Fast and slow self-propelled particles interacting with asymmetric obstacles: Wetting, segregation, rectification, and vorticity

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We study a mixture of “fast” and “slow” self-propelled particles in the presence of a regular array of large asymmetric obstacles. For this purpose, simulations of active Brownian particles interacting with a half-disk obstacle are performed in 2D with periodic boundary conditions. The system has two particle types, each of them characterized by its own self-propulsion speed. To isolate the effects of such “speed diversity”, the system-average self-propulsion speed is kept unvaried as the degree of speed diversity is tuned. Because of their persistent motion, particles accumulate around the obstacle in a wetting phenomenon. Stationary segregation arises since faster particles are more likely to occupy new available spaces. For degrees of speed diversity \( \geq 40\% \), we observe a transition where the self-propulsion of the slower particles becomes too weak and thus these particles start to accumulate more easily over a “layer” of faster particles rather than near the wall. Also, particles traveling from the curved to the flat side of the obstacle spend less time trapped than in the opposite direction. As a result, directed motion emerges spontaneously. We find that the corresponding rectification current is amplified when the degree of speed diversity is increased. In the passive-active limit, the passive particles still undergo directed motion dragged by the active ones. Due to rectification, segregation profiles are different between the curved and flat sides. Near the obstacle corners, pairs of vortices that further contribute to rectification are observed. Their vorticities also increase with speed diversity. Our results provide useful insights into the behavior of active matter in complex environments.

I. INTRODUCTION

Self-propelled particles—such as bacteria, tissue cells, and autophoretic colloids—have the ability to spontaneously accumulate around obstacles even in the absence of attractive forces [1]. Similarly to motility-induced phase separation (MIPS) [2], such active wetting arises because active particles have a direction of motion that evolves stochastically but slowly, i.e., their direction of motion is persistent [3–5]. For sufficiently large persistence times or densities, particles do not have time to find an escape route and thus become trapped between obstacles and other particles [6]. Active wetting helps control surface adhesion and capillary properties of bacterial biofilms [7–9], whose formation makes bacterial colonies more resilient against antibiotics [10].

In the case of asymmetric obstacles, simulations and experiments show that active particles undergo directed motion [11], in addition to accumulation. The spontaneous emergence of net particle transport due to environmental asymmetries, i.e., “rectification” currents, has constituted a central topic in both conceptual and technological contexts for decades [12]. More recently, research on rectification of self-propelled particles has gained momentum [13–17]. In Ref. [18], an initially homogeneous collection of active Brownian particles in 2D was simulated in a regular array of half-disk rigid obstacles oriented in the same fixed direction. The stationary average speed of the particles was found to be nonzero: instead, an effective rectification current emerges since particles traveling from the curved to the flat side of the obstacle spend less time trapped than those in the opposite direction. A similar behavior was observed for an irregular array of randomly-located obstacles oriented in the same fixed direction [19]. The sizes of the obstacles and accumulation layers directly affect the intensity of such rectification currents. Rectification by half-disk obstacles shows that no cavity is needed to trap particles, meaning that the existence of convex surfaces with distinct curvatures is sufficient to generate currents.

The authors of Ref. [18] considered identical active particles, i.e., particles with the same self-propulsion speed, rotational diffusion coefficient, and size. However, in natural colonies of bacteria and other microorganisms, a broad dispersion of motility parameters exists due to different ages, reproduction stages, shapes, sizes, and running modes [20–23]. For either passive or active fluids, it is known that “diversity” of some particle attribute generates several new phase behavior phenomena, including changing the nature and loci of phase diagram boundaries and introducing particle-type spatial segregation [1–24]. Still, it remains unclear what are the effects of particle diversity on active rectification by convex asymmetric obstacles. This is important because, in complex bio-
logical environments, active matter commonly interacts with obstacles like that, as for example bacteria swimming around the internal structures of the host body where they live \cite{12}.

In this work, we use 2D simulations to investigate a mixture of “fast” and “slow” active Brownian particles in a regular array of half-disk obstacles. No external fields, hydrodynamic effects, or imposed alignment rules are present. Our main motivation is to understand how “self-propulsion speed diversity” (hereafter just speed diversity) couples with the presence of asymmetric convex obstacles and thus alters rectification currents as well as accumulation profiles. In particular, we discuss how these effects are connected with the emergence of segregation \cite{13, 14} and vortices \cite{15, 16} near the obstacle corners.

