{1}{1+q} \nabla_R^2 + \frac{1+q}{q} \nabla_r^2 \right) \boldsymbol{\sigma} - \frac{1}{2\gamma} \left(\frac{1}{1+q} \nabla_R + \nabla_r \right) \cdot (f_s \boldsymbol{\mu}). \quad (\text{SI 8})$$

Finally, we can consider the inner product with the nematic tensor \mathbf{Q} to get:

$$\left\{ \frac{\partial}{\partial t} + 4D_R \right\} \boldsymbol{\mu} = -\frac{1}{\gamma} \frac{1+q}{q} \nabla_r \cdot (\mathbf{F} \boldsymbol{\mu}) + \frac{T}{\gamma} \left(\frac{1}{1+q} \nabla_R^2 + \frac{1+q}{q} \nabla_r^2 \right) \boldsymbol{\mu} \\ - \frac{2}{\pi\gamma} \left[\left(\frac{1}{1+q} \nabla_R + \nabla_r \right) f_s \boldsymbol{\sigma} \right] : \langle \mathbf{Q}, \mathbf{Q} \rangle - \frac{2}{\pi} \omega \langle \mathbf{Q}, \partial_\theta P \rangle \\ - \frac{2}{\pi\gamma} \left(\frac{1}{1+q} \nabla_R + \nabla_r \right) \cdot \langle f_s \mathbf{p} \mathbf{Q}, \Theta(P) \rangle. \quad (\text{SI 9})$$

The equations (SI 7), (SI 8) and (SI 9), together with the evolution equations for higher order expansion coefficients, form a hierarchical structure and exactly determine the full probability distribution $P(\mathbf{R}, \mathbf{r}, \theta, t)$. Unfortunately, such a hierarchy cannot be solved exactly. However, we will see in the following, this hierarchy can be closed by employing the small gradients approximation, which implies that all terms involving the nematic tensor are of order at least $\mathcal{O}(\nabla_R^2)$ and thus can be ignored.

3 Eliminating the bond coordinate

As we are interested in the marginal distribution of the position of the center of mass, we integrate out the information about the relative distance between the chiral active particle and the passive particle. This results in a continuity equation for the probability distribution $\rho(\mathbf{R}) = 2\pi \int d\mathbf{r} \phi(\mathbf{R}, \mathbf{r}, t)$ of the collective coordinate \mathbf{R} . This is done as follows:

$$\frac{\partial}{\partial t} \int d\mathbf{r} \phi(\mathbf{R}, \mathbf{r}, t) = \frac{T}{\gamma} \frac{1}{1+q} \nabla_R^2 \int d\mathbf{r} \phi - \frac{1}{1+q} \frac{1}{2\gamma} \int d\mathbf{r} \nabla_R \cdot (f_s \boldsymbol{\sigma}) \\ - \int d\mathbf{r} \left\{ \nabla_r \cdot \left[\frac{1}{2\gamma} f_s \boldsymbol{\sigma} + \frac{1+q}{q} \frac{1}{\gamma} \mathbf{F} \phi - \frac{T}{\gamma} \frac{1+q}{q} \nabla_r \phi \right] \right\}. \quad (\text{SI 10})$$

Under periodic boundary conditions, the above equation reduces to the continuity equation:

$$\frac{\partial}{\partial t} \rho = -\nabla_R \cdot \mathbf{J}, \quad (\text{SI 11})$$

where the probability current can be broken down into a part due to diffusion and a part due to the polarization:

$$\mathbf{J} = \mathbf{J}_D + \mathbf{J}_\sigma, \quad (\text{SI 12})$$

with

$$\mathbf{J}_D = -\frac{T}{\gamma} \frac{1}{1+q} \nabla_R \rho, \quad (\text{SI 13})$$

and

$$\mathbf{J}_\sigma = \frac{2\pi}{1+q} \frac{1}{2\gamma} \int d\mathbf{r} f_s \boldsymbol{\sigma}. \quad (\text{SI 14})$$

4 Approximations

To find the steady state density distribution $\rho(\mathbf{R})$ from eq. (SI 11), we need to calculate \mathbf{J}_σ , which involves closing the hierarchy in eqs. (SI 7), (SI 8) and (SI 9). To do so, we employ two approximations that are central to this analysis. These are the adiabatic approximation and the small gradients approximation.

