Motility versus fluctuations: Mixtures of self-propelled and passive particles

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Although many biological systems consist of both self-propelled and passive agents that may be crucial for overall functionality, there are but a few studies concerning the properties of such mixtures. Here we formulate a model for mixtures of self-motile and passive agents and show that the model gives rise to three different dynamical phases: a disordered mesoturbulent phase, a polar flocking phase, and a vortical phase characterized through two large-scale counterrotating vortices. We use numerical simulations to construct a phase diagram and discuss the relation between the statistical properties of the different phases and self-motile bacterial suspensions. Our findings afford specific insights regarding the interaction of microorganisms and passive particles and provide novel strategic guidance for the efficient technological realization of artificial active matter.

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In both bacterial suspensions and protein filaments propelled by molecular motors as well as in the swarming, herding, and flocking behavior of animal colonies such as fish and fowl, the self-motility of individual agents appears to provide the key ingredient needed to achieve remarkable properties and phenomena. Such phenomena include polar ordering, large-scale correlated motion, and intriguing rheological properties [1]. However, biological systems often consist of several different species which differ in their motilities and other properties. For example, in microbial biofilms heterogeneous populations arise with the emergence of different phenotypes [2–6]. Further, individual agents in biological systems also die, malfunction, or lose their flagella and thereby become partially or completely immotile. Despite the ubiquity of systems with heterogeneous motility properties, such mixtures have received little attention. Apart from the work of McCandlish et al. [7], who report spontaneous segregation in simulations of self-motile and passive rod-shaped agents, studies of the properties of mixtures of active and passive agents appear to be unavailable.

Yet, insights regarding biological and mechanical interactions in such systems are of great relevance in understanding biological systems and might enable progress in potential technological applications and, in particular, in the design of artificial active matter systems. For example, the fabrication of bacterial strains with engineered gene-regulation circuits that produce predefined spatial and temporal patterns is possible with techniques of synthetic biology and systems biology [8–13]. Similarly, artificial self-propelled agents can be realized through analytically driven Janus particles [14–18]. From a technological perspective, it would be of key importance to know whether it is possible to use a small number of these potentially difficult to manufacture agents to drive other passive agents and thereby generate desirable flow patterns. Knowing how many active agents are required for such a principle seems particularly crucial, as does knowing how such a principle might be realized most efficiently.

In the present letter we study the criteria for which different dynamical phases may be observed in dense mixtures of self-propelled and passive spherical soft-core agents. The motion of an agent \(i\) with constant mass \(m^i\) in a system of \(N\) agents is governed by Newton’s equations including the interaction force \(f^{ij} = -f^{ji}\) between agents \(i\) and \(j\), and the external force \(f^i_\text{e}\) exerted on agent \(i\). For \(f^{ij}\), the short-range interaction forces of dissipative particle dynamics (DPD) are used. Working with reduced units and using the standard parameter values [19] for a passive DPD fluid, we set \(k_BT = 1.0, r_c = 1.0, A = 25.0, \gamma = 4.5, \) and \(\rho_{2D} = \frac{N}{L^2} = 2.5\) (two-dimensional analog of \(\rho_{3D} = 4.0\)), where \(L = 100r_c\) is the dimensionless edge length of the square computational domain. Apart from standard DPD forces, we incorporate self-propulsion through a flocking term \(f^i_\text{f} = (\alpha - \beta|v^i|^2)v^i\), with \(\alpha \geq 0\) the constant self-propulsion force parameter and \(\beta \geq 0\) the constant Rayleigh friction parameter [20–25]. To model the features of a mixture, we apply \(f^i_\text{f}\) only on the fraction \(\phi\) of active agents and the random contribution of the DPD interactions \(f^i_R\) only between pairs of the fraction \(1-\phi\) of passive agents.

We performed simulations with LAMMPS [26, 27] using periodic boundary conditions and the standard velocity-Verlet [28] time integration scheme with a dimensionless integration timestep of \(\Delta t = 3.0 \times 10^{-3}\). We run all simulations for \(2.0 \times 10^6\) timesteps to ensure that a steady-state is reached, as verified by monitoring the total energy of the system. Initially, we took all agents to be randomly distributed with zero initial velocities. Hav-
The order parameter and agent distribution fields. The symbol ■ marks the mesoturbulent phase (T), ▼ the vortical phase (V), and • the polar flocking phase (F) identified with criteria of Table I. (a) $P_v$ from theoretical estimates (4), (7), and (8). (b) $P_v$ from simulations. (g) $P_e$ from simulations. (c)–(f) Agent distribution fields.