This paper is organized as follows. In Section II our model and simulation setup is laid out. In Section III we present our results for wetting and spatial segregation. In Section IV we turn our attention to rectification effects and how they are connected with the appearance of circulating currents. Section V brings our concluding remarks.

II. MODEL

We consider a binary mixture in 2D composed of $N$ active Brownian disks labeled by $i$, where $N/2$ of them are “fast” particles, with self-propulsion speed $v_i = v_f \equiv v_0(1 + \delta)$, and the other $N/2$ are “slow” particles, with $v_i = v_s \equiv v_0(1 - \delta)$. The parameter $\delta \in [0,1]$ thus corresponds to the degree of speed diversity. For $\delta = 0$, all particles have identical self-propulsion speed and the system is called “monodisperse”. In the opposite limit, when $\delta = 1$, the mixture is passive-active. For simplicity, global compositions other than 50-50% are not considered, but generalization is straightforward. On varying $\delta$, the system-average self-propulsion speed is kept at $v_0$, which is constant and independent of $\delta$. By doing so, the effects of speed diversity can be isolated. To avoid undesired artificial crystallization \cite{17}, each particle is randomly assigned one of two diameters, $d_{\text{small}} = d_0$ and $d_{\text{large}} = 1.4d_0$, uncorrelated with particle types, where $d_0$ is the scale that fixes particle diameters. Therefore, there are actually four particle types, but we focus on the effects of speed diversity since both particle sizes are similar. The system is said to be just binary or “bidisperse”.

The dynamics of each particle’s position $\mathbf{r}_i$ is governed by the equations

$$\partial_t \mathbf{r}_i = \mathbf{v}_i + \mu \mathbf{F}_i, \quad \partial_t \theta_i = \eta_i(t),$$

where $\mathbf{v}_i = (\cos \theta_i, \sin \theta_i)$ determines the self-propulsion force direction and $\mu$ is the mobility, which we take equal to one, meaning that forces are expressed in units of velocity. Also, $\mathbf{F}_i = \sum_{j \neq i} \mathbf{F}_{ij} + \mathbf{F}_{\text{obst}}$ is the net force on particle $i$ due to interactions with other particles and with a half-disk obstacle, of radius $D/2$. The noise term $\eta_i(t)$ is Gaussian and white, with mean $\langle \eta_i(t) \rangle = 0$ and correlation $\langle \eta_i(t)\eta_j(t') \rangle = 2\eta\delta(t-t')$, where $\eta$ is the rotational diffusion coefficient.

The interparticle interactions are taken as a soft repulsive WCA-like potential \cite{18} defined in terms of the interparticle distance $r_{ij}$ as \cite{19}

$$U = \begin{cases} 2^4 \frac{\sigma_{ij}}{r_{ij}}^3 - 3 \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 + \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \frac{3}{4} & r_{ij} \leq 2^4 \sigma_{ij}, \\ 0 & r_{ij} > 2^4 \sigma_{ij} \end{cases}$$

with $\sigma_{ij} \equiv \frac{1}{2}(d_i + d_j)$, where $d_i$ is the particle diameter of particle $i$. For the particle-obstacle interaction between particle $i$ and the curved side,
The parameter distinguishing the particle types is the self-propulsion speed. We choose units and fixed parameters such that \( v_0 = 1 \) and the diameter scale is \( d_0 = 1 \). For the rotational diffusion coefficient and simulation time step, we take \( \eta = 5 \times 10^{-3} \) and \( \Delta t = 10^{-2} \), respectively. Initially, particles are distributed homogeneously at random positions with random velocity directions, independent of their types. The simulation is performed in a square box of side \( L = 200 \) (such that \( D = L/2 \)) and with periodic boundary conditions, simulating therefore an infinite regular array of identical obstacles. The centers of the flat side and of the simulation box coincide. The average free-particle persistence length is \( \ell = v_0/\eta = 200 \), which is comparable to the system and obstacle sizes. The occupied area fraction \( \phi \) is defined as the total area occupied by particles divided by the area of the simulation box minus the obstacle, i.e.,

\[
\phi = \frac{N}{2} \times \frac{\pi (d_{\text{small}}^2 + d_{\text{large}}^2)}{L^2 - \frac{\pi}{2} \left( \frac{d_0}{2} \right)^2}.
\]  