4.1 Adiabatic Approximation

We identify the position probability distribution $\phi(\mathbf{R}, \mathbf{r}, t)$ as the slowest mode of our dynamics. Indeed, $\phi(\mathbf{R}, \mathbf{r}, t)$ satisfies a continuity equation, meaning that it is locally conserved and decays on timescales which are $\mathcal{O}(\nabla_{\mathbf{R}}^{-1})$. Additionally, all the higher order moments decay at much faster timescales due to the presence of sink-terms in their dynamics. Thus, they are effectively quasi-static at the timescales at which our quantity of interest $\phi(\mathbf{R}, \mathbf{r}, t)$ evolves. In particular, $\boldsymbol{\sigma}$ decays on a timescale given by the eigenvalues of the matrix $(D_{\mathbf{R}} \mathbb{1} - \omega \boldsymbol{\varepsilon})^{-1} \equiv \mathbb{L}$ and $\boldsymbol{\mu}$ decays on timescales of the order of $(4D_{\mathbf{R}})^{-1}$. This allows us to set the time derivative terms in eq. (SI 8) and eq. (SI 9) to zero, giving us:

$$\boldsymbol{\sigma} = \mathbb{L} \cdot \left\{ -\frac{1}{\gamma} \left(\frac{1}{1+q} \nabla_{\mathbf{R}} + \nabla_{\mathbf{r}} \right) (f_s \phi) - \frac{1}{\gamma} \frac{1+q}{q} \nabla_{\mathbf{r}} \cdot (\mathbf{F} \boldsymbol{\sigma}) + \frac{T}{\gamma} \left(\frac{1}{1+q} \nabla_{\mathbf{R}}^2 + \frac{1+q}{q} \nabla_{\mathbf{r}}^2 \right) \boldsymbol{\sigma} - \frac{1}{2\gamma} \left(\frac{1}{1+q} \nabla_{\mathbf{R}} + \nabla_{\mathbf{r}} \right) \cdot (f_s \boldsymbol{\mu}) \right\} \quad (\text{SI } 15)$$

and

$$\boldsymbol{\mu} = \frac{1}{4D_r} \left\{ -\frac{1}{\gamma} \frac{1+q}{q} \nabla_{\mathbf{r}} \cdot (\mathbf{F} \boldsymbol{\mu}) + \frac{T}{\gamma} \left(\frac{1}{1+q} \nabla_{\mathbf{R}}^2 + \frac{1+q}{q} \nabla_{\mathbf{r}}^2 \right) \boldsymbol{\mu} - \frac{2}{\pi\gamma} \left[\left(\frac{1}{1+q} \nabla_{\mathbf{R}} + \nabla_{\mathbf{r}} \right) f_s \boldsymbol{\sigma} \right] : \langle \mathbf{Q}, \mathbf{Q} \rangle - \frac{2}{\pi} \omega \langle \mathbf{Q}, \partial_\theta P \rangle - \frac{2}{\pi\gamma} \left(\frac{1}{1+q} \nabla_{\mathbf{R}} + \nabla_{\mathbf{r}} \right) \cdot \langle f_s \mathbf{p} \mathbf{Q}, \Theta(P) \rangle \right\}. \quad (\text{SI } 16)$$

Plugging eq. (SI 15) back into eq. (SI 14), we get:

$$\mathbf{J}_\sigma = 2\pi \mathbb{L} \cdot \left\{ -\frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \int d\mathbf{r} f_s \nabla_{\mathbf{R}} (f_s \phi) - \frac{1}{1+q} \frac{1}{2\gamma^2} \int d\mathbf{r} f_s \nabla_{\mathbf{r}} (f_s \phi) - \frac{1}{q} \frac{1}{2\gamma^2} \int d\mathbf{r} f_s \nabla_{\mathbf{r}} \cdot (\mathbf{F} \boldsymbol{\sigma}) + \frac{1}{(1+q)} \frac{T}{2\gamma^2} \int d\mathbf{r} f_s \left[\frac{1}{(1+q)} \nabla_{\mathbf{R}} \cdot (\nabla_{\mathbf{R}} \boldsymbol{\sigma}) + \frac{(1+q)}{q} \nabla_{\mathbf{r}} \cdot (\nabla_{\mathbf{r}} \boldsymbol{\sigma}) \right] - \frac{1}{1+q} \frac{1}{4\gamma^2} \int d\mathbf{r} f_s \left(\frac{1}{1+q} \nabla_{\mathbf{R}} + \nabla_{\mathbf{r}} \right) \cdot (f_s \boldsymbol{\mu}) \right\}. \quad (\text{SI } 17)$$

4.2 Small Gradients Approximation

Next, we are interested in the limits where the gradients in the activity field are small compared to the persistence length of the chiral active particle as well as small compared to the separation between the active and the passive particles. This approximation will allow us to decouple eq. (SI 11), (SI 12) and (SI 17) to get a closed form solution of the marginal probability density $\rho(\mathbf{R})$.

