Emergent collective dynamics of hydrodynamically coupled micro-rotors

Kyongmin Yeo\(^1\), Enkeleida Lushi\(^3\), Petia M. Vlahovska\(^3\)

\(^1\)IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA
\(^2\)Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912, USA
\(^3\)School of Engineering, Brown University, 182 Hope Street, Providence, Rhode Island 02912, USA

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We examine the collective dynamics of a monolayer of rotating particles immersed in viscous fluid. Each rotor is driven by a constant magnitude torque perpendicular to the monolayer. The rotors interact with each other through soft repulsions but can also be advected and rotated by fluid flow generated by the other rotors. We show here that this hydrodynamic coupling gives rise to structures and phase behavior unobserved in rotor suspensions with only steric repulsion. Our findings underscore the importance of inclusion of the many-body and long-range hydrodynamic interactions in predicting the phase behavior of active systems.

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Systems of motile, interacting units may exhibit many fascinating non-equilibrium phenomena such as self-organisation and directed motion at large scales \([1]\). Theoretical studies of active matter report clustering \([2]\), phase separations \([3]\) and rotating structures \([4]\). Some of these phenomena have been observed in experiments of bacterial suspensions \([5]\) or chemically-activated motile colloids \([6]\).

The collective motion of translating units such as bacteria has received much interest \([1]\). On the other hand, little is known about spinning units, partly because such systems were realized experimentally only recently. Active rotation of particles can be achieved using external forcing such as rotating magnetic fields \([8, 9]\), optical tweezers \([10]\) or uniform electric fields (the Quincke rotation effect) \([11]\). Self-assembly from polymers by motile bacteria can create micro-rotors \([11]\). In biological systems, the dancing volvox \([12]\) or uniflagellar algae \(C. Rheinhardtii\) \([13]\) behave rotor-like. Raising interest in rotor systems generated theoretical studies exploring rotors pair dynamics \([15, 16]\), self-assembly \([17]\), dynamics at interfaces \([18, 19]\), and rheology of suspensions \([20, 21]\).

Recently, Nguyen \textit{et al.} \([7]\) simulated a 2D monolayer of spinning gear-like particles that interact only sterically and predicted variety of phases: frozen state, separated fluid phases, and crystals of co-rotating particles. Notable in their study is the absence of hydrodynamic coupling: in a fluid environment, a moving particle generates flow, which drags other particles into motion. This hydrodynamic interaction is long-range and especially important in systems of microparticles, where inertia is negligible. Hydrodynamically interacting self-propelling particles have been extensively studied \([22]\), but only recently the combined effect of finite particle size (causing the near-contact steric repulsion) and long-range hydrodynamic interactions has been appreciated \([23]\), and shown to be essential to explain structures seen in experiments with bacterial suspensions \([24]\).

The studies on linearly propelled units raise the question: How sensitive is the phase behavior of a suspension of rotors to hydrodynamic interactions?

![FIG. 1: (Color online) Snapshots of simulations (50-50 mixture) with total rotor density $\phi=0.20, 0.40, 0.50, 0.54$. Black and red circles denote rotors spinning clockwise and counterclockwise, respectively.](image)

In this Letter, we show that fluid flows generated by the rotors play a crucial role in their collective dynamics and phase behavior. To allow comparison with the case where the fluid environment is neglected \([7]\), we consider a monolayer of counter-rotating spherical rotors suspended in a liquid. Figure 1.a illustrates the suspension behavior with increasing rotor density. At low densities, Figure 1.a, a gas like phase is observed unlike the frozen state found by \([7]\). As particle density increases, the populations of co-rotating rotors start to phase-separate and large rotating clusters emerge, seen in Figure 1.b-c. However, past a critical rotor density, such rotating clusters disappear and crystals composed of counter-rotating rotors form, Figure 1.d. In contrast, in the absence of hydrodynamic interactions, rotating crystals of co-rotating spinners are predicted \([7]\). In this Letter, we analyze how these collective dynamics and structures emerge from the
fluid mediated long-range multi-body hydrodynamic interactions and near-contact lubrication effects.