![FIG. 1: Coarse-grained velocity field $\boldsymbol{u}_M$ for $\beta = 2.25$ and representative choices of $\phi$ and $Pe$. (a) Arises for small $\phi$ in combination with small $Pe$; (b) arises for intermediate and large $\phi$ in combination with large $Pe$; (c) arises for small $\phi$ and $Pe > 1$.](image)

![TABLE I: Summary of criteria used to identify different phases.](table)

| Phase                | $P_e$ | $P_v$ | Snapshot       |
|----------------------|-------|-------|----------------|
| Mesoturbulent (T)    | $P_v \to 1$ | $P_e \to 0$ | Figure 1 (a)  |
| Polar flock (F)      | $P_v \to 0$ | $P_e \to 0$ | Figure 1 (b)  |
| Vortical (V)         | $P_v \to 1$ | $P_e > 0$ | Figure 1 (c)  |

phase diagram. Let

$$Pe = \frac{\alpha}{2\beta}/k_B T \quad (1)$$

denote a dimensionless Pécel number characterizing the ratio of the self-propulsion energy to the energy of random fluctuations. Depending on the values of $Pe$ and $\phi$, the system develops three different phases: a disordered mesoturbulent phase, a polar flocking phase, and a vortical phase characterized through two large-scale counter-rotating vortices (Fig. 1). Importantly, no segregation is observed (Fig. 2 (c)–(f)). We use order parameters based on the agent velocities $\mathbf{v}$ and the coarse-grained vorticity $\omega = \text{curl} \, \mathbf{u}_M$ to quantify the influence of $\phi$ and $Pe$ on phase emergence. The coarse-grained velocity $\mathbf{u}_M(x_M) = \frac{1}{N} \sum_{i=1}^{N} \mathbf{v}(x_M - x_i)$ is computed on a uniform grid with equidistant spacing in both coordinate directions, where $\psi$ is a sufficiently rapidly decaying filtering kernel and $n$ is the number of agents for which $\psi \neq 0$. For simplicity, we use a Gaussian filter with non-dimensional filter width $\epsilon = 15.0$. The order parameters $P_e$ and $P_v$ are defined as

$$P_v = \frac{\langle |\mathbf{v}|^2 \rangle_i - \langle \mathbf{v} \rangle_i^2}{\langle |\mathbf{v}|^2 \rangle_i} \quad \text{and} \quad P_\omega = \langle |\omega|^2 \rangle - \langle \omega \rangle^2 \quad , (2)$$

where $\langle \cdot \rangle_i$ denotes the spatial average over all agents in the computational domain and $\langle \cdot \rangle$ denotes the spatial average over all points $x_M$. Whereas $P_v$ distinguishes between polar and non-polar states, $P_\omega$ distinguishes between non-polar phases exhibiting large-scale vortical motion and non-polar mesoturbulent phases. The associated limiting cases are summarized in Table I. We determine the order parameters numerically and show them as 2D contour plots in the $(\phi, Pe)$–plane (Fig. 2). The phases in the $(\phi, Pe)$–plane are marked using the identification criteria summarized in Table I. The vortical phase arises for small $\phi$ and $Pe > 1$ (Fig. 2 (g)). The mesoturbulent phase appears to develop in a triangular region enclosed by the origin, a point near $\phi \to 0$ and $Pe \approx 1$, and a point near $\phi \to 1$ and $Pe \to 0$. Heuristically, the mesoturbulent phase is thus observed for parameter values of $\phi$ and $Pe$ satisfying

$$Pe \lesssim 1 - \eta \phi, \quad (3)$$

where $\eta$ is an empirical parameter describing the slope of the line in the $(\phi, Pe)$–plane below which the mesoturbulent phase prevails. To understand (3), consider a comparison between the (kinetic) energies $E_a$ and $E_p$ of the active and passive agents. The system is expected to exhibit the mesoturbulent phase for $E_a \lesssim E_p$. The energy $E_p$ estimated from the input parameter $k_B T$ is $E_p \approx (1 - \phi)k_B T$. Further, assuming that $E_a$ is independent of $\phi$ and approximately equal to the energy associated with the flocking term yields the estimate $E_a \approx \frac{\phi}{2}$.

