Electronic Supplementary Material (ESI) for Soft Matter

Equations of motion for non-spherical particles

In modelling the chiral particles, we use a so-called bead model [1] and assemble them from $N = 7$ identical spherical beads which are rigidly connected and where two neighbouring beads touch each other (see Fig. 1a). The equation of motion of such structured particle is obtained by transforming the coupled set of equations for the single component beads to generalized coordinates, i.e. centre motion and rotational degrees of freedom of the particle as a whole. Neglecting inertia effects, and also thermal noise for a moment, the component beads (numbered by i) obey the equations

$$\dot{\vec{r}}_i = \vec{v}(\vec{r}_i) + \sum_j \mu_{ij}^{tt}\, \vec{F}(\vec{r}_j) + \sum_j \mu_{ij}^{tr}\, \vec{T}(\vec{r}_j) \tag{1}$$

$$\dot{\vec{\varphi}}_i = \vec{\omega}(\vec{r}_i) + \sum_j \mu_{ij}^{rt}\, \vec{F}(\vec{r}_j) + \sum_j \mu_{ij}^{rr} \vec{T}(\vec{r}_j), \tag{2}$$

where $\vec{r}_i$ is the position of bead i, $\vec{\varphi}_i$ its rotational position, $\vec{v}(\vec{r})$ is the "externally" imposed flow velocity of the fluid, $\omega(\vec{r}) = [\vec{\nabla} \times \vec{v}(\vec{r})]/2$ half its vorticity, and $\vec{F}(\vec{r})$ and $\vec{T}(\vec{r})$ collect all forces and torques on the beads which are not imposed by the fluid (also, thermal noise effects are not included here). In particular, $\vec{F}$ and $\vec{T}$ contain the à priori unknown constraining forces and torques which maintain the rigid structure of the chiral particles. The 3×3 tensors μ_{ij}^{tt}, μ_{ij}^{tr}, μ_{ij}^{rt}, μ_{ij}^{rr} model the hydrodynamic interactions between the component beads, by quantifying the perturbations of the fluid flow at the position of bead i due to the presence of another bead at position $\vec{r}_j$.

Defining the particle centre by $\vec{r} = \sum_i \vec{r}_i / N$, its rotational degrees of freedom by $\vec{\varphi}$, and the positions of the component beads relative to the center by $\vec{s}_i = \vec{r}_i - \vec{r}$, we can write $\dot{\vec{r}}_i = \dot{\vec{r}} + \dot{\vec{\varphi}} \times \vec{s}_i$ and $\dot{\vec{\varphi}}_i = \dot{\vec{\varphi}}$, and obtain by a calculation similar to the one outlined in [1] (details will be given elsewhere) the deterministic equation of motion for a chiral particle in an external fluid flow

$$\begin{pmatrix} \dot{\vec{r}} \\ \dot{\vec{\varphi}} \end{pmatrix} = \begin{pmatrix} \mu^{tt} & \mu^{tr} \\ \mu^{rt} & \mu^{rr} \end{pmatrix} \begin{pmatrix} \vec{F} \\ \vec{T} \end{pmatrix}. \tag{3}$$

The final 3×3 mobility tensors μ^{tt}, μ^{tr}, μ^{rt}, μ^{rr} are given by

$$\begin{pmatrix} \mu^{tt} & \mu^{tr} \\ \mu^{rt} & \mu^{rr} \end{pmatrix} = \begin{pmatrix} \eta^{tt} & \eta^{tr} \\ \eta^{rt} & \eta^{rr} \end{pmatrix}^{-1}$$

with

$$\eta^{tt} = \sum_{i,j} \eta_{ij}^{tt}$$

$$\eta^{tr} = \sum_{i,j} \left(-\eta_{ij}^{tt} S_j + \eta_{ij}^{tr}\right)$$

$$\eta^{rt} = \sum_{i,j} \left(\eta_{ij}^{rt} + S_i \eta_{ij}^{tt}\right) = \left(\eta^{tr}\right)^T$$

$$\eta^{rr} = \sum_{i,j} \left(-\eta_{ij}^{rt} S_j - S_i \eta_{ij}^{tt} S_j + \eta_{ij}^{rr} + S_i \eta_{ij}^{tr}\right),$$

$$S_i := \begin{pmatrix} 0 & -s_{i,z} & s_{i,y} \\ s_{i,z} & 0 & -s_{i,x} \\ -s_{i,y} & s_{i,x} & 0 \end{pmatrix},$$

and

$$\begin{pmatrix} \eta_{11}^{tt} & \cdots & \eta_{1N}^{tt} & \eta_{11}^{tr} & \cdots & \eta_{1N}^{tr} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \eta_{N1}^{tt} & \cdots & \eta_{NN}^{tt} & \eta_{N1}^{tr} & \cdots & \eta_{NN}^{tr} \\ \eta_{11}^{rt} & \cdots & \eta_{1N}^{rt} & \eta_{11}^{rr} & \cdots & \eta_{1N}^{rr} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \eta_{N1}^{rt} & \cdots & \eta_{NN}^{rt} & \eta_{N1}^{rr} & \cdots & \eta_{NN}^{rr} \end{pmatrix} = \begin{pmatrix} \mu_{11}^{tt} & \cdots & \mu_{1N}^{tt} & \mu_{11}^{tr} & \cdots & \mu_{1N}^{tr} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mu_{N1}^{tt} & \cdots & \mu_{NN}^{tt} & \mu_{N1}^{tr} & \cdots & \mu_{NN}^{tr} \\ \mu_{11}^{rt} & \cdots & \mu_{1N}^{rt} & \mu_{11}^{rr} & \cdots & \mu_{1N}^{rr} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mu_{N1}^{rt} & \cdots & \mu_{NN}^{rt} & \mu_{N1}^{rr} & \cdots & \mu_{NN}^{rr} \end{pmatrix}^{-1}.$$