Model and Simulations. – We consider rotors whose size is such that inertia is unimportant (Stokes flow regime), e.g., colloidal spheres of radius 1μm suspended in water [11]. The force-coupling method is used to compute the full 3D hydrodynamic interactions between the rotors in the monolayer. The long-range multibody interactions are fully resolved by solving the Stokes equations with regularized low-order multipoles, while the short-range lubrication interactions are included from analytical solutions [24]. The force-coupling method has in the past been successfully applied for the study and analysis of magnetorheological flows [26, 27].

The numerical simulations of monolayer suspensions of spinners are performed in a computational domain of \( H_x \times H_y \times H_z = 80a \times 20a \times 80a \), in which \( a \) is the particle radius and \( y \) denotes the direction in which torques are applied. Periodic boundary conditions are used in the \( x \) and \( z \) directions. The particle monolayer is located at \( y = 0 \). The computational box is bounded by rigid walls located at \( y = \pm H_y/2 \). The vertical separation is chosen big enough to guarantee that the wall boundary does not affect the monolayer dynamics.

We consider a mixture of counter-rotating rotors with total volume fraction varying from \( \phi = 0.1 \) to 0.56. As we focus on monolayer suspensions, the volume fraction is defined as \( \phi = \left( \frac{4\pi a^3}{3} \right) N_p / (H_x \times H_y \times 2a) \), in which \( N_p \) is the number of the rotors. The number of the suspended rotors varies from \( N_p = 306 \) at \( \phi = 0.1 \) to \( N_p = 1,712 \) at \( \phi = 0.56 \). To model the active rotation, external torques are applied to the rotors in the vertical direction, so that the rotors have the angular velocity only in the vertical direction \( \Omega_y \) and the non-zero velocity components only in the horizontal directions \( (x, z) \). The volume fractions of the the counter-rotating rotors are set to be equal; \( \phi^+ = \phi^- = 0.5\phi \). The magnitude of the external torque normalized by the fluid viscosity \( \mu_o \) and a reference angular velocity \( \Omega_0 \) is \( T^* = T / (8\pi \mu_o \Omega_0 a^3) = 1 \). Note that due to the linearity of the Stokes flows any suspensions with two different species of rotors of equal volume fractions can be rescaled to this system. A short-range repulsion force is used when the separation between two particle surfaces \( (\text{ac}) \) becomes smaller than 0.002a [20]. The magnitude of the contact force is set to keep the minimum separation distance \( a_{\text{min}} \approx 0.001 \) in all simulations. Initial random configurations are generated by a molecular dynamics procedure. The suspension dynamics are studied after the suspensions reach a steady state, which usually takes about \( t \Omega_0 \approx O(1000) \) from the initial seeding.

Hydrodynamic Interactions. – A rotor in Stokes flow (rotlet) creates a flow with velocity decaying as \( \sim 1/r^2 \), in which \( r \) is the distance from the center of the rotlet. This flow drags other particles into motion. This is the essence of hydrodynamic interactions - a particle translates and rotates in response to the motion of another particle. Thus, the hydrodynamic interactions have two effects: modifying particle rotation rate and inducing particle translation.

The angular velocity of a rotor decreases with particle volume fraction [24]. To quantify the hydrodynamic resistance to the intrinsic torque, the angular velocity hindrance function is defined as \( \Psi = \langle |\Omega_y| \rangle / \Omega_0 \), in which \( \langle \cdot \rangle \) denote an ensemble average. Figure 2(a) shows that the angular velocity hindrance function \( (\Psi) \) monotonically decrease with the volume fraction \( \phi \).

Rotor translation due to hydrodynamic interactions, i.e., the conversion of the rotational kinetic energy supplied to the suspensions by an external or intrinsic torque into translational kinetic energy, is characterized by \( \kappa = E_{\text{rot}} / E_{\text{tot}} \), where the translation \( (E_{\text{rot}}) \) and rotational kinetic energies \( (E_{\text{rot}}) \) are defined as

\[
E_{\text{rot}} = \sum \frac{1}{2} m (\mathbf{u} \cdot \mathbf{u}), \quad E_{\text{rot}} = \sum \frac{1}{2} I (\Omega \cdot \Omega).
\]

