Supplementary Material — Hydrodynamically Induced Aggregation of Two Dimensional Oriented Active Particles

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1 Solving for the Streamfunction

Here we develop the equation for the Fourier components of ψ denoted by $B_n(r)$ from the flow equation given in the main text, and solve it. The right-hand-side is given by

$$\nabla^{\perp} \cdot \mathbf{f} = \frac{1}{R}\mathbf{f}_0 \cdot \nabla^{\perp}(\delta(r-R)F(\theta)) = \frac{1}{R}\,\mathrm{Re}\left\{\eta e^{i\theta}\left[\frac{1}{r}\delta(r-R)\frac{\partial}{\partial\theta} - i\frac{\partial\delta}{\partial r}(r-R)\right]F(\theta)\right\}, \tag{1.1}$$

where we used $\mathbf{f}_0 = f_0(\hat{x}\cos\varphi + \hat{y}\sin\varphi) = \mathrm{Re}\left\{(\hat{r}+i\hat{\theta})\eta e^{i\theta}\right\}$. Plugging in the Fourier sums, the left-hand-side is identified with $-\hat{O}_n^2 B_n$, as a result of the Laplacian in polar coordinates. Thus, the resulting equation is given by

$$\hat{O}_n^2 B_n(r) = \frac{1}{R} i\eta C_{n-1}\left[\frac{d}{dr}\delta(r-R) - \frac{n-1}{r}\delta(r-R)\right], \tag{1.2}$$

As mentioned in the main text, where we ignore the Re operator in Eq. (1.1) because the solution is now given by the real part of ψ. To solve this equation, one must first solve the homogeneous equation $\hat{O}_n^2 B_n(r) = 0$. This is an Euler equation, whose solutions are always given by monoms. Here, after plugin in $B_n = r^m$ we get $m = \pm n, 2 \pm n$. Thus, the solution to eq. (1.2) is given by:

$$B_n(r) = \frac{1}{R}\begin{cases} x_n\left(\frac{r}{R}\right)^{|n|} + y_n\left(\frac{r}{R}\right)^{|n|+2} & r < R \\ z_n\left(\frac{r}{R}\right)^{-|n|} + w_n\left(\frac{r}{R}\right)^{-|n|+2} & r > R \end{cases}, \tag{1.3}$$

as long as $n \neq 0, \pm 1$ which will be resolved later. The condition on the coefficients x_n, y_n, z_n, w_n are given by the behavior at $r = R$. B and B' must be continuous at $r = R$, because their discontinuity would result in higher derivatives of $\delta(r-R)$ in the equation. To obtain discontinuity constraints on B'' and B''' we first integrate over the equation from $R-\epsilon$ to $R+\epsilon$ and get one condition, and second we multiply both sides by $(r-R)$ and integrate over the same interval, getting the second condition

$$rB_n''(r)\Big|_{R-\epsilon}^{R+\epsilon} = i\eta C_{n-1},\; r^2 B_n'''(r)\Big|_{R-\epsilon}^{R+\epsilon} = -i\eta C_{n-1}(n+1). \tag{1.4}$$

After plugging in eq. (1.3), we get equations for the coefficients:

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ |n| & |n|+2 & |n| & |n|-2 \\ |n|(|n|-1) & (|n|+1)(|n|+2) & -|n|(|n|+1) & -(|n|-1)(|n|-2) \\ (|n|-1)(|n|-2) & (|n|+1)(|n|+2) & (|n|+1)(|n|+2) & (|n|-1)(|n|-2) \end{pmatrix} \begin{pmatrix} x_n \\ y_n \\ z_n \\ w_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -1 \\ \frac{n+1}{|n|} \end{pmatrix} i\eta C_{n-1} R \tag{1.5}$$

with the solution $z_n = \frac{1}{4(1+|n|)}\left(\frac{1}{|n|} + \Theta(n)\right) i\eta C_{n-1}R, w_n = \frac{1}{4(1-|n|)}\Theta(n) i\eta C_{n-1}R$, where Θ is the step function. When $n = -1$ the solution can be gained from a limit in n, since $w_n = 0$ for negative n. As mentioned in the main text, we don't concern ourselves with the case $n = 1$, and so $n = 0$ is the only special case. Its homogeneous solutions have a degeneracy, and so the general homogeneous solution is given as a linear combination of $1, r^2, \ln r, r^2 \ln r$. Applying the same continuity conditions gives the solution in the main text, where a global constant is ignored.

