J. Phys.: Condens. Matter 29 (2017) 115102 (7pp)

doi:10.1088/1361-648X/aa5a64

A 2D suspension of active agents: the role of fluid mediated interactions

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Received 13 November 2016, revised 3 January 2017 Accepted for publication 19 January 2017 Published 7 February 2017



Abstract

Taking into account both the Vicsek short-range ordering and the far-field hydrodynamic interactions mediated by the ambient fluid, we investigate the role of long-range interactions in the ordering phenomena in a quasi 2-dimensional active suspension. By studying the number fluctuations, the velocity correlation functions and cluster size distribution function, we show that depending on the number density of swimmers and the strength of noise, the hydrodynamic interactions can have significant effects in a suspension. For a fixed value of noise, at larger density of particles, long-range interactions enhance the particle pairing and cluster formation in the system.

Keywords: active suspension, hydrodynamic interactions, ordering

(Some figures may appear in colour only in the online journal)

1. Introduction

Active agents that can convert a non-mechanical form of energy to mechanical work, exhibit a wide range of interesting dynamical behaviors when they form a suspension [1–6]. Both at the scales of macro and micro, there are many examples of such systems that have attracted enormous interests recently. Schools of fishes and birds [7–10], bacterial suspensions [11, 12], gels of cytoplasmic polymers [13, 14], interacting active Janus particles [15] and swimmers in non newtonian fluids [16] are some relevant examples.

One of the main questions that needs to be answered, is the nature of ordered phases in such systems. In this article, we concentrate on the dynamics of micron-scale active agents. A wide class of works includes numerical simulations of micro-suspensions, based on phenomenological and simplified interaction terms between individual particles[17–22]. The well known model of Vicsek that can correctly account the local ordering of elongated objects, is the core of such studies [23]. Such simulations reveal how a local ordering rule can lead the system to reach a state with large scale ordered phases [24–28].

Continuum thermodynamic description of active suspensions, is another line of approach that can address some macroscopic features of the systems[29–34]. Dynamical equations for the

continuum fields, derived by symmetry arguments or obtained from statistical averaging over microscopic forces, can capture the physics of ordered phases developed in such systems.

In contrast to the above works, only a few studies have investigated the role of long-range hydrodynamic interactions (HD) between the particles [35–38]. Effects of such interactions is essential, specially in the case of micro-scale examples suspended in aqueous media. Fluid velocity produced by a moving particle, propagates instantaneously (a property of small scale hydrodynamic) through the medium and affects the motion of other particles. Some researchers, using a simple dipolar flow interaction mechanism, have concluded that HD may prevent the emergence of long-range order [39]. Cluster formation in bacterial suspension and its promotion with hydrodynamic interactions are among important results in active suspensions that needs more insight [40-42]. The aim of this article is to improve our understanding of the ordering phenomena and collective behavior in a suspension of active microscopic agents. To correctly account for such interactions, one needs to start from a hydrodynamic model that takes into account the internal structure of the swimmers. Starting from hydrodynamic interactions obtained from a generic microscopic model, we numerically study the statistical parameters, that can reflect the nature of ordering in a suspension of such micron scale swimmers.



Figure 1. The geometry and internal structure of two interacting swimmers are shown. Each swimmer, with two internal degrees of freedom, has an intrinsic swimming direction denoted by $\hat{\mathbf{t}}$.

2. Model

To study the dynamics of a two dimensional collection of \mathcal{N} interacting self propelled objects, we assume that the interaction between swimmers can be obtained from two-particle interactions. One should note that this is an approximation that permits us to simplify the problem and proceed. Hydrodynamic interactions between colloidal particles have contributions in the form of many body interaction potential. Considering the two-body interaction means that we are neglecting 3-body and more than 3-body correlations. Figure 1, shows a schematic view of two swimmers that interact through both short and long-range interactions. The position and the orientation of the *i*th swimmer is shown by \mathbf{r}_i and $\hat{\mathbf{t}}_i$, respectively. In addition to position and orientation, the internal structure of the swimmers is also important. Each swimmer has an internal structure, that allows it to swim. To model the internal structure of the swimmers, we use a minimal model with two internal degrees of freedom, namely the three beads connected by two arms [43, 44]. This is a generic model that can correctly explain the far field of both dipolar and quadrupolar swimmers. Denoting the lengths of front and back arms of a swimmer by $\ell_f^l(t)$ and $\ell_b^i(t)$ and the spheres radius by a, we can seek internal motions that are able to propel the swimmer. As it is verified experimentally, a simple harmonic undulating motion with a phase lag on arm lengths, is able to propel the swimmer at low Reynolds condition [44]. For identical swimmers, we choose an internal motion that is given by $\ell_f^i(t) = \ell + u \sin(\omega t)$ and $\ell_b^i(t) = \ell(1+\delta) + u\sin(\omega t + \varphi_i)$, where ℓ and $\ell(1+\delta)$ denote the average arm lengths, u denotes the undulation amplitude, the frequency is shown by ω and the phase difference between the arms is denoted by φ_i .