Here \( m \) and \( I \) are, respectively, the mass and the moment of inertia of the spherical rotor, and the total kinetic energy is \( E_{\text{tot}} = E_{\text{rot}} + E_{\text{rot}} \). Figure 2(b) shows that \( \kappa \) depends non-monotonically on volume fraction. The initial increase for \( \phi \leq 0.45 \) is due to the fact that as the particle separation decreases with \( \phi \) the translation-inducing hydrodynamic interactions become stronger. A peak of \( \kappa \) is observed around \( \phi = 0.45 \), followed by a sharp decrease of \( \kappa \) as \( \phi \) changes from 0.50 to 0.54 indicating a possible phase transition. The behavior of \( \kappa \) is very different from that of the non-hydrodynamic system in [7], where it is was predicted that the suspensions undergoes a phase transition from a frozen state to a phase-separated fluid state at a critical volume fraction, accompanied by a sharp increase of \( \kappa \). In contrast, in our hydrodynamic system, \( \kappa \) gradually increases with \( \phi \) and then drops rapidly at a volume fraction \( (\phi \approx 0.54) \). The different behavior stems from the way \( E_{\text{rot}} \) is converted to \( E_{\text{rot}} \). Contrary to the the non-hydrodynamic system of [7], where the energy conversion occurs only through pair-wise collisions, in the present...
hydrodynamic system there is a long-range multi-body hydrodynamic coupling between the rotors. Since the average separation distance decreases as $\phi$ increases, the conversion becomes more efficient (up to $\phi \sim 0.5$.) The sharp drop of $\kappa$ at the volume fraction about 0.5 suggests that there is a sudden change of suspension microstructure.

**Phase Behavior.**– Snapshots of the rotor suspension at different densities are shown in Figure 4 At $\phi = 0.20$, the suspension appears homogeneous, i.e., the counter-rotating rotor populations are in a well-mixed state. At $\phi = 0.40$ we notice that rotors of the same torque have aggregated to form clusters. The clustering is more clearly visible at $\phi = 0.50$. The suspensions at $\phi = 0.40$ and $\phi = 0.50$ show a qualitatively similar behavior to the phase-separated fluid state observed in [7]. However, at $\phi = 0.54$, the clustering becomes less pronounced and the suspension appears more homogeneous again.

To investigate the suspension microstructure, we compute the number density distribution of clockwise and counterclockwise rotors

$$\lambda^\pm(r) = \left\{ \frac{1}{N} \sum_{i=1}^{N} \left\{ \sum_{j=1,j \neq i}^{N} H(r - |\mathbf{d}_{ij}|) \delta(T_i \pm T_j) \right\} \right\}.$$  

Here $H(x)$ is the Heaviside function and $\delta(x)$ is the Dirac measure, $N$ is the number of the suspended rotors, and $|\mathbf{d}_{ij}|$ is the distance between the $i$–th and $j$–th rotors. In short, $\lambda^-(r)$ is the number density of the co-rotating rotors in a cylinder of radius $r$ and $\lambda^+(r)$ is that for the counter-rotating rotors. In Figure 3(a), $\lambda^\pm$ normalized by the bulk number density of the total rotors is shown for $\phi = 0.50$. We notice that at $\phi = 0.50$, $\lambda^-(r)$ is higher than $\lambda^+(r)$ for small $r$, implying more clustering of the co-rotating rotors (see inset for possible configurations). In the far field ($r > 20a$), eventually the number densities of the co- and counter-rotating rotors become almost the same.

In Figure 3(b), the difference between $\lambda^-$ and $\lambda^+$ are plotted for various volume fractions; $\Delta \lambda(r) = \lambda^-(r) - \lambda^+(r)$. As observed in figure 3(a), $\delta \lambda$ provides information about the clustering. It is interesting to find that, at low volume fractions ($\phi \leq 0.2$), $\Delta \lambda$ is negative indicating that there is a higher probability for counter-rotating rotors moving together. As noted in studies of rotor pairs [15, 16], two counter-rotating rotors achieve self-propulsion, as illustrated in the lower inset of Figure 3(a). For $\phi \geq 0.3$, the positive $\Delta \lambda$ suggests the clustering of the co-rotating rotors. However, for $\phi = 0.3$ and 0.4, $d\Delta \lambda/dr$ still remain positive similar to those at the lower volume fractions. The clustering seems to be most pronounced at $\phi = 0.50$ and afterward $\Delta \lambda$ for small $r$ starts to decrease. At $\phi = 0.54$, $\Delta \lambda$ becomes almost zero, suggesting there is no or very weak preferential aggregation of the rotors.

