

Orientational order in confined systems of self-driven spinners

Rushil Pingali 

Department of Materials Science and Engineering, [Northwestern University](#), Evanston, Illinois 60208, USA

Erik Luijten 

Departments of Materials Science and Engineering, Engineering Sciences and Applied Mathematics, Chemistry, and Physics & Astronomy, [Northwestern University](#), Evanston, Illinois 60208, USA



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Hydrodynamic interactions play a critical role in the collective behavior of active matter. Here, we investigate large systems of self-driven spinners confined over a substrate. Direct numerical simulation of three-dimensional hydrodynamics demonstrates that these systems generate unique flows from which spatial and orientational order emerges. We show that a transition in particle orientation accompanies the appearance of crystallinity as the packing fraction is increased. Further exploration reveals a rich, tunable state space, offering insights into the biophysics of natural microswimmers with rotational motion as well as into the design of synthetic spinner systems.

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Active matter systems are key drivers of biological dynamics at the microscale. The constituents of such systems consume energy to generate individual motion that in turn can give rise to out-of-equilibrium collective dynamics. Elucidating the principles that govern these dynamics is a prerequisite for understanding the origins and mechanics of complexity and self-organization in biological and bioinspired systems. For this reason, considerable attention has been devoted to developing theoretical models of microswimmers and, more recently, to computational studies of the dynamics of large systems thereof [1–10]. Although traditionally addressed through simple models of self-propelled particles, it has become clear that precise accounting of hydrodynamic interactions is crucial to accurate modeling of the collective behavior of swimmers. For “squirmers” microswimmers that propel themselves by generating a slip velocity [11,12], hydrodynamics has variously been shown to be responsible for polar order in isotropic suspensions [1], accumulation near obstacles [2] and walls [3,4], modulation of clustering and of motility-induced phase separation [5–9], and self-organization in active-passive mixtures [10]. Originally intended to represent low-Reynolds-number ciliates, the squirmer is now the standard for microswimmer models with force-dipole-like flows [13].

Nonetheless, real microswimmers do not always conform to the inherent simplicity of the squirmer [14]. Certain biological systems exhibit rotational motion, including “dancing” *Volvox* colonies [15], *Patiria miniata* starfish embryos that rotate while forming orientationally ordered “living chiral crystals” [16], and even aggregates of certain human cells

[17–19]. Likewise, efforts to produce synthetic active particles have yielded nanomotors with rotational degrees of freedom [20,21]. Recently, it has also been shown that grafting clusters of enzymatic motors onto a rigid structure such as a lipid vesicle enables the engineering of self-driven microscale spinners with independent axes of rotation [22]. A full understanding of how complexity emerges from motility in such systems must therefore incorporate the effects of rotational dynamics.

To shed light on this, we examine minimal, coarse-grained systems of spheres with *intrinsic* torque (and no other self-propulsion), aiming to provide generalizable insights into motile systems that exhibit rotation. Utilizing molecular dynamics simulations coupled with fully resolved three-dimensional (3D) hydrodynamics, we demonstrate that the flows generated by rotational motion alone suffice to induce translation, collective behavior, and spatial and orientational order in these “spinner” systems. Moreover, we examine how this order can be modulated with an eye toward advancing the development of synthetic spinners. Prior efforts have demonstrated hydrodynamically driven collective behavior in spinner systems but have focused on the Stokes regime [23,24], two dimensions [25,26], or externally driven particles with aligned torques [27–29]. Here, in contrast, we investigate self-driven inertial spinners capable of 3D reorientation, and thus of far richer collective behavior than externally driven systems.