The orientation of a swimmer in a two dimensional reference frame can be represented by a single angle θ_i . In this case we have: $\hat{\mathbf{t}}_i = (\cos \theta_i, \sin \theta_i)$. Detail hydrodynamic calculations (see appendix), show that the velocity of *i*th swimmer, moving in the presences of *j*th swimmer, can be written as [45, 46]:

$$\mathbf{V}_i = v \, \hat{\mathbf{t}}_i + \mathbf{V}_{ij}, \ \dot{\theta}_i = \Omega_{ij}$$

where the intrinsic swimming velocity of a swimmer depends on its internal structure as: $v = v(a, u, \omega, \ell, \delta)$ and, the interaction terms are functions of the distance $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and the orientation of swimmers: $\mathbf{V}_{ij} = \mathbf{V}_{ij}(v, \hat{\mathbf{t}}_i, \hat{\mathbf{t}}_j, \mathbf{r}_{ij})$ and $\Omega_{ij} = \Omega_{ij}(v, \hat{\mathbf{t}}_i, \hat{\mathbf{t}}_j, \mathbf{r}_{ij})$ (See appendix for details). The interaction terms, \mathbf{V}_{ij} and Ω_{ij} , obtained with this kind of modeling are valid only for very far swimmers: $r_{ij} \gg \ell$. Complexity of hydrodynamic equations, does not allow us to achieve analytical results for the shortrange part of the interactions between swimmers.

To overcome the complexity of short-range hydrodynamic interactions, we approximate the short-range part of the interactions by a very well known model of Vicsek that is essentially a phenomenological short-range interaction [23]. This interaction enforces an elongated object (like what we have shown by ellipsoids in figure 1) to change its direction according to the average orientations of its neighbors. The Vicsek model does not fully consider all features of the short-range hydrodynamic interaction, but as an approximation we neglect other details of short-range hydrodynamic interactions that are not included in Vicsek model. Vicsek's model mainly takes into account the steric interaction between the elongated objects. To simplify our study, we assume that there is a crossover length R_c that separates the short and longrange forces. Two objects with separation smaller than this crossover length, interact with short-range Vicsek model and beyond this length, the long-range hydrodynamic interactions are present. In our numerical scheme, we will assume that $R_c = 5\ell$. Emergent collective motions of the Vicsek model are clearly known and our combined model here, will show how HD interaction can affect such collective motions.

In order to numerically study the dynamics of a suspension, we write the discrete dynamics of the *i*th swimmer as:

$$\mathbf{r}_{i}(t+\delta t) = \mathbf{r}_{i}(t) + \delta t \left(v \mathbf{\hat{t}}_{i} + \sum_{j} \Theta(r_{ij} - R_{c}) \mathbf{V}_{ij} \right),$$

$$\theta_{i}(t+\delta t) = \theta_{i}(t) + \theta_{i}^{V} + \eta \xi_{i}(t) + \delta t \sum_{j} \Theta(r_{ij} - R_{c}) \Omega_{ij},$$

where Heaviside step function is $\Theta(x) = 1$ for $x \ge 0$ and it is 0 for x < 0. The short-range contribution to the dynamics is given by: $\theta_i^V = \arg \sum_j' e^{i\theta_j(t)}$, where the summation runs over all swimmers with $r_{ij} < R_c$. We assume that the fluctuations affect the dynamics of the swimmers, through a rotational noise represented by $\eta \xi_i(t)$. Here ξ is a random number with uniform probability in the interval $[-\pi, \pi]$ and the strength of noise η , can take any positive value.