**Crystal Structures.**– In higher density suspensions rotors form crystals, the smallest of which are characterized by a rotor having 6 neighbors. Figure 4 illustrates these crystals or hexagonal structures for $\phi = 0.54$ and 0.56. Note how the crystals are composed of rotors of either spin. The fraction of the domain that the crystals occupy grows with the volume fraction, from less than a quarter (at $\phi = 0.54$) to almost half ($\phi = 0.56$) of the computational domain. Hydrodynamically decoupled rotors [17] also form crystals, however they consist of co-rotating rotors. In the present study however the hexagonal structure consists of mixture of the counter-rotating rotors.

Figure 4(c) shows as a function of the density $\phi$ the hexagonal bond-orientational order parameter defined as:

$$\zeta_6 = \left( \frac{1}{N} \sum_i \left( \frac{1}{N_b} \sum_j N_i e^{6\theta_{ij}} \right) \right),$$

in which $\theta_{ij}$ is the azimuthal angle of $\mathbf{d}_{ij}$ and $N_b$ is the number of the rotors in the neighborhood ($|\mathbf{d}_{ij}| < 2.05a$). Clearly, $\zeta_6$ is zero for an isotropic system and one for a perfect crystal. It is shown that $\zeta_6$ is close to zero up to $\phi = 0.50$. $\zeta_6$ starts to increase rapidly from $\phi \sim 0.54$.
FIG. 4: (Color online) Hexagonal structures formed in a suspension with (a) $\phi = 0.54$ and (b) $\phi = 0.56$. The black and red circles denote the rotors rotating clockwise and counterclockwise respectively. (c) Hexagonal bond-orientational order parameter $\xi_6$ as a function the particle volume fraction. The critical volume fraction where the sudden drop of $\kappa$ is observed (see Figure 2(b)).

Discussion and Conclusion.– We presented a study of the dynamics and phase behavior of suspensions of counter-rotating spherical rotors immersed in viscous liquid. The numerical investigation is carried out by using the force-coupling method which accounts for the full hydrodynamic interactions between the rotors.

We showed that the conversion rate of the rotational to the translational kinetic energies ($\kappa$) initially increases with the particle volume fraction, and eventually exhibits a sudden drop at $\phi \simeq 0.54$. For $\phi \geq 0.54$, the active rotors start to form crystal structures, which are responsible for the sudden drop of $\kappa$. We found that the counter-rotating rotors tend to stay close at low $\phi$, whereas for $\phi \geq 0.40$ the co-rotating rotors form clusters.

The emerging behavior of the present system with hydrodynamic interactions is very different from that of the 2D non-hydrodynamic system recently studied by Nguyen et al. [7], which found monotonic increase of $\kappa$ with the volume fraction and predicted frozen state followed by separated fluid phases of co-rotating spinners and eventually rotating crystals. Our simulations show a gas phase at low particle density which becomes separated fluid phases consisting of large cluster of co-rotating spinners and eventually crystal structures composed of counter-rotating rotors. All of these suggest that multi-body hydrodynamic interactions play a significant role in the collective dynamics and phase behavior of suspensions of active rotors and these effects should not be neglected in studies of similar active systems. For example, they could influence or drive the formation of the peculiar dynamical structures experimentally observed at the interface of drops covered with colloidal particles [30, 31].

In this Letter we considered only torques that are perpendicular to the particle monolayer. Due to the symmetry of the generated flows, the particles remain confined to the monolayer and do not move transversely. In experimental systems, for example Quincke rotors [32, 33], it is not the case that torques stay in one direction or even constant, as the particle rotation is dependent on the full electro-hydrodynamics. Although, restricting the rotational motion to one direction in experiments is challenging, it is not impossible and our study suggests potentially intriguing experiments. Lastly, an area that remains relatively unexplored is that of using spinners and rotors for transport and mixture of passive tracers of the same size as the spinners [7], different sizes or even dye fields. We will address those questions in a future study.