2 Constraints on the Force Distribution

As mentioned in the main text, limiting the force distribution to a circle and to a constant direction does not constrain the solution of the flow given by the series solution. The coefficients in the series solution are given by:

$$D_{ji_1i_2\ldots i_n} = \frac{(-1)^n}{n!}\int_S f_j r_{i_1}\ldots r_{i_n} dA \tag{2.1}$$

where S is the region the force is applied. The series solution is given by a sum of the contraction between $\mathbf{D}_{n+1}$ and $\nabla^n \mathbf{G}$, in the from $D_{ji_1\cdots i_n}\partial_{i_1}\cdots\partial_{i_n}G_{jk}$. Now, we will show that the possible leading terms in a solution are independent of S in most cases, and indeed independent in our case, a circle. Because the permutation of i_p, i_q doesn't change the component of either tensor, $\mathbf{D}$ and $\nabla^n\mathbf{G}$, the contraction is of the form:

$$\begin{pmatrix} \binom{n}{0} D_{i11\cdots11} \\ \binom{n}{1} D_{i11\cdots12} \\ \vdots \\ \binom{n}{n} Di22\cdots22 \end{pmatrix} \cdot \begin{pmatrix} \partial_1^n\partial_2^0 G_{ij} \\ \partial_1^{n-1}\partial_2^1 G_{ij} \\ \vdots \\ \partial_1^0\partial_2^n G_{ij} \end{pmatrix} \tag{2.2}$$

where in the first line all $i_p = 1$, in the second line a single index is equal to 2 and so on. We now denote $D_{i\alpha}$ the components of $\mathbf{D}_n$ with α being the amount of $i_p = 1$. Since the derivative of the green function does not depend on S, to show the result space of Eq. 2.2 does not depend on S, it is enough to show that the possible space of $D_{i\alpha}$ does not depend on S (not a necessary but a sufficient condition). The components $D_{i\alpha}$ are defined as

$$D_{i\alpha} = \frac{(-1)^n}{n!}\int_S f_i x^\alpha y^{n-\alpha} dA = \langle f_i, b_\alpha \rangle_S, \tag{2.3}$$

where $\langle\cdot,\cdot\rangle_S$ is the standard inner product for function vector spaces, defined over S, and $b_\alpha = \frac{(-1)^n}{n!}x^\alpha y^{n-\alpha}$. First assume the direction of the force is fixed, say $f_2 = 0$. As long as $\mathcal{B} = \{b_\alpha | \alpha = 1\cdots n\}$ are linearly independent under S, for every $\mathbf{D}_n$ there exists $f_1 \in \text{span}\mathcal{B}$ such that Eq. (2.3) is satisfied. In particular, it is given by $f_1 = \sum_\alpha D_{1\alpha} b^*_\alpha$, where b^*_α are the dual basis of $\mathcal{B}$. In particular, when S is the unit circle, $b_\alpha = \cos^\alpha\theta \sin^{n-\alpha}\theta$ are linearly independent. Therefore, the possibilities of $\mathbf{D}_n$ are not limited by the choice that S is the unit circle, and therefore, the result of the series solution is not constrained by this choice. An example where the choice of S does matter is when $\mathcal{B}$ is linearly dependent, for instance, if S is a section of the line $y = x$.

However, the orientation of the force does matter. The solutions for the force that give a specific $D_{i\alpha}$ is $f_i = \sum D_{i\alpha} b_\alpha^*$. Because this force does not have a constant direction (in general), it is not possible to use the argument above here.

However, a solution for a general force distribution is given by the sum of two familiar solutions — one considering only the x-component of the force, and second only with the y-component. Therefore, the most general force distribution is given as a sum of the same terms discussed in the main text (ψ_{nm} in Sec. IIIB), just with different coefficients. As a result, the discussion on the dynamics in the main text applies to any force distribution. An example is given in the following section.

3 Constructing Multipoles with Point Forces

Here we highlight how to construct force distributions using point forces only, such that a specific multipole can be dominant. As mentioned in the main text, the term r^{-n} ($n > 0$) couples to the harmonics $\pm n, n+2$ in the streamfunction. These harmonics couple to the harmonics $\pm n-1, n+1$ of the force distribution. Therefore if the lowest (positive) harmonic in a force distribution is $n+1$ (which is accompanied by $-n-1$), then r^{-n} will be the leading term in the stream function.

$$\psi = \frac{R^{n+1}}{4r^n} \operatorname{Re}\left\{ -\frac{i\eta C_{n+1}}{n+1} e^{i(n+2)\theta} + \frac{i\eta C_{-n-1}}{n(n+1)} e^{-in\theta} \right\}, \tag{3.1}$$

where $C_{-n-1} = C_{n+1}^*$ because the force distribution is real. In order to accomplish Eq. (3.1) with point forces, a force distribution is given by

$$F(\theta) = \sum_{k=0}^{2n+1} (-1)^k \delta\left(\theta - \theta_0 + \frac{\pi k}{n+1}\right). \tag{3.2}$$

Intuitively, this function has a period of $2\pi/(n+1)$ and so its smallest harmonic must be $n+1$, and one can verify that using the Fourier expansion of the delta function, as well as the fact that the roots of $f(z) = 1 - z + z^2 - \cdots - z^{2n+1}$ are all the $2n+2$ roots of unity except -1. This distribution is used in the main text in Sec. IIIA with $n = 2$.