III. WETTING AND SEGREGATION

Movie 1 of the Supplementary Material [50] shows the dynamics between the initial state and the stationary state (\( t \geq 2000 \)) for \( \phi = 0.13 \) and \( \delta = 0.8 \). Snapshots of the initial and stationary states are shown in Figs. 1a and b. After particles quickly accumulate around the obstacle, the average thickness of the wetting layer stabilizes once the concentration of the “gas” (i.e., outside the layer) becomes sufficiently low that absorption and emission rates for the layer are equal. Because available spaces are more likely to be occupied by the faster particles (as they arrive there typically before the slower ones), segregation emerges. For larger area fractions, the wetting layer increases in size, as shown in Fig. 1c, for \( \phi = 0.26 \). In all cases studied below (\( \phi = 0.08, 0.13, \) and 0.26 for various values of \( \delta \)), the stationary gas concentration is sufficiently low such that no stationary clusters appear in the gas. That is, the residual gas density after the wetting layer has been formed is smaller than the necessary to produce MIPS [2]. Also, in the transient regime, the condensation by heterogeneous nucleation on the obstacle is faster than an eventual MIPS. Hence, the only condensed phase in the system is the wetting layer on the obstacle. Movies 2 [51] and 3 [52] of the Supplementary Material show, respectively, the transient and the steady state for \( \phi = 0.26 \) with \( \delta = 0.8 \).

Due to crowding, the dynamics inside the wetting cluster is much slower than that in the gas. Movie 1 also shows that the interface between the wetting layer and the gas fluctuates strongly. Presumably, this is a consequence of active capillary-like effects [53–54] enhanced by the fact that particles can escape from the cluster not only by rotational diffusion but also by reaching the end of the obstacle wall.

Fig. 2 shows the stationary concentration fields for the total, “slow”, and “fast” particles concentrations, denoted respectively by \( n_t(r), n_s(r), \) and \( n_f(r) \), for selected values of \( \phi \) and \( \delta \). They are defined similarly to the area fraction \( \phi \) but are calculated locally using coarse-graining square boxes of side 2.5. We counted the number of particle centers in each box, multiplied by the area of the corresponding particle, and then divided the result by the area of the coarse-graining box. For boxes that include a fraction of the obstacle, the available area was calculated using standard Monte Carlo integration.

Fig. 2a shows the monodisperse (\( \delta = 0 \)) scenario studied in Ref. [18]. The stationary accumulation is more pronounced for higher \( \phi \) and decays smoothly towards the gas. For \( \delta > 0 \), we observe that \( n_s(r) \) and \( n_f(r) \) are significantly different from each other as the faster particles dominate the occupation closer to the obstacle, whereas the slower particles accumulate less sharply.

Concentration profiles were obtained by averaging the concentration fields along the direction parallel to each wall. For the curved side, the concentration is plotted against the radial distance to the wall. The concentration of faster particles decays monotonically towards the gas irrespective of \( \delta \), for both the curved and flat sides (data not shown). Near the walls, the accumulation of faster particles becomes more pronounced for higher \( \delta \) as their incoming flux is naturally higher and also because a stronger self-propulsion means that the particle can open the way towards the obstacle by displacing other particles. Figure 3 shows concentration profiles of the slower particles for both sides and several values of \( \delta \). In this case, a peak located further away from the obstacle wall is clearly observed for \( \delta \geq 0.4 \). This transition occurs when the slower particles become sufficiently slow that they accumulate more easily on the boundary of the “layer” of faster particles than closer to the obstacle wall. Notice that the peak is less pronounced on the curved side.

To measure the degree of spatial segregation, we
FIG. 2. Stationary concentration fields for $\phi = 0.13$. (a) Monodisperse system ($\delta = 0$). (b) Slow and (c) fast particles for mixture case with $\delta = 0.8$.

calculate

$$\zeta = 1 - \frac{\int n_s(r)n_f(r)\,dx\,dy}{\sqrt{\int n_s^2(r)\,dx\,dy \int n_f^2(r)\,dx\,dy}}$$

(4)
a segregation parameter which takes into account

FIG. 3. Stationary concentration profiles of slow particles for various $\delta$ values and $\phi = 0.13$. (a) Curved and (b) flat side.

the overlapping between the concentration profiles. As such, $\zeta = 1$ implies complete segregation and $\zeta = 0$ means complete mixing, which in turn occurs only if $n_s(r) \propto n_f(r)$. Fig. 4 shows that the degree of segregation increases with speed diversity, but complete segregation is not obtained, not even in the passive-active limit. This has two causes. Firstly, not all active particles participate in the wetting cluster, as it stops increasing once the gas concentration is sufficiently low. Secondly, some passive particles remain trapped inside the wetting layer by the active ones. Furthermore, Fig. 4b shows that the degree of segregation in the low global concentration limit is almost independent of $\phi$.