This corresponds to the limiting minimal energy (active and passive) needed to form a polar flock. The mesoturbulent phase may thus be expected for $\frac{\phi}{2} \lesssim (1 - \phi)k_B T$ or, equivalently, for

$$Pe \lesssim 1 - \phi \quad (4)$$

where $\alpha$, $\beta$, and $\beta$ are the remaining free parameters.
on using (1). Comparison of (3) and (4) shows that the results from the numerical simulations agree qualitatively with the theoretical predictions and suggests that $\eta = 1$. However, the numerical results (Fig. 2 (b)) indicate that $\eta < 1$, resulting in transitions to the flocking phase for values of $\phi$ smaller than theoretically predicted. This effect can be explained by noting that the pairwise dissipative interactions between all agents results in an overall damping of the random fluctuations induced by the passive agents.

Next, we focus on the values of $P_v$ around the transition between the mesoturbulent and the flocking phases. The contour lines in Fig. 2 (b) indicate a discontinuous transition between these phases, resulting in abrupt changes near a threshold value of $P_v \approx 0.5$. To determine the values of $P_v$ for which transitions between the polar and non-polar states may be expected, consider the estimate of the energy in the polar state in terms of the mean velocity $\langle v^i \rangle_i$ and the fluctuating velocity $\langle v' \rangle = v^i - \langle v^i \rangle_i$, such that, without loss of generality,

$$\frac{1}{2} \langle |v'|^2 \rangle_i = \frac{1}{2} \langle v'^2 \rangle_i + \frac{1}{2} \langle |v''|^2 \rangle_i.$$  \hfill (5)

Transitions may be expected when the energies associated with the mean velocity and fluctuations are equal:

$$\langle v'^2 \rangle_i = \langle |v''|^2 \rangle_i.$$  \hfill (6)

By (2) and (5), and (6), we thus expect a transition between polar and non-polar phases near $P_v = 0.5$, which is consistent with the numerical results. In the flocking regime, $P_v$ exhibits a nonlinear but continuous dependence on $\phi$ and $Pe$ (Fig. 2 (b)). To understand how $P_v$ depends on $\phi$ and $Pe$, we estimate values of $P_v$ based on the relevant input parameters and compare them to numerical predictions. In the flocking regime, we estimate the terms entering the definition of the order parameter (2) as $\frac{1}{2} \langle |v'|^2 \rangle_i \approx \phi \frac{D_2}{2} + (1 - \phi) k_B T$ and $\frac{1}{2} \langle v'^2 \rangle_i \approx \phi \frac{D_4}{2}$. Consequently, we find that

$$P_v \approx \frac{1 - \phi}{\phi Pe + 1 - \phi}.$$  \hfill (7)

Importantly, (7) provides an estimate for the order parameter $P_v$ in the flocking regime of the $(Pe, \phi)$-plane. In view of the previous discussion, the transition between the polar flocking phase and the disordered phase is associated with $P_v \approx 0.5$, yielding a criterion similar to (4):

$$Pe \approx \frac{1 - \phi}{\phi}.$$  \hfill (8)

The good qualitative agreement between the theoretically estimated phase diagram and the numerical predictions (Fig. 2 (a)–(b)) confirms the validity of the criteria (4), (7), and (8) derived from the energy estimates. Mean-square displacement (MSD) and diffusion coefficients. The MSD $\langle (\Delta x_i)^2 \rangle_i = \langle (x_i(\tau) - x_i(0))^2 \rangle$ can be related to the diffusion through the Langevin equations. For a 2D system (cf., e.g., [29])

$$\langle (\Delta x_i)^2 \rangle_i = 4D_\xi \tau^\xi,$$  \hfill (9)