As mentioned in the main text, for $n = 2$ this distribution creates both second and forth harmonics in ψ. As mentioned earlier, using a force distribution with a varying direction, it is possible to achieve more varied linear combination of the terms. For example, we can sum two force distributions, each in a constant direction, in order to isolate only one of the harmonics. The distribution in Eq. (3.2) with $n = 2$ gives (as noted in the main text with $\theta_0 = 0, \mathbf{f}_0 = f_0\hat{x}, C_3 = \frac{3}{\pi}$)

$$\psi_{\text{oct}} = \frac{R^3}{4\pi r^2} f_0 \left(\sin 4\theta + \frac{1}{2}\sin 2\theta\right). \tag{3.3}$$

Now, to isolate only the forth harmonic, we rotate the force distribution (and $\mathbf{f}_0$) by $\pi/2$, creating a distribution with $\mathbf{f}_0 || \hat{y}$. These two distributions can be summed to create a distribution with a varying force direction. Summing Eq. (3.3) with itself after the transformation $\theta \to \theta + \frac{\pi}{2}$ gives

$$\psi = \frac{R^3}{2\pi r^2} f_0 \sin 4\theta. \tag{3.4}$$

Using this decomposition, any term we have mentioned ψ_{nm} can be dominant.

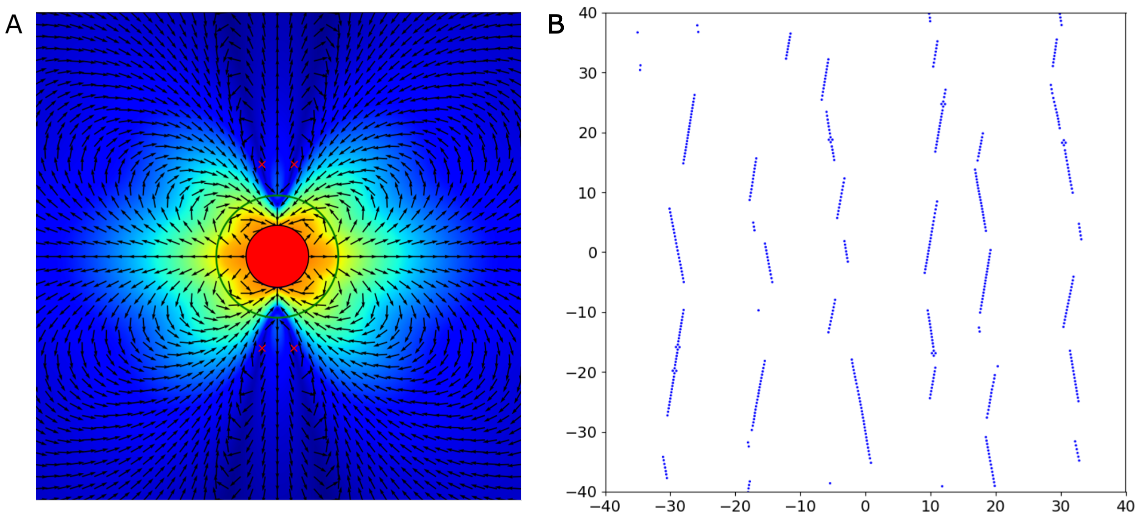

Figure 1: (a) The velocity field created by the stream function $\psi = (\frac{R^2}{3r^2} - \frac{R^4}{4r^4})\sin(4\theta) + \frac{R^2}{2r^2}\sin 2\theta$. The red circle marks the particle. The green circle has twice its radius, noting the closest distance another particle can approach before steric interactions take effect. The red crosses mark the extremum points. (b) The final state of a simulation of particles with this stream function. The particles clearly form lines tilted at the angles of the extrema. In addition, a few particles collide and form diamonds, similar to the clusters presented in the main text. It is possible that at even longer times, all the particles will form a single line.

4 Stream Functions that have Extrema

As mentioned in the main text, a simple example of a stream function with minima and maxima is given by a squirmer with $\psi = (\frac{R^2}{r^2} - \frac{R^4}{r^4})\sin(4\theta)$, which has extrema at $r = \sqrt{2}R$ and $\theta = \frac{\pi}{8}, \frac{3\pi}{8} \cdots \frac{15\pi}{8}$. In close range, the particles seem to exhibit mostly chaotic dynamics, with weak stability around the stream function's extrema.

Another examples is given by the stream function $\psi = (\frac{R^2}{3r^2} - \frac{R^4}{4r^4})\sin(4\theta) + \frac{R^2}{2r^2}\sin 2\theta$, generated by a particle with only a third harmonic in its force distribution, but with a varying force direction. Its velocity field is displayed in Fig.1. In a two-particle interaction, it is clear that most paths that $\mathbf{d}$ takes lead to the y-axis, and very few paths (that begin very close the the particle) result in collision and static stability. Once $\mathbf{d}$ reaches the y-axis, small perturbations will change its paths into orbits around the extrema points. Thus, particles are likely to be stable around the extrema in multi-particle interactions.

Indeed, simulating a multi-particle interaction, in a similar manner to the main text, shows dynamical stability in the formation of rods, angled according to the angle of the extrema, at $\approx \pm 9°$ measured from the y-axis. These structures, while relatively stable, are still much easier to change than the structures created by attraction of two particles at their boundary. In fact, while the rods can scatter and destroy each other, the rare crystallizations in this simulation remain uninterrupted.

This examples show that when extrema are present and crystallization is not forced, the dynamics can be very ordered or very chaotic, and a closer look is needed to understand close-range dynamics in general.