We explicitly solve for the incompressible fluid flows around spinners in 3D through direct numerical simulation of hydrodynamics. To do this, we adopt the smoothed profile method [30,31], in which the solid-fluid interface is modeled as a diffuse profile rather than a sharp boundary, eliminating the need to reconstruct meshes and enabling longer and more complex simulations. The solid-fluid interaction is treated as a body force $\mathbf{f}_p$ within the Navier-Stokes framework [32],

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$(\partial_t + \mathbf{u} \cdot \nabla) \mathbf{u} = \rho^{-1} \nabla \cdot \boldsymbol{\sigma} + \phi \mathbf{f}_p. \quad (2)$$

*Contact author: luijten@northwestern.edu

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Here, ρ is the fluid density, σ is the fluid stress tensor, and $\mathbf{u}$ is the global velocity field formed by coupling the fluid and particle velocity fields through no-slip boundary conditions and defining $\mathbf{u} = (1 - \varphi)\mathbf{u}_f + \varphi\mathbf{u}_p$, where φ varies smoothly from 0 in the fluid domain to 1 in the particle domain. Likewise, the hydrodynamic forces and torques on a particle are incorporated into the Newton-Euler equations of motion, which are concurrently integrated. Our computational domain has dimensions $l_x \times l_y \times l_z = 256\Delta \times 256\Delta \times 64\Delta$, where Δ is the discretization of the Fourier spectral scheme used to solve the fluid equations. (To exclude finite-size artifacts, we tested a $512\Delta \times 512\Delta \times 64\Delta$ domain and found qualitatively similar results; cf. S1 of the Supplemental Material [33].) The simulation cell is periodic in the x and y directions and bounded by smoothed-profile walls in the z direction, representing confinement of particles over a substrate. A large particle radius $a = 5\Delta$ is used; prior work on modeling active rotors using the smoothed profile method has shown this radius to sufficiently resolve near-field hydrodynamics [34]. Within a fluid of viscosity η , particles are driven by a constant intrinsic torque $L = 500\Delta\rho^{-1}\eta^2$ around independent, unconstrained axes. Their interactions are exclusively hydrodynamic, except for a short-ranged excluded-volume potential calibrated to prevent overlap,

$$U(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{36} - \left(\frac{\sigma}{r}\right)^{18}\right] + \varepsilon, & r < 2^{1/18}\sigma, \\ 0, & r \geq 2^{1/18}\sigma. \end{cases} \quad (3)$$

We set $\sigma = 2a = 10\Delta$, $\varepsilon = 50\Delta\rho^{-1}\eta^2$ for the interparticle potential and $\sigma = 5\Delta$, $\varepsilon = 100\Delta\rho^{-1}\eta^2$ for the particle-wall potential. Viscous damping arising from the hydrodynamics provides an effective thermostat equivalent to a zero-temperature Langevin environment. The particle Reynolds number (Re_0) is varied by adjusting viscosity ($\eta = 0.125, 0.25, 0.5, 1$) at fixed density ($\rho = 1$). We calculate $\text{Re}_0 = (\rho a^2 \Omega)/\eta$ for an isolated spinner in the bulk, as collective effects can cause the angular velocity Ω to vary. The resulting range of $4.5 \leq \text{Re}_0 \leq 86.0$ is realistic for micro- to milliscale swimmers [35].

In addition to the primary rotational flow, an isolated spinner at finite Re_0 induces a secondary flow directed inward to its poles and radially outward at its equator [36]. In the presence of a substrate normal to the rotation axis, this symmetry is broken and the inertial force of the unbalanced flow causes a polar attraction toward the substrate [Fig. 1(a)] that increases with Re_0 . Contrary to homochiral externally driven systems, a dilute randomly dispersed system of spinners thus forms a racemic monolayer over a substrate, with particles rotating around either the $+z$ axis (counterclockwise when viewed from above) or the $-z$ axis (clockwise). An isolated pair of like spinners (i.e., parallel axes) shows a stagnation region between them that causes the particles to orbit each other; the neighbor's presence also creates an unbalanced inertial force causing them to repel each other and spiral outward [Fig. 1(b) and S2 of the Supplemental Material [33]] [37]. This contrasts with the behavior of such spinners in the Stokes limit, where the absence of inertial repulsion allows stable orbiting [38]. However, it is possible for unlike spinner pairs (i.e., antiparallel axes) to form stable translating pairs, similar to those observed in the Stokes regime, as they