To apply this approximation, it is important to realize that, in the absence of gradients in the activity field, our system has no directional preferences and will be isotropic in space. This implies that the nematic tensor $\boldsymbol{\mu}$ and higher order moments are at least $\mathcal{O}(\nabla_{\mathbf{R}})$. This allows us to significantly simplify eq. (SI 17), wherein we only have to evaluate the first three terms. We will also convert the gradients in $\nabla_{\mathbf{r}}$ to gradients in $\nabla_{\mathbf{R}}$ by applying integration by parts:

$$\nabla_{\mathbf{r}} f_s(\mathbf{r}_1) = \frac{q}{1+q} \nabla_{\mathbf{R}} f_s(\mathbf{r}_1). \quad (\text{SI } 18)$$

We then get the following expression for $\mathbf{J}_{\boldsymbol{\sigma}}$:

$$\mathbf{J}_{\boldsymbol{\sigma}} = 2\pi\mathbb{L} \cdot \left\{ -\frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \int d\mathbf{r} f_s \nabla_{\mathbf{R}}(f_s \phi) + \frac{q}{(1+q)^2} \frac{1}{2\gamma^2} \int d\mathbf{r} \phi f_s \nabla_{\mathbf{R}} f_s + \frac{1}{1+q} \frac{1}{2\gamma^2} \mathbf{I} \right\}, \quad (\text{SI } 19)$$

where we have defined the quantity \mathbf{I} as:

$$\mathbf{I} = \int d\mathbf{r} (\mathbf{F} \cdot \nabla_{\mathbf{R}} f_s) \boldsymbol{\sigma}. \quad (\text{SI } 20)$$

We solve this integral as follows:

$$\begin{aligned} \mathbf{I} &= \int d\mathbf{r} (\mathbf{F} \cdot \nabla_{\mathbf{R}} f_s) \boldsymbol{\sigma} \\ &= -\frac{1}{\gamma} \mathbb{L} \cdot \int d\mathbf{r} [\mathbf{F} \cdot (\nabla_{\mathbf{R}} f_s) \nabla_{\mathbf{r}}] \cdot \left(\mathbf{1} \phi f_s + \frac{1+q}{q} \mathbf{F} \boldsymbol{\sigma} \right) + \mathcal{O}(\nabla_{\mathbf{R}}^2 f_s) \\ &= \frac{1}{\gamma} \mathbb{L} \cdot \int d\mathbf{r} \nabla_{\mathbf{r}} (\mathbf{F} \cdot \nabla_{\mathbf{R}} f_s) \cdot \left(\mathbf{1} \phi f_s + \frac{1+q}{q} \mathbf{F} \boldsymbol{\sigma} \right) + \mathcal{O}(\nabla_{\mathbf{R}}^2 f_s), \end{aligned} \quad (\text{SI } 21)$$

where we have used integration by parts in the last line. Now, we use

$$\nabla_{\mathbf{r}} (\mathbf{F} \cdot \nabla_{\mathbf{R}} f_s) = \nabla_{\mathbf{r}} \mathbf{F} \cdot \nabla_{\mathbf{R}} f_s + \mathcal{O}(\nabla_{\mathbf{R}}^2 f_s).$$

The interaction between the chiral active particle and the passive particle is modeled as a harmonic spring with rest length l_0 . So we can evaluate $\nabla_{\mathbf{r}} \mathbf{F}$ as:

$$\nabla_{\mathbf{r}} \mathbf{F} = -k \nabla_{\mathbf{r}} [(r - l_0) \hat{\mathbf{r}}] = -k \left[\hat{\mathbf{r}} \hat{\mathbf{r}} + (1 - l_0/r) (\mathbf{1} - \hat{\mathbf{r}} \hat{\mathbf{r}}) \right] \equiv -k \mathbb{A}, \quad \text{where } r = |\mathbf{r}|.$$