3. Two swimmer scattering

Before studying the case of many swimmers, it is instructive to start with two particles system. Rich behavior emerging from long-range hydrodynamic interaction, promises a non trivial behavior for the trajectories of two interacting swimmers. A plethora of behavior, repulsive, attractive and oscillating trajectories can be observed. The details of such behavior has been studied extensively before [45, 46].



Figure 2. Scattering of two individual swimmers are analyzed by their momentum change. Forward component of the change in total momentum, is plotted as a function of incoming angular separation Δ for different values of noise strength η . At very low noise, the isotropic state is not stable.

An important feature that one can learn from the two body system, is the stability of isotropic phase in a many swimmer system. In an isotropic phase, all swimmers move in random directions and no direction is preferred. Using a kinetics theory approach with two body scatterings, it is shown that for a dilute system, the nature of two body scattering is the essential mechanism that determines the stability of the isotropic state [47]. Denoting by **P** and δ **P**, the initial total momentum and the change in total momentum after a binary scattering, we define the average forward component of the momentum change in a binary scattering by: $\mu = \langle \mathbf{P} \cdot \delta \mathbf{P} \rangle_0$. Averaging is done over all impact parameters and as shown in figure 2(inset), the incoming angular separation is shown by Δ . Neglecting the self diffusion, for $\mu > 0$, the isotropic state is unstable and the interactions will eventually lead the system to reach a polar state [47]. For $\mu < 0$, the interaction between particles is not able to develop a polar state.

Figure 2, shows the forward component of averaged change in momentum as a function of incoming angular separation Δ . Here we have taken into account the HD interactions as described in the previous section. As one can see from this figure, for small noises, μ is positive for all Δ , and it reflects the instability of the isotropic state. Following such instability and for small noises, ordered state (anisotropis phase) emerges. In anisotropic phase, the rotational symmetry is spontaneously broken and all swimmers move in a preferred direction. Such an instability is a general feature of the Vicsek like interaction, and we see here that the long-range hydrodynamic interaction does not affect the instability. As one can see from the figure, by increasing the noise, μ starts to have negative values that reflects the stability of isotropic state. This means that, in the presence of HD, we expect to observe ordered (anisotropic) phase at small values of noise.

In the following parts we numerically investigate the detail role of HD in the ordering of a suspension.

4. Ordering

To investigate the role of hydrodynamic interaction in the long time behavior of a quasi 2D suspension, we proceed by numerically simulating the system. Along this path we study a set of order parameter and correlation functions. To quantify the polar order of the system, we define the polar order parameter as: $\psi = \frac{1}{N_{\nu}} |\sum_{i=1}^{N} \mathbf{V}_i|$. Fully polarized state (anisotropic phase) is given by $\psi = 1$ and the isotropic state corresponds to $\psi = 0$. Velocity autocorrelation and velocity–velocity correlation functions are defined as:

$$C_{a}(t) = \frac{1}{\mathcal{N}} \langle \sum_{i=1}^{\mathcal{N}} \frac{\mathbf{V}_{i}(0) \cdot \mathbf{V}_{i}(t)}{|\mathbf{V}_{i}(0)| |\mathbf{V}_{i}(t)|} \rangle,$$

$$C_{vv}(r) = \frac{1}{\mathcal{N}(\mathcal{N}-1)} \langle \sum_{i=1}^{\mathcal{N}} \sum_{j\neq i}^{\mathcal{N}} \frac{\mathbf{V}_{i}(t) \cdot \mathbf{V}_{j}(t)}{|\mathbf{V}_{i}(t)| |\mathbf{V}_{j}(t)|} \rangle.$$

where $\langle \cdots \rangle$ denotes averaging over all particles and also over time in a steady state regime. These two correlation functions contain information about correlation time and correlation length in a fluctuating system. Local spatial ordering and clustering in the system can be understood in terms of the radial distribution function g(r) that is defined by:

$$g(r) = \frac{\ell^2}{\mathcal{N}(\mathcal{N}-1)} \langle \sum_{i=1}^{\mathcal{N}} \sum_{j\neq i}^{\mathcal{N}} \delta(r - |\mathbf{r}_{ij}|) \rangle$$

The number fluctuation, is the other quantity that we can study in our simulations. Denoting the average number of particles by $\langle n \rangle$, we study its fluctuations: $\sigma = \langle n^2 \rangle - \langle n \rangle^2$. This is a statistical parameter that includes information about the non-equilibrium nature of a fluctuating system. The practical method which we use to calculate the number fluctuations is as follows. For a given total number of swimmers \mathcal{N} , we start by a small window in the middle of the simulation box and measure both average number of particles and its fluctuation inside this window. Then changing the size of this window will allow us to plot the number fluctuations as a function of average number.