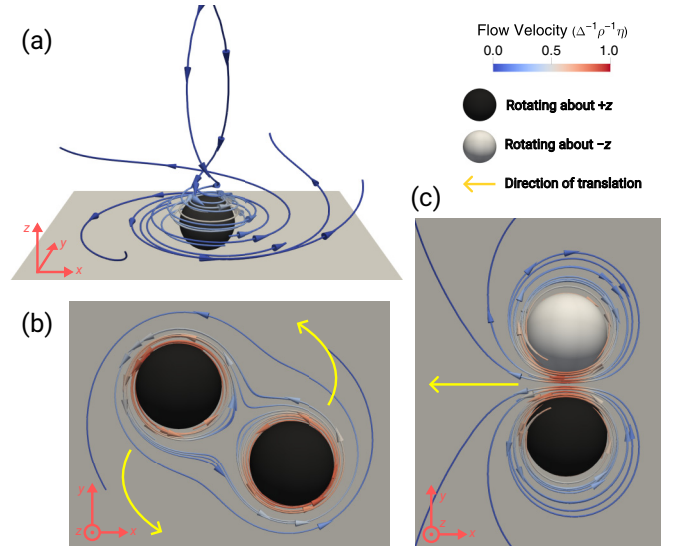


FIG. 1. Fluid streamlines showing flow generated by spinning particles driven by intrinsic torque. (a) Single particle spinning about the $+z$ axis experiences polar attraction toward the substrate. (b) Two spinners above a substrate with parallel axes of rotation ($+z$) orbit and repel at finite Re_0 ; (c) when the axes are antiparallel ($+z$ and $-z$), the spinners form a translating pair stabilized by high-velocity flow between them.

are stabilized by the attractive accelerated flow that develops between them [Fig. 1(c)] [39]. In this work, we apply a moderate gravitational force to ensure a smooth monolayer and to enable the study of packing fractions above those seen in a density-matched system. We choose a realistic particle mass density 1.5ρ , which corresponds to a net weight per particle of $262\rho^{-1}\eta^2$.

Proceeding to larger systems, we find that the dynamics observed in the simple two-particle systems remain instructive. For a scalar measure of the average spinner orientation, we employ the nematic order parameter $S_2 = \langle 3 \cos^2 \theta - 1 \rangle / 2$, where θ is the angle between the rotation axis and the z axis. We define the area packing fraction $\phi = \pi a^2 N / (l_x l_y)$, where N is the number of particles in the monolayer that forms after random dispersion and sedimentation. In Fig. 2(a), N ranges from ~ 120 to ~ 680 . At low ϕ , the spinners predominantly align their rotational axes with the z axis, reflected by S_2 being close to 1 [Fig. 2(a)]. They exhibit a disordered state, continuously forming and breaking translating pairs (S3 of the Supplemental Material [33]). The radial distribution function $g(r)$ of a representative system [Fig. 2(b)] confirms short-range order characterized by a preference for unlike nearest neighbors, consistent with the attraction between antiparallel pairs. A weaker second coordination shell of like neighbors is also evident before the short-range order dissipates. As ϕ increases above ~ 0.7 , the system undergoes two notable transitions. First, long-range spatial order emerges in the form of a two-dimensional hexagonal crystal, as would be expected for spherical particles at high ϕ . Second, this spatial arrangement induces a geometric frustration in the antialignment of neighboring spinners, which they resolve by reorienting their rotation axes parallel to the x - y plane, leading to a sharp decrease in S_2 toward its in-plane value -0.5 [Fig. 2(a)].