The segregation can also be quantified by the ratio between the slow and faster particles concentration profiles (Figs. 4b and c for the curved and flat side, respectively). For $\delta = 1$, there are almost no passive particles near the wall and the curved side concentration ratio is more than one order of magnitude bigger than for $\delta = 0.9$. This
reveals that the case $\delta = 0.9$ is not as close to a passive-active mixture as one might expect. In fact, Fig. 3 shows a significant difference in the behavior of the concentration profile between $\delta = 0.9$ and $\delta = 1.0$. This can be understood by noticing that for $\delta = 0.9$ the slow particles persistence length $v_s/\eta = v_0(1-\delta)/\eta = 20$ is still comparable to other relevant length scales such as the wetting layer thickness, the obstacle size, and the system size. We also notice that there is more segregation on the curved side than on the flat side as particles are less capable to penetrate and settle inside that layer. For slow particles, such “expulsion” becomes more pronounced. In fact, it is almost impossible for a particle with weak self-propulsion to remain near the wetting interface without being wiped out into the gas by the rectification “wind”. Conversely, particles on the flat side can accumulate closer to the wall since the particle current (see Section IV below) on the flat side near the interface is not sufficient to wipe them out. This can be confirmed by looking once again at the passive particles profile ($\delta = 1$) in Fig. 3, where the concentration near the wall is practically zero on the curved side but not so on the flat side.

IV. RECTIFICATION AND VORTICITY

The asymmetric shape of the obstacle implies that particles traveling from the curved to the flat side will spend less time to overcome it than those in the opposite direction. In the monodisperse case ($\delta = 0$), a rectifications current arises in the stationary state [18]. We now focus on the behavior for $\delta > 0$. Fig. 5 shows the total stationary current (vector) field $j(r) \equiv n(r)v(r)$, where $v(r)$ is the actual velocity field (not the self-propulsion velocity field). Global rectification along the $+x$ direction is indicated by the fact that most current arrows point to the right or have a large $+x$ component. Particles slide on the curved side towards the right and are subject to higher current than in the gas. In fact, the highest local current is observed near the corners. For the flat side, the local current is in the opposite direction, i.e., the $-x$ direction (reflecting the appearance of vortices, as discussed below), but near the obstacle it is constrained to the $y$-axis only. Far from the obstacle, the current field changes to the $+x$ direction again.

To investigate how rectification is affected by speed diversity, we show in Fig. 6a the mean velocity in $x$, $\langle v_x \rangle$, averaged over particles and time instants within the steady state, as a function of $\delta$. As a control, we also show that $\langle v_y \rangle$ is essentially zero, as expected. More importantly, $\langle v_x \rangle$ increases with $\delta$, indicating an amplification of rectification currents that is induced solely by speed diversity (remember that each type corresponds to 50% of all particles and the system-average self-propulsion speed does not change with $\delta$). By looking at $\langle v_x \rangle$ for each particle type in Fig. 6b, we see that, indeed, as $\delta$ increases, the faster particles undergo a rectification increase which is larger than...
FIG. 5. Total stationary current field \( j \) for \( \phi = 0.13 \) and \( \delta = 0.8 \). For clarity, the arrows have all the same size and only indicate the direction of the current, while the magnitude of \( j \) is given via the color legend.

The rectification decrease of the slower particles, even though their self-propulsion speeds were varied by the same amounts, in magnitude. Indeed, the average speed of fast particles is larger than the naïve dependence proportional to \( 1 + \delta \), a manifestation of significant interaction effects. The slow particles for low \( \phi \) do follow the naïve dependence proportional to \( 1 - \delta \), but as the density increases interactions take over and their rectified velocity increases.