Defining all the required statistical parameters of our system, we will study the thermodynamic state of our system in the next section. In our numerical study, we consider a two dimensional suspension of \mathcal{N} particles in a square box of length L with periodic boundary condition. To make the equations non dimensional, we use ℓ and v as characteristic length and velocity. In simulations, we choose a square box of size 50ℓ and change the particle numbers from 100 to 2000. The time step in dimensionless units is $\delta t = 0.001$ and a total number of $\sim 1.2 \times 10^6$ steps is necessary to reach steady state. To implement the periodic boundary conditions we use a single set of image particles beyond the walls of the box. The image system allows us to take into account the leading order contribution of the long-range hydrodynamic interaction.



Figure 3. Left: order parameter in terms of the number of swimmers. Right: density fluctuation as a function of average number is plotted for different strength of noise η . Results are compared for two cases where the hydrodynamic interaction is on or off (HD and NHD).



Figure 4. Velocity auto-correlation function $C_a(t)$ (left), velocity–velocity correlation function $C_{\nu\nu}$ (middle) and, radial distribution function g(r) (right) are plotted for a system with $\mathcal{N} = 2000$ and $\eta = 0.35$. At large noises, both correlation time and correlation length and also the pairing strength are enhanced by HD interactions.

5. Results and discussions

Swarming behavior in our model, results from interplay between hydrodynamic interactions, noise strength and number density of particles. As our main goal here is to investigate the role of hydrodynamic interactions, we repeat all simulations with and without hydrodynamic interactions. In the first set of simulations, we perform the simulations only with the Vicsek interaction then for the second set, we include the long-range interactions as well. Comparison between the results of these two sets of results will provide an understanding of the role of hydrodynamic interaction. All results marked by NHD are obtained by taking into account the Vicsek interaction and the results marked by HD, denote the cases where both Vicsek and long-range hydrodynamic interactions are present.

Figure 3(left) shows the polarization order parameter, ψ , as a function of number of the swimmers (for fixed box size). As we have expected from two-body scattering results, the results that have been obtained at previous section, for a fixed noise, increasing the density will result instability in the isotropic phase and a stable anisotropic polarized phase will appear. This is consistent with the results of previous section where, as we discussed, it is the short-range part of the interaction that dominates the instability mechanism.

Let us study the number fluctuation in the presence of hydrodynamic interactions. For a system that is in thermal equilibrium, we expect to see a relation like $\sigma \sim \langle n \rangle^{\frac{1}{2}}$. Figure 3(right) shows the results of numerical simulations, that as a result of particle's activity, deviate from equilibrium $\frac{1}{2}$ power law [48]. The results, indicate that by increasing the noise strength the system will tend to approach equilibrium power law (for larger noise, the slopes are smaller). But for a large and fixed noise strength, the HD curve has a slope smaller than the NHD curve. It turns out that for this condition, the HD interaction diminishes the out of equilibrium nature of the system. This result critically depends on the strength of noise, our simulations shows that for smaller noise the HD does not have any critical role in the behavior of number fluctuation.

Velocity auto-correlation function and velocity–velocity correlation function, are plotted in figure 4(left) and (middle). As one can see from the results, for large number density $\mathcal{N} = 2000$ and large noise $\eta = 0.35$, the HD interaction increases both the correlation time and correlation length. For small noise $\eta = 0.15$ (results are given only for autocorrelation function), the increase in correlation time is very small. Figure 4(right), shows the results for radial distribution function g(r). The height of peak in g(r) reflects the strength of two-particle pairing in the systems. As we can see from this figure, the strength of peak strongly depends on the interaction between particles. HD interactions increase the pairing and clustering in the system. This result, again verify the idea that the long-range interactions, inject more order to the suspension.



Figure 5. Up: two snapshots of the system for $\mathcal{N} = 1500$ with (left) and without (right) hydrodynamic interactions. Different colors denote different cluster and one can distinguish that HD strongly enhances the clustering mechanism. Down: cluster size distribution function for various particle number and noise strengths. For a large number of particles, having large clusters are most frequent in the case of HD.