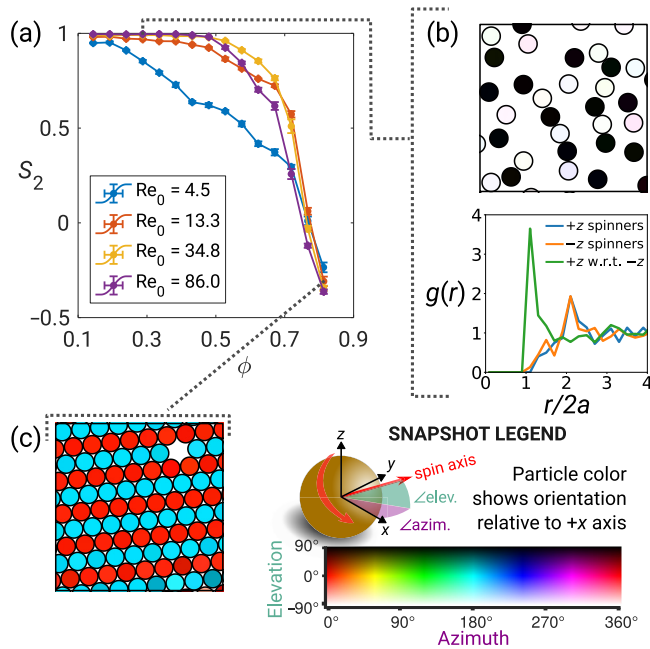


FIG. 2. Transition in spinner orientations. (a) Increasing the overall packing fraction ϕ causes a decrease in the nematic order parameter S_2 as spinners reorient to align their rotation axes with the substrate. (b) At low $\phi = 0.29$ and $Re_0 = 34.8$, spinners align with the wall-normal z axis; the radial distribution function $g(r)$ reveals a preference for antiparallel neighbors. (c) At high $\phi = 0.81$ and $Re_0 = 13.3$, spinners pack hexagonally and reorient their axes parallel to the substrate (cf. color coding for elevation of the rotation axis), forming “antiferromagnetic” stripes (cf. color coding for the azimuthal angle).

Moreover, the in-plane spinners align pole-to-pole into antiparallel stripes [Fig. 2(c)], redirecting their attractive polar hydrodynamic interactions toward neighboring particles instead of the substrate. The benefit of this reorientation is that equatorial neighbors can now spin around antiparallel axes, minimizing their repulsive interactions and stabilizing the in-plane antiferromagneticlike orientational order observed in the system.

Remarkably, the crystallization observed here is purely activity-driven. It occurs in the absence of Brownian forces—conditions under which a passive system would simply freeze into an amorphous, glassy state instead of achieving the ordered structures seen here. To further understand the dynamics of this crystallization, we quantitatively analyze the evolution of spatial order via the hexatic order parameter ψ_6 [40], whose magnitude measures the degree of sixfold rotational symmetry, with $|\psi_6| = 1$ representing perfect hexagonal order. The phase $\arg(\psi_6)$ corresponds to the orientation of the hexagonal grains (as opposed to the orientation of the individual rotation axes) relative to the reference x axis.

Figure 3(a) shows the progression of spinner orientations, $|\psi_6|$, and $\arg(\psi_6)$ over time at high $\phi = 0.81$, illustrating the nucleation and growth of hexagonally ordered grains (cf. S4 of the Supplemental Material [33] for the system’s full time evolution, elucidating the interplay between crystallization, grain reorientation, and adjustments of individual rotation axes). Point defects and grain boundaries are identifiable by low $|\psi_6|$. For a smaller grain (such as the central red domain in $\arg(\psi_6)$ at $t = 10\,000\Delta^2\rho\eta^{-1}$) to merge with a larger one, it must reorient to eliminate the difference in $\arg(\psi_6)$. However, a unique feature of our system is that the “antiferromagnetic” ordering of neighboring stripes must be maintained during grain growth. Thus, in addition to grains matching their lattice