This rectification amplification induced by speed diversity can be understood as follows. First, \( \langle v_x \rangle(\delta) \) must be an even function of \( \delta \) since \( \delta \to -\delta \) just relabels particle types and thus should have no physical consequence. Now, consider the monodisperse case of Ref. [18]. Fig. 3a therein suggests that the rectification current \( \langle v_x \rangle \sim \exp(-\eta d_0/v_0) \), where we remind that \( \eta \) is the rotational diffusion coefficient and we incorporated the self-propulsion speed \( v_0 \) and the particles’ diameter by dimensional analysis. This makes sense: by increasing the active speed \( v_0 \), activity-induced rectification ought to increase as well. We now assume that the qualitative behavior of \( \langle v_x \rangle(\delta) \) can be obtained simply from an arithmetic average between \( \exp(-\eta d_0/v_a) \) and \( \exp(-\eta d_0/v_t) \) (On the other hand, the quantitative behavior should require a more complicated analysis, as indicated, for example, by the \( \delta \)-dependence of motility-induced cluster sizes in a system of slow and fast run-and-tumble particles studied in Ref. [55].) Expanding in \( \delta \), indeed no linear \( \delta \) dependence survives, as anticipated. Also, for sufficiently high \( \eta \), \( \langle v_x \rangle(\delta) \) indeed increases with \( \delta \) as observed numerically.

FIG. 6. Stationary mean (actual) velocity averaged over particles and realizations as a function of \( \delta \) for \( \phi = 0.08 \) and 0.13. (a) Total mean velocity in \( x \) and in \( y \). (b) Mean velocity in \( x \) for slow and for fast particles. The case \( \phi = 0.26 \) has been included only for \( \delta = 1 \), avoiding an overcrowding of the figure. The dashed lines present the naïve dependence for the mean velocity of the fast and slow particles.

(The same qualitative analytical examination indicates that a transition for much lower \( \eta \) might exist in the simulations, through which \( \langle v_x \rangle(\delta) \) would become a decreasing function of \( \delta \). That is beyond our scope because the corresponding persistent lengths would be extremely large.)

Furthermore, Fig. 6a shows that \( \langle v_x \rangle \) for the slower particles does not vanish completely at the active-passive limit \( \delta = 1 \). In fact, the passive particles continue to contribute positively to the total \( \langle v_x \rangle \). Such behavior where the motion of passive particles is “enhanced” by active ones has been previously reported in the context of motility-induced phase separation: the presence of active particles in fact induces clustering for the passive ones [28, 30, 56]. Here, what we find is that the active particles induce a finite degree of rectification for the passive ones, which increases with \( \phi \).

Revisiting the current field for the active-active...
mixture case, we notice that the flat side has a nonvanishing total local current moving away from the obstacle center along the $y$-axis. This behavior is connected to the appearance of vortices. We define

$$\omega(r) \equiv \nabla \times j(r)$$

(5)

as a vorticity-like field (not exactly the vorticity since it is the curl of the current field, not of the velocity field) and plot its $z$ component in Fig. 7. We observe that one pair of vortices is formed around each obstacle corner.

For each pair, one of the vortices is produced by the particles that slide on the curved side and the other by those that slide on the flat side. The latter particles move away from the obstacle center, along the $y$-axis. For each side, once the obstacle wall ends, the particles start to interact directly with those that were sliding on the other side. As a consequence, velocities become reoriented, thus generating the corresponding vortices.

To see how vorticity changes with speed diversity, Fig. 8 shows the global vorticity magnitude, defined as $\Omega \equiv \int \omega_z(r) \, dx \, dy$, where we keep the signs in $\omega_z$. The intensity of the vorticity also increases with $\delta$: the particles that participate more in the vortices are those close to the obstacle and, as discussed above, these correspond to the faster particles.

V. CONCLUSIONS

Here we considered an active mixture of fast and slow swimmers in the presence of asymmetric obstacles (with a curved and a flat side). We identified wetting, segregation, rectification and vorticity. As such, this problem arises as an interesting playground for studying several phenomena. Using simulations, we showed how the degree of diversity of self-propulsion speeds alters these phenomena, both quantitatively and qualitatively.

The segregation profiles for speed diversity parameter $\delta = 0.9$ are significantly different from the $\delta = 1$ passive-active case. Also, for $\delta \geq 0.4$ a peak in the concentration profiles of the slower particles arises far from the wall and over the faster particles “layer”, as their self-propulsion becomes too “weak” to allow for accumulation near the wall.

Regarding rectification, our results complement the explanation given in Ref. [18] for monodisperse systems: particles coming from the left side become rectified when sliding along the curved side of the obstacle, whereas those coming from the right side are reoriented due to the formation of vortices which rotate favorably to the global current near the corners. Also, in the passive-active case, we observe that complete segregation is not achieved and that the passive particles continue to rectify as they are pushed by the active ones.

The present work provides a number of insights into the behavior of more realistic active matter systems such as bacterial fluids interacting with real surfaces. In the future, the effects of other active matter features and ingredients as well as distinct obstacle shapes would constitute an interesting research avenue.
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