With this, \mathbf{I} becomes

$$\begin{aligned} \mathbf{I} &= -\frac{k}{\gamma} \mathbb{L} \cdot \left[\int d\mathbf{r} \phi f_s \mathbb{A} \cdot \nabla_{\mathbf{R}} f_s + \frac{1+q}{q} \int d\mathbf{r} (\mathbf{F} \cdot \nabla_{\mathbf{R}} f_s) \boldsymbol{\sigma} \right] \\ &= -\frac{k}{\gamma} \mathbb{L} \cdot \left[\int d\mathbf{r} \phi f_s \mathbb{A} \cdot \nabla_{\mathbf{R}} f_s + \frac{1+q}{q} \mathbf{I} \right] \\ &= -\frac{qk}{\gamma} \mathbb{L} \cdot \left(q \mathbf{1} + \frac{(1+q)k}{\gamma} \mathbb{L} \right)^{-1} \int d\mathbf{r} \phi f_s \mathbb{A} \cdot \nabla_{\mathbf{R}} f_s \\ &= -\mathbb{B} \cdot \int d\mathbf{r} \phi f_s \mathbb{A} \cdot \nabla_{\mathbf{R}} f_s. \end{aligned} \quad (\text{SI } 22)$$

where we used the fact that the matrix \mathbb{A} is symmetric, the identity $\mathbb{A} \cdot \mathbf{F} = \mathbf{F}$ and we have simplified the notation by introducing the quantity \mathbb{B} :

$$\mathbb{B} = \frac{qk}{\gamma} \mathbb{L} \left(q \mathbf{1} + \frac{(1+q)k}{\gamma} \mathbb{L} \right)^{-1}.$$

We can now finally write the closed form expression for the polarisation current \mathbf{J}_σ

$$\mathbf{J}_\sigma = -\frac{2\pi}{(1+q)^2} \frac{1}{2\gamma^2} \mathbb{L} \cdot \left[\int d\mathbf{r} f_s \nabla_{\mathbf{R}}(f_s \phi) - q \int d\mathbf{r} \phi f_s \nabla_{\mathbf{R}} f_s + (1+q) \mathbb{B} \int d\mathbf{r} \phi f_s \mathbb{A} \cdot \nabla_{\mathbf{R}} f_s \right]. \quad (\text{SI } 23)$$

Now, we are in the position to get the expression of the steady state density distribution ρ . In particular, we analyze two specific forms of the force \mathbf{F} between the active particle and the passive particle: the rigid bond case and the harmonic potential with zero rest length. We do this in the following section.

5 Steady state density distribution

5.1 Spring with zero rest length

In this case, the quantity \mathbb{A} defined for the spring force is the identity matrix, i.e., $\mathbb{A}(l_0 = 0) = \mathbb{1}$. Since the spring has zero rest length, the separation between the active and passive particles is small compared to the gradients of the activity field, provided that k is not too small. So, we can approximate $\phi(\mathbf{R}, \mathbf{r}, t)$ as:

$$\phi(\mathbf{R}, \mathbf{r}, t) \approx \frac{1}{2\pi} \rho(\mathbf{R}) \delta(\mathbf{r}). \quad (\text{SI } 24)$$

Moreover, we can also Taylor-expand the activity field about the collective coordinate \mathbf{R} as:

$$f_s = f_s(\mathbf{r}_1) = f_s\left(\mathbf{R} + \mathbf{r} \frac{q}{1+q}\right) = f_s(\mathbf{R}) + \frac{q}{1+q} \mathbf{r} \cdot \nabla_{\mathbf{R}} f_s(\mathbf{R}), \quad (\text{SI } 25)$$

and thus move it out of the \mathbf{r} integral in all terms.

With these steps, we can write \mathbf{J}_σ as:

$$\begin{aligned} \mathbf{J}_\sigma &= -\frac{2\pi}{(1+q)^2} \frac{1}{2\gamma^2} \mathbb{L} \cdot \left[f_s^2 \nabla_{\mathbf{R}} \rho \int d\mathbf{r} \frac{1}{2\pi} \delta(\mathbf{r}) + \rho f_s \nabla_{\mathbf{R}} f_s \int d\mathbf{r} \frac{1}{2\pi} \delta(\mathbf{r}) \right. \\ &\quad \left. - q \rho f_s \nabla_{\mathbf{R}} f_s \int d\mathbf{r} \frac{1}{2\pi} \delta(\mathbf{r}) + (1+q) \mathbb{B} f_s \nabla_{\mathbf{R}} f_s \rho \int d\mathbf{r} \frac{1}{2\pi} \delta(\mathbf{r}) \right] + \mathcal{O}(\nabla_{\mathbf{R}}^2) \\ &= -\frac{1}{(1+q)^2} \frac{1}{2\gamma^2} f_s^2 \mathbb{L} \cdot \nabla_{\mathbf{R}} \rho - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \frac{\rho}{2} \mathbb{L} \left[(1-q) \mathbb{1} + (1+q) \mathbb{B} \right] \cdot \nabla_{\mathbf{R}} (f_s^2) + \mathcal{O}(\nabla_{\mathbf{R}}^2), \end{aligned} \quad (\text{SI } 26)$$

We can now evaluate the total flux up to the drift/diffusion order as:

$$\begin{aligned} \mathbf{J} &= \mathbf{J}_D + \mathbf{J}_\sigma \\ &= -\frac{1}{(1+q)} \frac{T}{\gamma} \nabla_{\mathbf{R}} \rho - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} f_s^2 \mathbb{L} \cdot \nabla_{\mathbf{R}} \rho - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \frac{\rho}{2} \mathbb{L} \left[(1-q) \mathbb{1} + (1+q) \mathbb{B} \right] \cdot \nabla_{\mathbf{R}} (f_s^2). \end{aligned} \quad (\text{SI } 27)$$

In particular, the total flux \mathbf{J} has the following structure

$$\mathbf{J} = \mathbf{V}(\mathbf{R}) \rho(\mathbf{R}) - \nabla_{\mathbf{R}} \cdot (\mathbb{D}(\mathbf{R}) \rho(\mathbf{R})), \quad (\text{SI } 28)$$

where the effective diffusion coefficient depends on \mathbf{R} and is given by:

$$\mathbb{D}(\mathbf{R}) = \frac{1}{1+q} \frac{T}{\gamma} \mathbb{1} + \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} f_s^2(\mathbf{R}) \mathbb{L}^T, \quad (\text{SI } 29)$$

and the effective drift $\mathbf{V}(\mathbf{R})$ can be written in terms of $\mathbb{D}(\mathbf{R})$ as:

$$\mathbf{V}(\mathbf{R}) = \left(\mathbb{1} - \frac{1}{2} \mathbb{L} \left[(1-q) \mathbb{1} + (1+q) \mathbb{B} \right] \mathbb{L}^{-1} \right) \nabla_{\mathbf{R}} \cdot \mathbb{D}(\mathbf{R}). \quad (\text{SI } 30)$$

In this study, the activity gradients are assumed to exist only in the x -direction. Since there is translational invariance in the y direction, the stationary density ρ has variations only along the x -direction. Thus, the stationary probability flux along the x -direction is given by:

$$\begin{aligned} J_x(x) &= -\frac{1}{(1+q)} \frac{T}{\gamma} \partial_x \rho(x) - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} f_s^2(x) \mathbb{L}_{xx} \partial_x \rho(x) \\ &\quad - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \frac{\rho(x)}{2} \left\{ \mathbb{L} \left[(1-q) \mathbb{1} + (1+q) \mathbb{B} \right] \right\}_{xx} \partial_x (f_s(x)^2) \\ &= -\frac{\epsilon}{2} \rho \partial_x \mathbb{D}_{xx} - \mathbb{D}_{xx} \partial_x \rho, \end{aligned} \quad (\text{SI } 31)$$

where we denoted with \mathbb{D}_{xx} the xx element of the effective diffusion coefficient. We define the quantity ϵ as the *tactic parameter*, which determines the accumulation behavior of the active-passive composite. Particularly, for $\epsilon < 0$, the composite accumulates in regions of high activity and vice-versa. Imposing a zero-flux condition along the direction of the activity gradient, we obtain the steady state density:

$$\rho(x) \propto \left[1 + \frac{D_R}{D_R^2 + \omega^2} \frac{1}{2\gamma T} \frac{1}{(1+q)} f_s^2(x) \right]^{-\epsilon/2}, \quad (\text{SI } 32)$$

where the tactic parameter enters as the exponent, and is dependent on the chiral torque Ω . Specifically, we get

$$\epsilon = 1 - q \frac{(1 + \Omega^2)(1 + \tau)}{\Omega^2 + (1 + \tau)^2}, \quad (\text{SI } 33)$$

where we have introduced the following non-dimensional parameters in units of the persistence time $\tau_p = D_R^{-1}$ of the active particle due to rotational diffusion,

$$\Omega = \omega \tau_p \quad \text{and} \quad \tau = \frac{(1+q)k\tau_p}{q\gamma}.$$