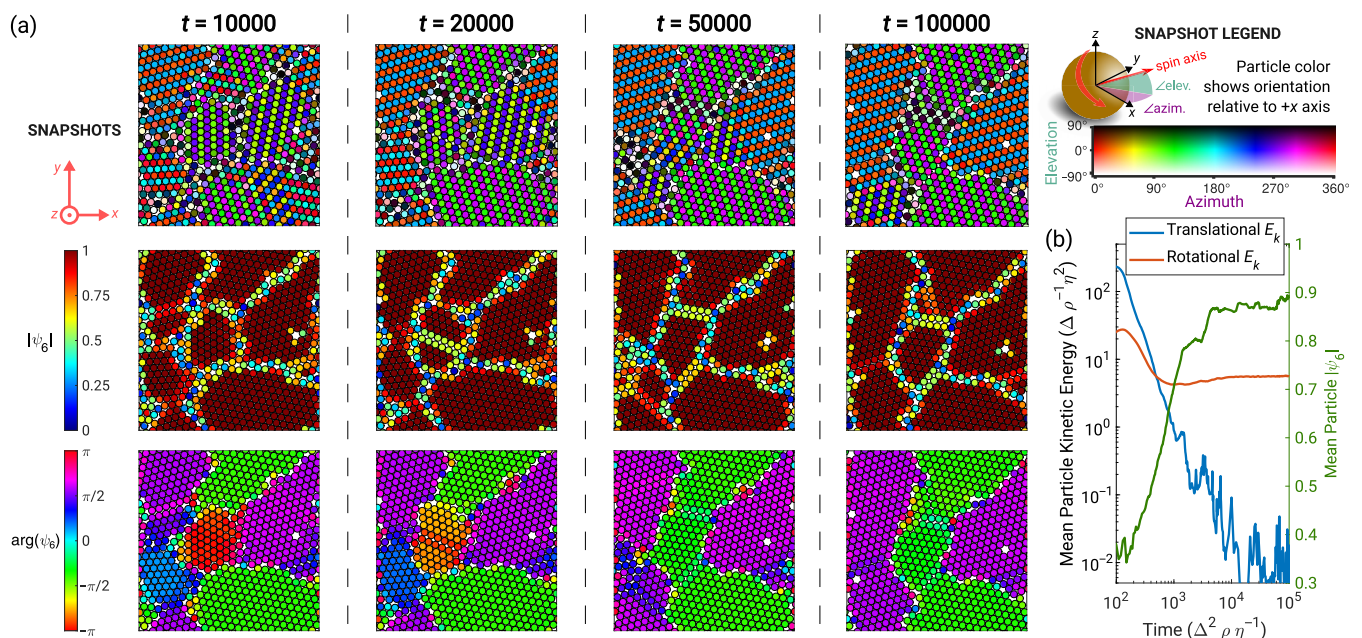


FIG. 3. Dynamics of polycrystalline grain growth in a $256\Delta \times 256\Delta$ periodic domain with $\phi = 0.81$ at times 10^4 – 10^5 ($\Delta^2\rho\eta^{-1}$). (a) Orientation (top row) and hexatic order parameter ψ_6 (middle and bottom rows) for each spinner. (b) Decrease in translational and rotational kinetic energy per particle (left-hand y axis) accompanies the increase in average $|\psi_6|$ (right-hand y axis).

vectors, constituent particles must have an orientation compatible with their counterparts across the grain growth front, presenting an additional energetic barrier due to spinner chirality. Consistent with this, we observe internal reorientation of spinners even within regions of the same lattice orientation [same $\arg(\psi_6)$], as well as the persistence of some grain boundaries during the later stages.

The ordering is accompanied by a decrease in mean *translational* kinetic energy [Fig. 3(b)] as the randomly dispersed spinners settle onto the substrate. Despite the constant applied torque, *rotational* kinetic energy is neither constant nor decreasing monotonically. Rather, it begins to decrease once the particles get closer and begin to experience hydrodynamic torques from their neighbors. Then, these very torques allow the spinners to explore orientational parameter space, stochastically driving their reorientation into antiferromagnetic stripes. In this state, the torques on the spinners are lower. Accordingly, they display a decreased propensity to reorient further, as well as a reduced resistance to angular motion. The angular velocity and the rotational kinetic energy therefore increase slightly as the system approaches its steady state.

Uncovering this interplay between spatial and orientational order prompts the question how it might be modulated, particularly in the context of designing synthetic spinner materials. Prior work has shown that the polar and equatorial hydrodynamic forces on a spinner depend on the distance to neighboring surfaces in the corresponding directions and on the Reynolds number [36]. While hydrodynamic flows in a large collective system cannot entirely be abstracted to pairwise attractive or repulsive forces, the framework of competing polar and equatorial interactions remains useful. Since we have already examined the system at different Re_0 , we now investigate whether tuning the particle-particle and particle-substrate separations can further control the emergent order. To avoid introducing nonhydrodynamic interactions, we test this hypothesis by introducing offsets to the excluded-volume potential, replacing the separation r in Eq. (3) with $r - \alpha$. For pairwise interactions between spinners, we impose a nonzero minimum separation distance α_{particle} by setting $\alpha = \alpha_{\text{particle}}\Delta$. Likewise, for the interaction between spinners and the substrate, we employ the same potential with $\alpha = \alpha_{\text{wall}}\Delta$. This approach retains a sharp repulsive profile, enabling direct comparison with previous results. In real systems, such separations might arise or be engineered from Coulombic interactions, steric constraints, or other hydrodynamic phenomena not modeled in our minimal system.