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[1] M. C. Marchetti, J. F. Joanny, S. Ramaswamy, T. B. Liverpool, J. Prost, M. Rao, and R. A. Simha, Rev. Mod. Phys. 85, 1143 (2013).
[2] F. Peruani, A. Deutsch, and M. Bar, Phys. Rev. E 74, 030904 (2006).
[3] Y. Fily, M.C. Marchetti Phys. Rev. Lett. 108, 235702 (2012).
[4] H. H. Wensink, V. Kantsler, R. E. Goldstein, and J. Dunkel, Phys. Rev. E 89, 010302(R) (2014).
[5] H.P. Zhang, A. Beer, E.-L. Florin, H.L. Swinney, Proc. Natl. Acad. Sci. USA 107, 13626 (2010).
[6] J. Palacci, C. Cottin-Bizonne, C. Ybert, and L. Bocquet, Phys. Rev. Lett. 105, 088304 (2010).
[7] N. H. P. Nguyen, D. Kloksa, M. Engel, and S. C. Glotzer, Phys. Rev. Lett. 112, 075701 (2014).
[8] B.S. Grzybowski, H.A. Stone, G.M. Whitesides, Nature 405, 1033 (2000).
[9] B. A. Grzybowski and G. M. Whitesides, Science 296, 718 (2002).
[10] D. G. Grier, Curr. Op. Coll. Int. Sci. 2, 264 (1997).
[11] A. Bricard, J.B. Caussin, N. Desreumaux, O. Dauchot, and D. Bartolo, Nature, 503, 95 (2013).
[12] K. Drescher, K. C. Leptos, I. Tuval, T. Ishikawa, T. J. Pedley, and R. E. Goldstein, Phys. Rev. Lett. 102, 168101 (2009).
[13] Private communication with J. Guasto, V. Kantsler, and M. Polin. A typically bi-flagellate algae such as *Chlamydomonas Rheinardtii* exhibits mostly rotational motion when one of the flagella is removed.
[14] J. Schwarz-Linek, C. Valeriani, A. Cacciuto, M. E. Cates, D. Marenduzzo, A. N. Morozov, and W. C. K. Poon, Proc. Natl. Acad. Sci. U. S. A. 109, 4052 (2012).
[15] M. Leoni and T. B. Liverpool, Europhys. Lett., 92, 64004 (2010).
[16] Y. Fily, A Baskaran, and M.C. Marchetti Soft Matter 8, 3002 (2012).
[17] E. Climent, K. Yeo, M. Maxey and G. Em. Karniadakis, J. Fluid Eng., 129, 379 (2007).
[18] I. Llopis and I. Pagonabarraga Eur. Phys. J. E 26, 103 (2008).
[19] P. Lenz, J.-F. Joanny, F. Julicher, and J. Prost, Phys. Rev. Lett. 91, 108104 (2003).
[20] K. Yeo and M. R. Maxey, Phys. Rev. E 81, 062501 (2010).
[21] L. Jibuti, S. Rafai, P. Peyla, J. Fluid. Mech. 63, 345 (2012).
[22] D. Saintillan and M.J. Shelley Phys. Rev. Lett. 99, 058102 (2007).
[23] A. Zottl and H. Stark, Phys. Rev. Lett. 112, 118101 (2014).
[24] E. Lushi, H. Wioland, and R.E. Goldstein, Proc. Natl. Acad. Sci. USA 111, 9733 (2014).
[25] K. Yeo and M. R. Maxey, J. Comput. Phys. 229, 2401 (2010).
[26] E. Climent, M. R. Maxey, and G. E. Karniadakis, Langmuir 20, 507 (2004).
[27] K. Yeo and M. R. Maxey, J. Fluid Mech. 649, 205 (2010).
[28] M. Marchioro, M. Tanksley, and A. Prosperetti, Int. J. Multiphase flow 26, 783 (2000).
[29] H. Brenner, Annu. Rev. Fluid Mech. 2, 137 (1970).
[30] P. Dommersnes, Z. Rozynek, K. Kjerstad, R. Castberg, A. Mikkelsen, K. Hersvik and J. O. Fossum, Nat. Commun. 4, 2066 (2013).
[31] M. Ouriemi and P.M. Vlahovska J. Fluid Mech. 751, 106 (2014).
[32] P.F. Salipante, P.M. Vlahovska Physical Review E 88, 043003 (2013).
[33] D. Das, D. Saintillan, Physical Review E, 87, 043014 (2013).