5.2 Infinitely stiff spring

This is implemented by taking the limit of the spring constant $k \rightarrow \infty$. The only term where the spring constant appears is \mathbb{B} and we can now evaluate it in this limit as:

$$\lim_{k \rightarrow \infty} (1+q) \mathbb{B} = \lim_{k \rightarrow \infty} \frac{q(1+q)k}{\gamma} \mathbb{L} \left(q \mathbb{1} + \frac{(1+q)k}{\gamma} \mathbb{L} \right)^{-1} = q \mathbb{1}. \quad (\text{SI } 34)$$

Note that in this limit, the spring force between the chiral active particle and the passive particle is so strong that the separation between them approximately remains the same as the spring rest length l_0 , i.e., $r' \approx l_0$ and so we can write:

$$\phi(\mathbf{R}, \mathbf{r}', t) \approx \frac{1}{2\pi} \frac{1}{2\pi l_0} \rho(\mathbf{R}, t) \delta(r' - l_0). \quad (\text{SI } 35)$$

Additionally, we can also Taylor-expand the activity field in the same way as Eq. (SI 25). With these steps, \mathbf{J}_σ now becomes

$$\begin{aligned}\mathbf{J}_\sigma &= -\frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \mathbb{L} \cdot \left[f_s^2 \nabla_{\mathbf{R}} \rho \int d\mathbf{r} \frac{1}{2\pi l_0} \delta(r-l_0) + \rho f_s \nabla_{\mathbf{R}} f_s \int d\mathbf{r} \frac{1}{2\pi l_0} \delta(r-l_0) \right. \\ &\quad \left. - q \rho f_s \nabla_{\mathbf{R}} f_s \int d\mathbf{r} \frac{1}{2\pi l_0} \delta(r-l_0) + q \mathbb{1} f_s \nabla_{\mathbf{R}} f_s \rho \int d\mathbf{r} \frac{1}{2\pi l_0} \delta(r-l_0) \hat{\mathbf{r}} \hat{\mathbf{r}} \right] + \mathcal{O}(\nabla_{\mathbf{R}}^2) \\ &= -\frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \mathbb{L} \cdot \left[f_s^2 \nabla_{\mathbf{R}} \rho + \frac{\rho}{2} \nabla_{\mathbf{R}} (f_s^2) - \frac{q\rho}{2} \nabla_{\mathbf{R}} (f_s^2) + \frac{q\rho}{4} \nabla_{\mathbf{R}} (f_s^2) \right] + \mathcal{O}(\nabla_{\mathbf{R}}^2),\end{aligned}\quad (\text{SI 36})$$

where we have used the normalization of the delta distribution and

$$\frac{1}{2\pi} \int d\mathbf{r} \hat{\mathbf{r}} \hat{\mathbf{r}} = \frac{\mathbb{1}}{2}.\quad (\text{SI 37})$$

The total flux then becomes:

$$\begin{aligned}\mathbf{J} &= \mathbf{J}_D + \mathbf{J}_\sigma, \\ &= -\frac{1}{(1+q)} \frac{T}{\gamma} \nabla_{\mathbf{R}} \rho - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} f_s^2 \mathbb{L} \cdot \nabla_{\mathbf{R}} \rho \\ &\quad - \left(1 - \frac{q}{2}\right) \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \frac{\rho}{2} \mathbb{L} \cdot \nabla_{\mathbf{R}} (f_s^2).\end{aligned}\quad (\text{SI 38})$$

Using this flux, we can write an effective drift-diffusion equation:

$$\mathbf{J} = \mathbf{V}(\mathbf{R})\rho(\mathbf{R}) - \nabla_{\mathbf{R}} \cdot (\mathbb{D}(\mathbf{R})\rho(\mathbf{R})),$$