Indeed, we find that α_{wall} and α_{particle} jointly span a state space for spinner systems at constant Re_0 and ϕ . Figure 4(a) presents state diagrams of the system, colored by the nematic order parameter S_2 , at fixed $\text{Re}_0 = 86$ for $\phi = 0.2, 0.5$, and 0.8 , where $\phi = \pi(a + \alpha_{\text{particle}}/2)^2 N / (l_x l_y)$. Here, $(\alpha_{\text{wall}} = 0, \alpha_{\text{particle}} = 0)$ corresponds to the baseline case where particles are allowed to closely approach each other as well as the substrate. As in Fig. 2, this system transitions from $S_2 \approx 1$ at low ϕ to $S_2 \approx -0.5$ at high ϕ as particles reorient their director parallel to the x - y plane.

At nonzero α , this behavior is not always observed. High interparticle separation α_{particle} at low particle-wall separation

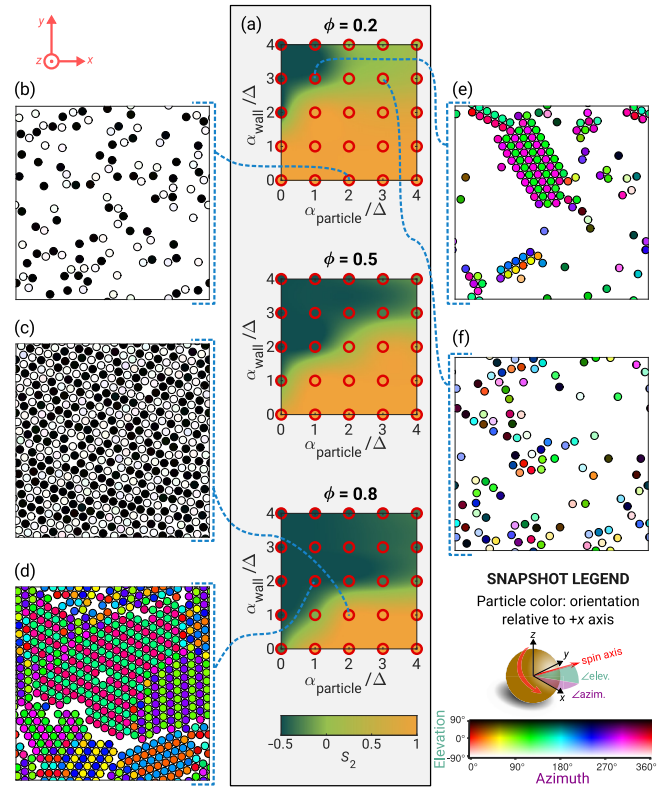


FIG. 4. (a) State diagrams of spinner structures at different combinations of minimum wall separation α_{wall} and interparticle separation α_{particle} . Nematic order parameter S_2 mapped at $t = 10^5 \Delta^2 \rho \eta^{-1}$ and $\text{Re}_0 = 86$ for $\phi = 0.2, 0.5$, and 0.8 . Red circles indicate systems simulated. Snapshots of final states: (b) disordered structure with rotation axes aligned with the z axis; (c) frustrated hexatic structure with axes aligned with the z axis; (d) hexagonal polycrystalline structure with axes in the x - y plane; (e) islands of hexagonal crystals; and (f) spatially and orientationally disordered system. Color coding of particles corresponds to the elevation and azimuthal angle of their rotation axes.