The force $\vec{F}$ and torque $\vec{T}$ in (3) are "effective" quantities resulting from the fluid velocity $\vec{v}$ and vorticity $\vec{\omega}$ and are given by

$$\vec{F} = \sum_{i,j} \left[\eta_{ij}^{tt} \vec{v}(\vec{r}_j) + \eta_{ij}^{tr} \vec{\omega}(\vec{r}_j)\right] \tag{4}$$

$$\vec{T} = \sum_{i,j} \left[\left(\eta_{ij}^{rt} + S_i \eta_{ij}^{tt}\right) \vec{v}(\vec{r}_j) + \left(\eta_{ij}^{rr} + S_i \eta_{ij}^{tr}\right) \vec{\omega}(\vec{r}_j)\right], \tag{5}$$

and thus depend on the positions of all the component beads.

Finally, to take into account thermal noise effects, we add unbiased Gaussian white noise sources to Eq. (3) and find the equation of motion

$$\begin{pmatrix} \dot{\vec{r}} \\ \dot{\vec{\varphi}} \end{pmatrix} = \begin{pmatrix} \mu^{tt} & \mu^{tr} \\ \mu^{rt} & \mu^{rr} \end{pmatrix} \begin{pmatrix} \vec{F} \\ \vec{T} \end{pmatrix} + \begin{pmatrix} \vec{\xi}_r(t) \\ \vec{\xi}_\varphi(t) \end{pmatrix}, \tag{6}$$

where we have to make sure that in equilibrium the Boltzmann distribution is approached so that we need to fulfil Einstein's relation. This dictates the noise correlations specified in the main text.

The dynamics of the chiral particles is computed in generalized coordinates, i.e. center of mass and rotational position, by discretizing the Langevin equation (6) according to the Euler algorithm. The positions $\vec{r}_i$ of the single beads, which are needed to calculate the net force $\vec{F}$ and torque $\vec{T}$ due to the flow field and its vorticity (see Eqs. (4), (5)), are determined from the generalized coordinates in every integration step.

Explicit expressions for the tensors μ^{tt}, μ^{tr}, μ^{rt}, μ^{rr} and the quantities involved in calculating $\vec{F}$ and $\vec{T}$, are obtained in a straightforward way once we specified the original hydrodynamic interactions tensors for the component beads μ_{ij}^{tt}, μ_{ij}^{tr}, μ_{ij}^{rt}, μ_{ij}^{rr}. For the simulations performed to study the chiral separation we used [1]

$$\mu_{ij}^{tt} = \delta_{ij}\frac{1}{6\pi\nu_0 a_i}\mathbb{I} + (1-\delta_{ij})\left[\frac{1}{8\pi\nu_0 r_{ij}}\left(\mathbb{I}+\mathbb{P}_{ij}\right) + \frac{a_i^2+a_j^2}{8\pi\nu_0 r_{ij}^3}\left(\mathbb{I}/3-\mathbb{P}_{ij}\right)\right]$$

$$\mu_{ij}^{tr} = \left(1-\delta_{ij}\right)\frac{1}{8\pi\nu_0 r_{ij}^3}\begin{pmatrix} 0 & -z_{ij} & y_{ij} \\ z_{ij} & 0 & -x_{ij} \\ -y_{ij} & x_{ij} & 0 \end{pmatrix}$$

$$\mu_{ij}^{rt} = \left(\mu_{ji}^{tr}\right)^T$$

$$\mu_{ij}^{rr} = \delta_{ij}\frac{1}{8\pi\nu_0 a_i^3}\mathbb{I} + \left(1-\delta_{ij}\right)\frac{1}{16\pi\nu_0 r_{ij}^3}\left(3\mathbb{P}_{ij}-\mathbb{I}\right),$$

where $\mathbb{I}$ is the 3×3 identity tensor, $\mathbb{P}_{ij}$ the projector $\mathbb{P}_{ij} = \vec{r}_{ij}\vec{r}_{ij}/r_{ij}^2$ onto the $\vec{r}_{ij}$ direction, with $\vec{r}_{ij} = \vec{r}_j - \vec{r}_i = \left(x_{ij}, y_{ij}, z_{ij}\right)$, $r_{ij} = \left|\vec{r}_{ij}\right|$, and where a_i is the radius of component bead i and $\nu_0 = 10^{-3}\,Ns/m^2$ is the dynamic viscosity of water at room temperature.

References

[1] B. Carrasco & J. García de la Torre, Improved hydrodynamic interaction in macro- molecular bead models. J. Chem. Phys. 111, 4817-4826 (1999).