where $D_\xi$ is the coefficient associated with the power-law exponent $\xi$. For classical diffusive Brownian motion $\xi = 1$ and $D_1$ is the diffusion coefficient [30], whereas for ballistic motion $\xi = 2$ and $D_2$ is proportional to a characteristic energy per unit mass. In the mesoturbulent phase, the present system exhibits ballistic motion at short times and diffusive motion at long times (Fig. 3.
In experiments with 2D bacterial baths with tracer particles, Wu and Libchaber [31–33] observed a similar crossover from superdiffusive motion with $\xi > 1$ to diffusive motion with $\xi \approx 1$. They found good fit of their experimental data with

$$\langle (\Delta x_i)^2 \rangle = 4D_2\tau(1 - \exp(-\tau/\tau_c)), \quad (10)$$

where $D$ is the diffusion coefficient and $\tau_c$ is the crossover time between two different asymptotic regimes; for $\tau \ll \tau_c$ the motion is ballistic and for $\tau \gg \tau_c$ the motion is diffusive. Least-squares fits of our simulation results (Fig. 3 (a)) show good agreement with (10), suggesting that the mesoturbulent phase exhibits statistical properties similar to those of 2D bacterial suspensions. Further, the diffusivity as well as the crossover time decrease with increasing $\phi$, indicating that the random fluctuations of the passive agents are mainly responsible for the diffusivity of the mixtures. At low $\phi$, the diffusivity associated with the passive agents is significantly higher than the diffusivity associated with the active agents (Fig. 3 (a.I)). This difference in diffusivities decreases for increasing $\phi$, signifying that the considered flocking mechanism effectively removes diffusivity, ultimately resulting in transitions to the polar flocking phase.

In contrast to the mesoturbulent phase, the flocking phase exhibits ballistic behavior on all timescales (Fig. 3 (b)). Consistent with this, the MSD scales with $\tau^2$. In the flocking phase, $D_2$ exhibits an increase with increasing $\phi$, approaching what appears to be an asymptotic value for large $\phi$ (Fig. 3 (b.I)). To understand this limiting behavior, consider the MSD over time, which may be estimated to be proportional to the characteristic flocking energy per unit mass $\langle (\Delta x_i)^2 \rangle \approx \xi^2 \tau^2 \approx \frac{\alpha}{\beta}$. In view of (9), $D_2 \approx \frac{\alpha}{\beta}$ for ballistic motion in the flocking phase as shown by the dashed line in Fig. 3 (b.I). Further, the ballistic coefficients associated with the active and passive agents are almost identical. This confirms that, in the flocking regime, the flocking term dominates and drives the passive agents.

In the vortical phase, the system exhibits ballistic motion at short and intermediate times and diffusive motion at long times (Fig. 3 (c)). Notice that, in contrast to the data appearing in Fig. 3 (a)–(b), the results in Fig. 3 (c) appear for different representative Péclet numbers and $\phi = 0.1$, since the vortical phase emerges only for low $\phi$. Similarly as in the mesoturbulent phase, the fit to (10) provides good agreement with the data (Fig. 3 (c)). The crossover times to diffusive motion are an order of magnitude higher than those of the mesoturbulent phase (Fig. 3 (c.I)). This is consistent with the presence of a pair of counterrotating vortices and suggests that this structure is coherent for much longer times than the small-scale swirls that distinguish the mesoturbulent phase. The short-time ballistic coefficient exhibits a linear increase with increasing Pe (Fig. 3 (c.II)). Since the ballistic coefficient is a measure for the characteristic energy per unit mass of the system, this demonstrates that the energy in the vortical phase depends linearly on Pe, even for small $\phi$.

**Discussion.** The current results have some key implications regarding the interactions of microorganisms with different motilities as well as artificial realizations of active matter and related technological applications. First, they suggest that all dynamical phases and the associated motion patterns may be achieved using a relatively low fraction of self-propelled agents. In scenarios where active matter is realized with artificial self-propelled agents such as, for example, catalytically driven Janus particles [14–18], this implies that a small number of these potentially difficult to manufacture agents should suffice to drive passive agents and generate large-scale flow patterns.

In a different scenario, the transition between mesoturbulent and the polar flocking phases might be controlled by adjusting the fraction of active agents, while keeping the parameters associated with self-propulsion constant. Technologically, this means that the emergence of either phase could be controlled by switching identical agents on and off to adjust the fraction of active agents. This strategy would make it unnecessary to adjust the parameters related to the magnitude of the self-propulsion. This potentially promising avenue remains to be investigated experimentally.

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