α_{wall} has the effect of weakening interparticle hydrodynamic interactions relative to particle-wall interactions. As a result, the spinners prefer to be z axis-aligned even as ϕ increases, resulting in regions of $S_2 \approx 1$ (bottom-right corners of the state diagrams). The resulting structures are disordered at low ϕ [Fig. 4(b)]. However, at high ϕ [Fig. 4(c)], an *out-of-plane* antiferromagnetic Ising-like structure is seen, with the relative proximity to the substrate forcing spinners to adopt a binary spin orientation on each site. The sites form a hexatic arrangement and adjacent sites are antiferromagnetically coupled, giving rise to frustrated patterns as the spinners try and fail to find a configuration where all nearest neighbors are antialigned.

Conversely, high α_{wall} at low α_{particle} allows interparticle hydrodynamics to dominate. As in Figs. 2(c) and 3(a), an *in-plane* antiferromagnetically ordered polycrystalline state is observed at high ϕ [Fig. 4(d)]. Surprisingly, the interparticle interactions are now strong enough to induce crystallization at low ϕ as well, resulting in isolated islands of antiferromagnetic hexagonal order [Fig. 4(e)]. This clustering demonstrates that orientational order in spinner systems is more than merely

a consequence of the spatial order demanded by sphere close packing—hydrodynamic interactions alone can induce spatial and orientational order, even at low ϕ . In this regime, the spinner axes lie in-plane; i.e., the elevation angle is effectively 0° , while the azimuthal angle spans the full color spectrum from 0° to 360° . This resembles a polar XY model, once again with antiferromagnetic nearest-neighbor interactions. In both Figs. 4(c) and 4(d), the underlying microscopic spin of a single particle remains a fully 3D (i.e., Heisenberg) spin, but the mere change of weakening wall interactions relative to interparticle interactions causes a hydrodynamically driven transition from a discrete (out-of-plane) symmetry to a continuous (in-plane) one.

Lastly, in the regime of high α_{particle} and α_{wall} at low ϕ , the spinners are far from any boundaries and from each other, and hydrodynamic effects are weakened to the point that any spatial or orientational order becomes negligible [Fig. 4(f)]. We conclude that the organization of spinner systems can be finely controlled by adjusting these parameters, demonstrating their utility for designing synthetic spinner materials with tunable properties. By balancing polar and equatorial interactions, it is possible to engineer diverse structural states, ranging from disordered monolayers to large crystals of spinners; our results therefore indicate that hydrodynamics alone offer a degree of control beyond what has been previously reported [23–29]. In light of recent experimental advances in the development of self-driven spinners with no external aligning field [22], our work illustrates what collective phenomena could be obtained by extending these efforts into the inertial regime.

From a statistical mechanics perspective, our system has the potential to act as a remarkably transparent and tunable platform for the exploration of diverse nonequilibrium phases and transitions within the same system. From an applications standpoint, self-driven spinners make it possible to write rapidly reprogrammable flow fields through patterned substrates, simply by modulating the substrate proximity, and thus the orientation, of different spatial regions of spinners. Potential applications include on-chip pumps, valves, and

mixers comprised of spinner building blocks, as well as energy transduction between chemical fuel, kinetic energy, and even electrolyte flows. This represents an improved level of control over microfluidic flows and presents an enabling technology for the emerging field of reconfigurable matter. Our study also demonstrates how spinner-based microrobots could exhibit hydrodynamically mediated behaviors such as translation, lane formation, avoidance of collisions or jamming, and eventual clustering into self-healing crystals where activity continuously attempts to minimize defects.

In conclusion, we have shown that confined systems of self-driven spinners can develop spatial and orientational order purely from hydrodynamic interactions. At high packing fractions, spinners display hexagonal crystalline arrangements, aligning their rotation axes and forming antiparallel stripes. Considering asymmetrical particle-substrate and particle-particle interactions expands the accessible state space further, making it possible to realize multiple forms of ordering through hydrodynamics. Many spin lattice concepts, such as frustration, antiferromagnetism, and domain coarsening, can be mapped onto this dissipative system. Our findings provide a framework for understanding the behavior of systems of rotating biological swimmers, as well as for optimizing the collective dynamics of synthetic active particles for microfluidics, microrobotics, biomedicine, and self-assembled hierarchical materials.

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Data availability. The data that support the findings of this Letter are openly available [41].

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