Size distribution function of clusters is another important quantity that can help us in correctly analyzing the swarming behavior in a suspension. In a many body system of active agents, clusters of different sizes intermittently form and break. As a results of particle exchange between different clusters, a power law distribution function can be expected [25]. Intuitively, if two particles are within the alignment zone, they are considered to belong to a same cluster. Size of a cluster *n*, is defined as the number of particles that belong to a same cluster. Examples of system snapshots, with and without HD interactions are shown figure 5(up), left and right, respectively. In similar conditions, for the case where the HD interaction is on, the clusters are finely distinguishable. Denoting by P(n), the probability to have a cluster with size n, we study this function for different values of number density and a fixed strength of noise $\eta = 0.35$ in figure 5(down). Cluster formation in bacterial suspensions have been studied experimentally where, results similar to figure 5(down) are reported [49, 50]. Having clusters with large sizes, depends strongly on the interaction and the number density. For larger densities, HD interaction increases the probability of finding large clusters, but by decreasing the density of particles, the HD may change its role. Consistence with the previous result, at small densities, the hydrodynamic interactions do not show any observable effects in our simulations. Promotion of cluster formation by hydrodynamic interaction can be understood by studying the case of two swimmers. Extensive investigations have shown that depending on the conditions, such long-range interactions can mediate effective attraction between two hydrodynamic swimmers [45, 46]. Depending on initial conditions of two swimmers (their impact parameter and velocities), their scattering shows a rich behavior. Interestingly they can capture each other or show oscillatory trajectories. These are manifestations of such effective attraction. Such phenomena can be a potential description for the cluster formation in a many body system.

In conclusion, we have numerically studied the effects of longrange hydrodynamic interactions in the ordering phenomena in an active suspension of micro-particles. The system that we have considered is quasi 2 dimensional in a sense that the swimmers are allowed to move in a two dimensional plane but the three dimensional fluid dynamic equations are used to derive the longrange interactions. In active systems, one does not expect to see a sharp differences between the results of 2 and 3 dimensional systems similar to what have been seen in classical equilibrium systems. In equilibrium systems with short-range interactions, the fluctuations will destroy any order in 2D systems. The situation is different here, particles are active and their directed motion will allow them to move and see more particles and interact with them. This effect can be seen as an effective long-range interaction and in such 2D systems ordered states can be formed. We have shown that depending on the strength of noise and number density of particles, the interactions have critical effects on the number fluctuations, correlation functions and clustering phenomena. We should stress here that the value of order parameter shows some dependence to the hydrodynamic interactions. Simulations with a large number of particles are necessary to study the role of long-range interactions in the order parameter. Along this work, we are studying the effects of interplay between internal phases of the swimmers (here, we have assumed that all swimmer are in phase). Coherent effects observed in small systems [51], promise us to see interesting effects in suspensions.

Acknowledgment

We benefited from useful discussions with S Ramaswamy. We also acknowledge Farideh Khalili and Mohsen Yarifard for their helps at the early stages of this work.

Appendix

In this appendix, we briefly present the analytical results for the hydrodynamic interactions between two model microswimmers. Following the method given in [45, 46], the intrinsic velocity of a single swimmer and it's hydrodynamic interaction with second swimmer can be written as:

$$v = \frac{7}{24} \left(\frac{a}{\ell^2}\right) (1+\delta) (u^2 \omega) \sin \varphi_i,$$
$$\mathbf{V}_{ij} = \alpha_1 \left(\frac{\ell}{r_{ij}}\right)^2 \mathbf{T} + \left(\frac{\ell}{r_{ij}}\right)^3 [\alpha_2 \mathbf{D} + \alpha_3 \mathbf{E}],$$
$$\mathbf{\Omega}_{ij} = \beta_1 \left(\frac{\ell}{r_{ij}}\right)^3 \mathbf{F} + \left(\frac{\ell}{r_{ij}}\right)^4 [\beta_2 \mathbf{G} + \beta_3 \mathbf{H}].$$