We again consider activity to be varying only along the x -direction with the stationary flux given by:

$$\begin{aligned}J_x(x) &= -\frac{1}{(1+q)} \frac{T}{\gamma} \partial_x \rho(x) - \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \frac{D_R}{D_R^2 + \omega^2} f_s^2(x) \partial_x \rho(x) \\ &\quad - \frac{1}{2} \left(1 - \frac{q}{2}\right) \frac{1}{(1+q)^2} \frac{1}{2\gamma^2} \frac{D_R}{D_R^2 + \omega^2} \partial_x (f_s^2(x)) \\ &= -\frac{\epsilon}{2} \rho \partial_x \mathbb{D}_{xx} - \mathbb{D}_{xx} \partial_x \rho,\end{aligned}\quad (\text{SI 39})$$

Similar to the previous case, we find that the effective drift and diffusion coefficient are related by a derivative relation. Upon imposing a zero-flux condition, we obtain the same structure for the steady state density:

$$\rho(x) \propto \left[1 + \frac{D_R}{D_R^2 + \omega^2} \frac{1}{2\gamma T} \frac{1}{(1+q)} f_s^2(x) \right]^{-\epsilon/2},\quad (\text{SI 40})$$

However, the tactic parameter ϵ is now given by:

$$\epsilon = 1 - \frac{q}{2}.\quad (\text{SI 41})$$

We see that the tactic parameter ϵ is only dependent on the size of the passive particle via q .

6 Chiral Active Chains

In the case of monomers and chains of chiral active particles without passive particles attached, we observe a dependence of chemotactic behavior on the chiral torque Ω . Figure SI 1 shows as Ω increases, monomers and dimers exhibit a reduction in antichemotaxis, but this effect does not vanish entirely. However, for trimers, a transition occurs at sufficiently high Ω , where chains accumulate in the high-activity regions. This trend becomes even more pronounced in tetramers, where even low-chirality chains have a tendency to accumulate in high-activity regions.

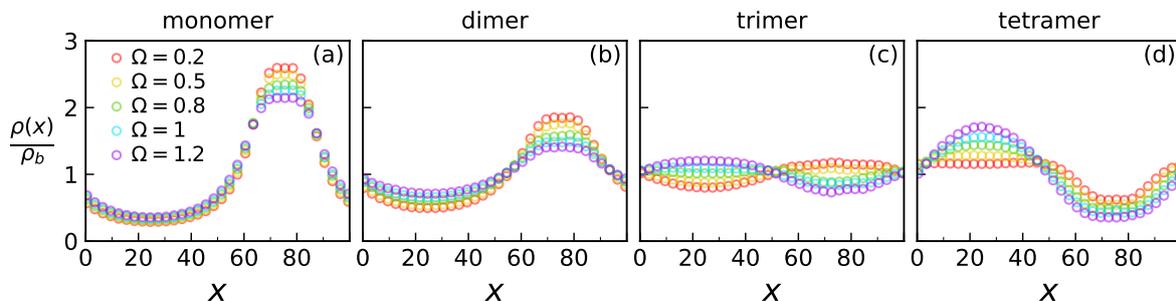


Figure SI 1: The steady state density distribution of active (a) monomers, (b) dimers, (c) trimers, and (d) tetramers connected via a spring with $\ell_0 = 1.5$ and $k = 30$. The y -axis is normalized by the bulk density ρ_b . The sinusoidal activity field is the same as in Fig. (2) of main manuscript, given by $f_s(x) = 20(1 + \sin(2\pi x/L))$. The accumulation behavior of the chains is influenced by the strength of the chiral torque Ω . The parameters of the simulation are $k_B T = 1.0$, $\gamma = 1.0$, $D_R = 10.0$, and the integration time step $\Delta t = 5D_R \times 10^{-6}$.

7 Simulation Details

The chiral active particle and the passive particle were simulated using Langevin dynamics: The equations of motion (eq. (1) in the main text) were first discretized up to linear order in the integration time-step using the Euler method. The increments at each time-step were then summed up using the Itó rule with a time-step size of $dt = D_R \times 10^{-5}$ for the case of harmonic spring with zero rest length and $dt = 5D_R \times 10^{-6}$ for the case of the infinitely stiff spring. The simulation box size was chosen to be $L = 100$ with periodic boundary conditions. The activity field was also chosen to be periodic with sinusoidal variations.

References

- [1] Vuijk HD, Merlitz H, Lang M, Sharma A, Sommer JU. Chemotaxis of Cargo-Carrying Self-Propelled Particles. *Phys Rev Lett*. 2021 May;126(20):208102. Available from: <https://link.aps.org/doi/10.1103/PhysRevLett.126.208102>.