The above results are obtained by averaging over a complete period of internal motion $(2\pi/\omega)$. In terms of $\epsilon = \frac{a}{\ell^2}u^2\omega$ and $\varphi_{ij} = \varphi_i - \varphi_j$, the parameters are given by:

$$\begin{split} \alpha_1 &= \frac{29}{64} \left(\frac{a \, \delta \epsilon}{\ell} \right) \, \sin \varphi_j, \quad \alpha_2 = -\frac{\epsilon}{4} \left(\delta + 2 \right) \, \sin \varphi_j, \\ \alpha_3 &= \frac{\epsilon}{24} \left[(3+\delta) \, \sin \varphi_i + (3+2\delta) \left(\sin \varphi_j + \sin \varphi_{ij} \right) \right], \\ \beta_1 &= -\frac{29}{64} \left(\frac{a \, \delta \epsilon}{\ell^2} \right) \, \sin \varphi_j, \quad \beta_2 = \frac{3}{8} \left(\frac{\epsilon}{\ell} \right) \, \sin \varphi_j \left(2 - \delta \right), \\ \beta_3 &= \frac{7}{48} \left(\frac{\epsilon}{\ell} \right) \, \left[(3-\delta) \, \sin \varphi_i + (3-2\delta) (\sin \varphi_j + \sin \varphi_{ij}) \right] \end{split}$$

and

$$\begin{split} \mathbf{T} &= -3[M_{mn}\hat{t}_{jm}\hat{t}_{jn}]\,\hat{r}_{ij} \\ \mathbf{D} &= -\frac{3}{2}[M_{mn}\hat{t}_{jm}\hat{t}_{jn}]\,\hat{t}_{j} + \frac{3}{2}[M_{mnk}\hat{t}_{jm}\hat{t}_{jn}\hat{t}_{jk}]\,\hat{r}_{ij} \\ \mathbf{E} &= -3[M_{mn}\hat{t}_{jm}\hat{t}_{jn}]\,\hat{t}_{i} + 3[M_{mnk}\hat{t}_{jm}\hat{t}_{jn}\hat{t}_{ik}]\,\hat{r}_{ij} \\ \mathbf{F} &= 3[M_{mnk}\,\hat{t}_{jm}\,\hat{t}_{jn}\,\hat{t}_{ik}]\,(\hat{r}_{ij}\times\hat{t}_{i}), \\ \mathbf{G} &= [M_{mnk}\hat{t}_{jm}\hat{t}_{jn}\hat{t}_{ik}]\,(\hat{t}_{j}\times\hat{t}_{i}) - 5[M_{mnkl}\hat{t}_{jm}\hat{t}_{jn}\hat{t}_{jk}\hat{t}_{il}]\,(\hat{r}_{ij}\times\hat{t}_{i}), \\ \mathbf{H} &= -\frac{15}{2}[M_{mnkl}\hat{t}_{jm}\hat{t}_{jn}\hat{t}_{ik}\hat{t}_{il}]\,(\hat{r}_{ij}\times\hat{t}_{i}), \end{split}$$

where \hat{t}_i represents the director of *i*th swimmer and \hat{t}_{ik} stands for its *k*th component. In above relations, summation over indices *m*, *n*, *k*, *l* are assumed. The symmetric and traceless tensors used at the above equations, are given by:

$$\begin{split} M_{ij}(\hat{r}) &= \hat{r}_{i}\hat{r}_{j} - \frac{1}{2}\delta_{ij}, \\ M_{ijk}(\hat{r}) &= 4\hat{r}_{i}\hat{r}_{j}\hat{r}_{k} - (\delta_{jk}\hat{r}_{i} + \delta_{ik}\hat{r}_{j} + \delta_{ij}\hat{r}_{k}), \\ M_{ijkl}(\hat{r}) &= 6\hat{r}_{i}\hat{r}_{j}\hat{r}_{k}\hat{r}_{l} + \frac{1}{4}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ - (\delta_{ij}\hat{r}_{k}\hat{r}_{l} + \delta_{kl}\hat{r}_{i}\hat{r}_{j} + \delta_{kl}\hat{r}_{i}\hat{r}_{l} + \delta_{il}\hat{r}_{j}\hat{r}_{k} + \delta_{jk}\hat{r}_{i}\hat{r}_{l} + \delta_{il}\hat{r}_{i}\hat{r}_{k}). \end{split}$$

The above equations are valid for two swimmers that are moving inside a 2D plane. For numerical calculations we have set all phases to $\varphi_i = \pi/2$ and $\delta = 0.1$.

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